Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 01:41 AM EDT

PDB ID	:	5W5O
Title	:	Identification of potent and selective RIPK2 inhibitors for the treatment of inflammatory diseases.
Authors	:	Kreusch, A.; Spraggon, G.
Deposited on	:	2017-06-15
Resolution	:	2.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

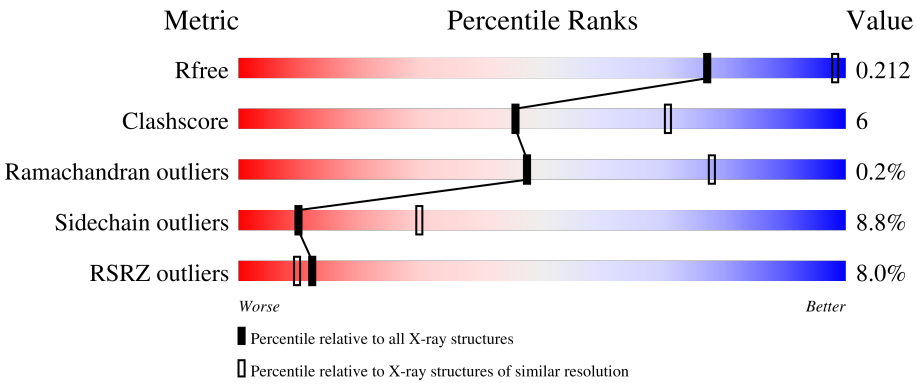
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	310	6% 69% 19% 11%
1	B	310	7% 67% 20% • 11%
1	C	310	8% 64% 21% • 11%
1	D	310	8% 68% 18% • 11%
1	E	310	6% 70% 17% • 11%

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Mol	Chain	Length	Quality of chain
1	F	310	5% 69% 18% 11%
1	G	310	5% 69% 19% 11%
1	H	310	6% 70% 17% 11%
1	I	310	9% 72% 16% 11%
1	J	310	8% 70% 18% 11%
1	K	310	7% 68% 18% 11%
1	L	310	10% 72% 16% 11%
1	M	310	7% 72% 17% 11%
1	N	310	6% 67% 18% 12%
1	O	310	7% 72% 15% 11%
1	P	310	7% 67% 22% 11%

2 Entry composition (i)

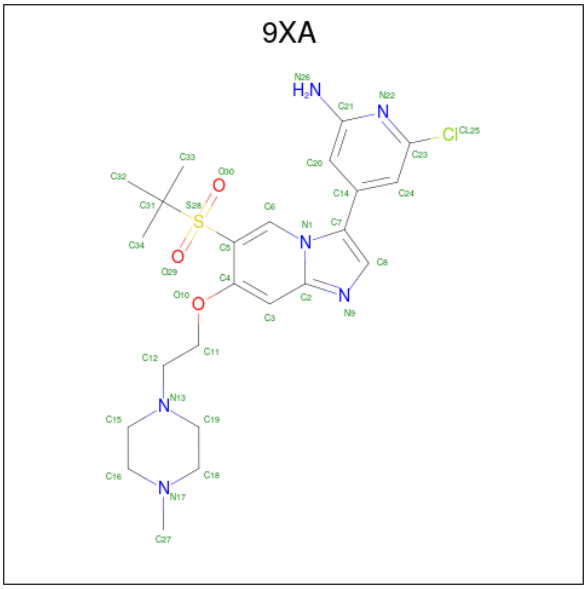
There are 3 unique types of molecules in this entry. The entry contains 35681 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Receptor-interacting serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	2165	1401	365	391	8	0	0	0
1	B	275	2177	1408	370	391	8	0	0	0
1	C	275	2170	1406	368	388	8	0	0	0
1	D	275	2174	1408	372	386	8	0	0	0
1	E	275	2197	1422	373	394	8	0	0	0
1	F	275	2184	1413	373	390	8	0	0	0
1	G	275	2198	1420	374	396	8	0	0	0
1	H	275	2188	1416	372	392	8	0	0	0
1	I	275	2176	1410	372	386	8	0	0	0
1	J	275	2199	1421	377	393	8	0	0	0
1	K	275	2198	1418	373	399	8	0	0	0
1	L	275	2182	1412	369	393	8	0	0	0
1	M	276	2159	1398	365	388	8	0	0	0
1	N	272	2118	1376	357	377	8	0	0	0
1	O	276	2185	1414	369	394	8	0	0	0
1	P	275	2163	1401	362	392	8	0	0	0

- Molecule 2 is 4-{6-(tert-butylsulfonyl)-7-[2-(4-methylpiperazin-1-yl)ethoxy]imidazo[1,2-a]pyridin-3-yl}-6-chloropyridin-2-amine (three-letter code: 9XA) (formula: $C_{23}H_{31}ClN_6O_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
2	A	1	34	23	1	6	3	1	0	0
2	B	1	34	23	1	6	3	1	0	0
2	C	1	34	23	1	6	3	1	0	0
2	D	1	34	23	1	6	3	1	0	0
2	E	1	34	23	1	6	3	1	0	0
2	F	1	34	23	1	6	3	1	0	0
2	G	1	34	23	1	6	3	1	0	0
2	H	1	34	23	1	6	3	1	0	0
2	I	1	34	23	1	6	3	1	0	0
2	J	1	34	23	1	6	3	1	0	0
2	K	1	34	23	1	6	3	1	0	0
2	L	1	34	23	1	6	3	1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
2	M	1	34	23	1	6	3	1	0	0
2	N	1	34	23	1	6	3	1	0	0
2	O	1	34	23	1	6	3	1	0	0
2	P	1	34	23	1	6	3	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	13	13	13	0	0
3	B	20	20	20	0	0
3	C	15	15	15	0	0
3	D	25	25	25	0	0
3	E	16	16	16	0	0
3	F	20	20	20	0	0
3	G	16	16	16	0	0
3	H	24	24	24	0	0
3	I	23	23	23	0	0
3	J	19	19	19	0	0
3	K	19	19	19	0	0
3	L	12	12	12	0	0
3	M	15	15	15	0	0
3	N	25	25	25	0	0
3	O	16	16	16	0	0

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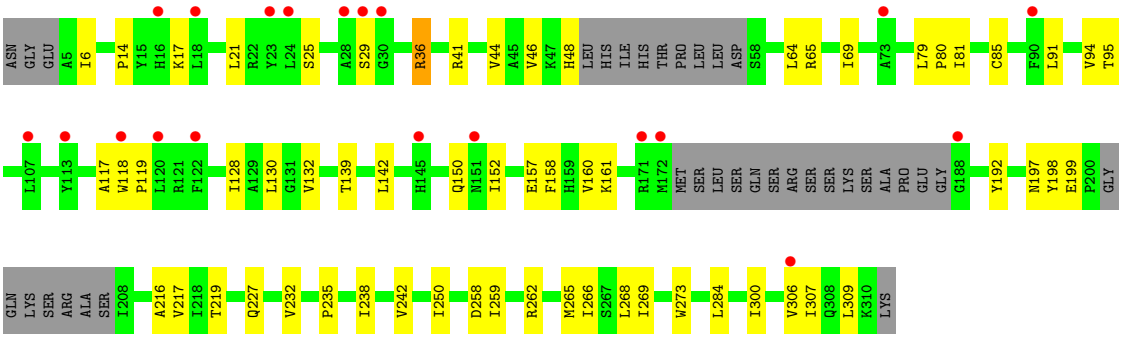
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	P	26	26	26	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

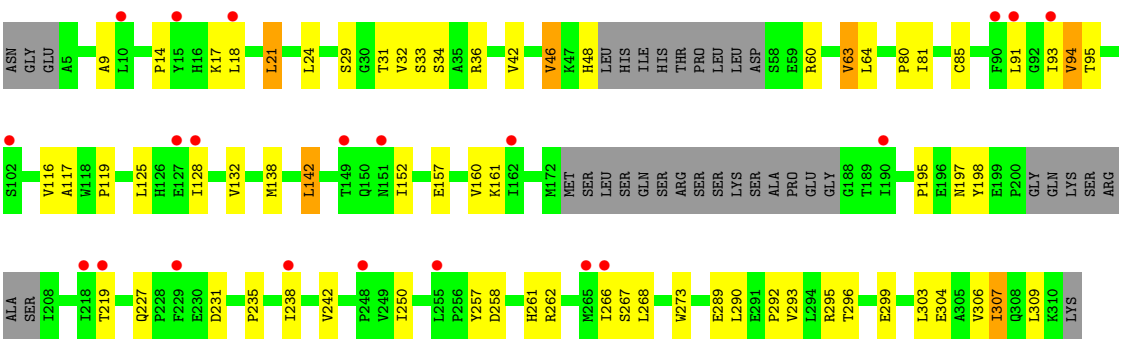
• Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

Chain A:



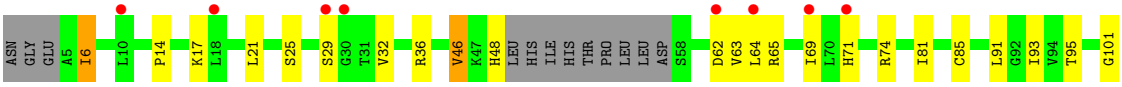
• Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

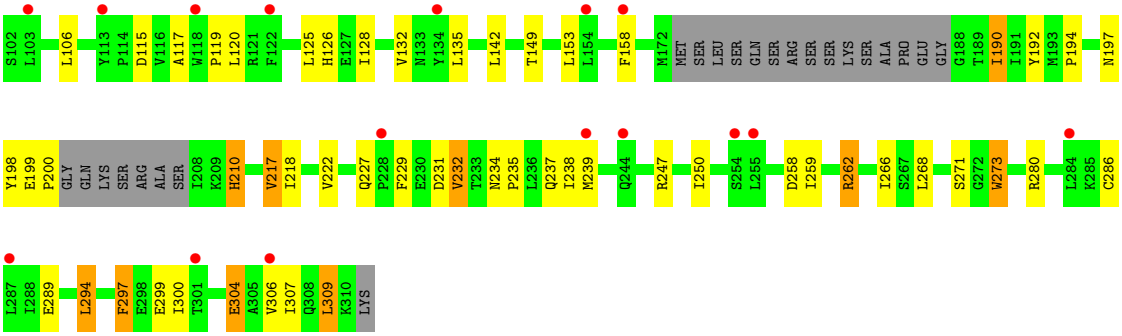
Chain B:



• Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

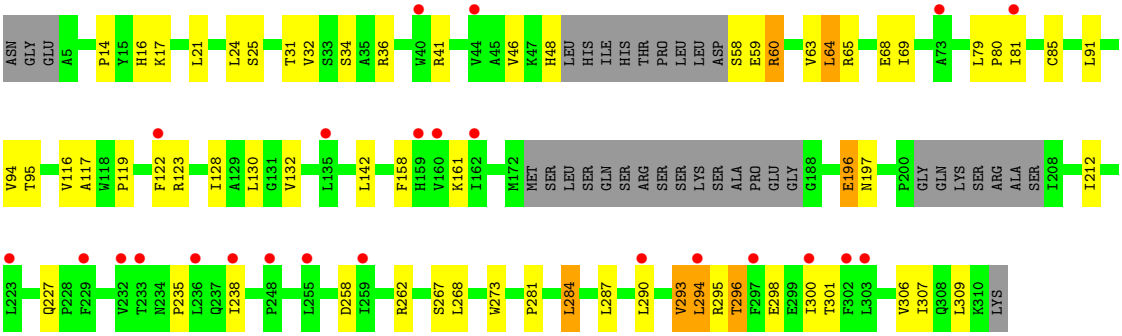
Chain C:





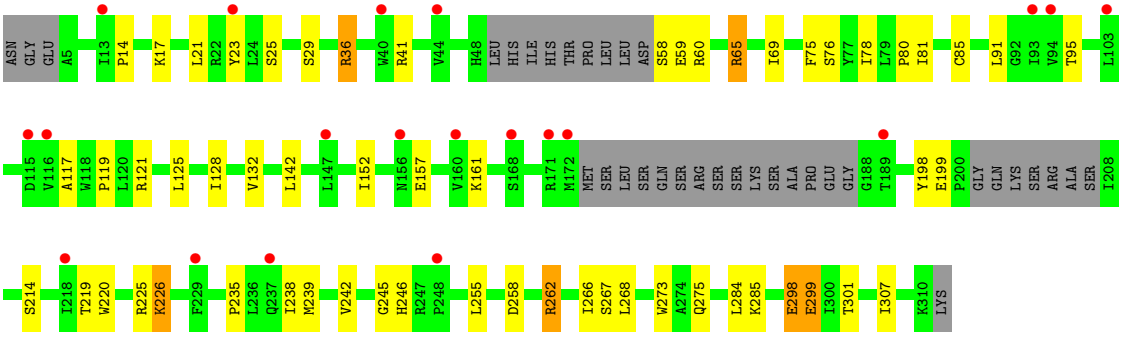
• Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

Chain D:



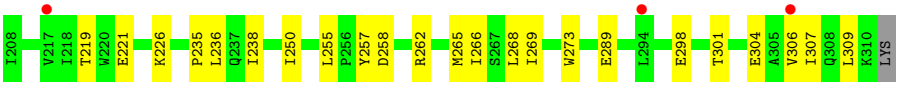
• Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

Chain E:



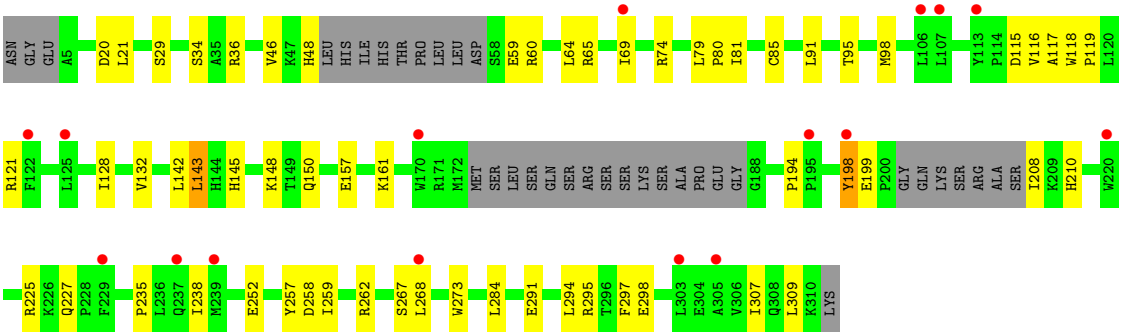
• Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

Chain F:



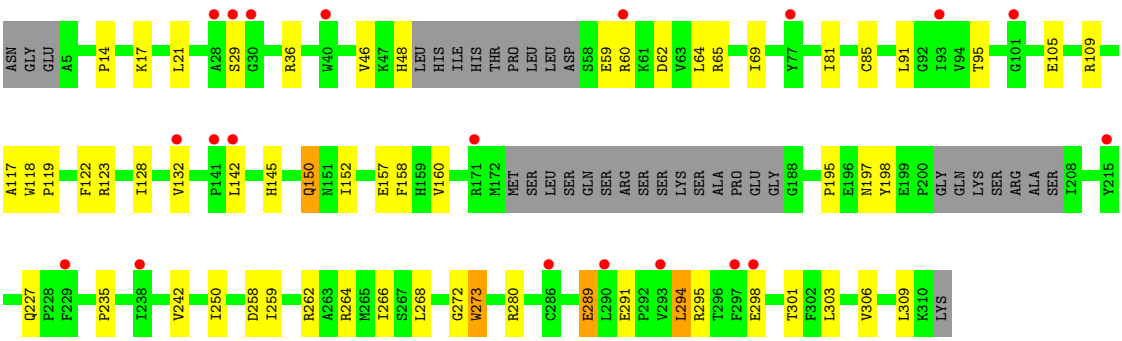
• Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

Chain G:



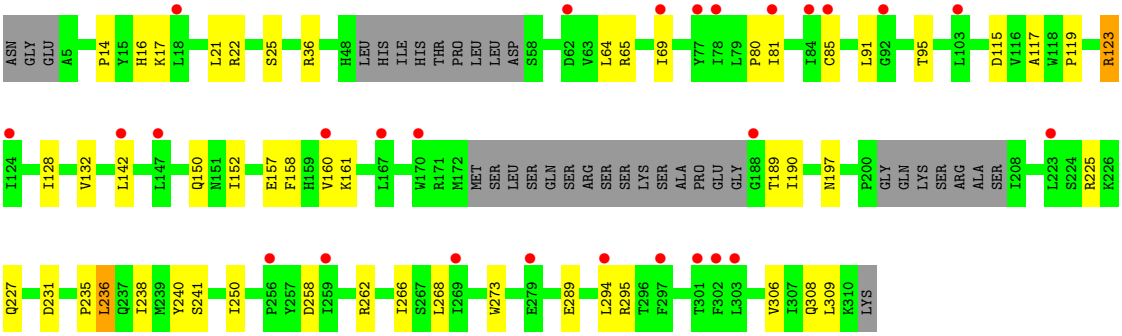
• Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

Chain H:



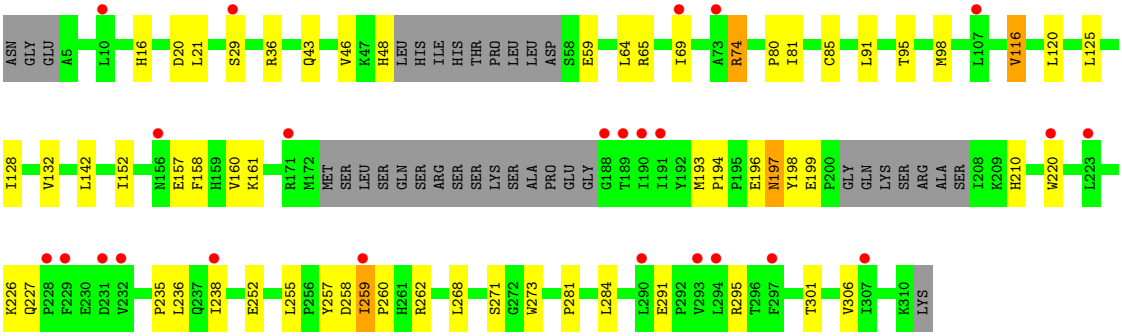
• Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

Chain I:



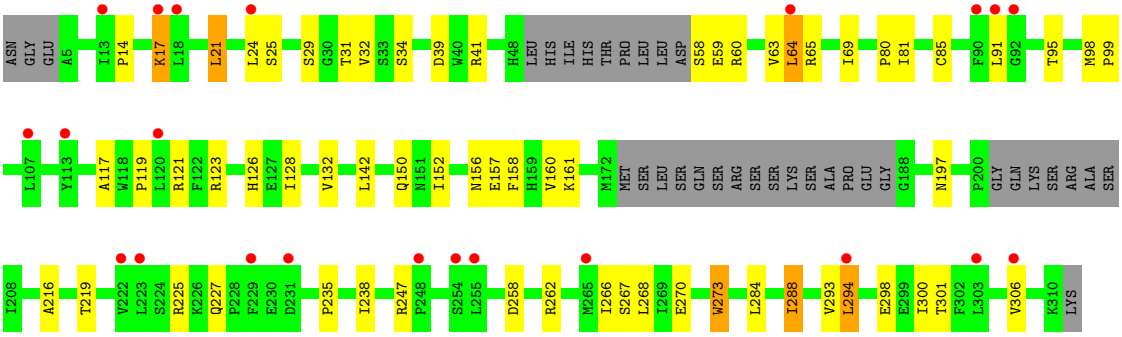
• Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

Chain J:



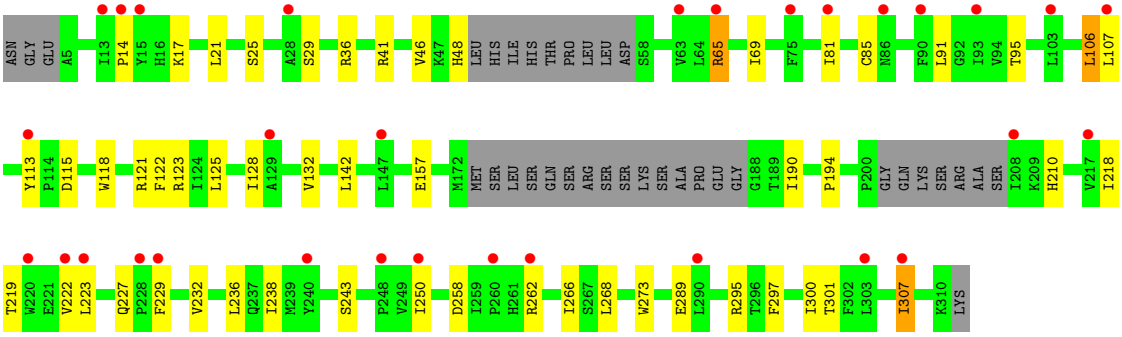
• Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

Chain K:



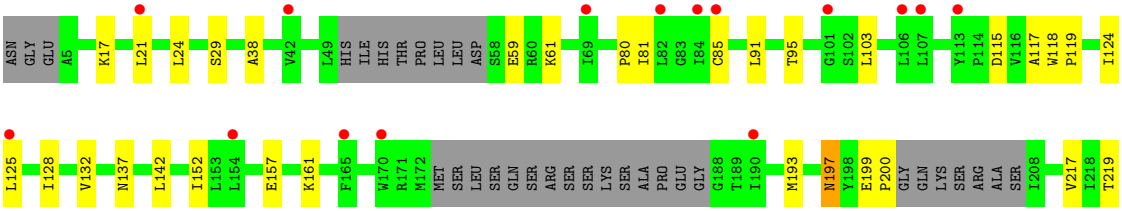
• Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

Chain L:



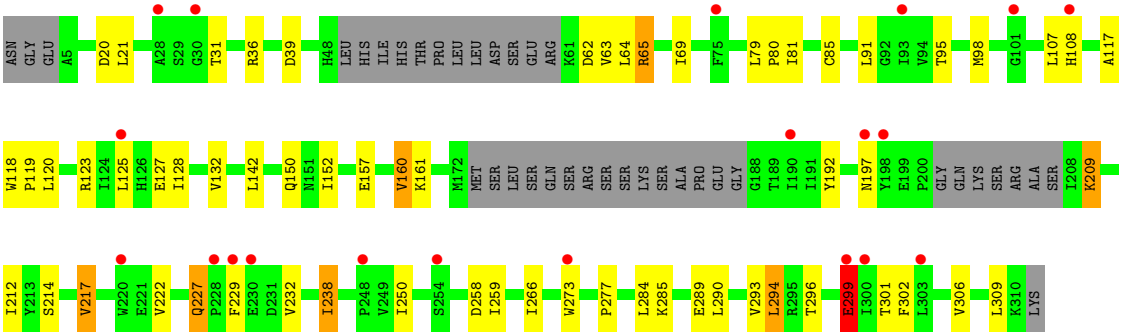
• Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

Chain M:



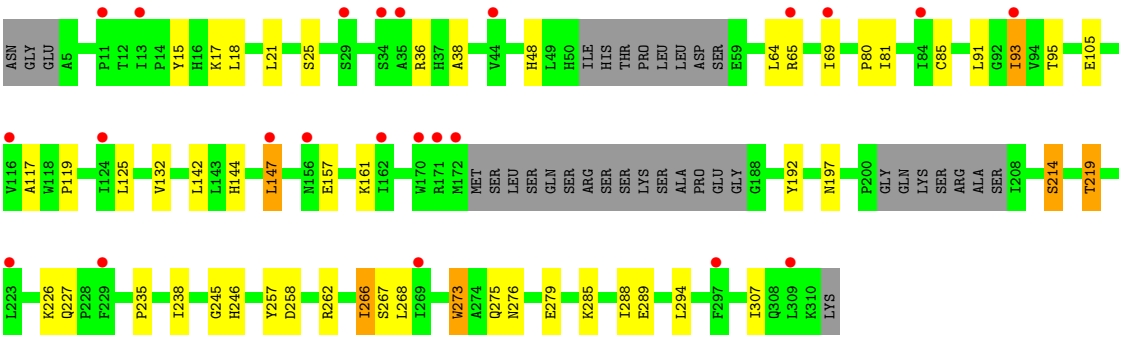
• Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

Chain N:



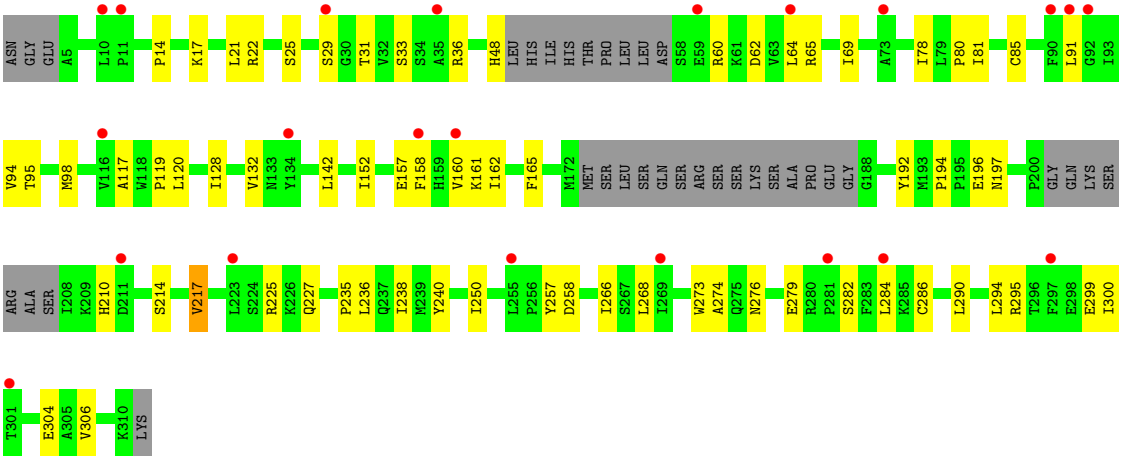
• Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

Chain O:



• Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	80.31Å 107.47Å 210.19Å 90.15° 89.77° 89.96°	Depositor
Resolution (Å)	47.90 – 2.89 47.90 – 2.89	Depositor EDS
% Data completeness (in resolution range)	88.4 (47.90-2.89) 87.8 (47.90-2.89)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.217 , 0.252 0.184 , 0.212	Depositor DCC
R_{free} test set	6905 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	73.9	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.366 for h,-k,-l 0.370 for -h,k,-l 0.417 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	35681	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 9XA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.53	0/2224	0.69	0/3040
1	B	0.51	0/2237	0.67	0/3056
1	C	0.52	0/2230	0.71	0/3048
1	D	0.53	0/2234	0.68	0/3052
1	E	0.54	0/2257	0.69	0/3079
1	F	0.52	0/2244	0.67	0/3063
1	G	0.51	0/2258	0.69	0/3082
1	H	0.50	0/2248	0.65	0/3069
1	I	0.52	0/2236	0.67	0/3054
1	J	0.51	0/2259	0.68	0/3081
1	K	0.52	0/2258	0.69	0/3081
1	L	0.51	0/2242	0.67	0/3063
1	M	0.51	0/2218	0.68	0/3033
1	N	0.51	0/2177	0.69	0/2981
1	O	0.52	0/2244	0.69	0/3064
1	P	0.52	0/2223	0.70	0/3040
All	All	0.52	0/35789	0.68	0/48886

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2165	0	2091	34	0
1	B	2177	0	2105	38	0
1	C	2170	0	2101	40	0
1	D	2174	0	2111	31	0
1	E	2197	0	2148	25	0
1	F	2184	0	2123	27	0
1	G	2198	0	2139	30	0
1	H	2188	0	2131	30	0
1	I	2176	0	2119	18	0
1	J	2199	0	2150	31	0
1	K	2198	0	2131	34	0
1	L	2182	0	2115	19	0
1	M	2159	0	2073	27	0
1	N	2118	0	2035	34	0
1	O	2185	0	2122	27	0
1	P	2163	0	2078	27	0
2	A	34	0	0	0	0
2	B	34	0	0	2	0
2	C	34	0	0	5	0
2	D	34	0	0	2	0
2	E	34	0	0	0	0
2	F	34	0	0	1	0
2	G	34	0	0	0	0
2	H	34	0	0	0	0
2	I	34	0	0	0	0
2	J	34	0	0	0	0
2	K	34	0	0	1	0
2	L	34	0	0	0	0
2	M	34	0	0	1	0
2	N	34	0	0	0	0
2	O	34	0	0	0	0
2	P	34	0	0	0	0
3	A	13	0	0	0	0
3	B	20	0	0	1	0
3	C	15	0	0	0	0
3	D	25	0	0	0	0
3	E	16	0	0	0	0
3	F	20	0	0	0	0
3	G	16	0	0	0	0
3	H	24	0	0	3	0
3	I	23	0	0	0	0
3	J	19	0	0	0	0
3	K	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	12	0	0	0	0
3	M	15	0	0	1	0
3	N	25	0	0	1	0
3	O	16	0	0	3	0
3	P	26	0	0	0	0
All	All	35681	0	33772	444	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (444) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:125:LEU:HD22	1:M:219:THR:HG22	1.47	0.95
1:J:236:LEU:HD21	1:M:235:PRO:HB2	1.50	0.93
1:N:290:LEU:O	1:N:293:VAL:HG12	1.77	0.85
1:A:157:GLU:HG2	1:B:157:GLU:HG2	1.56	0.85
1:M:157:GLU:HG2	1:N:157:GLU:HG2	1.61	0.83
1:I:157:GLU:HG2	1:J:157:GLU:HG2	1.61	0.82
1:A:219:THR:HG23	1:A:269:ILE:HG12	1.64	0.80
1:O:157:GLU:HG2	1:P:157:GLU:HG2	1.64	0.79
1:B:60:ARG:HG2	1:B:91:LEU:HD22	1.65	0.79
1:D:32:VAL:HG11	2:D:401:9XA:O29	1.82	0.78
1:G:157:GLU:HG2	1:H:157:GLU:HG2	1.67	0.76
1:H:60:ARG:HG3	1:H:91:LEU:HD22	1.70	0.74
1:K:288:ILE:HG22	1:L:41:ARG:NH1	2.03	0.73
1:K:17:LYS:HE3	1:K:39:ASP:OD2	1.91	0.70
1:J:98:MET:HE2	1:J:161:LYS:HB2	1.72	0.70
1:E:284:LEU:HD23	1:J:284:LEU:HD23	1.73	0.69
1:K:98:MET:HE2	1:K:161:LYS:HB2	1.74	0.69
1:K:157:GLU:HG2	1:L:157:GLU:HG2	1.74	0.69
1:M:103:LEU:HD22	1:M:152:ILE:HD11	1.75	0.69
1:K:284:LEU:HD23	1:M:284:LEU:HD23	1.75	0.69
1:A:192:TYR:HD1	1:A:217:VAL:HG23	1.59	0.68
1:G:98:MET:HE2	1:G:161:LYS:HB2	1.75	0.68
1:N:81:ILE:HA	1:N:95:THR:HG22	1.77	0.67
1:P:78:ILE:HD12	1:P:165:PHE:HZ	1.60	0.66
1:D:81:ILE:HA	1:D:95:THR:HG22	1.78	0.66
1:F:87:GLU:HB2	1:F:88:PRO:HD2	1.76	0.66
1:I:81:ILE:HA	1:I:95:THR:HG22	1.77	0.66
1:C:235:PRO:HA	1:C:238:ILE:HD12	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ILE:HA	1:C:95:THR:HG22	1.79	0.65
1:G:81:ILE:HA	1:G:95:THR:HG22	1.79	0.65
1:H:81:ILE:HA	1:H:95:THR:HG22	1.79	0.65
1:A:284:LEU:HD23	1:G:284:LEU:HD23	1.78	0.64
1:O:262:ARG:O	1:O:266:ILE:HG23	1.97	0.64
1:C:234:ASN:HB3	1:C:237:GLN:HB2	1.78	0.64
1:C:125:LEU:HD21	1:C:222:VAL:HG21	1.78	0.64
1:E:81:ILE:HA	1:E:95:THR:HG22	1.80	0.64
1:L:81:ILE:HA	1:L:95:THR:HG22	1.79	0.64
1:J:128:ILE:O	1:J:132:VAL:HG12	1.96	0.63
1:J:81:ILE:HA	1:J:95:THR:HG22	1.81	0.63
1:A:81:ILE:HA	1:A:95:THR:HG22	1.81	0.62
1:A:128:ILE:HG12	1:A:152:ILE:HD12	1.81	0.62
1:P:81:ILE:HA	1:P:95:THR:HG22	1.81	0.62
1:O:81:ILE:HA	1:O:95:THR:HG22	1.81	0.62
1:F:81:ILE:HA	1:F:95:THR:HG22	1.82	0.62
1:C:306:VAL:HA	1:C:309:LEU:HD22	1.82	0.62
1:B:81:ILE:HA	1:B:95:THR:HG22	1.81	0.62
1:C:229:PHE:O	1:C:232:VAL:HG12	2.00	0.62
1:J:194:PRO:HB2	1:J:196:GLU:OE1	2.00	0.61
1:C:194:PRO:HD2	1:C:210:HIS:CD2	2.34	0.61
1:A:192:TYR:HA	1:A:217:VAL:HG21	1.81	0.61
1:P:98:MET:HE2	1:P:161:LYS:HB2	1.82	0.61
1:M:128:ILE:HD11	1:M:152:ILE:HD12	1.83	0.61
1:F:128:ILE:O	1:F:132:VAL:HG12	2.00	0.61
1:C:101:GLY:HA2	2:C:401:9XA:C11	2.31	0.60
1:M:81:ILE:HA	1:M:95:THR:HG22	1.83	0.60
1:M:128:ILE:CD1	1:M:152:ILE:HD12	2.31	0.60
1:D:293:VAL:O	1:D:296:THR:HB	2.01	0.60
1:P:128:ILE:HG12	1:P:152:ILE:HD12	1.82	0.60
1:J:220:TRP:HH2	1:J:226:LYS:HE3	1.67	0.60
1:N:192:TYR:HA	1:N:217:VAL:HG11	1.84	0.60
1:K:81:ILE:HA	1:K:95:THR:HG22	1.84	0.59
1:K:158:PHE:CD1	1:K:306:VAL:HG23	2.37	0.59
1:A:158:PHE:HD2	1:A:306:VAL:HG13	1.66	0.59
1:H:123:ARG:HA	1:H:294:LEU:HD21	1.83	0.59
1:O:17:LYS:HD3	1:O:38:ALA:HB3	1.83	0.59
1:F:235:PRO:HA	1:F:238:ILE:HD12	1.85	0.59
1:E:235:PRO:HA	1:E:238:ILE:HD12	1.85	0.59
1:O:125:LEU:HD22	1:O:219:THR:CG2	2.32	0.58
1:E:128:ILE:O	1:E:132:VAL:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:LEU:O	1:B:293:VAL:HG12	2.02	0.58
1:D:158:PHE:CD1	1:D:306:VAL:HG23	2.38	0.58
1:M:199:GLU:OE2	1:M:200:PRO:HD2	2.03	0.58
1:J:158:PHE:CD1	1:J:306:VAL:HG23	2.39	0.58
1:O:125:LEU:HD22	1:O:219:THR:HG22	1.86	0.58
1:O:307:ILE:HG13	1:P:300:ILE:HD11	1.85	0.58
1:O:48:HIS:HB2	3:O:505:HOH:O	2.03	0.57
1:O:273:TRP:O	1:O:273:TRP:CD1	2.57	0.57
1:A:235:PRO:HA	1:A:238:ILE:HD12	1.86	0.57
1:C:232:VAL:HG11	1:C:238:ILE:HG12	1.87	0.57
1:F:25:SER:HB3	2:F:401:9XA:C32	2.34	0.57
1:I:115:ASP:HB2	1:I:308:GLN:OE1	2.05	0.56
1:M:235:PRO:HA	1:M:238:ILE:HD12	1.87	0.56
1:O:235:PRO:HA	1:O:238:ILE:HD12	1.85	0.56
1:B:235:PRO:HA	1:B:238:ILE:HD12	1.87	0.56
1:D:59:GLU:O	1:D:63:VAL:HG23	2.04	0.56
1:H:145:HIS:CE1	3:H:502:HOH:O	2.58	0.56
1:I:128:ILE:O	1:I:132:VAL:HG23	2.05	0.56
1:G:128:ILE:O	1:G:132:VAL:HG23	2.06	0.56
1:K:32:VAL:HG11	2:K:401:9XA:O29	2.05	0.56
1:L:125:LEU:HD22	1:L:219:THR:HG22	1.87	0.56
1:F:31:THR:HG23	1:F:48:HIS:CD2	2.41	0.56
2:C:401:9XA:C34	2:C:401:9XA:C4	2.84	0.55
1:F:104:ASN:HB2	1:F:149:THR:HG23	1.88	0.55
1:H:128:ILE:O	1:H:132:VAL:HG23	2.06	0.55
1:B:128:ILE:O	1:B:132:VAL:HG23	2.07	0.55
1:D:60:ARG:O	1:D:64:LEU:HD12	2.07	0.55
1:A:36:ARG:HH11	1:A:41:ARG:HG2	1.70	0.55
1:C:304:GLU:HA	1:C:307:ILE:HG22	1.88	0.55
1:H:158:PHE:CD2	1:H:306:VAL:HG23	2.42	0.55
1:N:152:ILE:HG23	1:N:160:VAL:CG2	2.36	0.55
1:P:78:ILE:HD13	1:P:162:ILE:HB	1.89	0.55
1:B:267:SER:HA	1:J:16:HIS:HB2	1.89	0.55
1:P:235:PRO:HA	1:P:238:ILE:HD12	1.89	0.55
1:I:123:ARG:HA	1:I:294:LEU:HD21	1.89	0.54
1:K:60:ARG:NH2	1:K:91:LEU:HB2	2.22	0.54
1:L:128:ILE:O	1:L:132:VAL:HG23	2.06	0.54
1:G:98:MET:CE	1:G:161:LYS:HG3	2.38	0.54
1:C:125:LEU:HD11	1:C:222:VAL:HG21	1.90	0.54
1:H:150:GLN:H	1:H:150:GLN:HE21	1.55	0.54
1:P:192:TYR:HA	1:P:217:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:63:VAL:HG22	1:N:91:LEU:HD21	1.89	0.54
1:E:65:ARG:O	1:E:69:ILE:HG12	2.08	0.54
1:J:98:MET:CE	1:J:161:LYS:HG3	2.38	0.54
1:P:128:ILE:O	1:P:132:VAL:HG23	2.07	0.54
1:C:128:ILE:O	1:C:132:VAL:HG23	2.08	0.54
1:E:117:ALA:HB1	1:E:119:PRO:HD2	1.90	0.54
1:A:128:ILE:O	1:A:132:VAL:HG23	2.06	0.53
1:D:14:PRO:HD2	1:D:17:LYS:HE2	1.91	0.53
1:O:245:GLY:HA2	1:O:275:GLN:OE1	2.08	0.53
1:P:117:ALA:HB1	1:P:119:PRO:HD2	1.90	0.53
1:E:58:SER:HB3	1:E:60:ARG:HG2	1.90	0.53
1:C:117:ALA:HB1	1:C:119:PRO:HD2	1.89	0.53
1:J:36:ARG:HG2	1:J:43:GLN:HA	1.90	0.53
1:H:105:GLU:O	1:H:109:ARG:HB2	2.08	0.53
1:K:216:ALA:HA	1:K:219:THR:HG22	1.91	0.53
1:D:122:PHE:O	1:D:294:LEU:HD11	2.09	0.53
1:B:24:LEU:HD22	2:B:401:9XA:C11	2.38	0.53
1:E:128:ILE:HG12	1:E:152:ILE:HD12	1.91	0.53
1:J:271:SER:OG	1:J:281:PRO:HD3	2.10	0.52
1:N:125:LEU:HD11	1:N:222:VAL:CG1	2.40	0.52
1:D:130:LEU:HD23	1:D:287:LEU:HD21	1.89	0.52
1:F:24:LEU:HD11	1:F:34:SER:HB3	1.91	0.52
1:F:298:GLU:HG3	1:F:301:THR:HG23	1.91	0.52
1:N:80:PRO:HD3	1:N:161:LYS:HD2	1.92	0.52
1:K:21:LEU:HA	1:K:34:SER:O	2.10	0.52
1:P:78:ILE:HD12	1:P:165:PHE:CZ	2.41	0.52
1:G:235:PRO:HA	1:G:238:ILE:HD12	1.92	0.52
1:M:24:LEU:HG	2:M:401:9XA:O30	2.10	0.52
1:N:125:LEU:HD11	1:N:222:VAL:HG11	1.91	0.52
1:A:192:TYR:CD1	1:A:217:VAL:HG23	2.41	0.52
1:C:259:ILE:HB	1:C:262:ARG:HG3	1.90	0.52
1:D:60:ARG:HG3	1:D:91:LEU:HD22	1.91	0.52
1:N:128:ILE:O	1:N:132:VAL:HG23	2.10	0.52
1:C:192:TYR:HA	1:C:217:VAL:HG11	1.91	0.52
1:K:98:MET:CE	1:K:161:LYS:HG3	2.40	0.51
1:B:33:SER:HB2	1:B:48:HIS:HE1	1.75	0.51
1:C:6:ILE:HD13	1:D:68:GLU:HG3	1.91	0.51
1:N:20:ASP:HB2	1:N:36:ARG:HD3	1.92	0.51
1:H:118:TRP:CH2	1:H:259:ILE:HG12	2.45	0.51
1:E:121:ARG:HH12	1:E:225:ARG:NE	2.09	0.51
1:H:298:GLU:HG3	1:H:301:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:245:GLY:HA2	1:M:275:GLN:OE1	2.08	0.51
1:B:46:VAL:HA	1:B:93:ILE:O	2.10	0.51
1:G:121:ARG:HH22	1:G:225:ARG:HG3	1.76	0.51
1:O:93:ILE:HD12	1:O:95:THR:HG23	1.92	0.51
1:G:121:ARG:NH2	1:G:225:ARG:HG3	2.26	0.51
1:D:290:LEU:O	1:D:293:VAL:HG13	2.10	0.51
1:K:128:ILE:O	1:K:132:VAL:HG23	2.10	0.51
1:H:117:ALA:HB1	1:H:119:PRO:HD2	1.92	0.51
1:G:143:LEU:HD22	1:G:145:HIS:NE2	2.26	0.50
1:M:128:ILE:O	1:M:132:VAL:HG23	2.12	0.50
1:P:194:PRO:HG3	1:P:210:HIS:HA	1.93	0.50
1:C:271:SER:O	1:C:280:ARG:HA	2.12	0.50
1:M:199:GLU:CD	1:M:200:PRO:HD2	2.31	0.50
1:B:32:VAL:HG11	2:B:401:9XA:C6	2.41	0.50
1:F:117:ALA:HB1	1:F:119:PRO:HD2	1.93	0.50
1:O:273:TRP:O	1:O:273:TRP:HD1	1.95	0.50
1:E:307:ILE:CD1	1:F:307:ILE:HG21	2.42	0.50
1:D:46:VAL:HG12	1:D:48:HIS:HD2	1.76	0.50
1:M:117:ALA:HB1	1:M:119:PRO:HD2	1.93	0.50
1:N:209:LYS:O	1:N:212:ILE:HG22	2.12	0.50
1:O:65:ARG:O	1:O:69:ILE:HG12	2.10	0.50
1:L:107:LEU:HD11	1:L:222:VAL:HG22	1.94	0.50
1:F:148:LYS:HG2	1:F:151:ASN:ND2	2.27	0.49
1:L:229:PHE:HB3	1:L:232:VAL:HG22	1.92	0.49
1:G:65:ARG:O	1:G:69:ILE:HG12	2.13	0.49
1:J:220:TRP:NE1	1:J:255:LEU:HD11	2.27	0.49
1:N:65:ARG:O	1:N:69:ILE:HG12	2.13	0.49
1:N:214:SER:O	1:N:217:VAL:HG13	2.13	0.49
1:A:192:TYR:HD1	1:A:217:VAL:CG2	2.24	0.49
1:J:291:GLU:HB3	1:J:295:ARG:HH21	1.76	0.49
1:K:117:ALA:HB1	1:K:119:PRO:HD2	1.95	0.49
1:N:299:GLU:HA	1:N:302:PHE:CD2	2.47	0.49
1:O:117:ALA:HB1	1:O:119:PRO:HD2	1.95	0.49
1:I:117:ALA:HB1	1:I:119:PRO:HD2	1.93	0.49
1:K:284:LEU:O	1:K:288:ILE:HG23	2.13	0.49
1:K:298:GLU:HG2	1:K:301:THR:HG23	1.95	0.49
1:M:80:PRO:HD3	1:M:161:LYS:HD2	1.95	0.49
1:B:117:ALA:HB1	1:B:119:PRO:HD2	1.94	0.49
1:J:235:PRO:HA	1:J:238:ILE:HD12	1.94	0.49
1:P:214:SER:O	1:P:217:VAL:HG13	2.13	0.49
1:N:229:PHE:HB3	1:N:232:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:PRO:HD2	1:C:17:LYS:HG3	1.95	0.49
1:G:291:GLU:O	1:G:295:ARG:HG2	2.12	0.49
1:A:80:PRO:HD3	1:A:161:LYS:HD2	1.95	0.49
1:D:298:GLU:HG2	1:D:301:THR:HG23	1.94	0.49
1:H:59:GLU:HA	1:H:62:ASP:OD2	2.13	0.49
1:M:137:ASN:ND2	1:N:39:ASP:HB3	2.28	0.49
1:E:80:PRO:HD3	1:E:161:LYS:HD2	1.95	0.48
1:J:198:TYR:HB2	1:J:199:GLU:OE2	2.13	0.48
1:N:277:PRO:HB2	3:N:505:HOH:O	2.12	0.48
1:C:65:ARG:O	1:C:69:ILE:HG12	2.13	0.48
1:D:116:VAL:HG12	1:D:309:LEU:HD21	1.95	0.48
1:D:117:ALA:HB1	1:D:119:PRO:HD2	1.95	0.48
1:K:17:LYS:HE3	1:K:39:ASP:CG	2.32	0.48
1:G:148:LYS:HG3	1:G:150:GLN:HB2	1.94	0.48
1:A:117:ALA:HB1	1:A:119:PRO:HD2	1.96	0.48
1:D:235:PRO:HA	1:D:238:ILE:HD12	1.95	0.48
1:E:75:PHE:HB3	1:E:78:ILE:HG12	1.95	0.48
1:G:117:ALA:HB1	1:G:119:PRO:HD2	1.95	0.48
1:K:216:ALA:O	1:K:219:THR:HG22	2.13	0.48
1:L:46:VAL:HG12	1:L:48:HIS:HD2	1.79	0.48
1:O:15:TYR:HA	1:O:18:LEU:HD12	1.95	0.48
1:B:14:PRO:HD2	1:B:17:LYS:HG3	1.96	0.48
1:C:46:VAL:HG22	1:C:48:HIS:HD2	1.78	0.48
1:D:128:ILE:O	1:D:132:VAL:HG23	2.13	0.48
1:C:190:ILE:HD12	1:C:239:MET:SD	2.54	0.47
1:M:193:MET:HE2	1:M:197:ASN:HB3	1.95	0.47
1:G:116:VAL:HG12	1:G:309:LEU:HD21	1.95	0.47
1:B:257:TYR:HA	1:B:262:ARG:HD2	1.96	0.47
1:E:157:GLU:HB3	1:F:157:GLU:HG2	1.96	0.47
1:J:236:LEU:HD21	1:M:235:PRO:CB	2.35	0.47
1:G:198:TYR:O	1:G:199:GLU:HG3	2.14	0.47
1:H:46:VAL:HG12	1:H:48:HIS:HD2	1.79	0.47
1:H:122:PHE:O	1:H:294:LEU:HD11	2.15	0.47
1:A:157:GLU:HG2	1:B:157:GLU:CG	2.38	0.47
1:A:192:TYR:CD1	1:A:217:VAL:CG2	2.98	0.47
1:F:85:CYS:O	1:F:91:LEU:HA	2.15	0.47
1:H:235:PRO:HB2	1:P:236:LEU:HD22	1.96	0.47
1:A:157:GLU:CG	1:B:157:GLU:HG2	2.37	0.46
1:H:264:ARG:HH11	1:H:289:GLU:HG3	1.79	0.46
1:K:235:PRO:HA	1:K:238:ILE:HD12	1.96	0.46
1:B:24:LEU:HD11	1:B:34:SER:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:ARG:O	1:F:69:ILE:HG12	2.15	0.46
1:N:299:GLU:HA	1:N:302:PHE:HD2	1.80	0.46
1:K:247:ARG:HG3	1:K:273:TRP:CD1	2.50	0.46
1:O:257:TYR:HA	1:O:262:ARG:HD2	1.98	0.46
1:L:121:ARG:O	1:L:125:LEU:HG	2.15	0.46
1:L:218:ILE:O	1:L:222:VAL:HG23	2.16	0.46
1:N:85:CYS:O	1:N:91:LEU:HA	2.16	0.46
1:F:14:PRO:HD2	1:F:17:LYS:HG3	1.97	0.46
1:O:246:HIS:HA	3:O:507:HOH:O	2.15	0.46
1:B:138:MET:CE	1:B:142:LEU:HB3	2.46	0.46
1:C:158:PHE:CD2	1:C:306:VAL:HG13	2.51	0.46
1:I:14:PRO:HD2	1:I:17:LYS:HG3	1.98	0.46
1:N:98:MET:HE2	1:N:161:LYS:HB2	1.98	0.46
1:O:192:TYR:HB3	1:O:214:SER:HB3	1.98	0.46
1:B:18:LEU:HB3	1:B:21:LEU:HD12	1.98	0.46
1:N:127:GLU:HB3	1:N:160:VAL:CG1	2.46	0.46
1:H:14:PRO:HD2	1:H:17:LYS:HG3	1.98	0.46
1:L:14:PRO:HD2	1:L:17:LYS:HG3	1.98	0.46
1:N:119:PRO:HG2	1:N:301:THR:HG22	1.97	0.46
1:N:127:GLU:HB3	1:N:160:VAL:HG12	1.97	0.46
1:P:65:ARG:O	1:P:69:ILE:HG12	2.16	0.46
1:E:14:PRO:HD2	1:E:17:LYS:HG3	1.98	0.45
1:K:121:ARG:HH11	1:K:225:ARG:HD2	1.81	0.45
1:K:123:ARG:HA	1:K:294:LEU:HD21	1.98	0.45
1:P:152:ILE:HD13	1:P:162:ILE:HG12	1.98	0.45
1:E:36:ARG:NH2	1:E:41:ARG:HG2	2.31	0.45
1:H:85:CYS:O	1:H:91:LEU:HA	2.16	0.45
1:I:235:PRO:HA	1:I:238:ILE:HD12	1.97	0.45
1:O:85:CYS:O	1:O:91:LEU:HA	2.16	0.45
1:C:32:VAL:HG11	2:C:401:9XA:C6	2.47	0.45
1:E:245:GLY:HA2	1:E:275:GLN:OE1	2.17	0.45
1:G:194:PRO:HG3	1:G:210:HIS:HA	1.98	0.45
1:O:132:VAL:HG21	1:O:147:LEU:HD21	1.97	0.45
1:O:144:HIS:ND1	1:O:147:LEU:HD13	2.31	0.45
1:C:158:PHE:HD2	1:C:306:VAL:HG13	1.80	0.45
1:C:268:LEU:HD21	1:C:286:CYS:HA	1.98	0.45
1:I:158:PHE:CD2	1:I:306:VAL:HG23	2.52	0.45
1:N:232:VAL:HG21	1:N:238:ILE:HB	1.98	0.45
1:A:265:MET:O	1:A:269:ILE:HG13	2.16	0.45
1:E:85:CYS:O	1:E:91:LEU:HA	2.16	0.45
1:J:259:ILE:HA	1:J:260:PRO:HD3	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:60:ARG:O	1:K:64:LEU:HD12	2.17	0.45
1:P:250:ILE:HD13	1:P:266:ILE:HG23	1.98	0.45
1:D:65:ARG:O	1:D:69:ILE:HG12	2.17	0.45
1:D:80:PRO:HD3	1:D:161:LYS:HD2	1.99	0.45
1:E:198:TYR:CZ	1:E:239:MET:HG2	2.52	0.45
1:K:14:PRO:HD2	1:K:17:LYS:HG3	1.98	0.45
1:K:266:ILE:O	1:K:270:GLU:HG2	2.16	0.45
1:A:14:PRO:HD2	1:A:17:LYS:HG3	1.98	0.45
1:M:257:TYR:HA	1:M:262:ARG:HD2	1.99	0.45
1:G:294:LEU:HA	1:G:297:PHE:CD2	2.52	0.45
1:L:232:VAL:HG21	1:L:238:ILE:HG12	1.99	0.45
1:O:80:PRO:HD3	1:O:161:LYS:HD2	1.98	0.45
1:O:276:ASN:HB3	1:O:279:GLU:HB2	1.99	0.45
1:G:80:PRO:HD3	1:G:161:LYS:HD2	1.99	0.45
1:I:306:VAL:HA	1:I:309:LEU:HD12	1.99	0.45
1:J:252:GLU:HB3	1:J:257:TYR:CE1	2.52	0.45
1:P:33:SER:HB2	1:P:48:HIS:HE1	1.82	0.45
1:C:294:LEU:HA	1:C:297:PHE:CE2	2.52	0.45
1:K:65:ARG:O	1:K:69:ILE:HG12	2.17	0.44
1:A:6:ILE:O	1:B:9:ALA:HA	2.17	0.44
1:E:23:TYR:CD1	1:E:23:TYR:N	2.84	0.44
1:G:118:TRP:CH2	1:G:259:ILE:HG12	2.52	0.44
1:E:36:ARG:HH21	1:E:41:ARG:HG2	1.81	0.44
1:F:16:HIS:HE1	1:F:17:LYS:HE3	1.82	0.44
1:F:16:HIS:CE1	1:F:17:LYS:HE3	2.53	0.44
1:I:80:PRO:HD3	1:I:161:LYS:HD2	1.99	0.44
1:J:152:ILE:HG23	1:J:160:VAL:HG13	2.00	0.44
1:B:250:ILE:HD13	1:B:266:ILE:HG23	2.00	0.44
1:F:306:VAL:HA	1:F:309:LEU:HD12	2.00	0.44
1:K:98:MET:HE2	1:K:161:LYS:CB	2.45	0.44
1:B:261:HIS:ND1	1:B:293:VAL:HG23	2.33	0.44
1:B:29:SER:HB3	3:B:507:HOH:O	2.17	0.44
1:F:80:PRO:HD3	1:F:161:LYS:HD2	1.99	0.44
1:F:148:LYS:HB3	1:F:192:TYR:CD2	2.52	0.44
1:G:143:LEU:HD21	1:G:208:ILE:HA	2.00	0.44
1:G:294:LEU:HA	1:G:297:PHE:HD2	1.83	0.44
1:H:273:TRP:CD1	1:H:273:TRP:C	2.91	0.44
1:M:85:CYS:O	1:M:91:LEU:HA	2.17	0.44
1:I:16:HIS:CE1	1:I:17:LYS:HE2	2.53	0.44
1:K:300:ILE:HD11	1:L:307:ILE:HG13	1.99	0.44
1:P:152:ILE:HG23	1:P:160:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LEU:HD22	1:B:42:VAL:HG13	1.99	0.43
1:B:85:CYS:O	1:B:91:LEU:HA	2.17	0.43
1:C:273:TRP:O	1:C:273:TRP:CD1	2.71	0.43
1:D:85:CYS:O	1:D:91:LEU:HA	2.18	0.43
1:D:196:GLU:H	1:D:196:GLU:HG3	1.60	0.43
1:M:17:LYS:HD3	1:M:38:ALA:HB3	2.00	0.43
1:G:46:VAL:HG12	1:G:48:HIS:HD2	1.82	0.43
1:P:85:CYS:O	1:P:91:LEU:HA	2.18	0.43
1:B:46:VAL:HB	1:B:94:VAL:HB	2.01	0.43
1:D:32:VAL:CG1	2:D:401:9XA:O29	2.62	0.43
1:H:250:ILE:HD13	1:H:266:ILE:HG23	2.00	0.43
1:J:65:ARG:O	1:J:69:ILE:HG12	2.17	0.43
1:J:98:MET:HE2	1:J:161:LYS:CB	2.43	0.43
1:K:85:CYS:O	1:K:91:LEU:HA	2.17	0.43
1:P:276:ASN:HB3	1:P:279:GLU:HB2	1.99	0.43
1:H:306:VAL:HA	1:H:309:LEU:HD12	2.00	0.43
1:J:193:MET:CE	1:J:197:ASN:HB3	2.48	0.43
1:K:80:PRO:HD3	1:K:161:LYS:HD2	1.99	0.43
1:L:85:CYS:O	1:L:91:LEU:HA	2.17	0.43
1:N:79:LEU:HA	1:N:80:PRO:HD3	1.94	0.43
1:B:306:VAL:HA	1:B:309:LEU:HD12	2.01	0.43
1:C:135:LEU:HD22	1:C:142:LEU:HD12	1.99	0.43
1:D:16:HIS:HB2	1:N:285:LYS:HD3	2.01	0.43
1:D:212:ILE:HG12	1:D:281:PRO:O	2.19	0.43
1:I:85:CYS:O	1:I:91:LEU:HA	2.18	0.43
1:I:236:LEU:HD22	1:I:240:TYR:CE2	2.53	0.43
1:L:250:ILE:HD13	1:L:266:ILE:HG23	2.01	0.43
1:P:14:PRO:HD2	1:P:17:LYS:HG3	2.01	0.43
1:B:80:PRO:HD3	1:B:161:LYS:HD2	2.00	0.43
1:M:231:ASP:HA	3:M:509:HOH:O	2.18	0.43
1:N:117:ALA:HB1	1:N:119:PRO:HD2	1.99	0.43
1:P:80:PRO:HD3	1:P:161:LYS:HD2	2.00	0.43
1:B:292:PRO:HA	1:B:295:ARG:HB2	2.01	0.43
1:F:304:GLU:O	1:F:307:ILE:HG13	2.18	0.43
1:G:257:TYR:HA	1:G:262:ARG:HD2	2.01	0.43
1:A:85:CYS:O	1:A:91:LEU:HA	2.18	0.43
1:C:85:CYS:O	1:C:91:LEU:HA	2.18	0.43
1:A:250:ILE:HD13	1:A:266:ILE:HG23	2.00	0.43
1:B:116:VAL:HG12	1:B:309:LEU:HD21	2.01	0.43
1:C:125:LEU:HD11	1:C:222:VAL:CG2	2.49	0.43
1:F:250:ILE:HD13	1:F:266:ILE:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:16:HIS:HE1	1:I:17:LYS:HE2	1.83	0.43
1:L:118:TRP:O	1:L:122:PHE:HD2	2.01	0.43
1:B:195:PRO:HA	1:B:198:TYR:CE2	2.54	0.42
1:E:298:GLU:HG3	1:E:301:THR:HG23	2.01	0.42
1:G:252:GLU:HB3	1:G:257:TYR:CE1	2.54	0.42
1:A:79:LEU:HA	1:A:80:PRO:HD3	1.91	0.42
1:N:118:TRP:CH2	1:N:259:ILE:HG12	2.54	0.42
1:D:212:ILE:HD12	1:D:212:ILE:HA	1.94	0.42
1:A:216:ALA:HA	1:A:219:THR:HG22	2.00	0.42
1:B:60:ARG:O	1:B:63:VAL:HG13	2.19	0.42
1:B:304:GLU:O	1:B:307:ILE:HG22	2.19	0.42
1:A:46:VAL:HG12	1:A:48:HIS:HD2	1.84	0.42
1:B:299:GLU:H	1:B:299:GLU:CD	2.23	0.42
1:C:273:TRP:O	1:C:273:TRP:HD1	2.02	0.42
1:J:194:PRO:HG3	1:J:210:HIS:HA	2.00	0.42
1:E:125:LEU:HD13	1:E:219:THR:HG23	2.02	0.42
1:A:158:PHE:CD2	1:A:306:VAL:HG13	2.49	0.42
1:D:14:PRO:HD2	1:D:17:LYS:CE	2.48	0.42
1:F:149:THR:HG21	1:F:221:GLU:OE2	2.20	0.42
1:G:79:LEU:HA	1:G:80:PRO:HD3	1.90	0.42
1:B:125:LEU:HD13	1:B:219:THR:HG23	2.01	0.42
1:H:65:ARG:O	1:H:69:ILE:HG12	2.20	0.42
1:I:65:ARG:O	1:I:69:ILE:HG12	2.19	0.42
1:I:250:ILE:HD13	1:I:266:ILE:HG23	2.02	0.42
1:J:74:ARG:HE	1:J:74:ARG:HB3	1.47	0.42
1:M:277:PRO:HA	1:M:280:ARG:HE	1.84	0.42
1:J:193:MET:HE2	1:J:197:ASN:HB3	2.01	0.42
1:K:158:PHE:HD1	1:K:306:VAL:HG23	1.84	0.42
1:M:272:GLY:HA2	1:M:281:PRO:HD2	2.02	0.42
1:A:65:ARG:O	1:A:69:ILE:HG12	2.19	0.42
1:N:250:ILE:HD13	1:N:266:ILE:HG23	2.00	0.42
1:A:158:PHE:CZ	1:A:309:LEU:HD23	2.55	0.41
1:A:198:TYR:OH	1:A:242:VAL:HG21	2.20	0.41
1:C:101:GLY:HA2	2:C:401:9XA:C34	2.50	0.41
1:D:24:LEU:HD11	1:D:34:SER:HB3	2.02	0.41
1:H:272:GLY:O	1:H:280:ARG:HG2	2.20	0.41
1:C:149:THR:HG22	1:C:218:ILE:HG23	2.01	0.41
1:L:194:PRO:HG3	1:L:210:HIS:HA	2.01	0.41
1:M:118:TRP:CH2	1:M:259:ILE:HG12	2.56	0.41
1:O:125:LEU:HD22	1:O:219:THR:HG23	2.01	0.41
1:C:250:ILE:HD13	1:C:266:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:257:TYR:HA	1:F:262:ARG:HD2	2.02	0.41
1:G:98:MET:HE2	1:G:161:LYS:CB	2.46	0.41
1:C:153:LEU:HD11	2:C:401:9XA:C20	2.50	0.41
1:E:262:ARG:O	1:E:266:ILE:HG12	2.20	0.41
1:F:265:MET:O	1:F:269:ILE:HG13	2.20	0.41
1:G:85:CYS:O	1:G:91:LEU:HA	2.20	0.41
1:J:46:VAL:HG12	1:J:48:HIS:HD2	1.85	0.41
1:L:106:LEU:HA	1:L:113:TYR:CD2	2.55	0.41
1:B:152:ILE:HG23	1:B:160:VAL:HG13	2.03	0.41
1:E:220:TRP:CH2	1:E:226:LYS:HG3	2.55	0.41
1:G:307:ILE:HD12	1:H:303:LEU:HB3	2.03	0.41
1:H:195:PRO:HB3	1:H:242:VAL:HG12	2.02	0.41
1:B:198:TYR:HE2	1:B:242:VAL:CG2	2.34	0.41
1:H:291:GLU:HB3	3:H:520:HOH:O	2.20	0.41
1:C:199:GLU:HB2	1:C:200:PRO:HD2	2.03	0.41
1:J:80:PRO:HD3	1:J:161:LYS:HD2	2.02	0.41
1:A:152:ILE:HG23	1:A:160:VAL:HG13	2.02	0.41
1:H:152:ILE:HG23	1:H:160:VAL:HG13	2.02	0.41
1:C:71:HIS:ND1	1:C:74:ARG:NH2	2.69	0.41
1:C:190:ILE:H	1:C:190:ILE:HG12	1.65	0.41
1:D:123:ARG:HA	1:D:294:LEU:HD21	2.02	0.41
1:E:242:VAL:HA	1:E:246:HIS:O	2.21	0.41
1:J:85:CYS:O	1:J:91:LEU:HA	2.20	0.41
1:N:107:LEU:HD21	1:N:222:VAL:HG23	2.01	0.41
1:N:123:ARG:HA	1:N:294:LEU:HD21	2.03	0.41
1:N:306:VAL:HA	1:N:309:LEU:HD12	2.03	0.41
1:O:192:TYR:HB2	3:O:512:HOH:O	2.20	0.41
1:I:152:ILE:HG23	1:I:160:VAL:HG13	2.03	0.41
1:K:152:ILE:HG23	1:K:160:VAL:HG13	2.03	0.41
1:L:65:ARG:O	1:L:69:ILE:HG12	2.20	0.41
1:N:108:HIS:CE1	1:N:227:GLN:HE21	2.39	0.41
1:P:158:PHE:CD1	1:P:306:VAL:HG13	2.56	0.41
1:C:46:VAL:HA	1:C:93:ILE:O	2.21	0.40
1:P:286:CYS:O	1:P:290:LEU:HD12	2.20	0.40
1:A:118:TRP:CH2	1:A:259:ILE:HG12	2.56	0.40
1:D:284:LEU:HD21	1:O:288:ILE:HD13	2.04	0.40
1:G:21:LEU:HA	1:G:34:SER:O	2.22	0.40
1:H:198:TYR:HB3	1:P:240:TYR:CD2	2.56	0.40
1:A:307:ILE:HG22	1:B:303:LEU:HB3	2.03	0.40
1:F:125:LEU:HD13	1:F:219:THR:HG23	2.03	0.40
1:J:116:VAL:HG12	1:J:120:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:99:PRO:HG2	1:K:156:ASN:HB2	2.04	0.40
1:K:126:HIS:HB2	1:K:294:LEU:HD11	2.02	0.40
1:D:79:LEU:HA	1:D:80:PRO:HD3	1.92	0.40
1:M:103:LEU:HD21	1:M:222:VAL:HG22	2.03	0.40
1:C:126:HIS:HB2	1:C:294:LEU:HD11	2.01	0.40
1:H:145:HIS:HE1	3:H:502:HOH:O	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	267/310 (86%)	255 (96%)	12 (4%)	0	100	100
1	B	267/310 (86%)	255 (96%)	12 (4%)	0	100	100
1	C	267/310 (86%)	256 (96%)	9 (3%)	2 (1%)	22	54
1	D	267/310 (86%)	260 (97%)	7 (3%)	0	100	100
1	E	267/310 (86%)	255 (96%)	11 (4%)	1 (0%)	34	66
1	F	267/310 (86%)	254 (95%)	12 (4%)	1 (0%)	34	66
1	G	267/310 (86%)	258 (97%)	9 (3%)	0	100	100
1	H	267/310 (86%)	257 (96%)	10 (4%)	0	100	100
1	I	267/310 (86%)	255 (96%)	12 (4%)	0	100	100
1	J	267/310 (86%)	258 (97%)	9 (3%)	0	100	100
1	K	267/310 (86%)	256 (96%)	11 (4%)	0	100	100
1	L	267/310 (86%)	259 (97%)	8 (3%)	0	100	100
1	M	268/310 (86%)	257 (96%)	10 (4%)	1 (0%)	34	66
1	N	264/310 (85%)	252 (96%)	10 (4%)	2 (1%)	19	51
1	O	268/310 (86%)	259 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	267/310 (86%)	255 (96%)	10 (4%)	2 (1%)	22	54
All	All	4271/4960 (86%)	4101 (96%)	161 (4%)	9 (0%)	47	78

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	61	LYS
1	P	299	GLU
1	N	209	LYS
1	C	198	TYR
1	C	299	GLU
1	E	299	GLU
1	N	299	GLU
1	F	61	LYS
1	P	274	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/279 (83%)	212 (92%)	19 (8%)	11	32
1	B	232/279 (83%)	215 (93%)	17 (7%)	14	38
1	C	231/279 (83%)	202 (87%)	29 (13%)	4	13
1	D	231/279 (83%)	206 (89%)	25 (11%)	6	20
1	E	237/279 (85%)	217 (92%)	20 (8%)	11	31
1	F	233/279 (84%)	216 (93%)	17 (7%)	14	38
1	G	237/279 (85%)	220 (93%)	17 (7%)	14	39
1	H	235/279 (84%)	220 (94%)	15 (6%)	17	45
1	I	232/279 (83%)	210 (90%)	22 (10%)	8	26
1	J	237/279 (85%)	220 (93%)	17 (7%)	14	39
1	K	237/279 (85%)	214 (90%)	23 (10%)	8	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	234/279 (84%)	210 (90%)	24 (10%)	7 22
1	M	227/279 (81%)	211 (93%)	16 (7%)	15 41
1	N	222/279 (80%)	202 (91%)	20 (9%)	9 29
1	O	234/279 (84%)	213 (91%)	21 (9%)	9 29
1	P	230/279 (82%)	204 (89%)	26 (11%)	6 18
All	All	3720/4464 (83%)	3392 (91%)	328 (9%)	10 30

All (328) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	25	SER
1	A	29	SER
1	A	36	ARG
1	A	44	VAL
1	A	64	LEU
1	A	94	VAL
1	A	139	THR
1	A	142	LEU
1	A	150	GLN
1	A	197	ASN
1	A	199	GLU
1	A	227	GLN
1	A	232	VAL
1	A	258	ASP
1	A	262	ARG
1	A	268	LEU
1	A	273	TRP
1	A	300	ILE
1	B	21	LEU
1	B	31	THR
1	B	36	ARG
1	B	46	VAL
1	B	63	VAL
1	B	64	LEU
1	B	94	VAL
1	B	142	LEU
1	B	197	ASN
1	B	227	GLN
1	B	231	ASP

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Mol	Chain	Res	Type
1	B	258	ASP
1	B	268	LEU
1	B	273	TRP
1	B	289	GLU
1	B	296	THR
1	B	307	ILE
1	C	6	ILE
1	C	21	LEU
1	C	25	SER
1	C	29	SER
1	C	36	ARG
1	C	46	VAL
1	C	62	ASP
1	C	63	VAL
1	C	64	LEU
1	C	106	LEU
1	C	115	ASP
1	C	120	LEU
1	C	190	ILE
1	C	197	ASN
1	C	210	HIS
1	C	217	VAL
1	C	227	GLN
1	C	231	ASP
1	C	232	VAL
1	C	247	ARG
1	C	258	ASP
1	C	262	ARG
1	C	273	TRP
1	C	289	GLU
1	C	294	LEU
1	C	297	PHE
1	C	300	ILE
1	C	304	GLU
1	C	309	LEU
1	D	21	LEU
1	D	25	SER
1	D	31	THR
1	D	36	ARG
1	D	41	ARG
1	D	58	SER
1	D	60	ARG

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Mol	Chain	Res	Type
1	D	64	LEU
1	D	94	VAL
1	D	142	LEU
1	D	196	GLU
1	D	197	ASN
1	D	227	GLN
1	D	258	ASP
1	D	262	ARG
1	D	267	SER
1	D	268	LEU
1	D	273	TRP
1	D	284	LEU
1	D	293	VAL
1	D	294	LEU
1	D	295	ARG
1	D	296	THR
1	D	300	ILE
1	D	307	ILE
1	E	21	LEU
1	E	25	SER
1	E	29	SER
1	E	36	ARG
1	E	59	GLU
1	E	65	ARG
1	E	76	SER
1	E	142	LEU
1	E	199	GLU
1	E	214	SER
1	E	226	LYS
1	E	255	LEU
1	E	258	ASP
1	E	262	ARG
1	E	267	SER
1	E	268	LEU
1	E	273	TRP
1	E	285	LYS
1	E	298	GLU
1	E	299	GLU
1	F	20	ASP
1	F	21	LEU
1	F	29	SER
1	F	32	VAL

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Mol	Chain	Res	Type
1	F	64	LEU
1	F	87	GLU
1	F	115	ASP
1	F	132	VAL
1	F	142	LEU
1	F	148	LYS
1	F	226	LYS
1	F	236	LEU
1	F	255	LEU
1	F	258	ASP
1	F	268	LEU
1	F	273	TRP
1	F	289	GLU
1	G	20	ASP
1	G	29	SER
1	G	36	ARG
1	G	59	GLU
1	G	60	ARG
1	G	64	LEU
1	G	74	ARG
1	G	115	ASP
1	G	142	LEU
1	G	143	LEU
1	G	198	TYR
1	G	227	GLN
1	G	258	ASP
1	G	267	SER
1	G	268	LEU
1	G	273	TRP
1	G	298	GLU
1	H	21	LEU
1	H	29	SER
1	H	36	ARG
1	H	64	LEU
1	H	142	LEU
1	H	150	GLN
1	H	197	ASN
1	H	227	GLN
1	H	258	ASP
1	H	262	ARG
1	H	268	LEU
1	H	273	TRP

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Mol	Chain	Res	Type
1	H	289	GLU
1	H	294	LEU
1	H	295	ARG
1	I	21	LEU
1	I	22	ARG
1	I	25	SER
1	I	36	ARG
1	I	64	LEU
1	I	123	ARG
1	I	142	LEU
1	I	150	GLN
1	I	189	THR
1	I	190	ILE
1	I	197	ASN
1	I	225	ARG
1	I	227	GLN
1	I	231	ASP
1	I	236	LEU
1	I	241	SER
1	I	258	ASP
1	I	262	ARG
1	I	268	LEU
1	I	273	TRP
1	I	289	GLU
1	I	295	ARG
1	J	20	ASP
1	J	21	LEU
1	J	29	SER
1	J	59	GLU
1	J	64	LEU
1	J	74	ARG
1	J	116	VAL
1	J	125	LEU
1	J	142	LEU
1	J	197	ASN
1	J	227	GLN
1	J	258	ASP
1	J	259	ILE
1	J	262	ARG
1	J	268	LEU
1	J	273	TRP
1	J	301	THR

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Mol	Chain	Res	Type
1	K	17	LYS
1	K	21	LEU
1	K	24	LEU
1	K	25	SER
1	K	29	SER
1	K	31	THR
1	K	41	ARG
1	K	58	SER
1	K	59	GLU
1	K	63	VAL
1	K	64	LEU
1	K	142	LEU
1	K	150	GLN
1	K	197	ASN
1	K	227	GLN
1	K	258	ASP
1	K	262	ARG
1	K	267	SER
1	K	268	LEU
1	K	273	TRP
1	K	288	ILE
1	K	293	VAL
1	K	294	LEU
1	L	21	LEU
1	L	25	SER
1	L	29	SER
1	L	36	ARG
1	L	65	ARG
1	L	106	LEU
1	L	115	ASP
1	L	123	ARG
1	L	142	LEU
1	L	190	ILE
1	L	223	LEU
1	L	227	GLN
1	L	236	LEU
1	L	243	SER
1	L	258	ASP
1	L	262	ARG
1	L	268	LEU
1	L	273	TRP
1	L	289	GLU

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Mol	Chain	Res	Type
1	L	295	ARG
1	L	297	PHE
1	L	300	ILE
1	L	301	THR
1	L	307	ILE
1	M	21	LEU
1	M	29	SER
1	M	59	GLU
1	M	115	ASP
1	M	124	ILE
1	M	142	LEU
1	M	197	ASN
1	M	217	VAL
1	M	227	GLN
1	M	258	ASP
1	M	267	SER
1	M	268	LEU
1	M	273	TRP
1	M	285	LYS
1	M	289	GLU
1	M	299	GLU
1	N	21	LEU
1	N	31	THR
1	N	62	ASP
1	N	64	LEU
1	N	65	ARG
1	N	120	LEU
1	N	142	LEU
1	N	150	GLN
1	N	160	VAL
1	N	197	ASN
1	N	217	VAL
1	N	227	GLN
1	N	238	ILE
1	N	258	ASP
1	N	273	TRP
1	N	284	LEU
1	N	289	GLU
1	N	294	LEU
1	N	296	THR
1	N	299	GLU
1	O	21	LEU

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Mol	Chain	Res	Type
1	O	25	SER
1	O	36	ARG
1	O	64	LEU
1	O	93	ILE
1	O	105	GLU
1	O	142	LEU
1	O	147	LEU
1	O	197	ASN
1	O	214	SER
1	O	219	THR
1	O	226	LYS
1	O	227	GLN
1	O	258	ASP
1	O	266	ILE
1	O	267	SER
1	O	268	LEU
1	O	273	TRP
1	O	285	LYS
1	O	289	GLU
1	O	294	LEU
1	P	21	LEU
1	P	22	ARG
1	P	25	SER
1	P	29	SER
1	P	31	THR
1	P	36	ARG
1	P	60	ARG
1	P	62	ASP
1	P	64	LEU
1	P	94	VAL
1	P	120	LEU
1	P	142	LEU
1	P	196	GLU
1	P	197	ASN
1	P	217	VAL
1	P	225	ARG
1	P	227	GLN
1	P	257	TYR
1	P	258	ASP
1	P	268	LEU
1	P	273	TRP
1	P	282	SER

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Mol	Chain	Res	Type
1	P	284	LEU
1	P	294	LEU
1	P	295	ARG
1	P	304	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	C	210	HIS
1	C	244	GLN
1	D	108	HIS
1	D	151	ASN
1	D	227	GLN
1	F	151	ASN
1	F	197	ASN
1	G	108	HIS
1	G	210	HIS
1	G	227	GLN
1	H	16	HIS
1	H	104	ASN
1	H	150	GLN
1	I	104	ASN
1	I	150	GLN
1	I	244	GLN
1	K	150	GLN
1	M	43	GLN
1	M	48	HIS
1	M	108	HIS
1	M	137	ASN
1	M	227	GLN
1	N	108	HIS
1	N	150	GLN
1	N	227	GLN
1	N	237	GLN
1	P	137	ASN
1	P	197	ASN
1	P	261	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	9XA	B	401	-	35,37,37	2.64	9 (25%)	45,56,56	2.60	18 (40%)
2	9XA	A	401	-	35,37,37	2.66	9 (25%)	45,56,56	2.79	20 (44%)
2	9XA	L	401	-	35,37,37	2.54	8 (22%)	45,56,56	2.53	15 (33%)
2	9XA	H	401	-	35,37,37	2.69	11 (31%)	45,56,56	2.51	16 (35%)
2	9XA	C	401	-	35,37,37	2.82	13 (37%)	45,56,56	3.71	19 (42%)
2	9XA	K	401	-	35,37,37	2.52	7 (20%)	45,56,56	2.35	18 (40%)
2	9XA	N	401	-	35,37,37	2.61	9 (25%)	45,56,56	2.59	18 (40%)
2	9XA	I	401	-	35,37,37	2.66	10 (28%)	45,56,56	2.60	19 (42%)
2	9XA	J	401	-	35,37,37	2.71	10 (28%)	45,56,56	2.97	18 (40%)
2	9XA	G	401	-	35,37,37	2.67	8 (22%)	45,56,56	2.88	17 (37%)
2	9XA	E	401	-	35,37,37	2.70	9 (25%)	45,56,56	2.50	19 (42%)
2	9XA	F	401	-	35,37,37	2.60	9 (25%)	45,56,56	2.85	20 (44%)
2	9XA	O	401	-	35,37,37	2.59	9 (25%)	45,56,56	2.68	21 (46%)
2	9XA	D	401	-	35,37,37	2.53	9 (25%)	45,56,56	2.43	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	9XA	M	401	-	35,37,37	2.61	8 (22%)	45,56,56	2.69	20 (44%)
2	9XA	P	401	-	35,37,37	2.67	10 (28%)	45,56,56	2.56	18 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9XA	B	401	-	-	4/25/35/35	0/4/4/4
2	9XA	A	401	-	-	2/25/35/35	0/4/4/4
2	9XA	L	401	-	-	3/25/35/35	0/4/4/4
2	9XA	H	401	-	-	3/25/35/35	0/4/4/4
2	9XA	C	401	-	-	15/25/35/35	0/4/4/4
2	9XA	K	401	-	-	3/25/35/35	0/4/4/4
2	9XA	N	401	-	-	3/25/35/35	0/4/4/4
2	9XA	I	401	-	-	3/25/35/35	0/4/4/4
2	9XA	J	401	-	-	3/25/35/35	0/4/4/4
2	9XA	G	401	-	-	3/25/35/35	0/4/4/4
2	9XA	E	401	-	-	3/25/35/35	0/4/4/4
2	9XA	F	401	-	-	8/25/35/35	0/4/4/4
2	9XA	O	401	-	-	4/25/35/35	0/4/4/4
2	9XA	D	401	-	-	3/25/35/35	0/4/4/4
2	9XA	M	401	-	-	3/25/35/35	0/4/4/4
2	9XA	P	401	-	-	1/25/35/35	0/4/4/4

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	9XA	C2-N9	-11.05	1.23	1.33
2	H	401	9XA	C2-N9	-9.86	1.24	1.33
2	P	401	9XA	C2-N9	-9.68	1.24	1.33
2	I	401	9XA	C2-N9	-9.48	1.24	1.33
2	J	401	9XA	C2-N9	-9.40	1.25	1.33
2	F	401	9XA	C2-N9	-9.28	1.25	1.33
2	G	401	9XA	C2-N9	-9.26	1.25	1.33
2	N	401	9XA	C2-N9	-9.23	1.25	1.33
2	B	401	9XA	C2-N9	-9.17	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	401	9XA	C2-N9	-9.16	1.25	1.33
2	K	401	9XA	C2-N9	-9.16	1.25	1.33
2	A	401	9XA	C2-N9	-8.97	1.25	1.33
2	E	401	9XA	C2-N9	-8.96	1.25	1.33
2	M	401	9XA	C2-N9	-8.84	1.25	1.33
2	D	401	9XA	C2-N9	-8.82	1.25	1.33
2	O	401	9XA	C2-N9	-8.72	1.25	1.33
2	G	401	9XA	C4-C5	7.32	1.52	1.40
2	J	401	9XA	C4-C5	7.15	1.51	1.40
2	L	401	9XA	C4-C5	7.12	1.51	1.40
2	H	401	9XA	C4-C5	7.10	1.51	1.40
2	M	401	9XA	C4-C5	7.07	1.51	1.40
2	I	401	9XA	C4-C5	7.06	1.51	1.40
2	D	401	9XA	C4-C5	7.06	1.51	1.40
2	K	401	9XA	C4-C5	6.98	1.51	1.40
2	A	401	9XA	C4-C5	6.95	1.51	1.40
2	O	401	9XA	C4-C5	6.94	1.51	1.40
2	N	401	9XA	C4-C5	6.88	1.51	1.40
2	E	401	9XA	C4-C5	6.70	1.51	1.40
2	B	401	9XA	C4-C5	6.61	1.51	1.40
2	P	401	9XA	C4-C5	6.58	1.51	1.40
2	F	401	9XA	C4-C5	5.87	1.49	1.40
2	B	401	9XA	C3-C2	5.48	1.48	1.40
2	O	401	9XA	C3-C2	5.15	1.48	1.40
2	J	401	9XA	C3-C2	5.13	1.48	1.40
2	G	401	9XA	C3-C2	5.11	1.48	1.40
2	C	401	9XA	C31-S28	-5.01	1.77	1.82
2	M	401	9XA	C3-C2	4.92	1.47	1.40
2	F	401	9XA	C3-C2	4.90	1.47	1.40
2	E	401	9XA	C3-C2	4.89	1.47	1.40
2	A	401	9XA	C3-C2	4.82	1.47	1.40
2	P	401	9XA	C3-C2	4.70	1.47	1.40
2	K	401	9XA	C3-C2	4.68	1.47	1.40
2	D	401	9XA	C3-C2	4.68	1.47	1.40
2	N	401	9XA	C3-C2	4.61	1.47	1.40
2	F	401	9XA	O30-S28	4.53	1.48	1.44
2	I	401	9XA	C3-C2	4.53	1.47	1.40
2	C	401	9XA	C6-N1	-4.50	1.29	1.36
2	L	401	9XA	C3-C2	4.36	1.47	1.40
2	H	401	9XA	C3-C2	4.35	1.47	1.40
2	E	401	9XA	O30-S28	3.86	1.47	1.44
2	E	401	9XA	C8-N9	3.76	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	9XA	O30-S28	3.71	1.47	1.44
2	A	401	9XA	C8-N9	3.69	1.44	1.36
2	E	401	9XA	O29-S28	3.67	1.47	1.44
2	B	401	9XA	C14-C7	3.59	1.53	1.48
2	J	401	9XA	O29-S28	3.57	1.47	1.44
2	P	401	9XA	C14-C7	3.54	1.52	1.48
2	J	401	9XA	C8-N9	3.49	1.43	1.36
2	O	401	9XA	C8-N9	3.48	1.43	1.36
2	M	401	9XA	C8-N9	3.48	1.43	1.36
2	G	401	9XA	C8-N9	3.47	1.43	1.36
2	N	401	9XA	C8-N9	3.43	1.43	1.36
2	P	401	9XA	C8-N9	3.42	1.43	1.36
2	C	401	9XA	C21-N22	-3.42	1.30	1.35
2	L	401	9XA	C8-N9	3.33	1.43	1.36
2	D	401	9XA	C8-N9	3.31	1.43	1.36
2	B	401	9XA	O29-S28	3.30	1.46	1.44
2	I	401	9XA	C8-N9	3.30	1.43	1.36
2	E	401	9XA	C14-C7	3.30	1.52	1.48
2	B	401	9XA	C8-N9	3.28	1.43	1.36
2	K	401	9XA	C8-N9	3.27	1.43	1.36
2	C	401	9XA	O30-S28	-3.27	1.41	1.44
2	H	401	9XA	C8-N9	3.25	1.43	1.36
2	C	401	9XA	C3-C2	3.22	1.45	1.40
2	H	401	9XA	C14-C7	3.21	1.52	1.48
2	C	401	9XA	C5-S28	-3.20	1.73	1.78
2	N	401	9XA	O30-S28	3.16	1.46	1.44
2	I	401	9XA	C6-N1	-3.16	1.31	1.36
2	C	401	9XA	C4-C5	3.14	1.45	1.40
2	M	401	9XA	C14-C7	3.13	1.52	1.48
2	I	401	9XA	C14-C7	3.08	1.52	1.48
2	E	401	9XA	C6-N1	-3.06	1.31	1.36
2	A	401	9XA	C6-N1	-3.06	1.31	1.36
2	L	401	9XA	C14-C7	3.04	1.52	1.48
2	M	401	9XA	C6-N1	-3.04	1.31	1.36
2	F	401	9XA	C14-C7	3.04	1.52	1.48
2	F	401	9XA	C8-N9	3.02	1.42	1.36
2	O	401	9XA	C14-C7	3.01	1.52	1.48
2	C	401	9XA	C8-N9	3.01	1.42	1.36
2	G	401	9XA	C6-N1	-3.00	1.31	1.36
2	O	401	9XA	C6-N1	-2.99	1.32	1.36
2	H	401	9XA	C6-N1	-2.98	1.32	1.36
2	L	401	9XA	C6-N1	-2.97	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	9XA	C6-C5	-2.96	1.32	1.38
2	D	401	9XA	C14-C7	2.96	1.52	1.48
2	A	401	9XA	O29-S28	2.95	1.46	1.44
2	K	401	9XA	C6-N1	-2.94	1.32	1.36
2	K	401	9XA	C14-C7	2.94	1.52	1.48
2	M	401	9XA	O29-S28	2.92	1.46	1.44
2	G	401	9XA	C14-C7	2.91	1.52	1.48
2	F	401	9XA	C6-N1	-2.88	1.32	1.36
2	H	401	9XA	O30-S28	2.88	1.46	1.44
2	D	401	9XA	C6-N1	-2.88	1.32	1.36
2	N	401	9XA	C6-N1	-2.83	1.32	1.36
2	G	401	9XA	O29-S28	2.78	1.46	1.44
2	J	401	9XA	C6-N1	-2.77	1.32	1.36
2	F	401	9XA	O29-S28	2.77	1.46	1.44
2	P	401	9XA	C6-N1	-2.77	1.32	1.36
2	A	401	9XA	C14-C7	2.75	1.51	1.48
2	N	401	9XA	C14-C7	2.74	1.51	1.48
2	C	401	9XA	O10-C4	-2.67	1.32	1.37
2	N	401	9XA	O29-S28	2.66	1.46	1.44
2	C	401	9XA	C14-C7	2.64	1.51	1.48
2	P	401	9XA	O29-S28	2.62	1.46	1.44
2	A	401	9XA	C23-N22	2.60	1.37	1.33
2	C	401	9XA	C8-C7	-2.59	1.33	1.38
2	I	401	9XA	O29-S28	2.59	1.46	1.44
2	B	401	9XA	C31-S28	2.58	1.85	1.82
2	J	401	9XA	C14-C7	2.58	1.51	1.48
2	H	401	9XA	C32-C31	2.52	1.57	1.52
2	I	401	9XA	O30-S28	2.44	1.46	1.44
2	B	401	9XA	O30-S28	2.42	1.46	1.44
2	O	401	9XA	C31-S28	2.40	1.84	1.82
2	H	401	9XA	C16-N17	2.38	1.51	1.46
2	O	401	9XA	O29-S28	2.38	1.46	1.44
2	G	401	9XA	C18-N17	2.35	1.51	1.46
2	P	401	9XA	O30-S28	2.31	1.46	1.44
2	E	401	9XA	C23-N22	2.31	1.37	1.33
2	I	401	9XA	C32-C31	2.30	1.56	1.52
2	L	401	9XA	O30-S28	2.30	1.46	1.44
2	H	401	9XA	O29-S28	2.30	1.46	1.44
2	J	401	9XA	C18-N17	2.27	1.51	1.46
2	I	401	9XA	C23-N22	2.25	1.37	1.33
2	N	401	9XA	C23-N22	2.24	1.37	1.33
2	K	401	9XA	C32-C31	2.16	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	401	9XA	O30-S28	2.14	1.45	1.44
2	D	401	9XA	O29-S28	2.14	1.45	1.44
2	D	401	9XA	C32-C31	2.14	1.56	1.52
2	F	401	9XA	C23-N22	2.09	1.36	1.33
2	P	401	9XA	C23-N22	2.08	1.36	1.33
2	J	401	9XA	C16-N17	2.07	1.50	1.46
2	M	401	9XA	C31-S28	2.05	1.84	1.82
2	H	401	9XA	C33-C31	2.05	1.56	1.52
2	O	401	9XA	C33-C31	2.04	1.56	1.52
2	D	401	9XA	C34-C31	2.02	1.56	1.52
2	P	401	9XA	C24-C23	2.02	1.41	1.38
2	B	401	9XA	C33-C31	2.02	1.56	1.52
2	L	401	9XA	C16-N17	2.02	1.50	1.46

All (294) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	9XA	C31-S28-C5	-14.24	98.47	107.78
2	C	401	9XA	C24-C23-CL25	9.50	130.73	118.88
2	J	401	9XA	C18-N17-C16	8.50	121.42	109.52
2	A	401	9XA	C23-N22-C21	8.45	122.58	116.72
2	M	401	9XA	C23-N22-C21	8.26	122.45	116.72
2	G	401	9XA	C18-N17-C16	8.06	120.80	109.52
2	F	401	9XA	C8-C7-C14	-7.99	118.83	128.47
2	I	401	9XA	C23-N22-C21	7.65	122.03	116.72
2	O	401	9XA	C23-N22-C21	7.62	122.01	116.72
2	F	401	9XA	C23-N22-C21	7.54	121.95	116.72
2	P	401	9XA	C23-N22-C21	7.39	121.85	116.72
2	P	401	9XA	C8-C7-C14	-7.29	119.68	128.47
2	N	401	9XA	C23-N22-C21	7.24	121.75	116.72
2	E	401	9XA	C23-N22-C21	7.21	121.72	116.72
2	C	401	9XA	C14-C20-C21	7.08	123.04	117.38
2	B	401	9XA	C8-C7-C14	-7.01	120.02	128.47
2	J	401	9XA	C23-N22-C21	6.92	121.52	116.72
2	C	401	9XA	C24-C14-C7	6.81	133.32	120.06
2	D	401	9XA	C8-C7-C14	-6.77	120.30	128.47
2	L	401	9XA	C23-N22-C21	6.76	121.41	116.72
2	H	401	9XA	C18-N17-C16	6.70	118.90	109.52
2	H	401	9XA	C23-N22-C21	6.66	121.34	116.72
2	D	401	9XA	C23-N22-C21	6.64	121.33	116.72
2	K	401	9XA	C23-N22-C21	6.52	121.24	116.72
2	N	401	9XA	C8-C7-C14	-6.49	120.64	128.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	401	9XA	C8-C7-C14	-6.47	120.67	128.47
2	J	401	9XA	C8-C7-C14	-6.43	120.72	128.47
2	I	401	9XA	C8-C7-C14	-6.42	120.73	128.47
2	M	401	9XA	C18-N17-C16	6.39	118.46	109.52
2	B	401	9XA	C23-N22-C21	6.35	121.13	116.72
2	A	401	9XA	C24-C23-N22	-6.15	118.75	125.50
2	G	401	9XA	C23-N22-C21	6.14	120.98	116.72
2	L	401	9XA	C8-C7-C14	-6.14	121.06	128.47
2	O	401	9XA	C18-N17-C16	6.14	118.11	109.52
2	A	401	9XA	C8-C7-C14	-6.14	121.07	128.47
2	E	401	9XA	C8-C7-C14	-6.09	121.12	128.47
2	H	401	9XA	C8-C7-C14	-6.09	121.13	128.47
2	N	401	9XA	C12-N13-C19	6.04	126.69	111.23
2	G	401	9XA	C8-C7-C14	-6.04	121.19	128.47
2	G	401	9XA	C19-C18-N17	6.03	117.62	110.80
2	O	401	9XA	C8-C7-C14	-5.95	121.30	128.47
2	M	401	9XA	C8-C7-C14	-5.86	121.40	128.47
2	L	401	9XA	C18-N17-C16	5.48	117.18	109.52
2	C	401	9XA	C23-N22-C21	5.48	120.52	116.72
2	G	401	9XA	C15-C16-N17	5.17	116.64	110.80
2	J	401	9XA	C19-C18-N17	5.16	116.64	110.80
2	G	401	9XA	C27-N17-C18	5.15	118.36	110.66
2	B	401	9XA	C18-N17-C16	5.12	116.69	109.52
2	J	401	9XA	C15-C16-N17	5.00	116.45	110.80
2	C	401	9XA	C20-C14-C7	-4.99	110.35	120.06
2	F	401	9XA	C14-C20-C21	4.90	121.30	117.38
2	M	401	9XA	C24-C23-N22	-4.80	120.23	125.50
2	B	401	9XA	C14-C20-C21	4.80	121.22	117.38
2	D	401	9XA	C24-C23-N22	-4.62	120.43	125.50
2	N	401	9XA	C24-C23-N22	-4.60	120.45	125.50
2	O	401	9XA	C24-C23-N22	-4.57	120.48	125.50
2	P	401	9XA	C14-C7-N1	4.57	130.71	122.93
2	C	401	9XA	C4-C3-C2	-4.57	114.97	120.12
2	C	401	9XA	CL25-C23-N22	-4.53	104.98	115.44
2	P	401	9XA	C18-N17-C16	4.53	115.85	109.52
2	K	401	9XA	C24-C23-N22	-4.50	120.56	125.50
2	H	401	9XA	C14-C20-C21	4.46	120.95	117.38
2	A	401	9XA	C12-N13-C15	4.46	122.63	111.23
2	J	401	9XA	C27-N17-C18	4.44	117.30	110.66
2	C	401	9XA	C6-C5-S28	4.43	123.97	118.53
2	J	401	9XA	C24-C23-N22	-4.36	120.71	125.50
2	F	401	9XA	C12-N13-C19	4.36	122.38	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	401	9XA	C24-C23-N22	-4.34	120.73	125.50
2	P	401	9XA	C24-C23-N22	-4.34	120.74	125.50
2	E	401	9XA	C14-C20-C21	4.33	120.85	117.38
2	E	401	9XA	C24-C23-N22	-4.33	120.74	125.50
2	F	401	9XA	C14-C7-N1	4.32	130.28	122.93
2	E	401	9XA	C15-C16-N17	-4.31	105.94	110.80
2	I	401	9XA	C14-C20-C21	4.31	120.83	117.38
2	O	401	9XA	C14-C20-C21	4.27	120.80	117.38
2	B	401	9XA	C14-C7-N1	4.25	130.16	122.93
2	O	401	9XA	C19-C18-N17	4.23	115.58	110.80
2	F	401	9XA	C7-C8-N9	-4.22	100.45	109.11
2	M	401	9XA	C14-C20-C21	4.20	120.74	117.38
2	L	401	9XA	O30-S28-O29	-4.13	114.44	118.98
2	F	401	9XA	C6-C5-S28	4.12	123.59	118.53
2	P	401	9XA	C14-C20-C21	4.07	120.64	117.38
2	A	401	9XA	C18-N17-C16	4.06	115.21	109.52
2	N	401	9XA	C19-N13-C15	4.03	117.91	108.83
2	J	401	9XA	C14-C20-C21	4.02	120.60	117.38
2	B	401	9XA	C24-C23-N22	-4.02	121.09	125.50
2	B	401	9XA	C19-N13-C15	3.97	117.76	108.83
2	G	401	9XA	C14-C20-C21	3.96	120.55	117.38
2	I	401	9XA	C7-C8-N9	-3.93	101.03	109.11
2	O	401	9XA	O30-S28-O29	-3.92	114.67	118.98
2	H	401	9XA	C24-C23-N22	-3.91	121.21	125.50
2	D	401	9XA	C7-C8-N9	-3.88	101.14	109.11
2	I	401	9XA	C24-C23-N22	-3.86	121.27	125.50
2	G	401	9XA	C24-C23-N22	-3.83	121.30	125.50
2	K	401	9XA	C7-C8-N9	-3.81	101.30	109.11
2	A	401	9XA	C7-C8-N9	-3.80	101.31	109.11
2	L	401	9XA	C19-N13-C15	3.78	117.34	108.83
2	B	401	9XA	C7-C8-N9	-3.77	101.37	109.11
2	E	401	9XA	C7-C8-N9	-3.77	101.37	109.11
2	H	401	9XA	C7-C8-N9	-3.75	101.41	109.11
2	J	401	9XA	C14-C7-N1	3.75	129.31	122.93
2	N	401	9XA	C14-C7-N1	3.75	129.31	122.93
2	K	401	9XA	C14-C7-N1	3.71	129.24	122.93
2	F	401	9XA	C34-C31-S28	3.71	116.07	107.72
2	F	401	9XA	C19-N13-C15	3.69	117.14	108.83
2	I	401	9XA	C16-C15-N13	3.69	118.21	110.64
2	H	401	9XA	C14-C7-N1	3.69	129.20	122.93
2	J	401	9XA	O30-S28-O29	-3.68	114.94	118.98
2	A	401	9XA	C14-C7-N1	3.67	129.17	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	9XA	C14-C7-N1	3.67	129.16	122.93
2	E	401	9XA	C18-N17-C16	3.66	114.64	109.52
2	F	401	9XA	C18-N17-C16	3.65	114.63	109.52
2	F	401	9XA	O30-S28-C31	-3.64	104.26	107.97
2	D	401	9XA	C18-N17-C16	3.64	114.61	109.52
2	G	401	9XA	C14-C7-N1	3.62	129.09	122.93
2	L	401	9XA	C7-C8-N9	-3.62	101.67	109.11
2	M	401	9XA	C15-C16-N17	3.60	114.88	110.80
2	O	401	9XA	C7-C8-N9	-3.60	101.73	109.11
2	I	401	9XA	C14-C7-N1	3.59	129.04	122.93
2	J	401	9XA	C7-C8-N9	-3.58	101.76	109.11
2	E	401	9XA	C14-C7-N1	3.58	129.01	122.93
2	M	401	9XA	C14-C7-N1	3.56	128.99	122.93
2	I	401	9XA	C18-N17-C16	3.56	114.51	109.52
2	O	401	9XA	C15-C16-N17	3.56	114.82	110.80
2	L	401	9XA	C14-C7-N1	3.54	128.96	122.93
2	C	401	9XA	C7-C8-N9	-3.54	101.85	109.11
2	N	401	9XA	C7-C8-N9	-3.53	101.86	109.11
2	M	401	9XA	C7-C8-N9	-3.52	101.88	109.11
2	K	401	9XA	C18-N17-C16	3.50	114.41	109.52
2	L	401	9XA	C15-C16-N17	3.48	114.74	110.80
2	O	401	9XA	C14-C7-N1	3.43	128.76	122.93
2	A	401	9XA	C15-C16-N17	-3.42	106.94	110.80
2	P	401	9XA	C7-C8-N9	-3.42	102.10	109.11
2	I	401	9XA	C19-N13-C15	3.42	116.52	108.83
2	G	401	9XA	C7-C8-N9	-3.41	102.12	109.11
2	C	401	9XA	C27-N17-C16	3.36	115.69	110.66
2	D	401	9XA	C19-N13-C15	3.35	116.38	108.83
2	D	401	9XA	C14-C20-C21	3.30	120.02	117.38
2	L	401	9XA	C14-C20-C21	3.29	120.02	117.38
2	J	401	9XA	C27-N17-C16	3.24	115.51	110.66
2	A	401	9XA	C27-N17-C18	3.24	115.51	110.66
2	A	401	9XA	C23-C24-C14	3.21	120.36	117.76
2	F	401	9XA	C27-N17-C18	3.20	115.44	110.66
2	F	401	9XA	C24-C23-N22	-3.17	122.01	125.50
2	E	401	9XA	O30-S28-O29	-3.16	115.51	118.98
2	A	401	9XA	O30-S28-O29	-3.15	115.52	118.98
2	G	401	9XA	C12-N13-C19	3.14	119.27	111.23
2	P	401	9XA	C19-C18-N17	3.13	114.34	110.80
2	D	401	9XA	C27-N17-C18	3.13	115.35	110.66
2	C	401	9XA	C19-N13-C15	3.13	115.88	108.83
2	A	401	9XA	C14-C20-C21	3.13	119.88	117.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	401	9XA	O30-S28-O29	-3.12	115.55	118.98
2	N	401	9XA	C27-N17-C18	3.09	115.28	110.66
2	M	401	9XA	C19-C18-N17	3.09	114.29	110.80
2	A	401	9XA	CL25-C23-N22	3.09	122.56	115.44
2	B	401	9XA	C27-N17-C18	3.08	115.27	110.66
2	I	401	9XA	C27-N17-C16	3.08	115.27	110.66
2	H	401	9XA	O30-S28-O29	-3.06	115.62	118.98
2	L	401	9XA	C32-C31-S28	3.02	114.53	107.72
2	H	401	9XA	C15-C16-N17	3.02	114.22	110.80
2	F	401	9XA	C4-C3-C2	-3.00	116.74	120.12
2	G	401	9XA	O10-C4-C5	3.00	121.43	116.68
2	P	401	9XA	C19-N13-C15	2.98	115.55	108.83
2	M	401	9XA	O30-S28-O29	-2.98	115.70	118.98
2	N	401	9XA	C14-C20-C21	2.98	119.77	117.38
2	C	401	9XA	C8-C7-C14	-2.96	124.90	128.47
2	A	401	9XA	C27-N17-C16	2.96	115.09	110.66
2	C	401	9XA	O29-S28-C5	2.95	114.87	107.98
2	J	401	9XA	C12-N13-C19	2.95	118.77	111.23
2	M	401	9XA	C12-N13-C19	2.93	118.74	111.23
2	K	401	9XA	O30-S28-O29	-2.92	115.77	118.98
2	J	401	9XA	O10-C4-C5	2.91	121.29	116.68
2	E	401	9XA	C27-N17-C18	2.91	115.01	110.66
2	B	401	9XA	O30-S28-O29	-2.89	115.80	118.98
2	C	401	9XA	C34-C31-S28	2.89	114.22	107.72
2	I	401	9XA	C27-N17-C18	2.88	114.97	110.66
2	P	401	9XA	O30-S28-O29	-2.84	115.86	118.98
2	N	401	9XA	C16-C15-N13	2.83	116.45	110.64
2	E	401	9XA	C27-N17-C16	2.82	114.89	110.66
2	D	401	9XA	O10-C4-C5	2.82	121.14	116.68
2	P	401	9XA	C12-N13-C19	2.82	118.44	111.23
2	A	401	9XA	C4-C3-C2	-2.78	116.99	120.12
2	F	401	9XA	N26-C21-N22	2.78	120.88	116.49
2	B	401	9XA	C19-C18-N17	2.77	113.94	110.80
2	D	401	9XA	C12-N13-C19	2.76	118.30	111.23
2	G	401	9XA	O30-S28-O29	-2.76	115.95	118.98
2	K	401	9XA	O29-S28-C31	-2.75	105.17	107.97
2	H	401	9XA	C19-C18-N17	2.74	113.90	110.80
2	M	401	9XA	O10-C4-C5	2.73	121.01	116.68
2	C	401	9XA	C16-C15-N13	2.72	116.22	110.64
2	B	401	9XA	O30-S28-C31	-2.71	105.21	107.97
2	D	401	9XA	CL25-C23-N22	2.71	121.69	115.44
2	O	401	9XA	O10-C4-C5	2.70	120.97	116.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	401	9XA	C15-C16-N17	-2.69	107.76	110.80
2	N	401	9XA	CL25-C23-N22	2.67	121.59	115.44
2	A	401	9XA	C11-O10-C4	2.64	124.15	117.69
2	L	401	9XA	O10-C4-C5	2.64	120.86	116.68
2	K	401	9XA	C14-C20-C21	2.64	119.49	117.38
2	H	401	9XA	C27-N17-C16	2.62	114.58	110.66
2	I	401	9XA	C15-C16-N17	2.61	113.76	110.80
2	K	401	9XA	O10-C4-C5	2.61	120.81	116.68
2	F	401	9XA	C31-S28-C5	2.60	109.48	107.78
2	G	401	9XA	C4-C3-C2	-2.59	117.20	120.12
2	O	401	9XA	C4-C3-C2	-2.59	117.20	120.12
2	K	401	9XA	C19-N13-C15	2.59	114.66	108.83
2	D	401	9XA	C34-C31-S28	2.58	113.53	107.72
2	B	401	9XA	C34-C31-C33	-2.58	106.02	111.04
2	P	401	9XA	C4-C3-C2	-2.57	117.23	120.12
2	F	401	9XA	C27-N17-C16	2.55	114.47	110.66
2	H	401	9XA	O10-C4-C5	2.54	120.71	116.68
2	K	401	9XA	CL25-C23-N22	2.52	121.26	115.44
2	E	401	9XA	C4-C3-C2	-2.52	117.29	120.12
2	J	401	9XA	N26-C21-N22	2.51	120.45	116.49
2	E	401	9XA	O10-C4-C5	2.50	120.64	116.68
2	P	401	9XA	C31-S28-C5	2.50	109.42	107.78
2	I	401	9XA	C12-N13-C19	2.50	117.62	111.23
2	G	401	9XA	C6-C5-S28	-2.49	115.48	118.53
2	E	401	9XA	C19-N13-C15	2.49	114.42	108.83
2	M	401	9XA	C4-C3-C2	-2.48	117.33	120.12
2	I	401	9XA	CL25-C23-N22	2.48	121.16	115.44
2	A	401	9XA	O10-C4-C5	2.48	120.61	116.68
2	O	401	9XA	N26-C21-N22	2.48	120.41	116.49
2	M	401	9XA	C11-O10-C4	2.48	123.75	117.69
2	N	401	9XA	C27-N17-C16	2.45	114.32	110.66
2	M	401	9XA	N26-C21-N22	2.45	120.36	116.49
2	A	401	9XA	C19-N13-C15	2.44	114.32	108.83
2	O	401	9XA	C11-O10-C4	2.44	123.65	117.69
2	D	401	9XA	N26-C21-N22	2.43	120.33	116.49
2	E	401	9XA	C11-O10-C4	2.41	123.59	117.69
2	K	401	9XA	C27-N17-C18	2.41	114.26	110.66
2	B	401	9XA	C23-C24-C14	2.40	119.70	117.76
2	D	401	9XA	O30-S28-O29	-2.40	116.34	118.98
2	N	401	9XA	O10-C4-C5	2.40	120.48	116.68
2	I	401	9XA	C32-C31-S28	2.39	113.10	107.72
2	G	401	9XA	C11-O10-C4	2.39	123.53	117.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	401	9XA	C11-O10-C4	2.38	123.50	117.69
2	I	401	9XA	O10-C4-C5	2.37	120.44	116.68
2	K	401	9XA	C11-O10-C4	2.37	123.47	117.69
2	A	401	9XA	C32-C31-S28	2.36	113.04	107.72
2	O	401	9XA	C32-C31-S28	2.36	113.03	107.72
2	N	401	9XA	C4-C3-C2	-2.36	117.47	120.12
2	H	401	9XA	C32-C31-S28	2.35	113.01	107.72
2	D	401	9XA	C23-C24-C14	2.35	119.66	117.76
2	B	401	9XA	C16-C15-N13	2.34	115.44	110.64
2	J	401	9XA	C11-O10-C4	2.33	123.39	117.69
2	N	401	9XA	O30-S28-O29	-2.32	116.43	118.98
2	J	401	9XA	C4-C3-C2	-2.32	117.51	120.12
2	O	401	9XA	C6-C5-S28	-2.31	115.70	118.53
2	A	401	9XA	N26-C21-N22	2.31	120.14	116.49
2	C	401	9XA	C12-N13-C19	2.30	117.13	111.23
2	E	401	9XA	CL25-C23-N22	2.30	120.74	115.44
2	I	401	9XA	C11-O10-C4	2.29	123.28	117.69
2	D	401	9XA	C11-O10-C4	2.27	123.24	117.69
2	F	401	9XA	O30-S28-O29	-2.27	116.49	118.98
2	B	401	9XA	C34-C31-S28	2.27	112.83	107.72
2	L	401	9XA	O30-S28-C31	2.26	110.27	107.97
2	F	401	9XA	C34-C31-C33	-2.24	106.68	111.04
2	N	401	9XA	N26-C21-N22	2.23	120.01	116.49
2	E	401	9XA	C34-C31-S28	2.21	112.70	107.72
2	P	401	9XA	C33-C31-C32	-2.20	106.75	111.04
2	H	401	9XA	CL25-C23-N22	2.20	120.52	115.44
2	L	401	9XA	C27-N17-C16	2.17	113.91	110.66
2	K	401	9XA	N26-C21-N22	2.17	119.92	116.49
2	P	401	9XA	C3-C2-N9	-2.17	126.50	130.55
2	M	401	9XA	C34-C31-S28	2.16	112.59	107.72
2	M	401	9XA	CL25-C23-N22	2.16	120.42	115.44
2	B	401	9XA	C18-C19-N13	2.16	115.07	110.64
2	F	401	9XA	CL25-C23-N22	2.15	120.40	115.44
2	M	401	9XA	C6-C5-S28	-2.15	115.90	118.53
2	G	401	9XA	O10-C4-C3	-2.14	121.57	125.19
2	C	401	9XA	O30-S28-O29	-2.13	116.64	118.98
2	J	401	9XA	O10-C4-C3	-2.13	121.59	125.19
2	H	401	9XA	C11-O10-C4	2.13	122.89	117.69
2	B	401	9XA	C4-C3-C2	-2.13	117.72	120.12
2	M	401	9XA	C32-C31-S28	2.12	112.50	107.72
2	E	401	9XA	C32-C31-S28	2.12	112.48	107.72
2	I	401	9XA	C18-C19-N13	2.11	114.98	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	401	9XA	C23-C24-C14	2.09	119.45	117.76
2	E	401	9XA	C23-C24-C14	2.09	119.45	117.76
2	M	401	9XA	O10-C4-C3	-2.08	121.67	125.19
2	N	401	9XA	C32-C31-S28	2.07	112.38	107.72
2	O	401	9XA	CL25-C23-N22	2.07	120.21	115.44
2	O	401	9XA	C23-C24-C14	2.06	119.42	117.76
2	H	401	9XA	C34-C31-C33	-2.05	107.04	111.04
2	N	401	9XA	C11-O10-C4	2.05	122.71	117.69
2	O	401	9XA	C34-C31-S28	2.05	112.34	107.72
2	D	401	9XA	O10-C4-C3	-2.05	121.73	125.19
2	P	401	9XA	N26-C21-N22	2.03	119.70	116.49
2	P	401	9XA	O10-C4-C5	2.03	119.89	116.68
2	K	401	9XA	C12-N13-C19	2.02	116.39	111.23
2	L	401	9XA	C23-C24-C14	2.01	119.39	117.76
2	O	401	9XA	C27-N17-C16	2.01	113.67	110.66
2	O	401	9XA	O10-C4-C3	-2.01	121.79	125.19
2	C	401	9XA	C3-C2-N9	-2.01	126.80	130.55

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	9XA	C4-C5-S28-O29
2	B	401	9XA	C5-C4-O10-C11
2	C	401	9XA	C32-C31-S28-C5
2	C	401	9XA	C33-C31-S28-C5
2	C	401	9XA	C34-C31-S28-C5
2	C	401	9XA	C32-C31-S28-O29
2	C	401	9XA	C33-C31-S28-O29
2	C	401	9XA	C34-C31-S28-O29
2	C	401	9XA	C32-C31-S28-O30
2	C	401	9XA	C33-C31-S28-O30
2	C	401	9XA	C34-C31-S28-O30
2	E	401	9XA	C4-C5-S28-O29
2	F	401	9XA	C11-C12-N13-C19
2	F	401	9XA	C4-C5-S28-O30
2	F	401	9XA	C4-C5-S28-C31
2	F	401	9XA	C6-C5-S28-O30
2	F	401	9XA	C6-C5-S28-C31
2	G	401	9XA	C4-C5-S28-O29
2	H	401	9XA	C4-C5-S28-O29
2	I	401	9XA	C4-C5-S28-O29

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Mol	Chain	Res	Type	Atoms
2	J	401	9XA	C4-C5-S28-O29
2	L	401	9XA	C4-C5-S28-O29
2	M	401	9XA	C4-C5-S28-O29
2	N	401	9XA	C11-C12-N13-C19
2	N	401	9XA	C4-C5-S28-O29
2	O	401	9XA	C4-C5-S28-O29
2	O	401	9XA	O10-C11-C12-N13
2	C	401	9XA	O10-C11-C12-N13
2	C	401	9XA	C12-C11-O10-C4
2	G	401	9XA	C11-C12-N13-C19
2	J	401	9XA	C11-C12-N13-C19
2	K	401	9XA	C11-C12-N13-C19
2	L	401	9XA	C11-C12-N13-C15
2	B	401	9XA	C3-C4-O10-C11
2	F	401	9XA	C11-C12-N13-C15
2	I	401	9XA	C11-C12-N13-C19
2	M	401	9XA	C11-C12-N13-C19
2	D	401	9XA	C11-C12-N13-C19
2	O	401	9XA	C11-C12-N13-C15
2	P	401	9XA	O10-C11-C12-N13
2	C	401	9XA	C24-C14-C7-C8
2	F	401	9XA	C3-C4-O10-C11
2	E	401	9XA	C11-C12-N13-C19
2	H	401	9XA	C11-C12-N13-C19
2	O	401	9XA	C11-C12-N13-C19
2	F	401	9XA	C5-C4-O10-C11
2	B	401	9XA	C12-C11-O10-C4
2	B	401	9XA	C11-C12-N13-C15
2	D	401	9XA	C11-C12-N13-C15
2	L	401	9XA	C11-C12-N13-C19
2	H	401	9XA	C11-C12-N13-C15
2	K	401	9XA	C11-C12-N13-C15
2	C	401	9XA	C20-C14-C7-C8
2	E	401	9XA	C11-C12-N13-C15
2	M	401	9XA	C11-C12-N13-C15
2	C	401	9XA	C5-C4-O10-C11
2	A	401	9XA	C11-C12-N13-C19
2	G	401	9XA	C11-C12-N13-C15
2	J	401	9XA	C11-C12-N13-C15
2	C	401	9XA	C3-C4-O10-C11
2	I	401	9XA	C11-C12-N13-C15
2	D	401	9XA	C4-C5-S28-O29

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Mol	Chain	Res	Type	Atoms
2	K	401	9XA	C4-C5-S28-O29
2	N	401	9XA	C11-C12-N13-C15

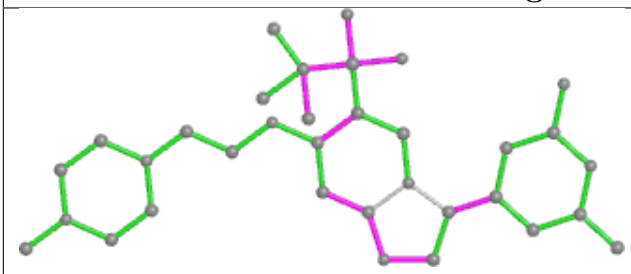
There are no ring outliers.

6 monomers are involved in 12 short contacts:

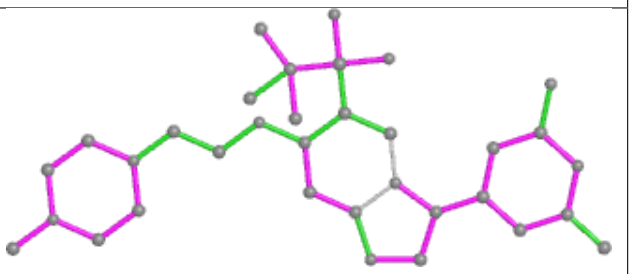
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	9XA	2	0
2	C	401	9XA	5	0
2	K	401	9XA	1	0
2	F	401	9XA	1	0
2	D	401	9XA	2	0
2	M	401	9XA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

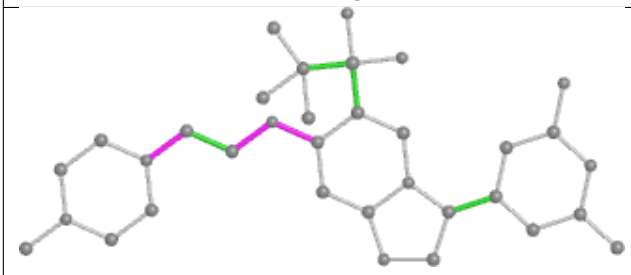
Ligand 9XA B 401



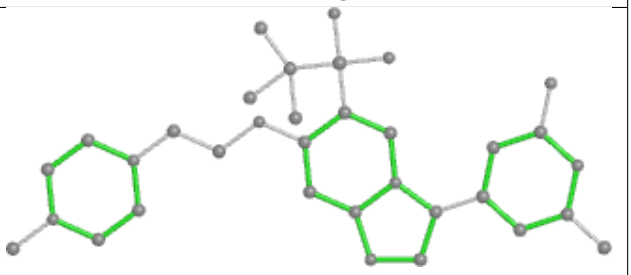
Bond lengths



Bond angles

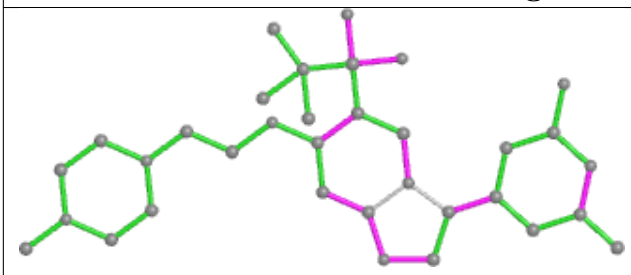


Torsions



Rings

Ligand 9XA A 401



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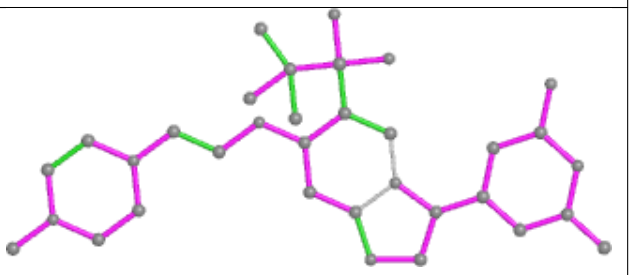

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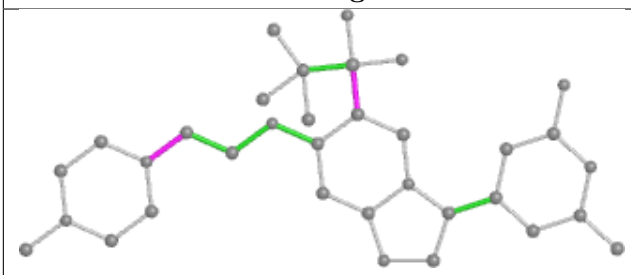

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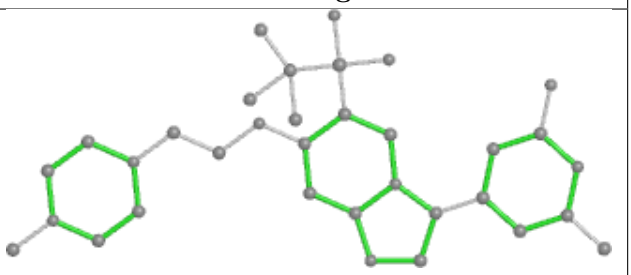
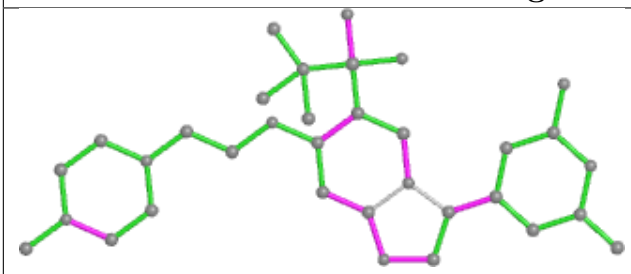


Rings

Ligand 9XA L 401



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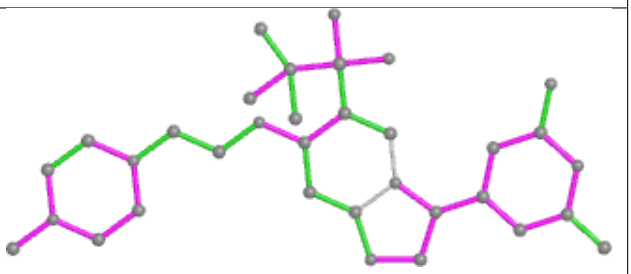

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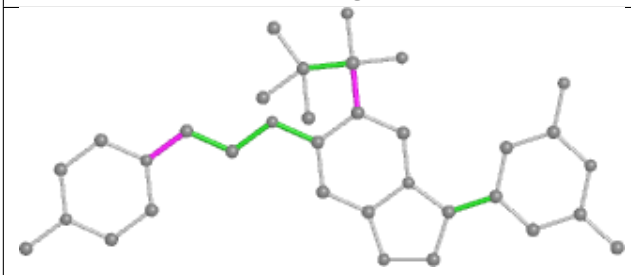

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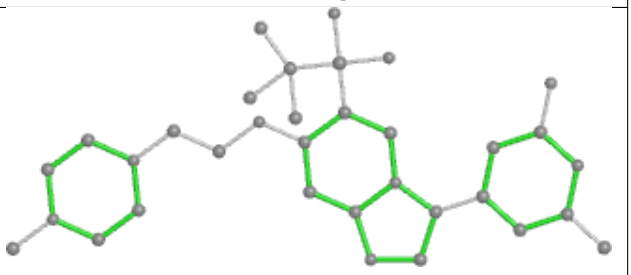
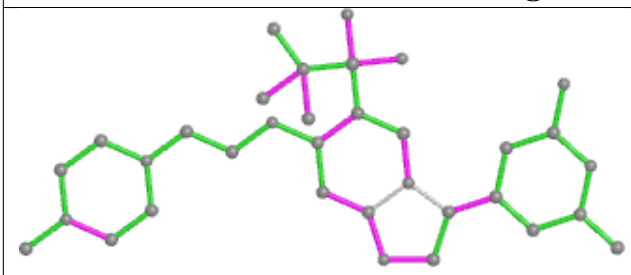


Rings

Ligand 9XA H 401



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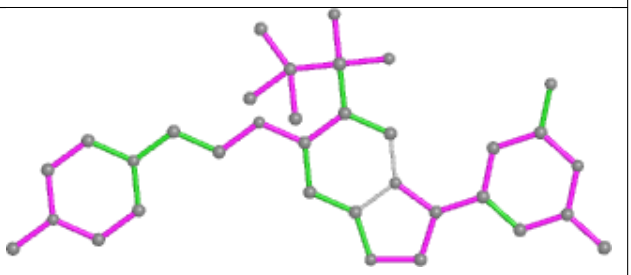

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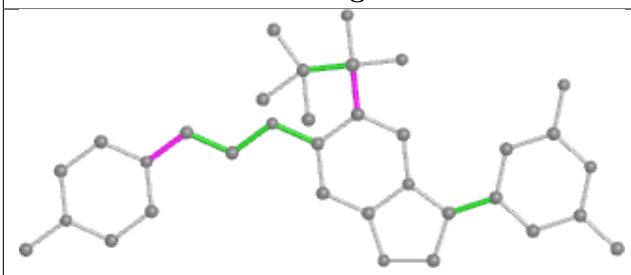

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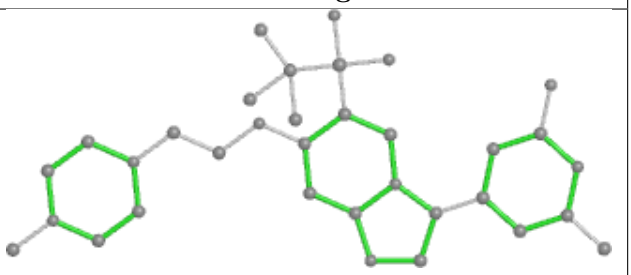
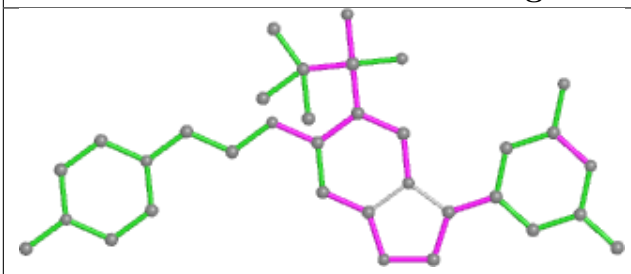


Rings

Ligand 9XA C 401



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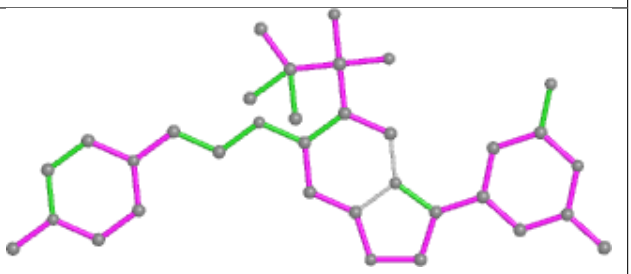
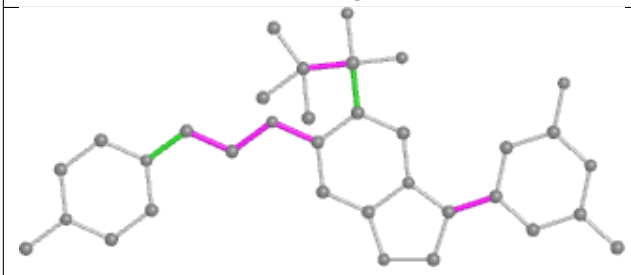


Bond angles



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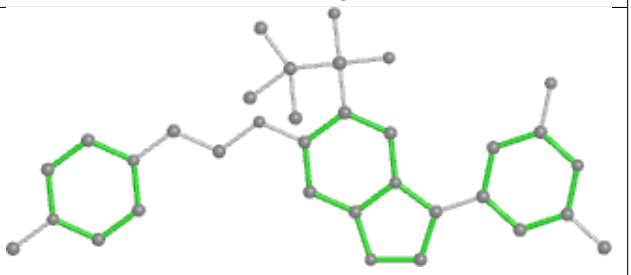

Rings

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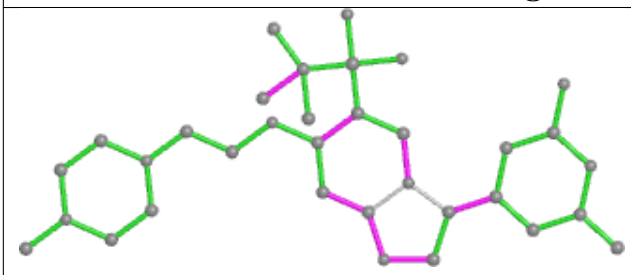

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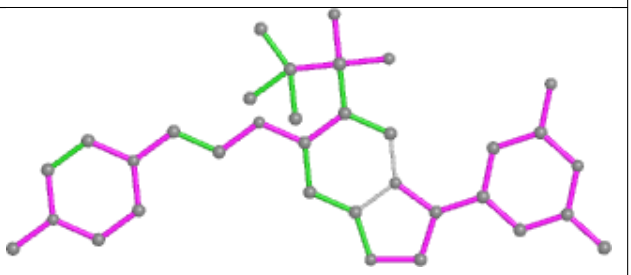
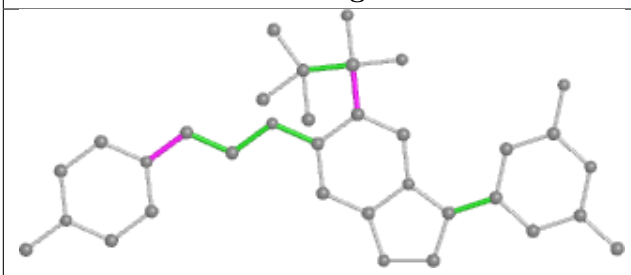


Bond angles



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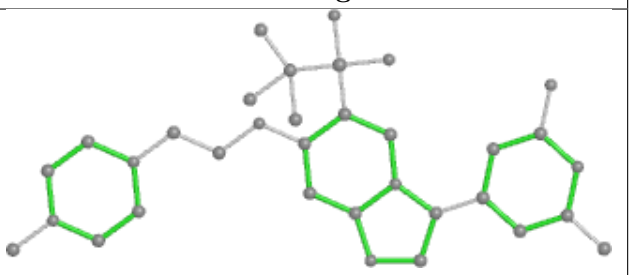

Rings

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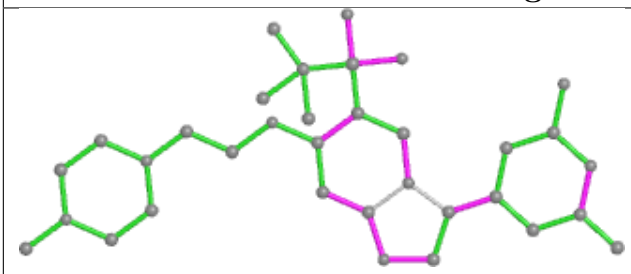
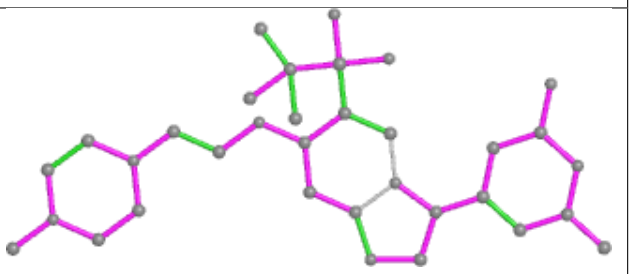
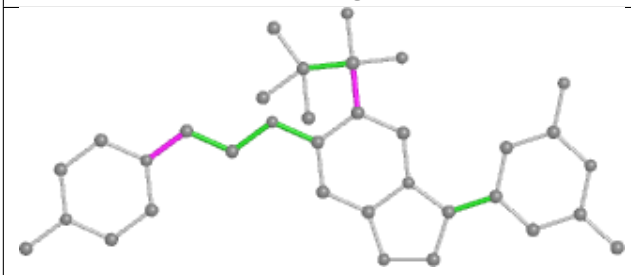


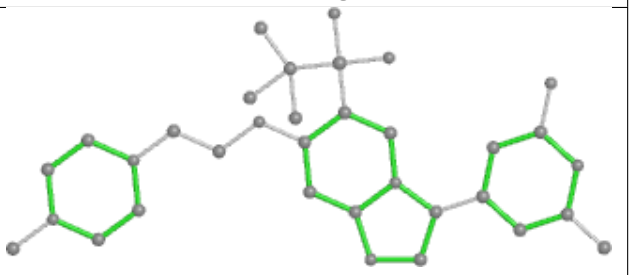
Bond lengths



Bond angles

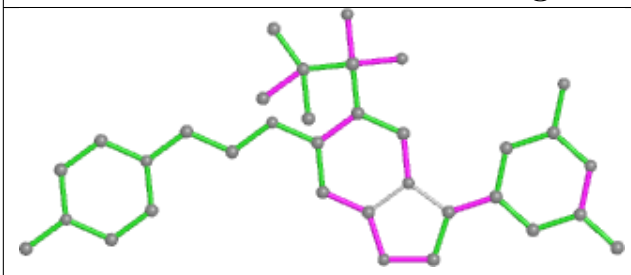


Torsions

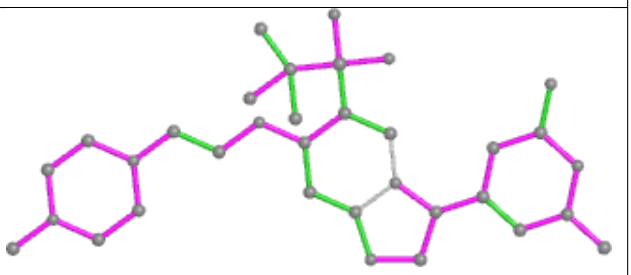


Rings

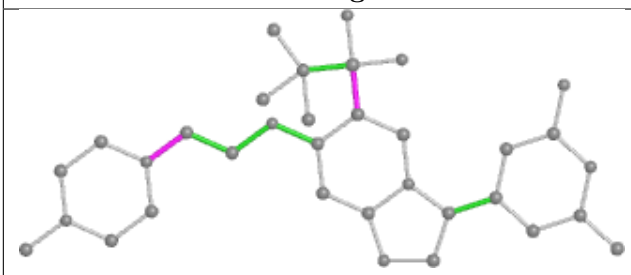
Ligand 9XA I 401



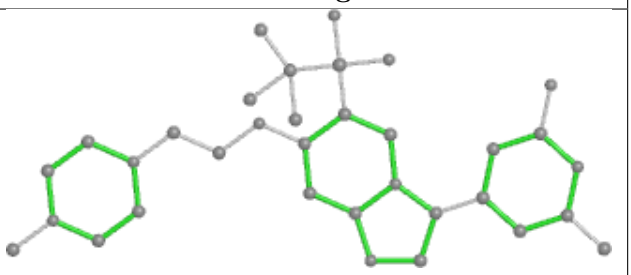
Bond lengths



Bond angles

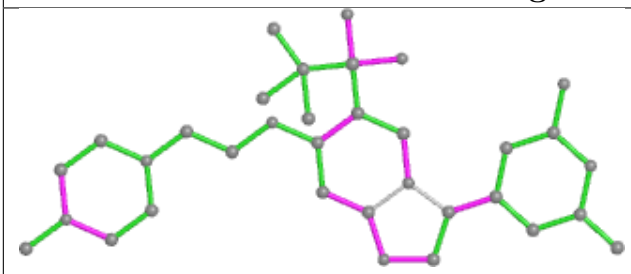


Torsions

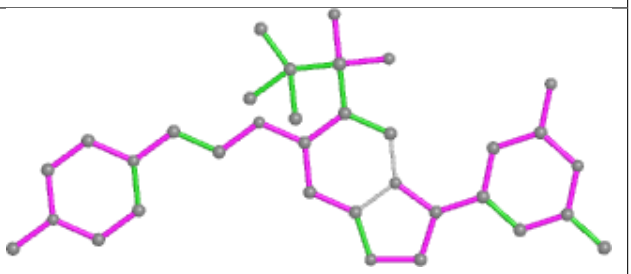


Rings

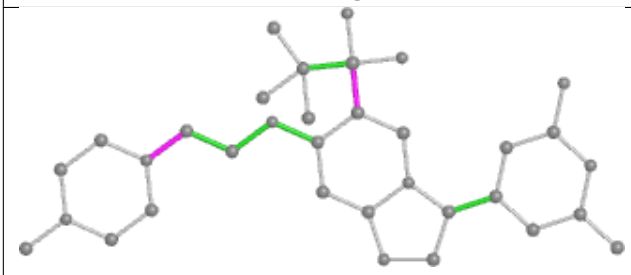
Ligand 9XA J 401



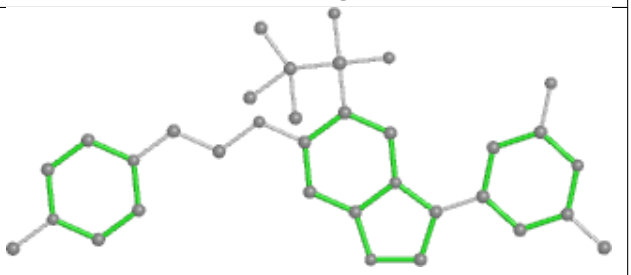
Bond lengths



Bond angles

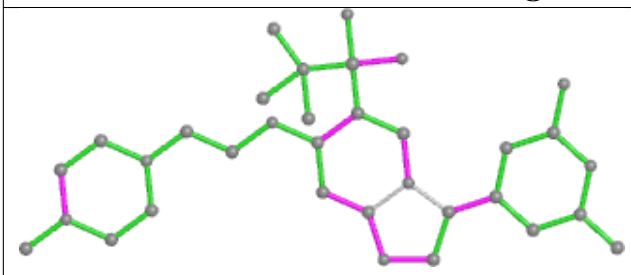


Torsions

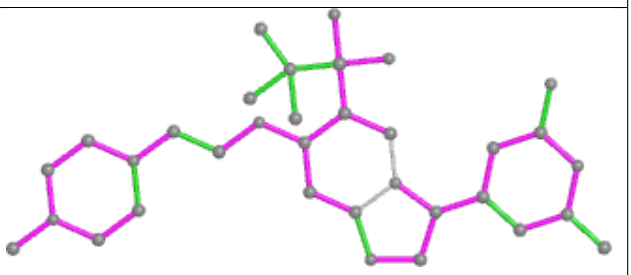


Rings

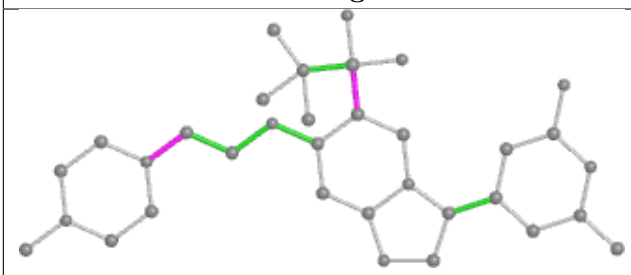
Ligand 9XA G 401



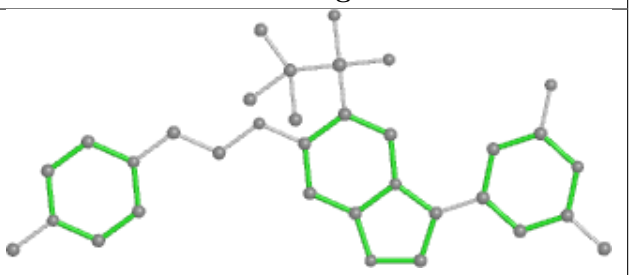
Bond lengths



Bond angles

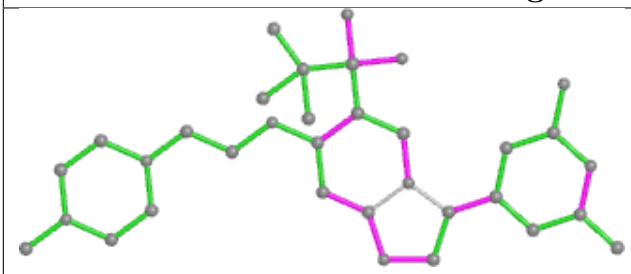


Torsions



Rings

Ligand 9XA E 401



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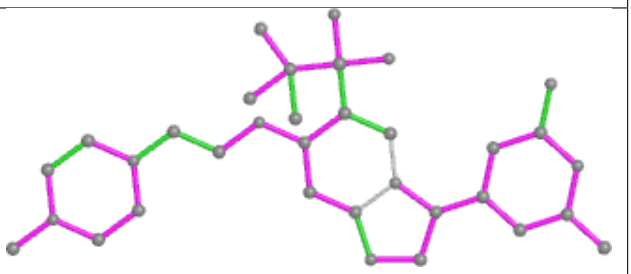
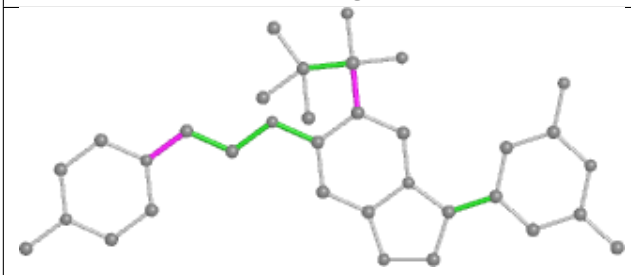
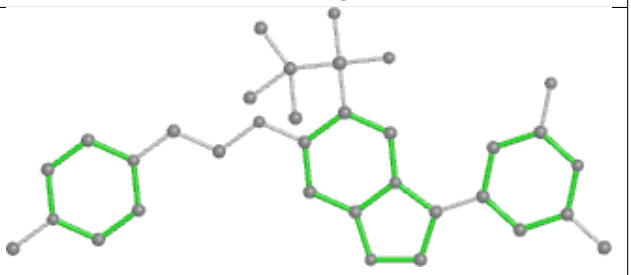


Bond angles

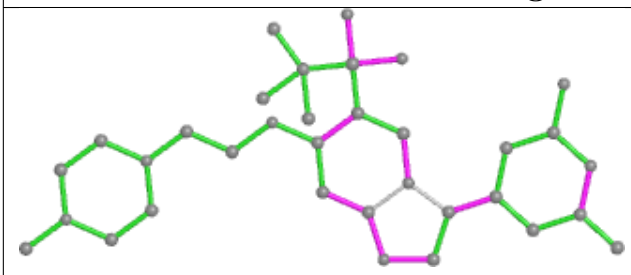


Torsions

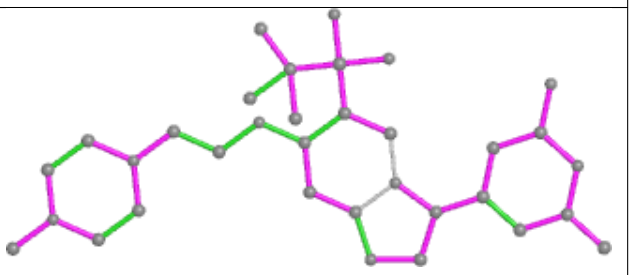


Rings

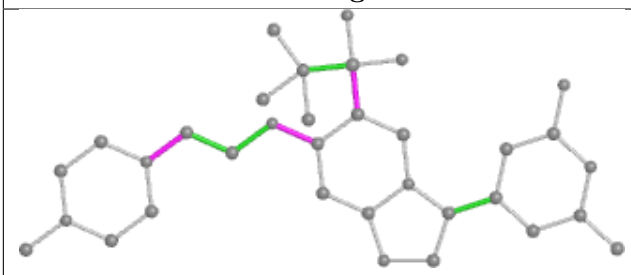
Ligand 9XA F 401



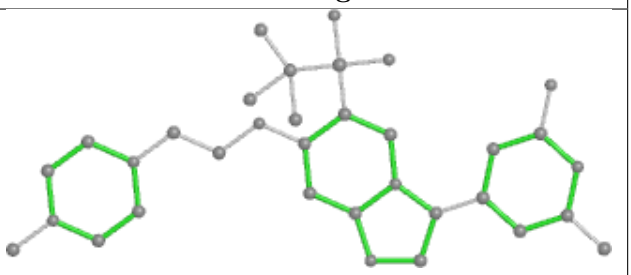
Bond lengths



Bond angles

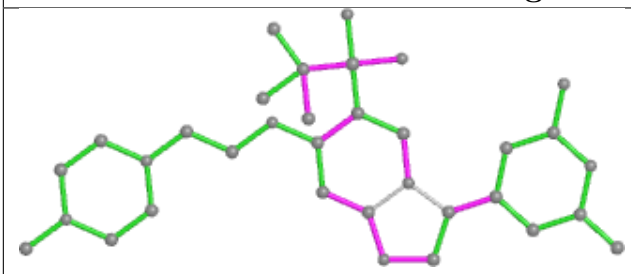


Torsions



Rings

Ligand 9XA O 401



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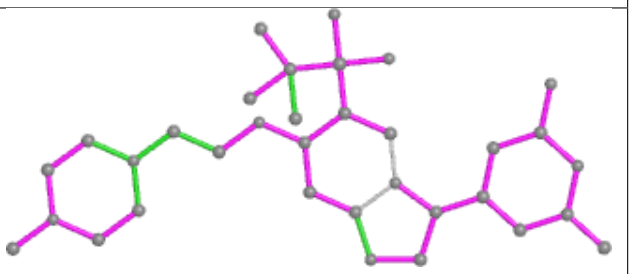
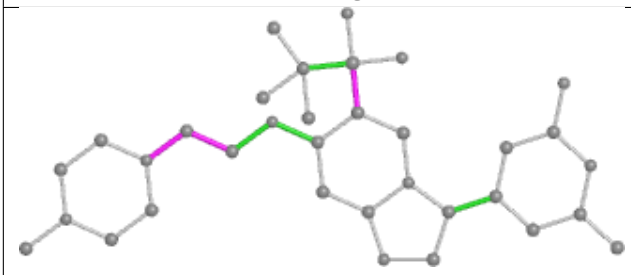
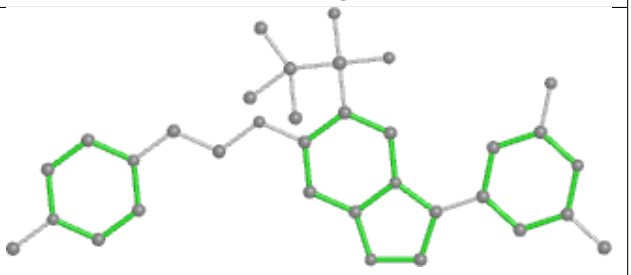


Bond angles

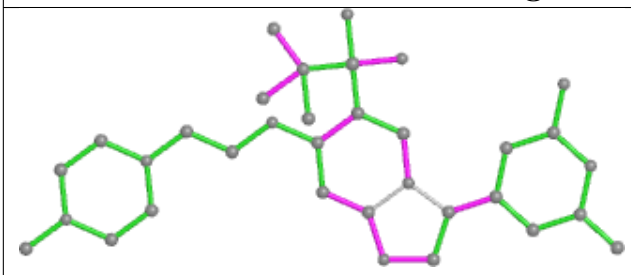


Torsions

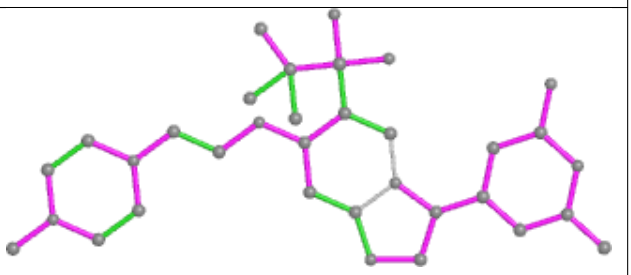


Rings

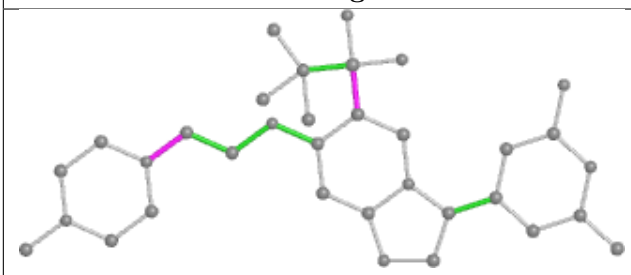
Ligand 9XA D 401



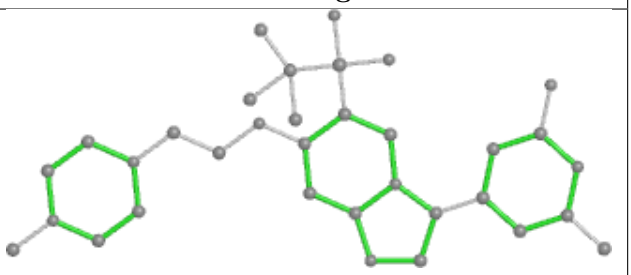
Bond lengths



Bond angles

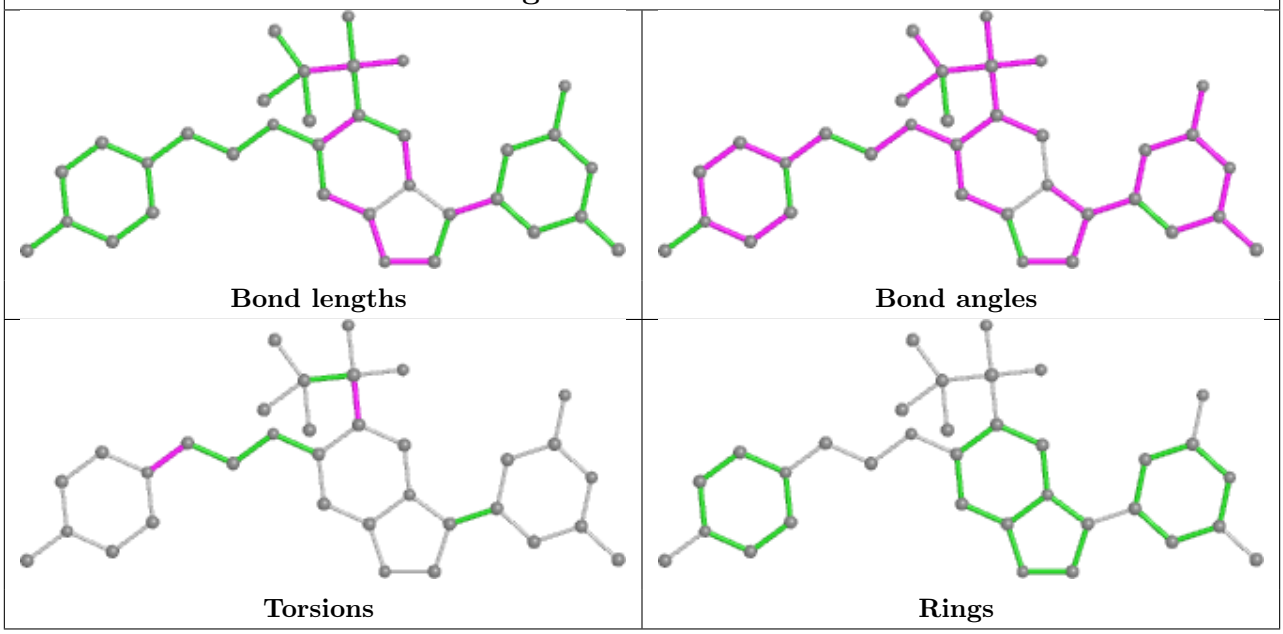


Torsions

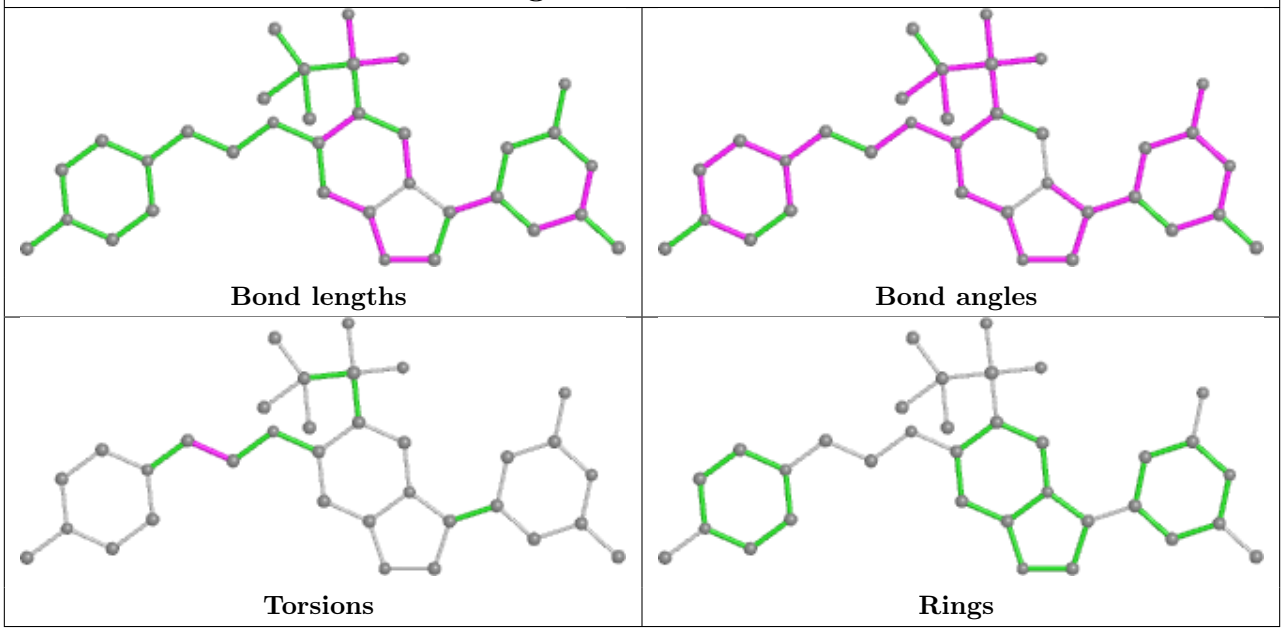


Rings

Ligand 9XA M 401



Ligand 9XA P 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	275/310 (88%)	0.50	20 (7%)	15	11	48, 78, 106, 141	0
1	B	275/310 (88%)	0.53	21 (7%)	13	10	51, 82, 109, 128	0
1	C	275/310 (88%)	0.64	24 (8%)	10	7	59, 91, 121, 133	0
1	D	275/310 (88%)	0.60	24 (8%)	10	7	47, 83, 110, 126	0
1	E	275/310 (88%)	0.56	20 (7%)	15	11	51, 78, 106, 121	0
1	F	275/310 (88%)	0.49	17 (6%)	20	16	54, 81, 107, 132	0
1	G	275/310 (88%)	0.47	16 (5%)	23	19	51, 77, 107, 125	0
1	H	275/310 (88%)	0.55	20 (7%)	15	11	50, 82, 114, 139	0
1	I	275/310 (88%)	0.56	27 (9%)	7	5	53, 82, 110, 127	0
1	J	275/310 (88%)	0.56	24 (8%)	10	7	53, 80, 106, 130	0
1	K	275/310 (88%)	0.54	22 (8%)	12	9	54, 83, 109, 121	0
1	L	275/310 (88%)	0.55	31 (11%)	5	4	62, 92, 123, 140	0
1	M	276/310 (89%)	0.51	23 (8%)	11	8	55, 85, 112, 128	0
1	N	272/310 (87%)	0.52	20 (7%)	14	11	62, 91, 117, 129	0
1	O	276/310 (89%)	0.60	23 (8%)	11	8	56, 85, 111, 131	0
1	P	275/310 (88%)	0.54	22 (8%)	12	9	59, 91, 111, 138	0
All	All	4399/4960 (88%)	0.55	354 (8%)	12	9	47, 84, 112, 141	0

All (354) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	172	MET	10.6
1	E	172	MET	9.0
1	O	171	ARG	8.4
1	A	172	MET	6.7
1	D	229	PHE	5.8

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Mol	Chain	Res	Type	RSRZ
1	D	232	VAL	5.8
1	J	297	PHE	5.6
1	E	171	ARG	5.5
1	N	220	TRP	5.4
1	C	30	GLY	5.1
1	J	229	PHE	5.0
1	I	188	GLY	5.0
1	P	29	SER	4.7
1	J	29	SER	4.6
1	M	101	GLY	4.5
1	N	254	SER	4.5
1	K	113	TYR	4.4
1	L	229	PHE	4.4
1	N	228	PRO	4.3
1	D	233	THR	4.3
1	L	28	ALA	4.3
1	H	290	LEU	4.3
1	F	29	SER	4.3
1	C	10	LEU	4.2
1	C	122	PHE	4.1
1	J	10	LEU	4.1
1	K	92	GLY	4.0
1	B	15	TYR	4.0
1	O	269	ILE	4.0
1	O	13	ILE	4.0
1	D	294	LEU	4.0
1	C	71	HIS	3.9
1	L	13	ILE	3.9
1	G	107	LEU	3.9
1	D	44	VAL	3.9
1	F	28	ALA	3.9
1	I	269	ILE	3.9
1	L	93	ILE	3.9
1	A	16	HIS	3.8
1	N	303	LEU	3.8
1	N	30	GLY	3.8
1	K	18	LEU	3.8
1	L	220	TRP	3.8
1	D	73	ALA	3.8
1	I	84	ILE	3.7
1	C	239	MET	3.7
1	C	29	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	168	SER	3.7
1	A	28	ALA	3.7
1	N	125	LEU	3.7
1	D	223	LEU	3.7
1	J	223	LEU	3.6
1	A	30	GLY	3.6
1	P	301	THR	3.6
1	A	24	LEU	3.5
1	O	35	ALA	3.5
1	E	116	VAL	3.5
1	D	236	LEU	3.5
1	E	147	LEU	3.5
1	L	129	ALA	3.5
1	O	297	PHE	3.5
1	B	91	LEU	3.4
1	M	106	LEU	3.4
1	B	190	ILE	3.4
1	H	101	GLY	3.4
1	I	223	LEU	3.4
1	C	306	VAL	3.4
1	H	132	VAL	3.4
1	L	81	ILE	3.4
1	P	73	ALA	3.3
1	I	294	LEU	3.3
1	K	303	LEU	3.3
1	L	290	LEU	3.3
1	K	222	VAL	3.3
1	O	170	TRP	3.3
1	B	128	ILE	3.3
1	O	84	ILE	3.3
1	L	248	PRO	3.3
1	B	151	ASN	3.2
1	L	15	TYR	3.2
1	J	189	THR	3.2
1	P	35	ALA	3.2
1	E	160	VAL	3.2
1	K	107	LEU	3.2
1	I	92	GLY	3.2
1	P	11	PRO	3.2
1	M	309	LEU	3.2
1	I	160	VAL	3.2
1	I	256	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	306	VAL	3.2
1	N	108	HIS	3.1
1	M	85	CYS	3.1
1	N	28	ALA	3.1
1	H	141	PRO	3.1
1	A	18	LEU	3.1
1	K	294	LEU	3.1
1	P	281	PRO	3.1
1	C	64	LEU	3.1
1	M	222	VAL	3.1
1	L	223	LEU	3.1
1	F	198	TYR	3.1
1	J	190	ILE	3.1
1	C	158	PHE	3.1
1	N	299	GLU	3.0
1	B	90	PHE	3.0
1	J	107	LEU	3.0
1	L	147	LEU	3.0
1	H	30	GLY	3.0
1	I	69	ILE	3.0
1	M	293	VAL	3.0
1	B	149	THR	3.0
1	F	217	VAL	3.0
1	E	218	ILE	3.0
1	K	223	LEU	3.0
1	A	120	LEU	2.9
1	G	268	LEU	2.9
1	J	228	PRO	2.9
1	D	300	ILE	2.9
1	A	107	LEU	2.9
1	J	171	ARG	2.9
1	C	69	ILE	2.9
1	P	223	LEU	2.9
1	G	237	GLN	2.9
1	F	122	PHE	2.9
1	P	116	VAL	2.9
1	A	188	GLY	2.9
1	I	167	LEU	2.9
1	K	91	LEU	2.9
1	O	223	LEU	2.9
1	D	248	PRO	2.9
1	C	103	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	O	309	LEU	2.9
1	D	160	VAL	2.9
1	F	18	LEU	2.9
1	L	262	ARG	2.9
1	O	147	LEU	2.9
1	P	269	ILE	2.8
1	C	255	LEU	2.8
1	M	21	LEU	2.8
1	C	254	SER	2.8
1	E	23	TYR	2.8
1	K	90	PHE	2.8
1	J	290	LEU	2.8
1	C	244	GLN	2.8
1	B	229	PHE	2.8
1	J	232	VAL	2.8
1	F	92	GLY	2.8
1	J	188	GLY	2.8
1	P	59	GLU	2.8
1	K	64	LEU	2.8
1	L	222	VAL	2.8
1	M	42	VAL	2.8
1	M	125	LEU	2.7
1	G	122	PHE	2.7
1	P	255	LEU	2.7
1	G	229	PHE	2.7
1	J	238	ILE	2.7
1	O	116	VAL	2.7
1	M	165	PHE	2.7
1	O	156	ASN	2.7
1	B	18	LEU	2.7
1	C	118	TRP	2.7
1	J	293	VAL	2.7
1	H	298	GLU	2.7
1	F	147	LEU	2.7
1	L	103	LEU	2.7
1	I	85	CYS	2.7
1	A	29	SER	2.7
1	K	120	LEU	2.7
1	I	18	LEU	2.7
1	L	250	ILE	2.7
1	O	162	ILE	2.7
1	J	231	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	P	211	ASP	2.7
1	G	170	TRP	2.6
1	K	229	PHE	2.6
1	N	101	GLY	2.6
1	F	13	ILE	2.6
1	L	303	LEU	2.6
1	O	44	VAL	2.6
1	L	90	PHE	2.6
1	B	93	ILE	2.6
1	N	75	PHE	2.6
1	N	229	PHE	2.6
1	D	162	ILE	2.6
1	H	293	VAL	2.6
1	K	231	ASP	2.6
1	G	220	TRP	2.6
1	K	24	LEU	2.6
1	P	10	LEU	2.6
1	D	297	PHE	2.6
1	P	158	PHE	2.6
1	J	191	ILE	2.6
1	N	190	ILE	2.6
1	O	124	ILE	2.6
1	I	124	ILE	2.5
1	G	106	LEU	2.5
1	A	23	TYR	2.5
1	E	13	ILE	2.5
1	M	84	ILE	2.5
1	D	290	LEU	2.5
1	K	17	LYS	2.5
1	C	62	ASP	2.5
1	O	229	PHE	2.5
1	A	145	HIS	2.5
1	G	69	ILE	2.5
1	K	248	PRO	2.5
1	L	107	LEU	2.5
1	J	73	ALA	2.5
1	B	248	PRO	2.4
1	C	284	LEU	2.5
1	J	307	ILE	2.5
1	M	303	LEU	2.5
1	L	75	PHE	2.4
1	P	160	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	237	GLN	2.4
1	B	218	ILE	2.4
1	C	287	LEU	2.4
1	J	220	TRP	2.4
1	E	103	LEU	2.4
1	H	142	LEU	2.4
1	I	259	ILE	2.4
1	H	77	TYR	2.4
1	E	229	PHE	2.4
1	H	29	SER	2.4
1	N	197	ASN	2.4
1	J	69	ILE	2.4
1	M	190	ILE	2.4
1	N	300	ILE	2.4
1	P	64	LEU	2.4
1	L	217	VAL	2.4
1	K	265	MET	2.4
1	D	81	ILE	2.4
1	D	238	ILE	2.4
1	G	195	PRO	2.4
1	L	65	ARG	2.4
1	O	29	SER	2.4
1	I	170	TRP	2.4
1	E	156	ASN	2.4
1	K	254	SER	2.4
1	J	156	ASN	2.4
1	H	171	ARG	2.4
1	M	154	LEU	2.4
1	F	90	PHE	2.3
1	L	63	VAL	2.3
1	N	248	PRO	2.3
1	J	294	LEU	2.3
1	M	283	PHE	2.3
1	N	198	TYR	2.3
1	D	255	LEU	2.3
1	F	294	LEU	2.3
1	I	81	ILE	2.3
1	M	107	LEU	2.3
1	P	284	LEU	2.3
1	C	228	PRO	2.3
1	F	107	LEU	2.3
1	O	65	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	297	PHE	2.3
1	A	118	TRP	2.3
1	H	40	TRP	2.3
1	G	239	MET	2.3
1	I	142	LEU	2.3
1	L	208	ILE	2.3
1	E	115	ASP	2.3
1	F	91	LEU	2.3
1	A	151	ASN	2.2
1	H	286	CYS	2.2
1	B	10	LEU	2.2
1	K	255	LEU	2.2
1	B	266	ILE	2.2
1	N	93	ILE	2.2
1	L	86	ASN	2.2
1	D	303	LEU	2.2
1	G	305	ALA	2.2
1	E	93	ILE	2.2
1	I	302	PHE	2.2
1	G	113	TYR	2.2
1	L	240	TYR	2.2
1	N	273	TRP	2.2
1	P	92	GLY	2.2
1	H	238	ILE	2.2
1	L	260	PRO	2.2
1	A	171	ARG	2.2
1	C	134	TYR	2.2
1	H	93	ILE	2.2
1	O	11	PRO	2.2
1	A	113	TYR	2.2
1	P	134	TYR	2.2
1	E	44	VAL	2.2
1	F	30	GLY	2.2
1	I	103	LEU	2.2
1	I	303	LEU	2.2
1	A	90	PHE	2.2
1	H	297	PHE	2.2
1	H	229	PHE	2.2
1	M	300	ILE	2.2
1	H	60	ARG	2.2
1	G	303	LEU	2.2
1	M	307	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	265	MET	2.2
1	D	122	PHE	2.1
1	G	125	LEU	2.1
1	D	259	ILE	2.1
1	L	307	ILE	2.1
1	B	102	SER	2.1
1	D	40	TRP	2.1
1	M	69	ILE	2.1
1	M	170	TRP	2.1
1	O	69	ILE	2.1
1	E	248	PRO	2.1
1	L	228	PRO	2.1
1	E	189	THR	2.1
1	I	301	THR	2.1
1	B	255	LEU	2.1
1	J	259	ILE	2.1
1	E	40	TRP	2.1
1	D	135	LEU	2.1
1	D	302	PHE	2.1
1	M	113	TYR	2.1
1	P	91	LEU	2.1
1	I	62	ASP	2.1
1	B	162	ILE	2.1
1	K	13	ILE	2.1
1	M	259	ILE	2.1
1	D	159	HIS	2.1
1	G	198	TYR	2.1
1	O	93	ILE	2.1
1	L	14	PRO	2.1
1	M	82	LEU	2.1
1	L	113	TYR	2.1
1	I	78	ILE	2.1
1	F	306	VAL	2.1
1	B	127	GLU	2.1
1	I	279	GLU	2.1
1	O	34	SER	2.1
1	P	90	PHE	2.1
1	B	219	THR	2.1
1	C	113	TYR	2.1
1	I	297	PHE	2.1
1	A	73	ALA	2.0
1	C	301	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	77	TYR	2.0
1	N	230	GLU	2.0
1	F	103	LEU	2.0
1	H	28	ALA	2.0
1	H	215	TYR	2.0
1	A	122	PHE	2.0
1	C	18	LEU	2.0
1	C	154	LEU	2.0
1	B	238	ILE	2.0
1	K	306	VAL	2.0
1	F	64	LEU	2.0
1	I	147	LEU	2.0
1	E	94	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	9XA	P	401	34/34	0.85	0.28	99,110,123,125	0
2	9XA	K	401	34/34	0.89	0.34	85,93,109,112	0
2	9XA	N	401	34/34	0.90	0.28	107,113,115,115	0
2	9XA	M	401	34/34	0.90	0.25	80,93,114,115	0
2	9XA	E	401	34/34	0.91	0.29	73,88,117,117	0
2	9XA	B	401	34/34	0.92	0.27	68,80,89,97	0
2	9XA	L	401	34/34	0.92	0.23	87,97,111,120	0
2	9XA	A	401	34/34	0.92	0.31	78,87,115,117	0
2	9XA	F	401	34/34	0.92	0.25	71,86,96,98	0
2	9XA	G	401	34/34	0.92	0.27	74,81,89,100	0

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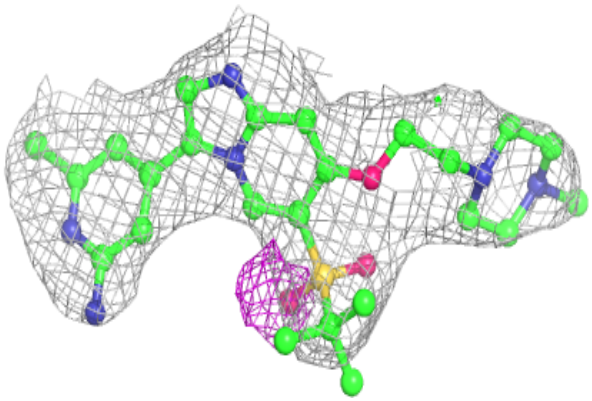
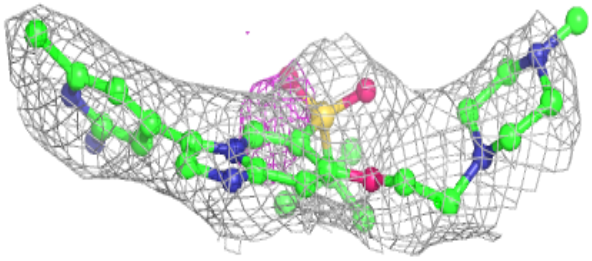
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	9XA	C	401	34/34	0.93	0.20	87,97,112,117	0
2	9XA	H	401	34/34	0.93	0.28	60,75,107,108	0
2	9XA	I	401	34/34	0.93	0.25	66,81,98,99	0
2	9XA	O	401	34/34	0.93	0.26	83,98,118,119	0
2	9XA	D	401	34/34	0.93	0.23	74,88,113,114	0
2	9XA	J	401	34/34	0.94	0.25	76,83,98,100	0

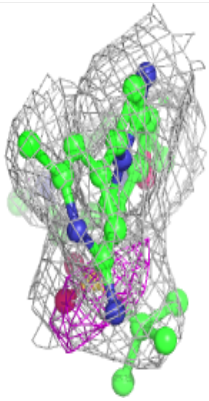
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 9XA P 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

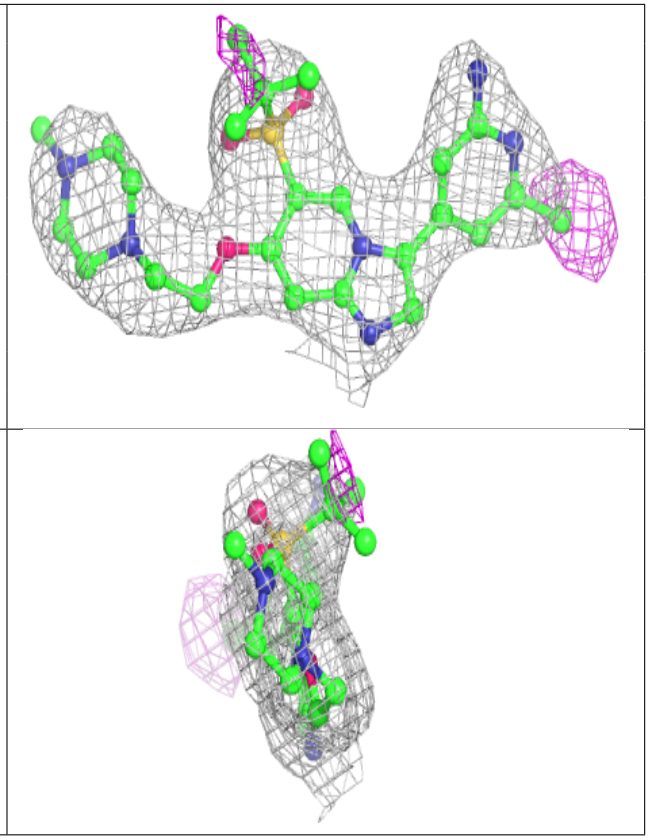






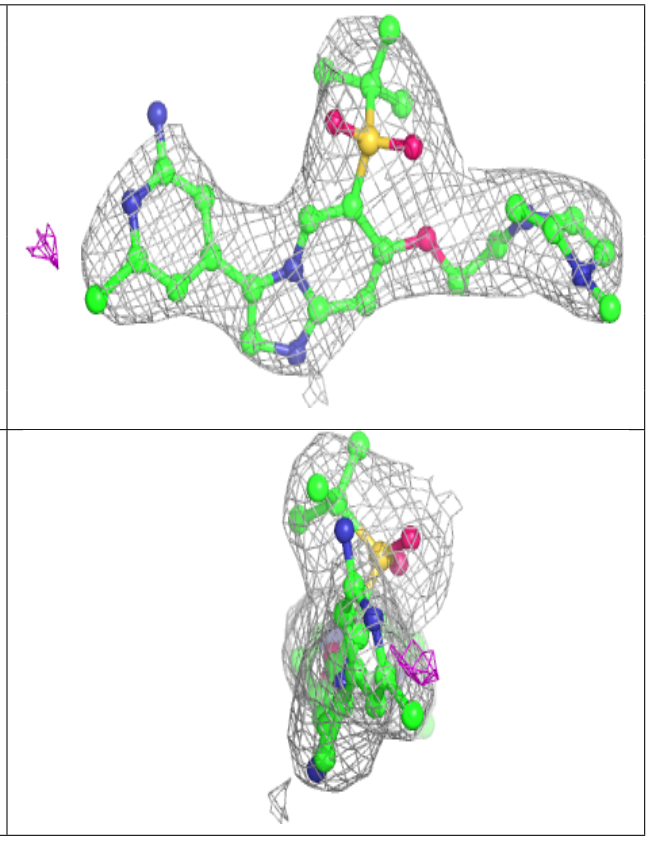
Electron density around 9XA K 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



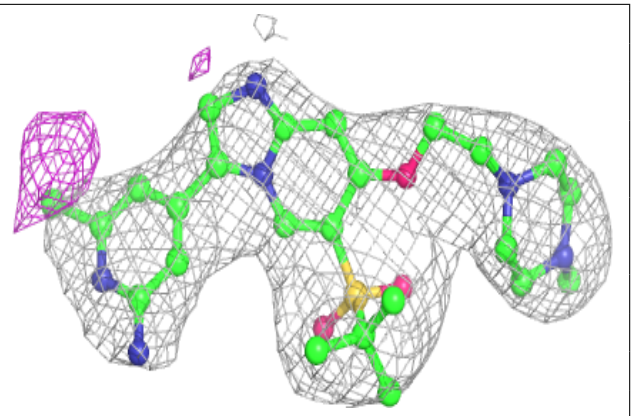
Electron density around 9XA N 401:

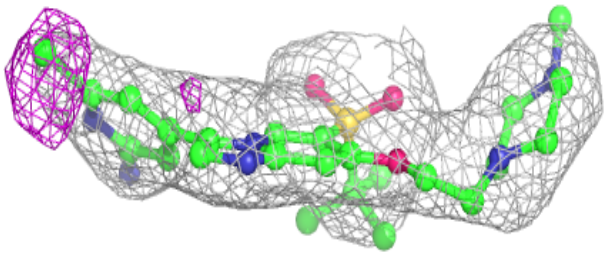
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

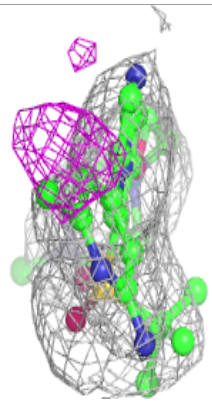


Electron density around 9XA M 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

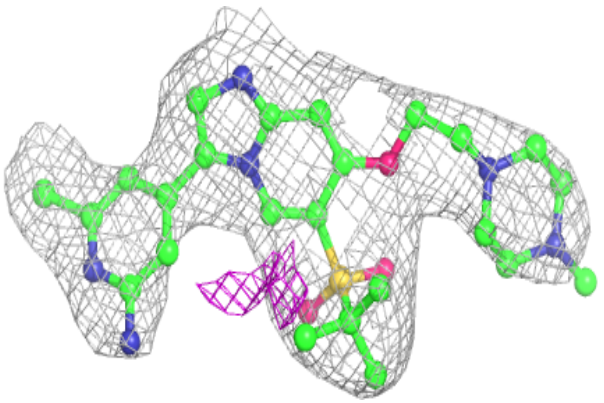


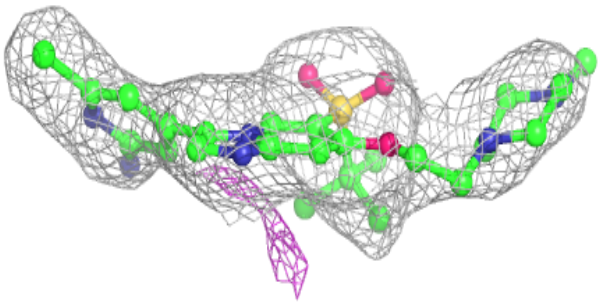


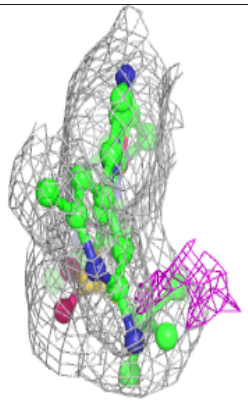


Electron density around 9XA E 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

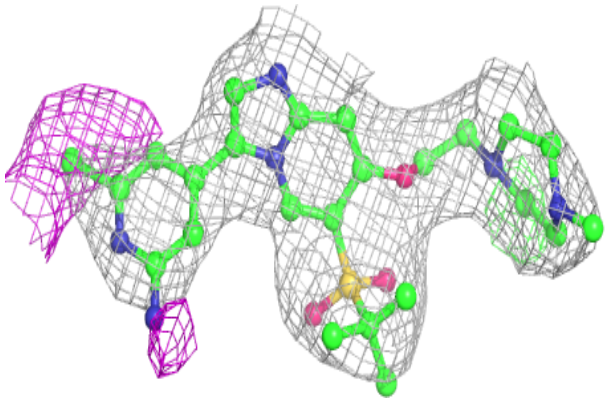


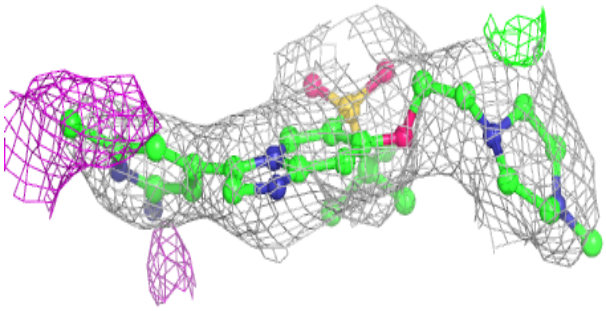


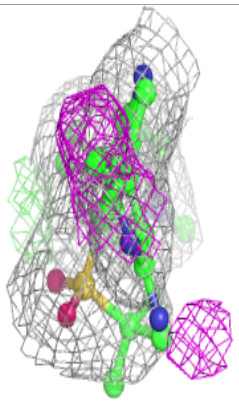


Electron density around 9XA B 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

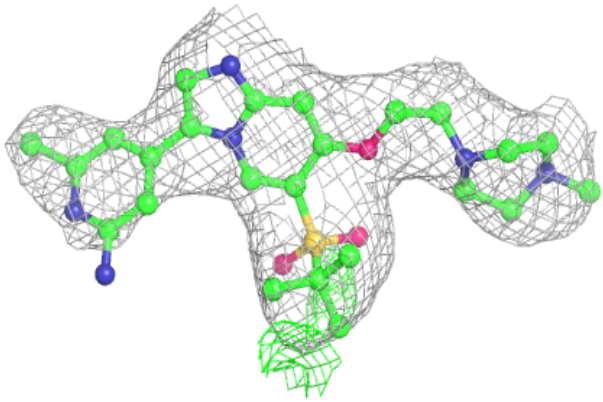


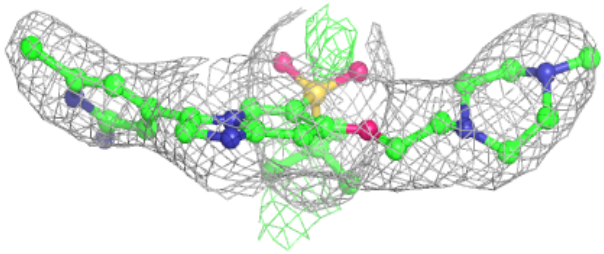


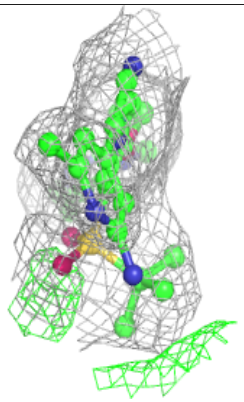


Electron density around 9XA L 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

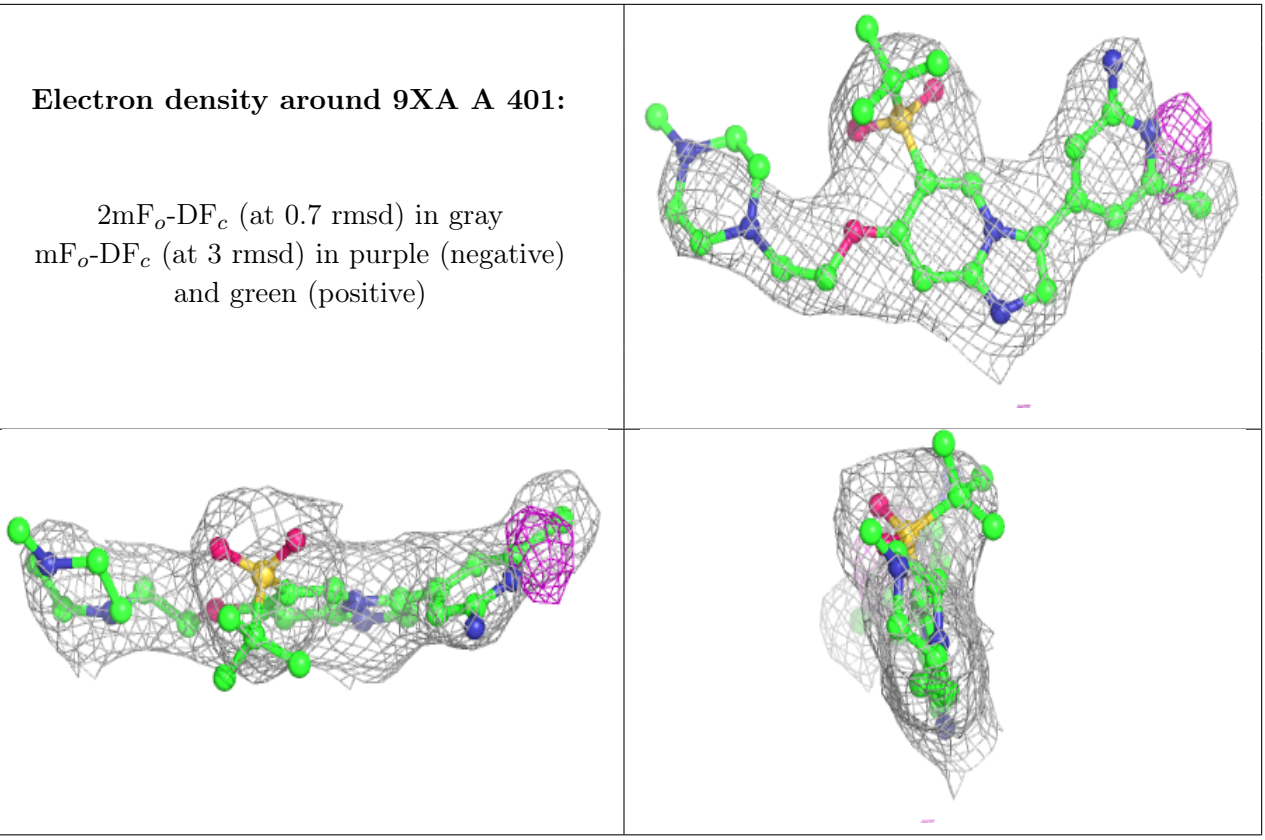






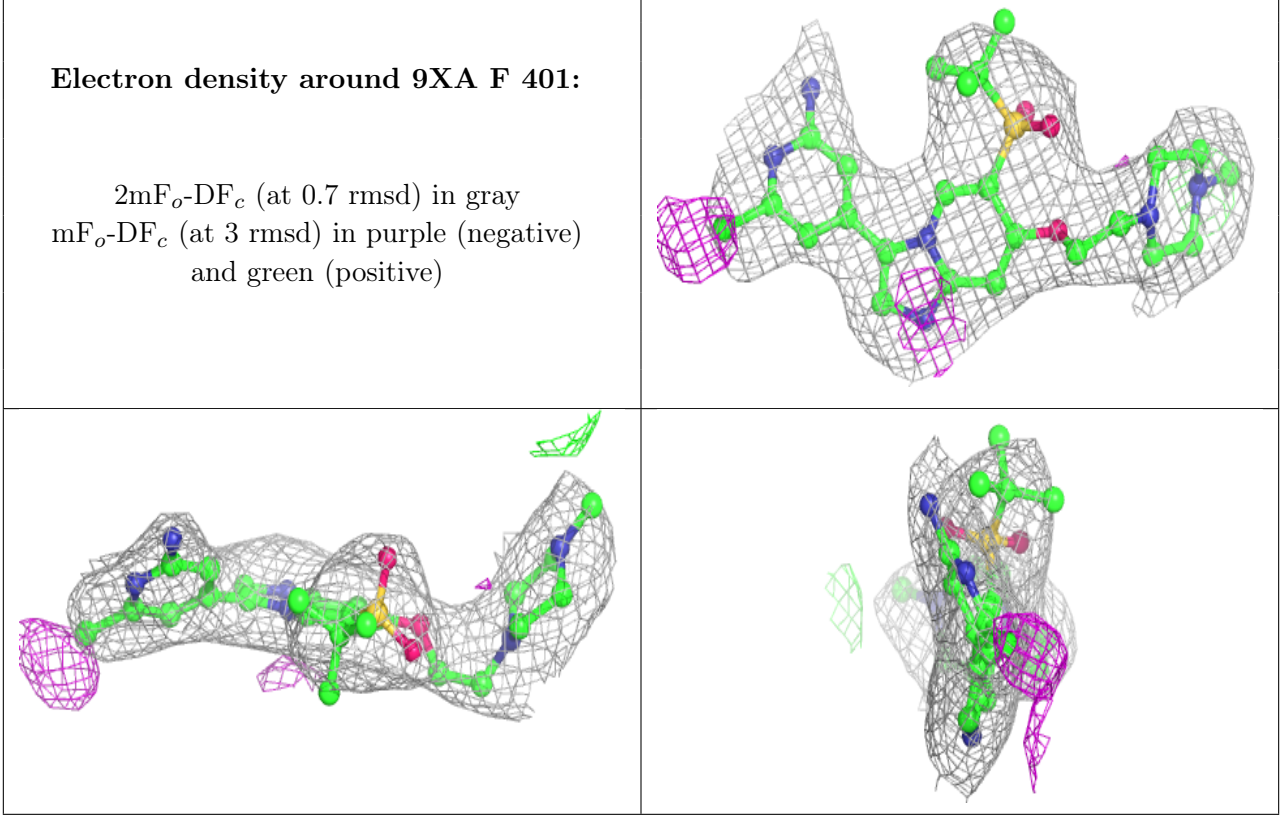
Electron density around 9XA A 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



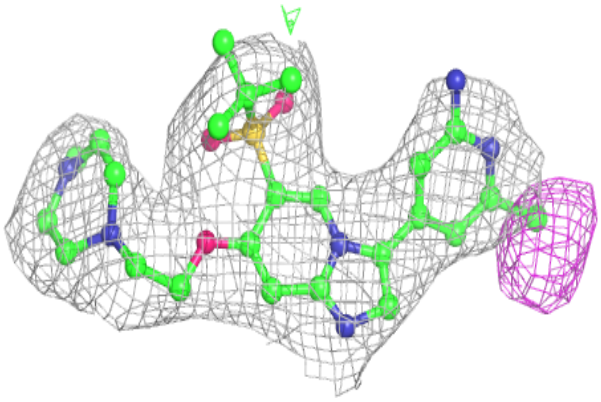
Electron density around 9XA F 401:

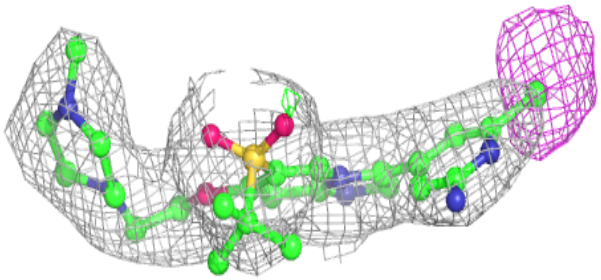
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

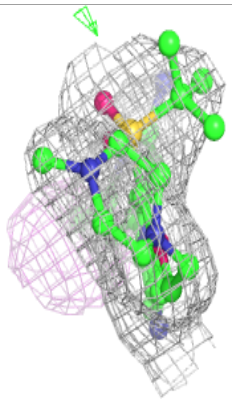


Electron density around 9XA G 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

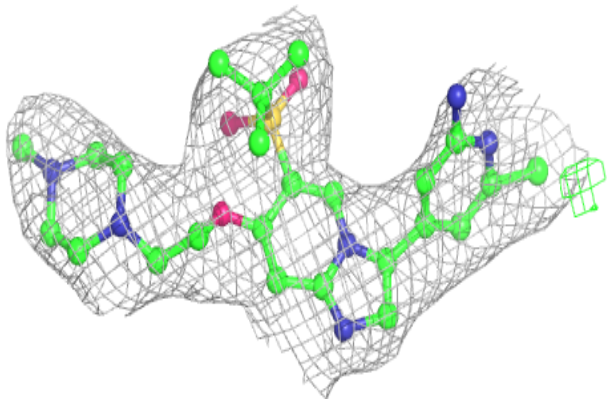


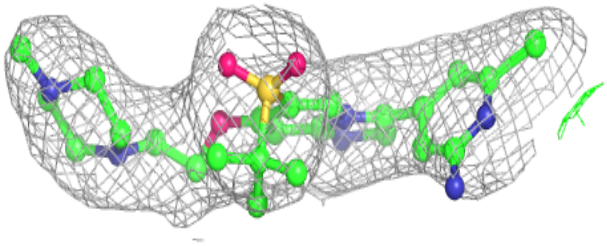


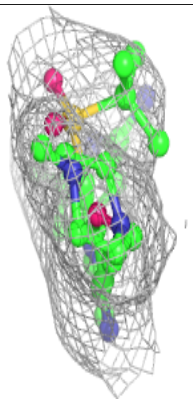


Electron density around 9XA C 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

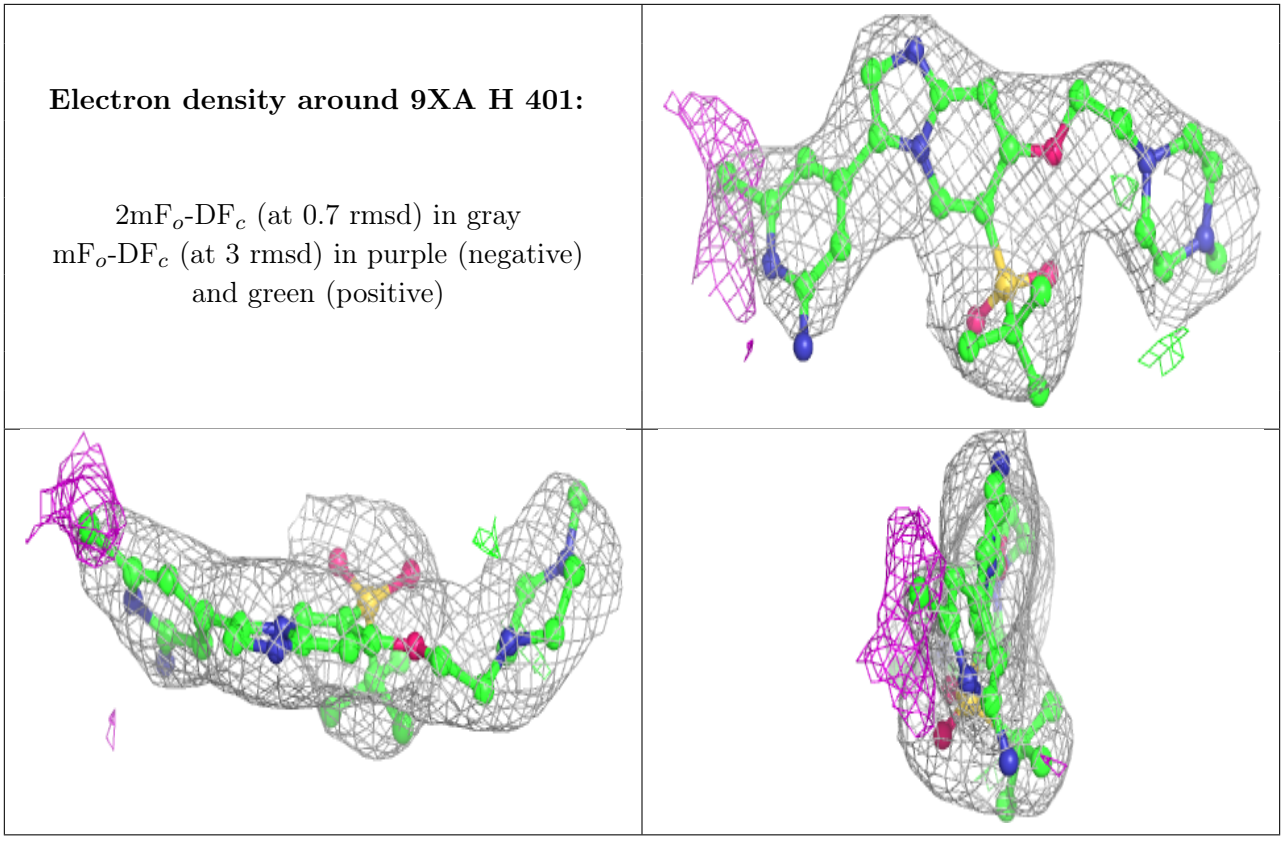






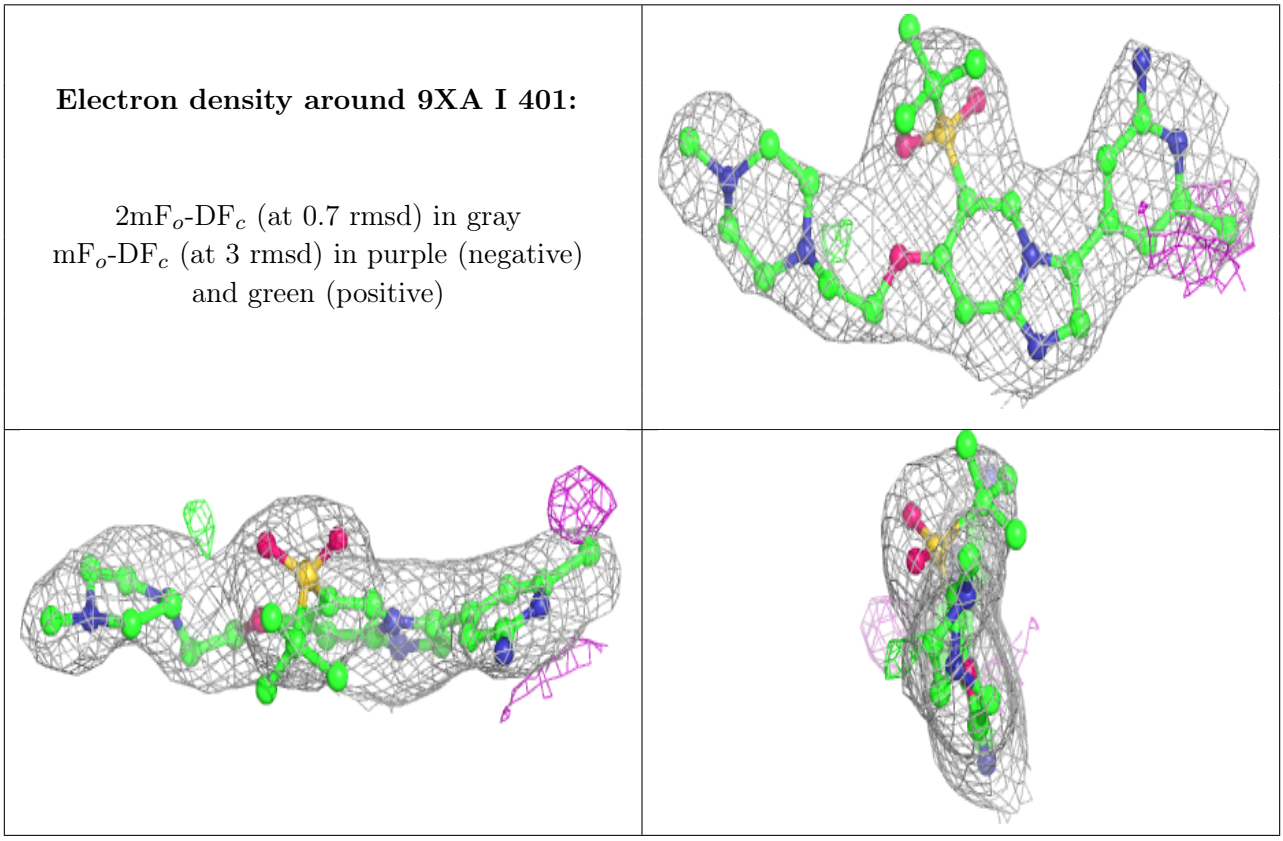
Electron density around 9XA H 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



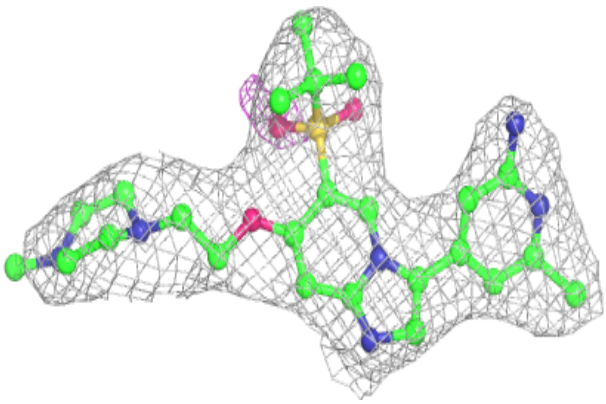
Electron density around 9XA I 401:

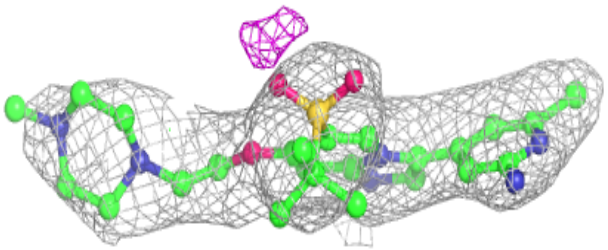
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

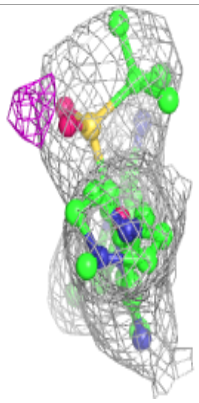


Electron density around 9XA O 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

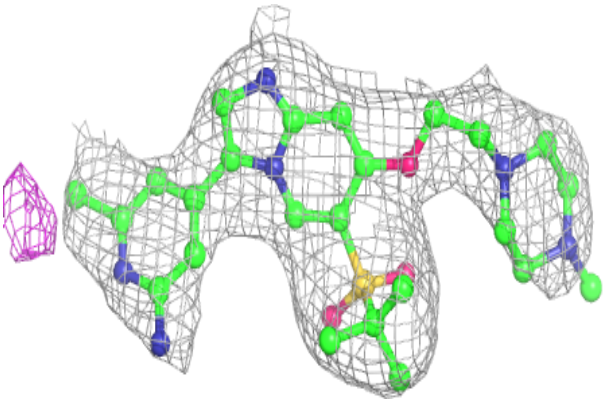


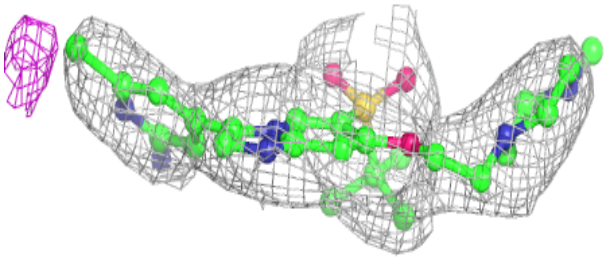


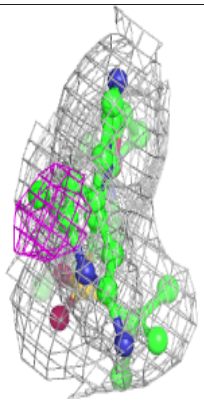


Electron density around 9XA D 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

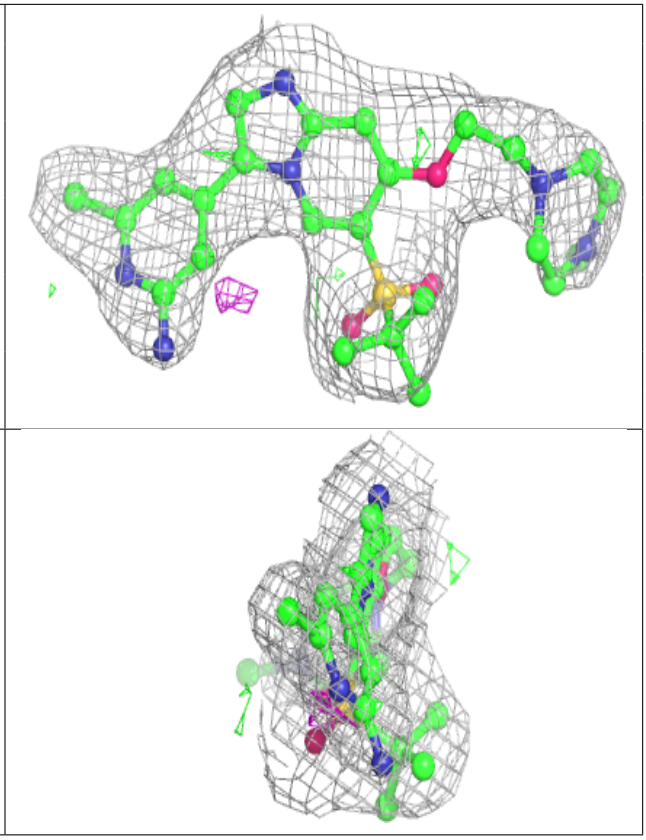






Electron density around 9XA J 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.