Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 12:13 PM EST

PDB ID	:	3SL5
Title	:	Crystal structure of the catalytic domain of PDE4D2 complexed with compound 10d
Authors	:	Feil, S.F.
Deposited on	:	2011-06-24
Resolution	:	2.65 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:

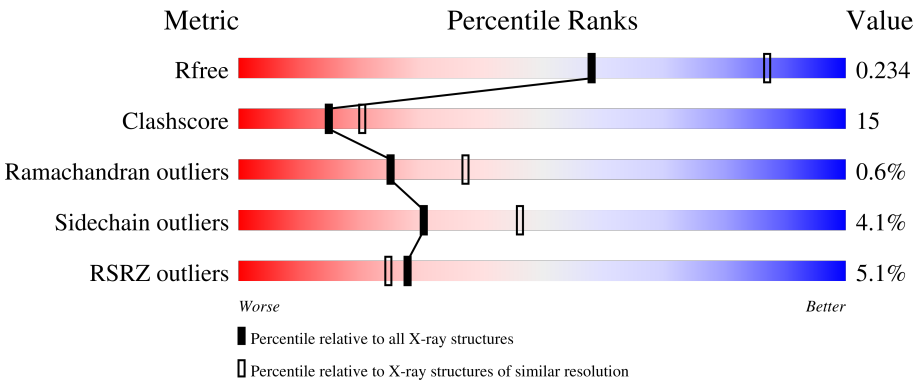
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	359	6% 65% 23% • 9%
1	B	359	2% 55% 32% • 9%
1	C	359	6% 61% 27% • 9%
1	D	359	4% 67% 20% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	J25	A	1	-	-	X	-
4	EDO	D	3	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11156 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.

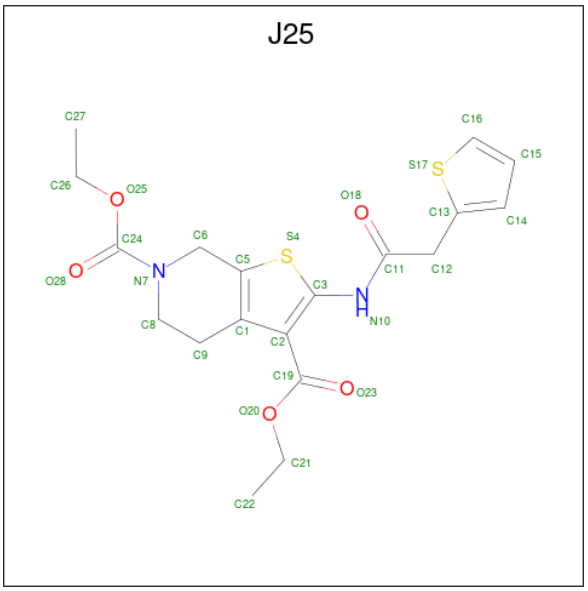
- Molecule 1 is a protein called cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	328	2651	1676	453	508	14	0	0	0
1	B	325	2631	1664	450	503	14	0	0	0
1	C	325	2631	1663	449	505	14	0	0	0
1	D	324	2622	1659	448	501	14	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

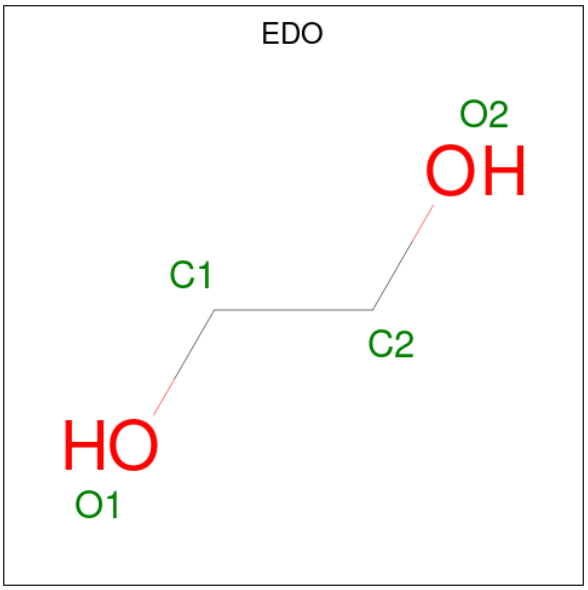
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0

- Molecule 3 is diethyl 2-[(thiophen-2-ylacetyl)amino]-4,7-dihydrothieno[2,3-c]pyridine-3,6(5H)-dicarboxylate (three-letter code: J25) (formula: $C_{19}H_{22}N_2O_5S_2$).



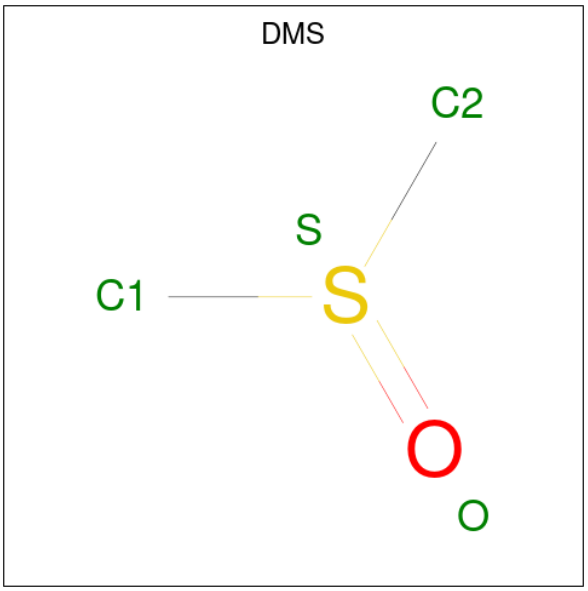
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	28	19	2	5	2	0	0
			Total	C	N	O	S		
3	B	1	28	19	2	5	2	0	0
			Total	C	N	O	S		
3	C	1	28	19	2	5	2	0	0
			Total	C	N	O	S		
3	D	1	28	19	2	5	2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



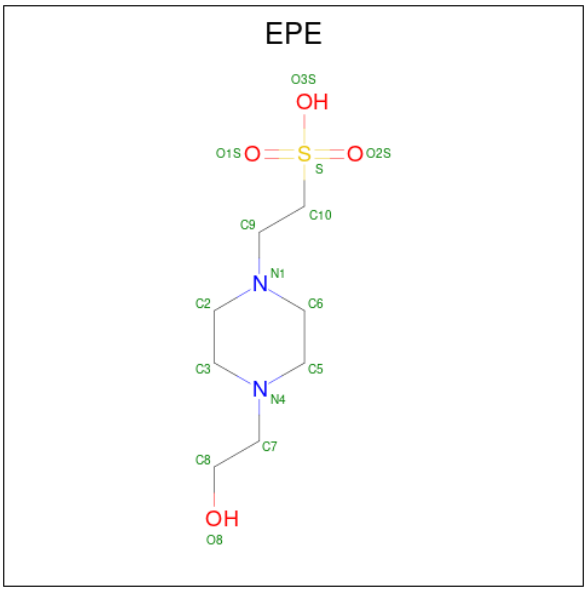
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0
			Total	C	O		
4	A	1	4	2	2	0	0
			Total	C	O		
4	B	1	4	2	2	0	0
			Total	C	O		
4	B	1	4	2	2	0	0
			Total	C	O		
4	C	1	4	2	2	0	0
			Total	C	O		
4	C	1	4	2	2	0	0
			Total	C	O		
4	C	1	4	2	2	0	0
			Total	C	O		
4	C	1	4	2	2	0	0
			Total	C	O		
4	C	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
5	A	1	4	2	1	1	0	0

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	C	1	15	8	2	4	1	0	0

- Molecule 7 is water.

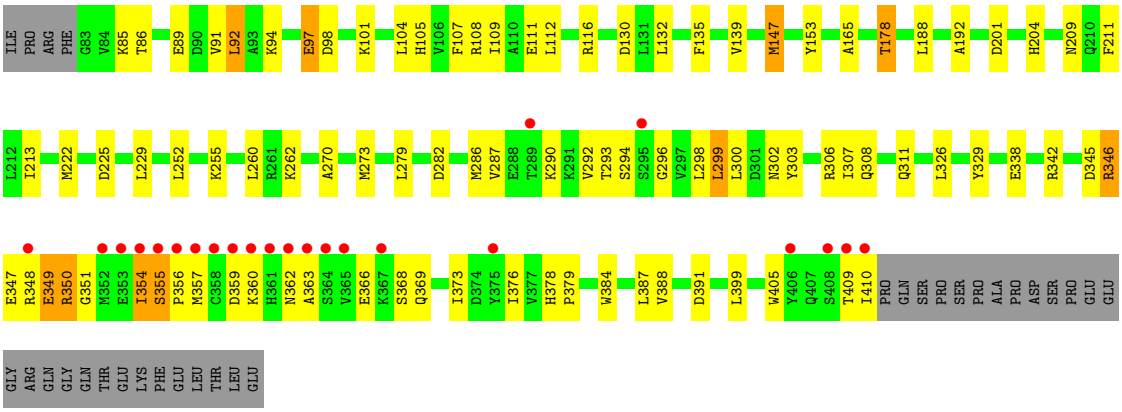
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	107	107	107	0	0
			Total	O		
7	B	92	92	92	0	0
			Total	O		
7	C	82	82	82	0	0
			Total	O		
7	D	133	133	133	0	0

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.

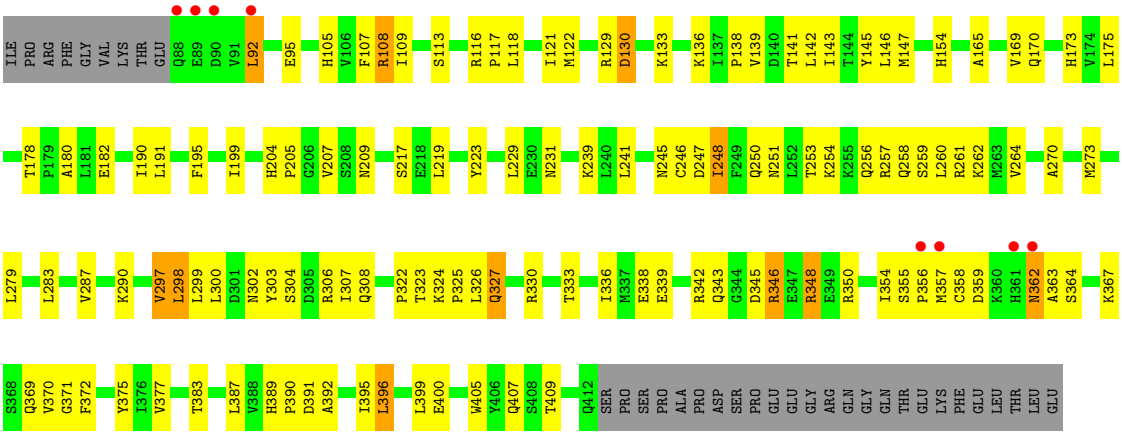
• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain A: 6% 65% 23% • 9%



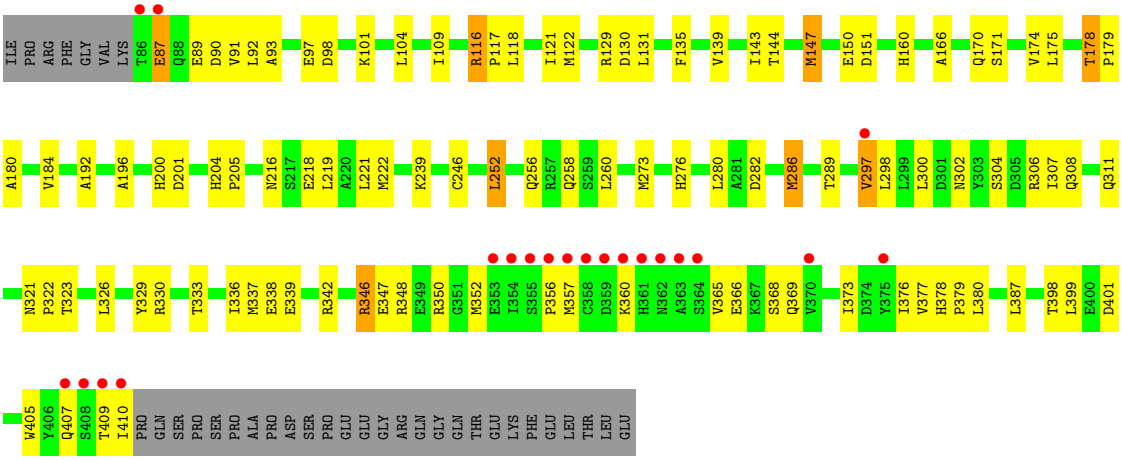
• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain B: 2% 55% 32% • 9%



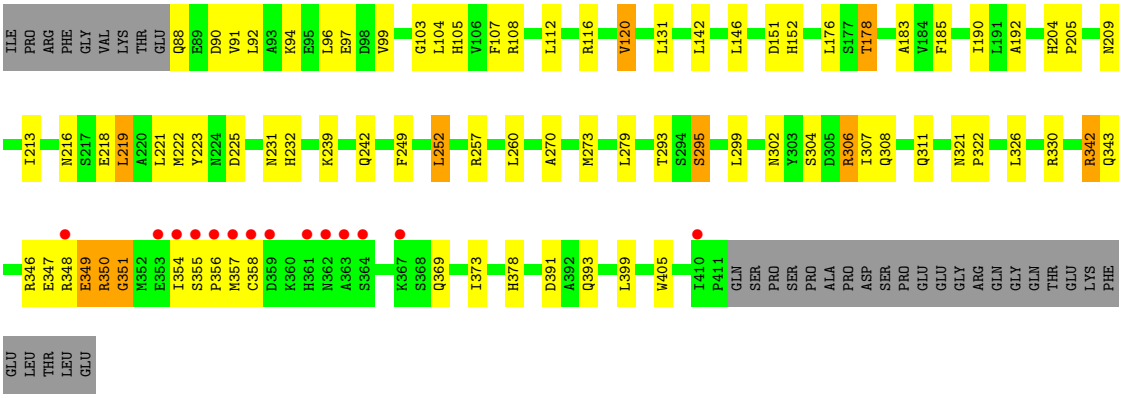
• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain C: 6% 61% 27% • 9%



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.39Å 109.97Å 159.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.73 – 2.65 61.73 – 2.65	Depositor EDS
% Data completeness (in resolution range)	91.3 (61.73-2.65) 91.3 (61.73-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	3.62 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.171 , 0.242 0.162 , 0.234	Depositor DCC
R_{free} test set	2365 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11156	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: J25, ZN, EPE, EDO, DMS

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	0.39	0/2704	0.52	0/3672
1	B	0.37	0/2685	0.53	0/3648
1	C	0.38	0/2684	0.53	0/3646
1	D	0.42	0/2676	0.54	0/3636
All	All	0.39	0/10749	0.53	0/14602

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	2651	0	2609	85	0
1	B	2631	0	2586	104	0
1	C	2631	0	2584	77	0
1	D	2622	0	2578	60	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	28	0	22	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	22	7	0
3	C	28	0	22	6	0
3	D	28	0	22	4	0
4	A	8	0	12	1	0
4	B	8	0	12	3	0
4	C	20	0	30	2	0
4	D	32	0	48	6	0
5	A	4	0	6	0	0
6	C	15	0	17	0	0
7	A	107	0	0	5	0
7	B	92	0	0	7	0
7	C	82	0	0	3	0
7	D	133	0	0	3	0
All	All	11156	0	10570	324	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 15.

All (324) 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:A:368:SER:HB3	3:A:1:J25:H22	1.40	1.00
1:C:368:SER:HB3	3:C:1:J25:H22	1.47	0.95
1:B:348:ARG:HG3	1:B:354:ILE:HD11	1.55	0.86
1:B:108:ARG:HG3	1:B:108:ARG:HH11	1.37	0.86
1:D:273:MET:HG3	3:D:1:J25:H6	1.55	0.86
1:D:304:SER:O	1:D:308:GLN:HG3	1.75	0.85
1:A:273:MET:HG3	3:A:1:J25:H6	1.58	0.85
3:A:1:J25:H26	3:A:1:J25:H6A	1.58	0.85
1:B:108:ARG:HH11	1:B:108:ARG:CG	1.90	0.84
1:A:86:THR:OG1	1:A:89:GLU:HG3	1.79	0.83
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.43	0.83
1:B:182:GLU:O	1:B:297:VAL:HG21	1.77	0.82
1:A:116:ARG:HE	1:A:147:MET:HE2	1.43	0.81
3:B:1:J25:H8	3:B:1:J25:H26A	1.63	0.79
1:C:135:PHE:HA	4:C:2:EDO:H21	1.62	0.79
1:D:190:ILE:HD11	4:D:3:EDO:H21	1.63	0.79
1:B:105:HIS:CE1	1:B:107:PHE:HB2	2.19	0.77
1:D:88:GLN:HB3	1:D:91:VAL:HG23	1.67	0.77
1:A:338:GLU:O	1:A:342:ARG:HG3	1.87	0.75
1:D:185:PHE:H	4:D:3:EDO:H11	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ARG:HG2	1:C:147:MET:HE1	1.70	0.73
1:A:132:LEU:HD22	1:A:139:VAL:HG12	1.70	0.72
1:C:337:MET:HG3	1:C:365:VAL:HG22	1.72	0.72
1:B:253:THR:HG23	1:B:256:GLN:OE1	1.91	0.71
1:B:254:LYS:O	1:B:258:GLN:HG3	1.90	0.71
1:D:326:LEU:O	1:D:330:ARG:HG3	1.90	0.71
1:D:321:ASN:HB2	1:D:322:PRO:HD3	1.74	0.69
1:A:366:GLU:HG2	1:A:409:THR:CG2	2.22	0.69
1:C:180:ALA:O	1:C:297:VAL:HG22	1.93	0.69
1:C:347:GLU:HG2	1:C:352:MET:HE2	1.74	0.68
1:A:369:GLN:O	1:A:373:ILE:HG13	1.94	0.68
1:A:292:VAL:CG1	1:A:296:GLY:HA2	2.24	0.68
1:B:217:SER:HB2	7:D:527:HOH:O	1.94	0.67
3:B:1:J25:H26A	3:B:1:J25:C8	2.25	0.66
1:A:104:LEU:HD11	1:A:109:ILE:HD11	1.78	0.66
1:A:287:VAL:O	1:A:290:LYS:HB2	1.96	0.66
1:B:109:ILE:O	1:B:113:SER:HB2	1.96	0.65
1:A:354:ILE:HG21	1:A:359:ASP:HA	1.79	0.65
1:D:348:ARG:HB3	1:D:354:ILE:HD11	1.78	0.65
1:A:270:ALA:HB1	1:A:279:LEU:HD11	1.79	0.64
1:A:369:GLN:NE2	3:A:1:J25:H21	2.13	0.64
1:C:330:ARG:HD3	1:C:405:TRP:CH2	2.33	0.64
1:C:273:MET:HE2	3:C:1:J25:O28	1.98	0.63
1:D:88:GLN:HG3	1:D:90:ASP:H	1.62	0.63
1:D:322:PRO:HG3	3:D:1:J25:H15	1.79	0.63
1:A:105:HIS:CD2	1:A:108:ARG:H	2.16	0.63
1:C:348:ARG:HH22	1:C:360:LYS:HE2	1.62	0.63
1:C:139:VAL:HG23	7:C:547:HOH:O	1.97	0.63
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.81	0.62
1:A:302:ASN:O	1:A:306:ARG:HG3	1.99	0.62
1:B:364:SER:HB2	7:B:529:HOH:O	1.99	0.62
1:B:298:LEU:HD11	1:B:387:LEU:HD11	1.81	0.62
1:B:372:PHE:HE2	3:B:1:J25:H14	1.64	0.62
1:A:345:ASP:O	1:A:349:GLU:HG3	1.99	0.62
1:A:116:ARG:HE	1:A:147:MET:CE	2.11	0.62
1:A:359:ASP:CG	1:A:362:ASN:HB2	2.20	0.62
1:A:292:VAL:HG12	1:A:293:THR:N	2.15	0.61
1:B:108:ARG:HG3	1:B:108:ARG:NH1	2.13	0.61
1:B:141:THR:HG22	1:B:248:ILE:HG22	1.82	0.61
1:C:302:ASN:HD22	1:C:304:SER:HB3	1.64	0.61
1:B:302:ASN:O	1:B:306:ARG:HG3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:HG2	1:A:108:ARG:NH1	2.16	0.60
1:A:366:GLU:HG2	1:A:409:THR:HB	1.83	0.60
1:C:116:ARG:CG	1:C:147:MET:HE1	2.31	0.60
1:B:129:ARG:HH12	1:B:190:ILE:HD13	1.66	0.59
1:C:369:GLN:O	1:C:373:ILE:HG13	2.02	0.59
1:D:270:ALA:HB1	1:D:279:LEU:HD11	1.85	0.59
1:C:184:VAL:HG11	1:C:300:LEU:HD12	1.85	0.59
1:B:396:LEU:O	1:B:400:GLU:HG3	2.03	0.59
1:A:85:LYS:HB3	1:A:89:GLU:HB2	1.84	0.58
1:B:372:PHE:CE2	3:B:1:J25:H14	2.38	0.58
1:C:87:GLU:O	1:C:91:VAL:HG23	2.03	0.58
1:D:223:TYR:CE1	1:D:231:ASN:HB3	2.39	0.57
1:A:369:GLN:HE22	3:A:1:J25:H21	1.69	0.57
1:B:338:GLU:OE2	1:B:342:ARG:NH2	2.37	0.57
1:D:94:LYS:O	1:D:97:GLU:HB2	2.05	0.57
1:C:282:ASP:HB3	1:C:308:GLN:NE2	2.20	0.57
1:A:105:HIS:HD2	1:A:108:ARG:H	1.52	0.57
1:B:355:SER:HB2	1:B:358:CYS:SG	2.45	0.57
1:C:222:MET:HG2	1:D:222:MET:CE	2.35	0.57
1:A:225:ASP:OD1	1:B:261:ARG:NH2	2.38	0.57
1:D:96:LEU:HD11	1:D:120:VAL:HG13	1.87	0.57
1:D:356:PRO:O	1:D:357:MET:HE2	2.05	0.57
1:D:192:ALA:HB2	1:D:260:LEU:HD12	1.87	0.56
3:A:1:J25:H26	3:A:1:J25:C6	2.34	0.56
1:A:307:ILE:O	1:A:311:GLN:HG3	2.04	0.56
1:C:304:SER:O	1:C:308:GLN:HB2	2.05	0.56
1:C:116:ARG:N	1:C:117:PRO:CD	2.68	0.56
1:C:160:HIS:ND1	1:C:339:GLU:OE2	2.31	0.56
1:D:219:LEU:HD21	1:D:232:HIS:CD2	2.41	0.56
1:C:121:ILE:HD12	1:C:166:ALA:HB1	1.88	0.56
1:C:129:ARG:HB2	1:C:131:LEU:HG	1.88	0.56
1:D:355:SER:HB2	1:D:358:CYS:SG	2.45	0.56
1:D:105:HIS:CE1	1:D:107:PHE:HB2	2.41	0.56
1:A:366:GLU:HG2	1:A:409:THR:HG21	1.88	0.55
1:B:326:LEU:HD21	1:B:405:TRP:CE2	2.41	0.55
1:B:116:ARG:N	1:B:117:PRO:CD	2.69	0.55
1:C:216:ASN:HB3	7:D:587:HOH:O	2.06	0.55
1:D:346:ARG:O	1:D:350:ARG:HG3	2.06	0.55
1:A:292:VAL:HG11	1:A:296:GLY:HA2	1.88	0.55
1:B:261:ARG:NH1	7:B:534:HOH:O	2.39	0.54
1:A:342:ARG:HD3	7:A:606:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLN:OE1	3:A:1:J25:H15	2.08	0.54
1:A:366:GLU:HG2	1:A:409:THR:CB	2.38	0.54
1:C:192:ALA:HB2	1:C:260:LEU:HD12	1.89	0.54
1:B:105:HIS:HE1	1:B:107:PHE:HB2	1.73	0.54
1:A:116:ARG:HG3	1:A:147:MET:HE3	1.90	0.53
1:B:92:LEU:HD22	1:B:92:LEU:O	2.07	0.53
1:B:223:TYR:CE1	1:B:231:ASN:HB3	2.43	0.53
1:C:398:THR:O	1:C:401:ASP:HB2	2.09	0.53
1:A:92:LEU:O	1:A:92:LEU:HD22	2.08	0.53
1:B:364:SER:OG	1:B:367:LYS:HB2	2.09	0.53
1:D:213:ILE:HD13	1:D:225:ASP:HB3	1.91	0.53
1:D:178:THR:OG1	4:D:6:EDO:H22	2.09	0.53
1:A:188:LEU:HD23	4:A:4:EDO:H21	1.90	0.52
1:A:298:LEU:HD21	1:A:387:LEU:O	2.10	0.52
1:C:171:SER:O	1:C:175:LEU:HG	2.09	0.52
1:C:376:ILE:CD1	3:C:1:J25:H26A	2.40	0.52
1:B:355:SER:HB3	1:B:356:PRO:HD2	1.92	0.52
1:A:349:GLU:C	1:A:351:GLY:H	2.13	0.51
1:C:298:LEU:HD11	1:C:387:LEU:HD11	1.93	0.51
1:D:176:LEU:HD13	1:D:190:ILE:HG23	1.92	0.51
1:A:357:MET:SD	3:A:1:J25:H22A	2.50	0.51
1:C:356:PRO:O	1:C:357:MET:HB2	2.10	0.51
1:C:326:LEU:HD21	1:C:405:TRP:CE2	2.45	0.51
1:B:304:SER:O	1:B:308:GLN:HG3	2.10	0.51
1:A:209:ASN:O	1:A:213:ILE:HG13	2.10	0.51
1:B:354:ILE:HG21	1:B:359:ASP:HB2	1.91	0.51
1:C:196:ALA:O	1:C:200:HIS:HB3	2.10	0.51
1:C:218:GLU:O	1:C:222:MET:HB2	2.11	0.51
1:B:118:LEU:O	1:B:122:MET:HB2	2.11	0.51
1:C:302:ASN:ND2	1:C:304:SER:HB3	2.25	0.51
1:B:143:ILE:O	1:B:147:MET:HG2	2.11	0.51
1:C:116:ARG:NH2	1:C:151:ASP:OD2	2.43	0.51
1:C:323:THR:HG22	1:C:399:LEU:HD13	1.92	0.51
1:A:384:TRP:O	1:A:388:VAL:HG22	2.11	0.50
1:B:389:HIS:CD2	1:B:390:PRO:HA	2.46	0.50
1:B:142:LEU:O	1:B:146:LEU:HG	2.11	0.50
1:A:282:ASP:HB3	1:A:308:GLN:OE1	2.11	0.50
1:C:93:ALA:O	1:C:97:GLU:HG3	2.12	0.50
1:B:239:LYS:HE2	1:D:218:GLU:CG	2.42	0.50
1:B:239:LYS:HE2	1:D:218:GLU:HG3	1.93	0.50
1:C:346:ARG:O	1:C:350:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:GLN:NE2	1:C:410:ILE:HD12	2.27	0.49
1:D:90:ASP:O	1:D:94:LYS:HD3	2.11	0.49
1:A:132:LEU:CD2	1:A:139:VAL:HG12	2.42	0.49
1:B:138:PRO:HG2	1:B:250:GLN:OE1	2.12	0.49
1:C:116:ARG:NH1	1:C:150:GLU:HG2	2.28	0.49
1:D:239:LYS:HE3	1:D:242:GLN:OE1	2.12	0.49
1:A:91:VAL:HG12	1:A:112:LEU:HD13	1.95	0.49
1:A:359:ASP:O	1:A:363:ALA:HB2	2.13	0.49
1:B:260:LEU:O	1:B:264:VAL:HG23	2.12	0.49
1:A:201:ASP:O	1:A:204:HIS:HB2	2.12	0.49
1:B:129:ARG:HE	1:B:173:HIS:CE1	2.31	0.49
1:C:366:GLU:CD	1:C:366:GLU:H	2.15	0.49
1:B:273:MET:HG3	3:B:1:J25:H6	1.94	0.48
1:B:283:LEU:O	1:B:287:VAL:HG23	2.13	0.48
1:C:273:MET:HG3	3:C:1:J25:H6	1.94	0.48
1:D:209:ASN:O	1:D:213:ILE:HG13	2.13	0.48
1:B:342:ARG:O	1:B:346:ARG:HG3	2.13	0.48
3:B:1:J25:S4	3:B:1:J25:O18	2.71	0.48
1:D:216:ASN:HD21	1:D:221:LEU:HD21	1.78	0.48
1:B:345:ASP:OD1	1:B:348:ARG:NH2	2.45	0.48
1:B:409:THR:O	1:B:409:THR:HG22	2.13	0.48
1:D:393:GLN:HG2	7:D:613:HOH:O	2.12	0.48
1:D:342:ARG:HD2	1:D:342:ARG:HA	1.60	0.48
1:A:409:THR:O	1:A:410:ILE:HG22	2.14	0.48
1:B:136:LYS:HB2	1:B:251:ASN:HB2	1.95	0.48
1:C:302:ASN:O	1:C:306:ARG:HG3	2.13	0.48
1:C:201:ASP:O	1:C:204:HIS:HB2	2.13	0.48
1:D:223:TYR:CD1	1:D:231:ASN:HB3	2.48	0.48
1:B:116:ARG:HD2	1:B:147:MET:SD	2.54	0.48
1:B:136:LYS:O	1:B:138:PRO:HD3	2.13	0.48
1:B:290:LYS:HD3	7:B:556:HOH:O	2.14	0.48
1:A:108:ARG:HH11	1:A:108:ARG:CG	2.22	0.48
1:B:362:ASN:H	1:B:362:ASN:ND2	2.12	0.48
1:B:257:ARG:HD3	7:B:536:HOH:O	2.14	0.47
1:B:333:THR:HA	1:B:336:ILE:HG22	1.96	0.47
1:C:118:LEU:O	1:C:122:MET:HB2	2.15	0.47
1:A:94:LYS:O	1:A:97:GLU:HB2	2.13	0.47
1:B:339:GLU:HG2	4:B:3:EDO:H21	1.96	0.47
1:A:346:ARG:O	1:A:350:ARG:HG3	2.15	0.47
1:B:121:ILE:HG21	1:B:170:GLN:HB2	1.97	0.47
1:D:252:LEU:HB2	1:D:257:ARG:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ASN:HB3	7:B:589:HOH:O	2.15	0.47
1:C:330:ARG:HD3	1:C:405:TRP:CZ3	2.49	0.47
1:C:333:THR:HA	1:C:336:ILE:HG22	1.96	0.47
1:D:108:ARG:HH21	1:D:112:LEU:HD21	1.80	0.47
1:D:252:LEU:N	1:D:252:LEU:HD23	2.30	0.47
1:C:116:ARG:HH22	1:C:151:ASP:CG	2.17	0.47
1:D:330:ARG:HD2	1:D:405:TRP:CZ3	2.49	0.47
1:B:333:THR:O	1:B:336:ILE:HG22	2.15	0.46
1:D:142:LEU:O	1:D:146:LEU:HG	2.15	0.46
1:D:302:ASN:O	1:D:306:ARG:HG3	2.15	0.46
1:B:165:ALA:O	1:B:169:VAL:HG23	2.15	0.46
1:B:246:CYS:O	1:B:248:ILE:HG23	2.14	0.46
1:B:195:PHE:CE2	1:B:199:ILE:HD13	2.51	0.46
1:C:321:ASN:OD1	3:C:1:J25:H12	2.15	0.46
1:A:292:VAL:CG1	1:A:293:THR:N	2.78	0.46
1:B:191:LEU:HD23	1:B:260:LEU:CD1	2.45	0.46
1:C:184:VAL:CG1	1:C:300:LEU:HD12	2.45	0.46
1:D:321:ASN:CB	1:D:322:PRO:HD3	2.43	0.46
1:D:369:GLN:O	1:D:373:ILE:HG13	2.15	0.46
1:A:153:TYR:CZ	1:A:165:ALA:HB2	2.51	0.46
1:B:327:GLN:NE2	1:B:327:GLN:HA	2.31	0.46
1:A:104:LEU:HD21	1:A:109:ILE:HD12	1.97	0.45
1:B:245:ASN:ND2	7:B:532:HOH:O	2.49	0.45
1:B:130:ASP:OD2	1:B:133:LYS:HB2	2.16	0.45
1:C:143:ILE:O	1:C:147:MET:HG2	2.16	0.45
1:A:178:THR:OG1	1:A:391:ASP:HB3	2.17	0.45
1:D:307:ILE:O	1:D:311:GLN:HG3	2.17	0.45
1:A:345:ASP:O	1:A:348:ARG:HG2	2.17	0.45
1:B:346:ARG:NH1	1:D:151:ASP:OD1	2.50	0.45
1:B:348:ARG:HH11	1:B:354:ILE:HD11	1.81	0.45
1:C:130:ASP:HA	7:C:516:HOH:O	2.17	0.45
1:D:299:LEU:C	1:D:299:LEU:HD13	2.37	0.45
1:C:239:LYS:HG3	7:C:575:HOH:O	2.17	0.45
1:B:129:ARG:NH1	1:B:190:ILE:HD13	2.31	0.45
1:B:204:HIS:HA	1:B:205:PRO:HD3	1.86	0.45
1:C:98:ASP:HA	1:C:101:LYS:NZ	2.31	0.45
1:B:327:GLN:NE2	7:B:548:HOH:O	2.38	0.44
1:C:170:GLN:O	1:C:174:VAL:HG23	2.17	0.44
1:D:185:PHE:H	4:D:3:EDO:C1	2.28	0.44
1:D:349:GLU:C	1:D:351:GLY:H	2.21	0.44
1:A:255:LYS:HA	7:A:542:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:LEU:HD22	1:B:247:ASP:O	2.17	0.44
1:B:371:GLY:O	1:B:375:TYR:HD1	1.99	0.44
1:B:247:ASP:O	1:B:248:ILE:HG12	2.16	0.44
1:B:298:LEU:HD23	1:B:298:LEU:HA	1.87	0.44
1:A:135:PHE:HB3	1:A:252:LEU:HD11	2.00	0.44
1:A:368:SER:HB3	3:A:1:J25:C22	2.28	0.44
1:D:249:PHE:CZ	1:D:260:LEU:HD21	2.53	0.44
1:B:191:LEU:HD23	1:B:260:LEU:HD13	1.99	0.44
1:C:221:LEU:HD13	1:C:221:LEU:C	2.38	0.44
1:C:366:GLU:HG2	1:C:409:THR:CG2	2.48	0.44
1:A:107:PHE:O	1:A:111:GLU:HG3	2.18	0.44
1:A:262:LYS:HE3	7:A:563:HOH:O	2.18	0.44
1:A:378:HIS:HA	1:A:399:LEU:HD21	2.00	0.43
1:A:355:SER:HB3	1:A:356:PRO:CD	2.48	0.43
1:D:183:ALA:N	4:D:3:EDO:H12	2.33	0.43
1:A:299:LEU:HD22	1:A:300:LEU:N	2.34	0.43
1:C:329:TYR:HE1	3:C:1:J25:H15	1.83	0.43
1:D:103:GLY:O	1:D:104:LEU:C	2.55	0.43
1:D:357:MET:HE1	3:D:1:J25:H9	2.00	0.43
1:A:192:ALA:HB2	1:A:260:LEU:HD12	2.01	0.43
1:A:354:ILE:H	1:A:354:ILE:HG13	1.62	0.43
1:A:356:PRO:O	1:A:357:MET:HB2	2.19	0.43
1:B:300:LEU:O	1:B:306:ARG:NH1	2.50	0.43
1:B:348:ARG:HH11	1:B:354:ILE:CD1	2.32	0.43
1:B:355:SER:HB3	1:B:356:PRO:CD	2.49	0.43
1:B:342:ARG:O	1:B:346:ARG:CG	2.67	0.43
1:A:225:ASP:CG	1:B:261:ARG:NH2	2.72	0.43
1:A:279:LEU:HD23	1:A:279:LEU:HA	1.83	0.43
1:A:303:TYR:O	1:A:307:ILE:HG22	2.19	0.43
1:C:144:THR:HG22	1:C:246:CYS:SG	2.58	0.43
1:A:329:TYR:HE1	3:A:1:J25:H15	1.84	0.43
1:B:324:LYS:O	1:B:325:PRO:C	2.57	0.43
1:B:369:GLN:OE1	3:B:1:J25:H15	2.19	0.43
1:A:342:ARG:HB3	7:A:606:HOH:O	2.18	0.42
1:A:360:LYS:C	1:A:362:ASN:H	2.22	0.42
1:C:104:LEU:HD11	1:C:109:ILE:HD11	2.01	0.42
1:A:349:GLU:HG3	1:A:349:GLU:H	1.49	0.42
1:D:152:HIS:CE1	4:D:2:EDO:H11	2.55	0.42
1:B:339:GLU:OE2	4:B:3:EDO:H21	2.20	0.42
1:B:392:ALA:O	1:B:395:ILE:HB	2.20	0.42
1:C:286:MET:HE2	1:C:286:MET:HB2	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASP:HA	7:A:553:HOH:O	2.18	0.42
1:A:355:SER:HB3	1:A:356:PRO:HD2	2.01	0.42
1:B:154:HIS:N	1:B:154:HIS:CD2	2.87	0.42
1:B:323:THR:HG22	1:B:399:LEU:HD13	2.00	0.42
1:B:389:HIS:HA	1:B:390:PRO:HA	1.78	0.42
1:D:322:PRO:HG3	3:D:1:J25:C15	2.49	0.42
1:A:98:ASP:OD1	1:A:101:LYS:HD2	2.20	0.42
1:D:204:HIS:HA	1:D:205:PRO:HD3	1.85	0.42
1:A:326:LEU:HD21	1:A:405:TRP:CE2	2.55	0.42
1:B:283:LEU:HG	1:B:383:THR:HG22	2.02	0.42
1:B:370:VAL:HG11	1:B:407:GLN:OE1	2.19	0.42
1:C:373:ILE:HA	1:C:377:VAL:HB	2.01	0.42
1:A:292:VAL:HG12	1:A:293:THR:H	1.84	0.42
1:C:348:ARG:NH2	1:C:360:LYS:HE2	2.32	0.42
1:D:178:THR:OG1	1:D:391:ASP:HB3	2.20	0.42
1:B:359:ASP:O	1:B:363:ALA:HB2	2.18	0.41
1:B:108:ARG:CG	1:B:108:ARG:NH1	2.61	0.41
1:C:204:HIS:HA	1:C:205:PRO:HD3	1.82	0.41
1:C:338:GLU:OE2	1:C:342:ARG:HD2	2.20	0.41
1:C:378:HIS:HB3	1:C:379:PRO:HD3	2.02	0.41
1:C:322:PRO:HA	1:C:329:TYR:CD2	2.55	0.41
1:A:342:ARG:O	1:A:346:ARG:HD2	2.20	0.41
1:B:326:LEU:HD21	1:B:405:TRP:CD2	2.55	0.41
1:C:321:ASN:HB2	1:C:322:PRO:HD3	2.03	0.41
1:A:108:ARG:NH1	1:A:108:ARG:CG	2.82	0.41
1:A:376:ILE:O	1:A:379:PRO:HD2	2.20	0.41
1:A:116:ARG:HG3	1:A:147:MET:CE	2.51	0.41
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.81	0.41
1:C:273:MET:HE3	1:C:276:HIS:HB2	2.02	0.41
1:B:95:GLU:HG3	1:B:108:ARG:HD3	2.01	0.41
1:B:229:LEU:HD23	1:B:229:LEU:HA	1.86	0.41
1:B:346:ARG:O	1:B:350:ARG:HD2	2.20	0.41
1:B:145:TYR:CE1	1:B:241:LEU:HD23	2.56	0.41
1:D:343:GLN:O	1:D:347:GLU:HG3	2.21	0.41
1:A:348:ARG:HG3	1:A:349:GLU:N	2.35	0.41
1:B:180:ALA:HB2	1:B:391:ASP:OD2	2.21	0.41
1:B:262:LYS:HE3	1:B:303:TYR:CE2	2.56	0.41
1:B:307:ILE:HD12	1:B:307:ILE:HA	1.86	0.41
1:B:326:LEU:O	1:B:330:ARG:HG3	2.21	0.41
1:C:218:GLU:HG2	1:C:222:MET:CE	2.51	0.41
1:C:252:LEU:HD13	1:C:256:GLN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:LEU:HD13	1:C:380:LEU:HA	2.03	0.41
1:C:311:GLN:NE2	4:C:7:EDO:H22	2.36	0.41
1:C:337:MET:HG3	1:C:365:VAL:CG2	2.48	0.41
1:A:211:PHE:HE2	1:A:347:GLU:HG3	1.85	0.40
1:C:322:PRO:HA	1:C:329:TYR:CG	2.56	0.40
1:D:96:LEU:HD11	1:D:120:VAL:CG1	2.51	0.40
1:D:378:HIS:HA	1:D:399:LEU:HD21	2.03	0.40
1:A:204:HIS:NE2	1:A:229:LEU:HD13	2.36	0.40
1:B:396:LEU:O	1:B:399:LEU:HB3	2.21	0.40
1:B:204:HIS:CE1	4:B:3:EDO:H12	2.56	0.40
1:B:207:VAL:HA	1:B:343:GLN:OE1	2.22	0.40
1:C:222:MET:HG2	1:D:222:MET:HE2	2.02	0.40
1:C:307:ILE:HG23	1:C:308:GLN:N	2.35	0.40
1:D:293:THR:O	1:D:295:SER:O	2.39	0.40
1:C:178:THR:HA	1:C:179:PRO:HD3	1.96	0.40
1:B:322:PRO:HG2	1:B:377:VAL:HG21	2.03	0.40
1:D:131:LEU:HD23	1:D:131:LEU:HA	1.93	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	326/359 (91%)	308 (94%)	14 (4%)	4 (1%)	13 19
1	B	323/359 (90%)	303 (94%)	19 (6%)	1 (0%)	41 56
1	C	323/359 (90%)	306 (95%)	17 (5%)	0	100 100
1	D	322/359 (90%)	310 (96%)	9 (3%)	3 (1%)	17 26
All	All	1294/1436 (90%)	1227 (95%)	59 (5%)	8 (1%)	25 37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	SER
1	B	248	ILE
1	D	349	GLU
1	D	350	ARG
1	A	350	ARG
1	D	351	GLY
1	A	354	ILE
1	A	355	SER

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	299/327 (91%)	290 (97%)	9 (3%)	41	59
1	B	297/327 (91%)	281 (95%)	16 (5%)	22	34
1	C	297/327 (91%)	283 (95%)	14 (5%)	26	40
1	D	296/327 (90%)	286 (97%)	10 (3%)	37	53
All	All	1189/1308 (91%)	1140 (96%)	49 (4%)	30	46

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
1	A	97	GLU
1	A	147	MET
1	A	178	THR
1	A	222	MET
1	A	286	MET
1	A	299	LEU
1	A	346	ARG
1	A	349	GLU
1	B	92	LEU
1	B	108	ARG
1	B	130	ASP
1	B	139	VAL
1	B	178	THR

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Mol	Chain	Res	Type
1	B	219	LEU
1	B	259	SER
1	B	297	VAL
1	B	298	LEU
1	B	299	LEU
1	B	327	GLN
1	B	346	ARG
1	B	348	ARG
1	B	357	MET
1	B	362	ASN
1	B	396	LEU
1	C	87	GLU
1	C	89	GLU
1	C	90	ASP
1	C	92	LEU
1	C	116	ARG
1	C	147	MET
1	C	178	THR
1	C	219	LEU
1	C	252	LEU
1	C	258	GLN
1	C	286	MET
1	C	289	THR
1	C	297	VAL
1	C	346	ARG
1	D	92	LEU
1	D	99	VAL
1	D	116	ARG
1	D	120	VAL
1	D	178	THR
1	D	219	LEU
1	D	252	LEU
1	D	295	SER
1	D	306	ARG
1	D	342	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	123	HIS
1	A	216	ASN

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Mol	Chain	Res	Type
1	A	245	ASN
1	A	407	GLN
1	B	245	ASN
1	B	258	GLN
1	B	327	GLN
1	B	362	ASN
1	B	389	HIS
1	C	245	ASN
1	C	250	GLN
1	C	258	GLN
1	C	308	GLN
1	D	123	HIS
1	D	127	GLN
1	D	216	ASN
1	D	245	ASN
1	D	278	ASN
1	D	389	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)

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 for Mogul analysis.

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	$\#\|Z\| > 2$
4	EDO	D	6	-	3,3,3	0.51	0	2,2,2	0.34	0
4	EDO	D	5	-	3,3,3	0.55	0	2,2,2	0.32	0
4	EDO	D	2	-	3,3,3	0.63	0	2,2,2	0.04	0
4	EDO	C	6	-	3,3,3	0.52	0	2,2,2	0.22	0
4	EDO	A	4	-	3,3,3	0.45	0	2,2,2	0.48	0
3	J25	C	1	-	28,30,30	2.17	4 (14%)	24,41,41	3.50	9 (37%)
4	EDO	C	7	-	3,3,3	0.55	0	2,2,2	0.32	0
5	DMS	A	3	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
3	J25	D	1	-	28,30,30	2.23	4 (14%)	24,41,41	3.64	9 (37%)
4	EDO	A	2	-	3,3,3	0.45	0	2,2,2	0.35	0
4	EDO	C	3	-	3,3,3	0.53	0	2,2,2	0.11	0
4	EDO	D	9	-	3,3,3	0.55	0	2,2,2	0.20	0
4	EDO	D	8	-	3,3,3	0.61	0	2,2,2	0.20	0
4	EDO	C	2	-	3,3,3	0.37	0	2,2,2	0.55	0
3	J25	A	1	-	28,30,30	2.26	4 (14%)	24,41,41	3.47	9 (37%)
4	EDO	B	2	-	3,3,3	0.44	0	2,2,2	0.43	0
4	EDO	D	7	-	3,3,3	0.45	0	2,2,2	0.40	0
4	EDO	B	3	-	3,3,3	0.55	0	2,2,2	0.10	0
6	EPE	C	5	-	15,15,15	0.79	1 (6%)	18,20,20	2.06	5 (27%)
4	EDO	D	3	-	3,3,3	0.48	0	2,2,2	0.34	0
3	J25	B	1	-	28,30,30	2.19	4 (14%)	24,41,41	4.24	9 (37%)
4	EDO	D	4	-	3,3,3	0.49	0	2,2,2	0.48	0
4	EDO	C	4	-	3,3,3	0.45	0	2,2,2	0.39	0

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
4	EDO	D	6	-	-	1/1/1/1	-
4	EDO	D	5	-	-	1/1/1/1	-
4	EDO	D	2	-	-	1/1/1/1	-
4	EDO	C	6	-	-	0/1/1/1	-
4	EDO	A	4	-	-	0/1/1/1	-
3	J25	C	1	-	-	8/18/31/31	0/3/3/3
4	EDO	C	7	-	-	0/1/1/1	-
3	J25	D	1	-	-	8/18/31/31	0/3/3/3
4	EDO	A	2	-	-	0/1/1/1	-
4	EDO	C	3	-	-	0/1/1/1	-
4	EDO	D	9	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	8	-	-	0/1/1/1	-
4	EDO	C	2	-	-	0/1/1/1	-
3	J25	A	1	-	-	12/18/31/31	0/3/3/3
4	EDO	B	2	-	-	0/1/1/1	-
4	EDO	D	7	-	-	0/1/1/1	-
4	EDO	B	3	-	-	0/1/1/1	-
6	EPE	C	5	-	-	7/9/19/19	0/1/1/1
4	EDO	D	3	-	-	0/1/1/1	-
3	J25	B	1	-	-	9/18/31/31	0/3/3/3
4	EDO	D	4	-	-	1/1/1/1	-
4	EDO	C	4	-	-	0/1/1/1	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	J25	O25-C24	6.87	1.47	1.34
3	A	1	J25	O25-C24	6.86	1.47	1.34
3	B	1	J25	O25-C24	6.79	1.47	1.34
3	D	1	J25	C2-C1	6.61	1.51	1.39
3	C	1	J25	O25-C24	6.26	1.46	1.34
3	C	1	J25	C2-C1	6.19	1.50	1.39
3	A	1	J25	C2-C1	6.01	1.50	1.39
3	B	1	J25	C2-C1	5.58	1.49	1.39
3	C	1	J25	O20-C19	4.83	1.45	1.33
3	B	1	J25	O20-C19	4.81	1.45	1.33
3	A	1	J25	O20-C19	4.62	1.45	1.33
3	D	1	J25	O20-C19	4.60	1.45	1.33
3	A	1	J25	C2-C3	4.48	1.50	1.41
5	A	3	DMS	O-S	4.47	1.80	1.50
3	B	1	J25	C2-C3	4.20	1.50	1.41
3	C	1	J25	C2-C3	3.99	1.49	1.41
3	D	1	J25	C2-C3	3.51	1.48	1.41
6	C	5	EPE	C10-S	2.67	1.81	1.77

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1	J25	C5-C6-N7	-13.80	98.28	112.72
3	D	1	J25	C15-C16-S17	-9.18	105.53	112.98
3	A	1	J25	C15-C16-S17	-9.11	105.59	112.98
3	C	1	J25	O25-C24-N7	9.03	122.74	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1	J25	O25-C24-N7	9.00	122.71	111.66
3	D	1	J25	O25-C24-N7	8.91	122.60	111.66
3	C	1	J25	C5-C6-N7	-8.80	103.52	112.72
3	B	1	J25	C15-C16-S17	-7.86	106.60	112.98
3	C	1	J25	C15-C16-S17	-7.81	106.64	112.98
3	B	1	J25	O25-C24-N7	7.79	121.22	111.66
3	D	1	J25	C5-C6-N7	-7.52	104.85	112.72
3	B	1	J25	C26-O25-C24	6.55	125.42	115.59
3	A	1	J25	C9-C8-N7	5.87	116.96	110.04
3	D	1	J25	C26-O25-C24	5.43	123.74	115.59
3	A	1	J25	C26-O25-C24	5.19	123.38	115.59
3	D	1	J25	O25-C24-O28	-4.90	116.44	124.78
6	C	5	EPE	O2S-S-C10	4.79	112.68	106.92
3	C	1	J25	O25-C24-O28	-4.53	117.07	124.78
3	B	1	J25	O25-C24-O28	-4.47	117.17	124.78
3	C	1	J25	C26-O25-C24	4.21	121.91	115.59
3	A	1	J25	O25-C24-O28	-4.10	117.79	124.78
3	D	1	J25	O20-C19-C2	4.03	121.41	112.33
6	C	5	EPE	C5-N4-C3	3.99	117.82	108.83
3	B	1	J25	C9-C8-N7	-3.92	105.43	110.04
3	B	1	J25	C8-C9-C1	-3.41	106.03	111.63
6	C	5	EPE	C7-N4-C3	3.27	119.59	111.23
3	D	1	J25	C9-C8-N7	3.18	113.79	110.04
3	A	1	J25	O28-C24-N7	-2.88	119.50	124.32
6	C	5	EPE	C7-N4-C5	2.79	118.36	111.23
3	C	1	J25	O20-C19-C2	2.69	118.38	112.33
3	A	1	J25	C5-C6-N7	-2.67	109.93	112.72
3	B	1	J25	C13-C12-C11	-2.49	108.44	113.39
3	C	1	J25	O28-C24-N7	-2.48	120.17	124.32
3	A	1	J25	O20-C19-C2	2.45	117.84	112.33
3	A	1	J25	C6-N7-C8	2.39	122.70	115.57
3	C	1	J25	C3-N10-C11	-2.39	119.12	124.36
6	C	5	EPE	C9-N1-C6	-2.33	105.29	111.23
3	B	1	J25	O20-C19-C2	2.24	117.36	112.33
3	C	1	J25	C21-O20-C19	2.12	121.38	116.46
3	D	1	J25	O20-C19-O23	-2.07	119.48	123.67
3	D	1	J25	O28-C24-N7	-2.01	120.95	124.32

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	J25	O25-C24-N7-C6
3	A	1	J25	O28-C24-N7-C6
3	A	1	J25	O25-C24-N7-C8
3	A	1	J25	O28-C24-N7-C8
3	A	1	J25	C12-C11-N10-C3
3	A	1	J25	O18-C11-N10-C3
3	A	1	J25	N7-C24-O25-C26
3	A	1	J25	O28-C24-O25-C26
3	B	1	J25	N7-C24-O25-C26
3	B	1	J25	O28-C24-O25-C26
3	C	1	J25	C12-C11-N10-C3
3	C	1	J25	O18-C11-N10-C3
3	C	1	J25	N7-C24-O25-C26
3	C	1	J25	O28-C24-O25-C26
3	D	1	J25	O25-C24-N7-C6
3	D	1	J25	O28-C24-N7-C6
3	D	1	J25	O25-C24-N7-C8
3	D	1	J25	O28-C24-N7-C8
3	D	1	J25	N7-C24-O25-C26
3	D	1	J25	O28-C24-O25-C26
6	C	5	EPE	C8-C7-N4-C3
3	C	1	J25	C2-C19-O20-C21
3	C	1	J25	O23-C19-O20-C21
3	B	1	J25	O25-C24-N7-C6
3	A	1	J25	C2-C19-O20-C21
4	D	2	EDO	O1-C1-C2-O2
4	D	5	EDO	O1-C1-C2-O2
4	D	4	EDO	O1-C1-C2-O2
6	C	5	EPE	C9-C10-S-O3S
3	A	1	J25	O18-C11-C12-C13
3	A	1	J25	O23-C19-O20-C21
3	B	1	J25	O28-C24-N7-C6
3	B	1	J25	O25-C24-N7-C8
6	C	5	EPE	C10-C9-N1-C2
6	C	5	EPE	C10-C9-N1-C6
3	B	1	J25	O18-C11-C12-C13
3	A	1	J25	N10-C11-C12-C13
3	C	1	J25	O18-C11-C12-C13
3	D	1	J25	O18-C11-C12-C13
3	B	1	J25	O28-C24-N7-C8
3	B	1	J25	N10-C11-C12-C13
3	D	1	J25	N10-C11-C12-C13
6	C	5	EPE	N4-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
3	C	1	J25	N10-C11-C12-C13
3	B	1	J25	C22-C21-O20-C19
4	D	6	EDO	O1-C1-C2-O2
4	D	9	EDO	O1-C1-C2-O2
6	C	5	EPE	C9-C10-S-O1S
6	C	5	EPE	C9-C10-S-O2S

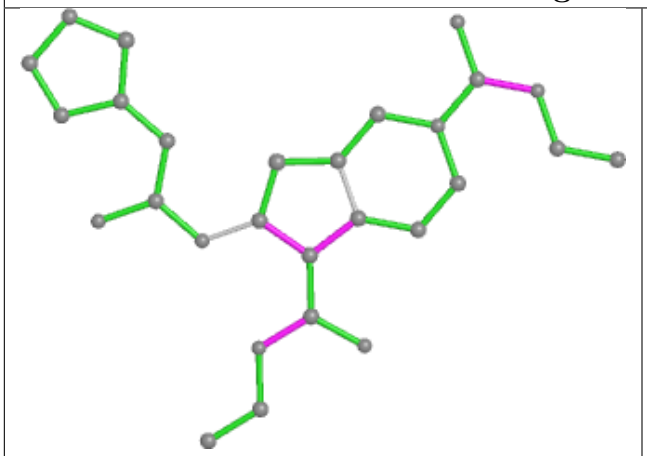
There are no ring outliers.

11 monomers are involved in 39 short contacts:

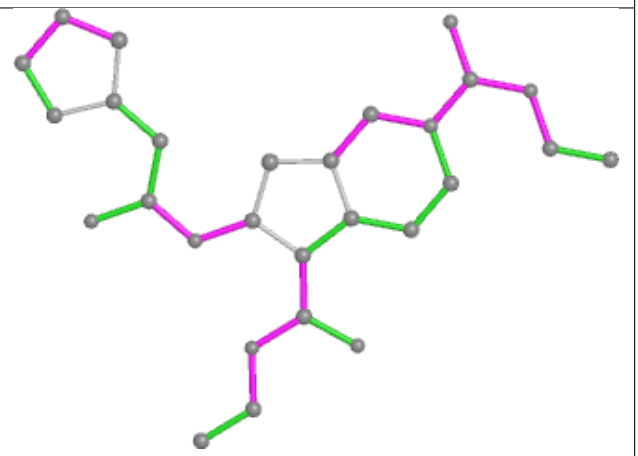
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	6	EDO	1	0
4	D	2	EDO	1	0
4	A	4	EDO	1	0
3	C	1	J25	6	0
4	C	7	EDO	1	0
3	D	1	J25	4	0
4	C	2	EDO	1	0
3	A	1	J25	10	0
4	B	3	EDO	3	0
4	D	3	EDO	4	0
3	B	1	J25	7	0

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.

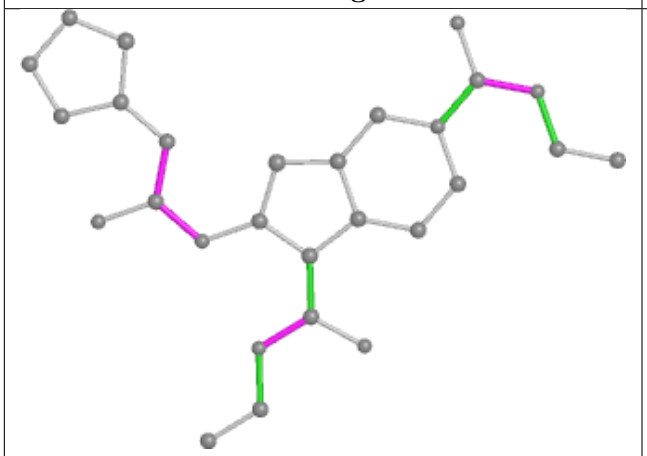
Ligand J25 C 1



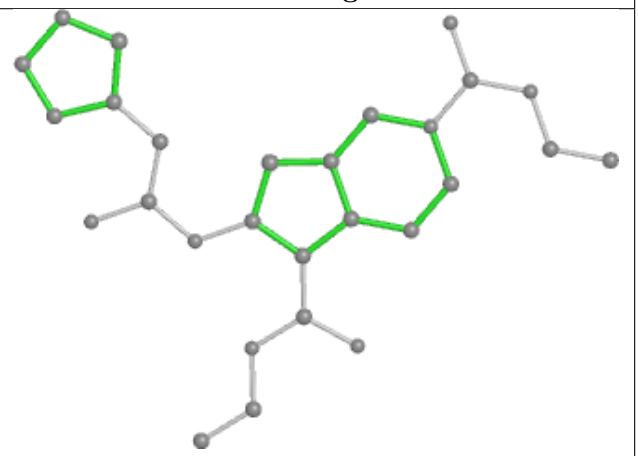
Bond lengths



Bond angles

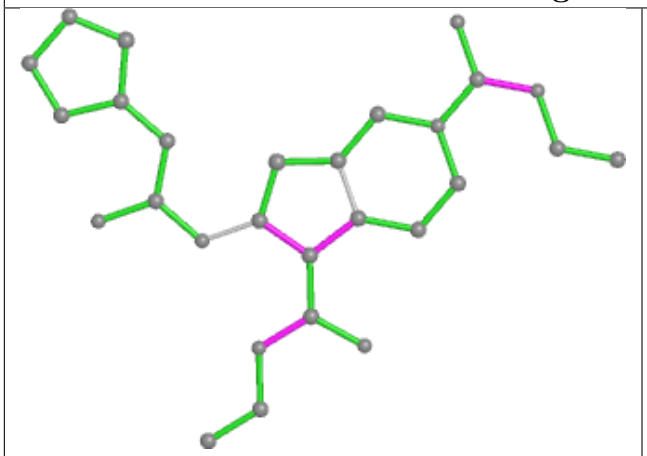


Torsions

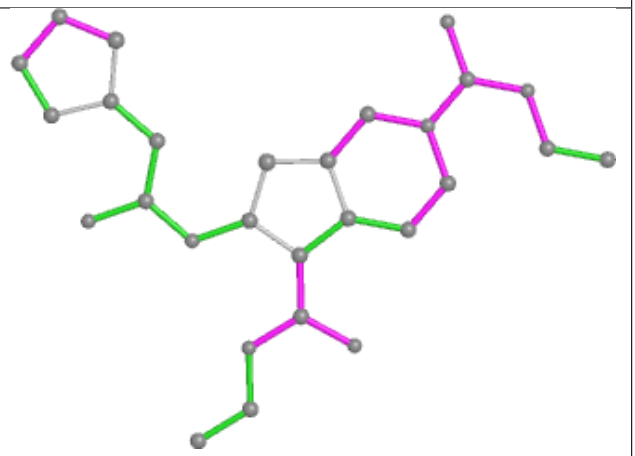


Rings

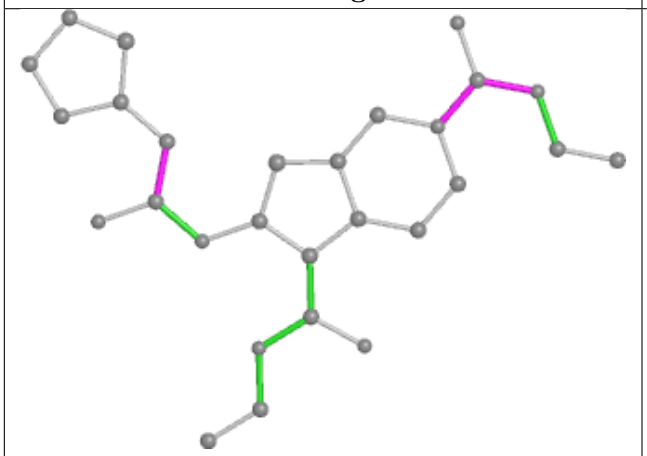
Ligand J25 D 1



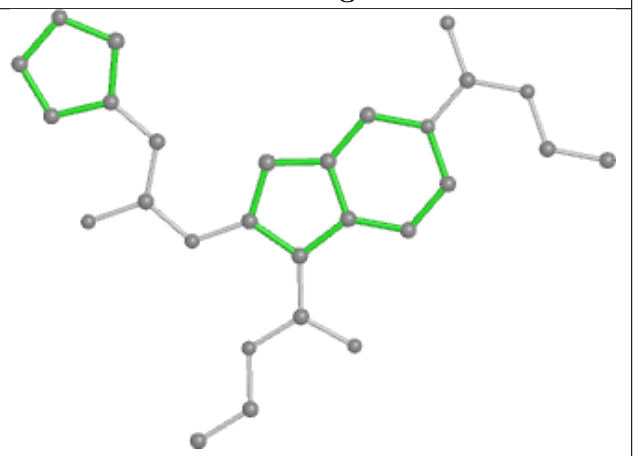
Bond lengths



Bond angles

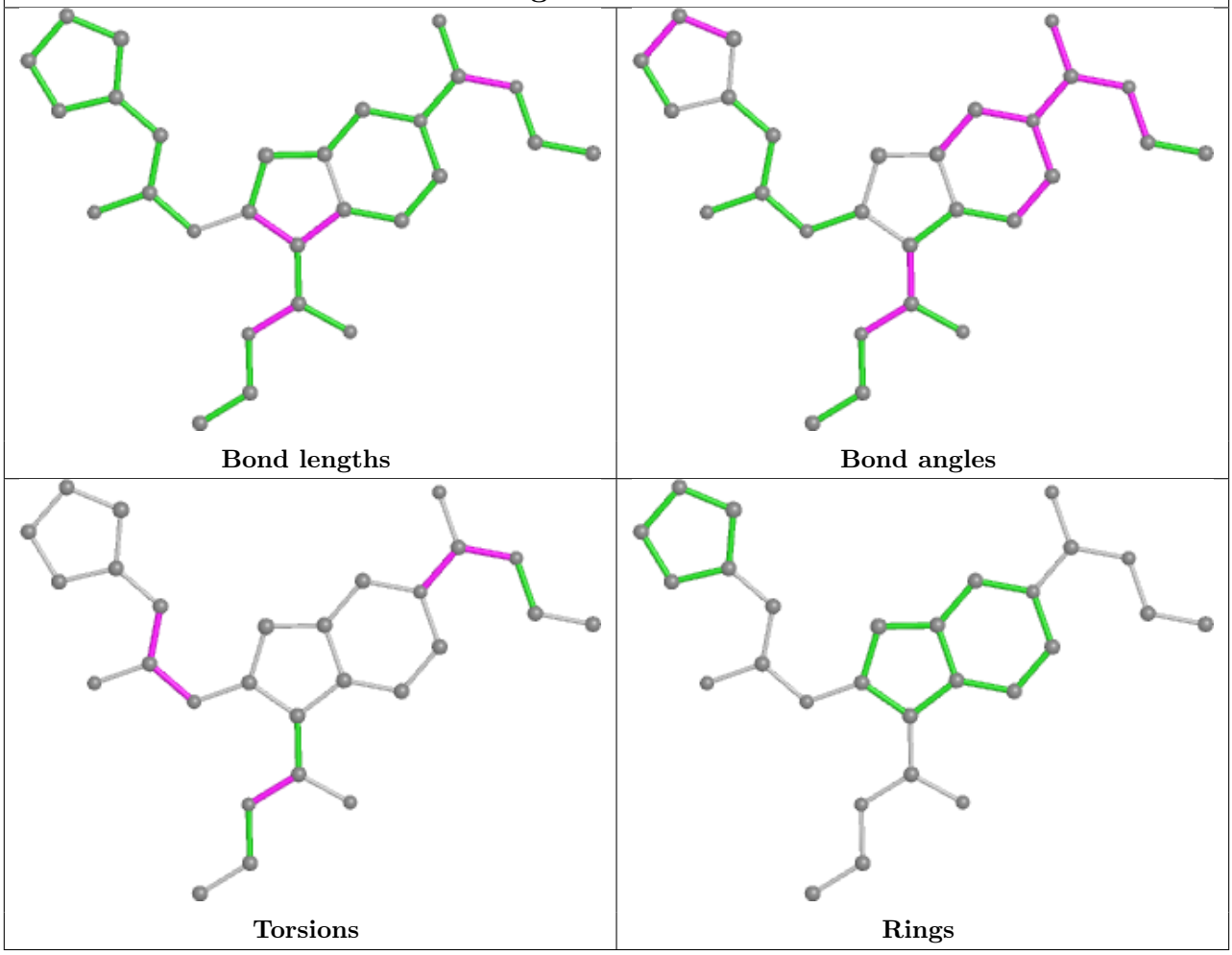


Torsions

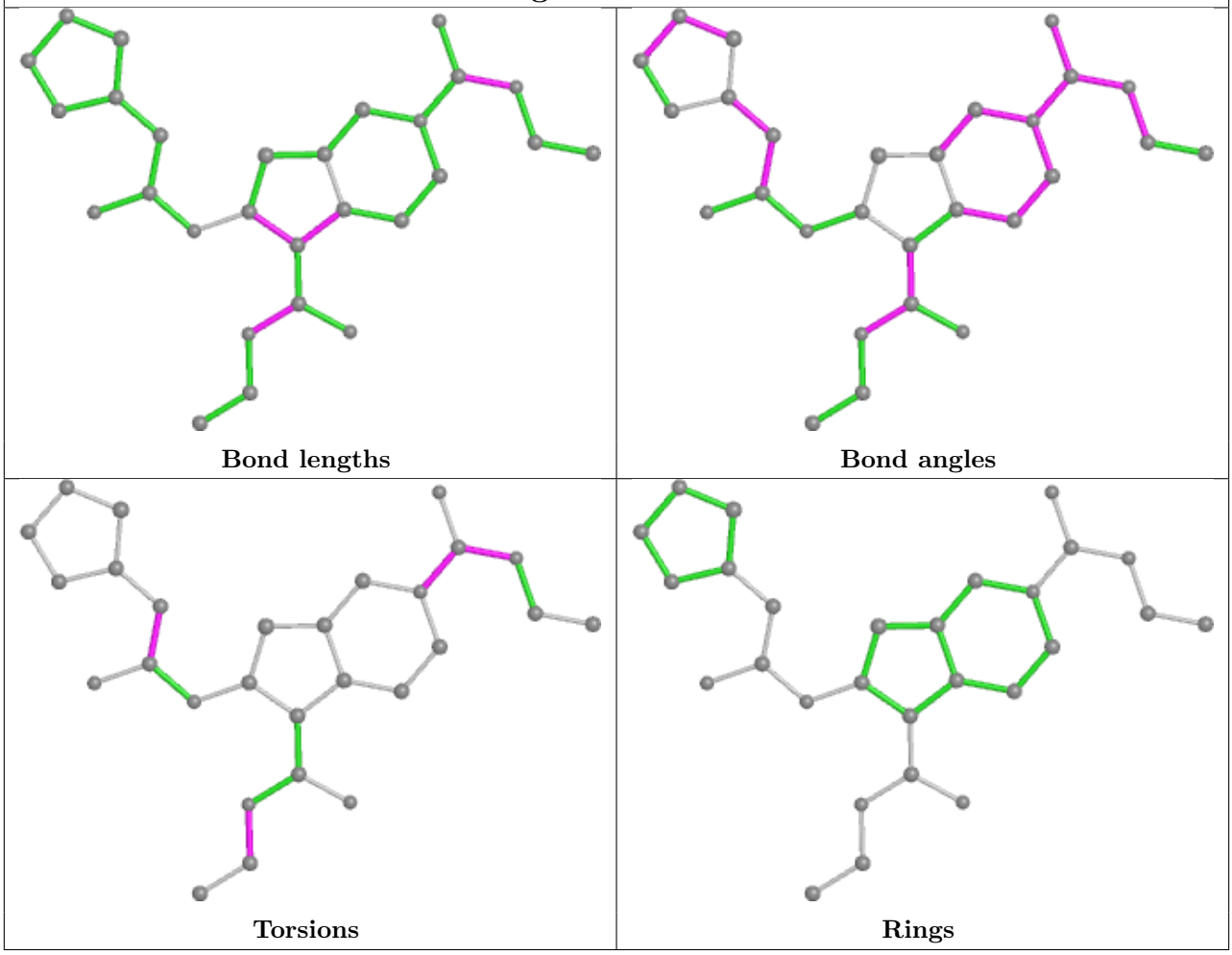


Rings

Ligand J25 A 1



Ligand J25 B 1



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	328/359 (91%)	0.15	23 (7%)	16	13	11, 23, 65, 96	0
1	B	325/359 (90%)	-0.06	8 (2%)	57	53	14, 29, 49, 79	0
1	C	325/359 (90%)	0.10	21 (6%)	18	16	12, 27, 62, 99	0
1	D	324/359 (90%)	-0.14	14 (4%)	35	31	9, 19, 48, 77	0
All	All	1302/1436 (90%)	0.02	66 (5%)	28	25	9, 25, 57, 99	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	ALA	6.5
1	C	357	MET	6.4
1	C	356	PRO	6.2
1	C	362	ASN	6.0
1	A	354	ILE	5.6
1	C	363	ALA	5.4
1	D	362	ASN	5.2
1	D	356	PRO	5.0
1	A	355	SER	4.9
1	A	356	PRO	4.9
1	B	356	PRO	4.6
1	A	359	ASP	4.6
1	C	355	SER	4.5
1	D	357	MET	4.4
1	D	361	HIS	4.4
1	A	362	ASN	4.3
1	D	354	ILE	4.2
1	A	353	GLU	4.1
1	D	363	ALA	3.8
1	A	361	HIS	3.8
1	D	359	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	357	MET	3.7
1	A	375	TYR	3.5
1	D	355	SER	3.5
1	C	361	HIS	3.4
1	C	359	ASP	3.4
1	B	89	GLU	3.3
1	A	352	MET	3.3
1	A	348	ARG	3.3
1	B	361	HIS	3.3
1	C	87	GLU	3.2
1	A	406	TYR	3.0
1	A	295	SER	3.0
1	C	408	SER	3.0
1	D	364	SER	3.0
1	D	367	LYS	3.0
1	B	362	ASN	2.9
1	C	410	ILE	2.9
1	A	289	THR	2.9
1	A	358	CYS	2.9
1	B	88	GLN	2.8
1	A	360	LYS	2.7
1	D	358	CYS	2.7
1	A	367	LYS	2.7
1	A	410	ILE	2.7
1	D	353	GLU	2.6
1	C	360	LYS	2.5
1	C	409	THR	2.5
1	B	90	ASP	2.5
1	A	408	SER	2.5
1	C	354	ILE	2.5
1	C	375	TYR	2.4
1	D	410	ILE	2.4
1	A	365	VAL	2.4
1	C	353	GLU	2.4
1	C	358	CYS	2.3
1	A	364	SER	2.3
1	C	364	SER	2.2
1	A	409	THR	2.2
1	C	370	VAL	2.2
1	C	407	GLN	2.2
1	C	297	VAL	2.2
1	C	86	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	92	LEU	2.1
1	D	348	ARG	2.1
1	B	357	MET	2.1

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
3	J25	A	1	28/28	0.85	0.54	35,53,67,78	0
4	EDO	D	5	4/4	0.86	0.24	34,35,37,38	0
4	EDO	C	7	4/4	0.89	0.20	34,37,40,45	0
4	EDO	C	3	4/4	0.90	0.21	28,31,32,41	0
3	J25	C	1	28/28	0.92	0.36	33,48,55,57	0
4	EDO	C	6	4/4	0.92	0.22	42,46,46,49	0
4	EDO	C	4	4/4	0.93	0.12	34,37,38,40	0
4	EDO	B	2	4/4	0.93	0.35	21,22,32,44	0
4	EDO	D	6	4/4	0.93	0.18	15,17,19,21	0
4	EDO	D	2	4/4	0.94	0.21	18,22,22,27	0
3	J25	D	1	28/28	0.94	0.23	24,38,51,57	0
3	J25	B	1	28/28	0.94	0.32	26,39,51,55	0
4	EDO	D	7	4/4	0.94	0.18	23,23,24,35	0
4	EDO	A	4	4/4	0.95	0.19	24,25,28,30	0
4	EDO	B	3	4/4	0.95	0.19	25,25,30,31	0
4	EDO	D	9	4/4	0.95	0.15	27,29,33,35	0
4	EDO	C	2	4/4	0.97	0.18	27,30,30,36	0
4	EDO	D	3	4/4	0.97	0.16	16,17,25,30	0
4	EDO	D	4	4/4	0.97	0.12	16,21,21,23	0
5	DMS	A	3	4/4	0.97	0.14	33,35,39,48	0

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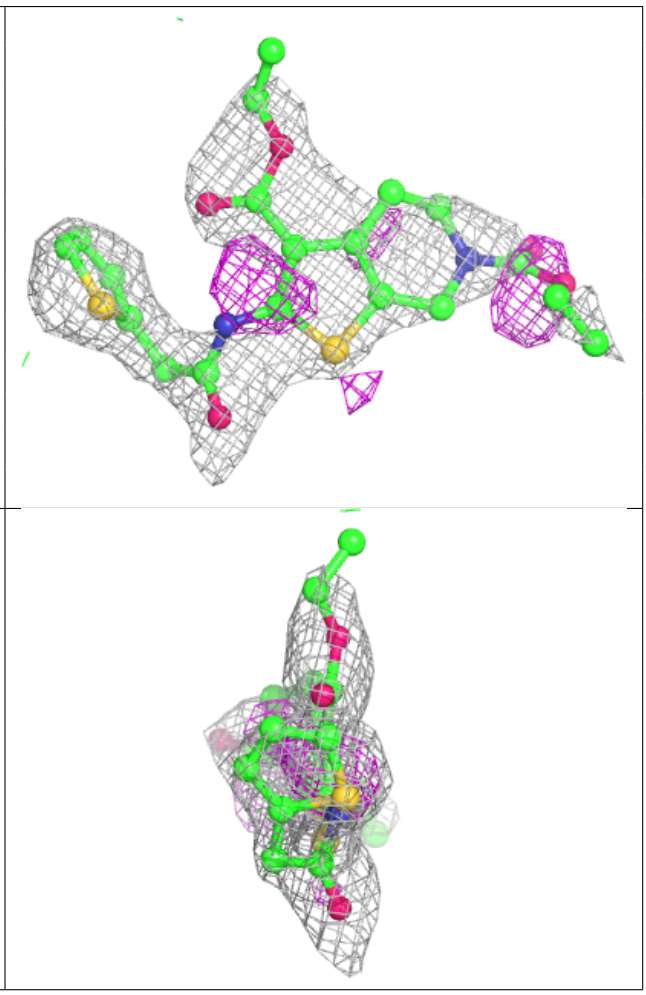
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	2	4/4	0.98	0.15	17,18,18,22	0
2	ZN	C	439	1/1	0.98	0.08	37,37,37,37	0
4	EDO	D	8	4/4	0.98	0.14	16,17,20,21	0
6	EPE	C	5	15/15	0.98	0.25	26,32,52,53	0
2	ZN	D	439	1/1	0.99	0.10	40,40,40,40	0
2	ZN	B	439	1/1	0.99	0.08	47,47,47,47	0
2	ZN	A	439	1/1	0.99	0.07	39,39,39,39	0
2	ZN	A	438	1/1	1.00	0.13	18,18,18,18	0
2	ZN	C	438	1/1	1.00	0.10	19,19,19,19	0
2	ZN	B	438	1/1	1.00	0.09	24,24,24,24	0
2	ZN	D	438	1/1	1.00	0.12	16,16,16,16	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.

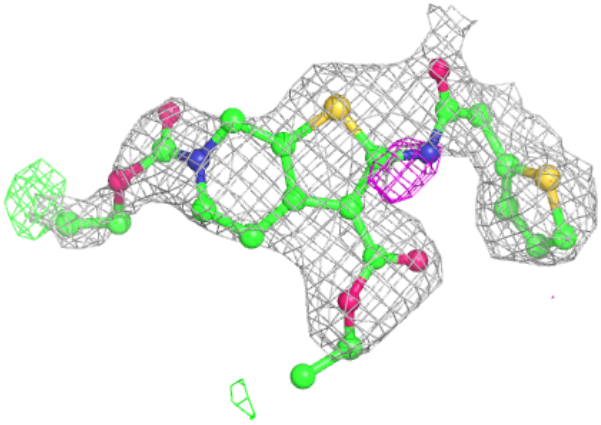
Electron density around J25 A 1:

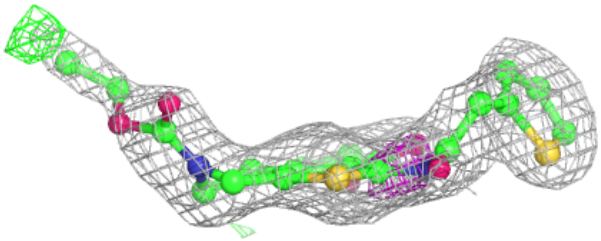
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

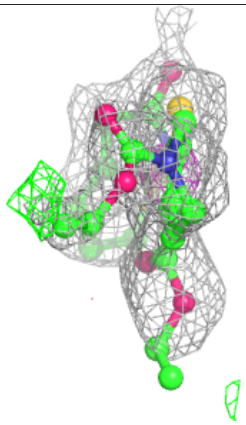


Electron density around J25 C 1:

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

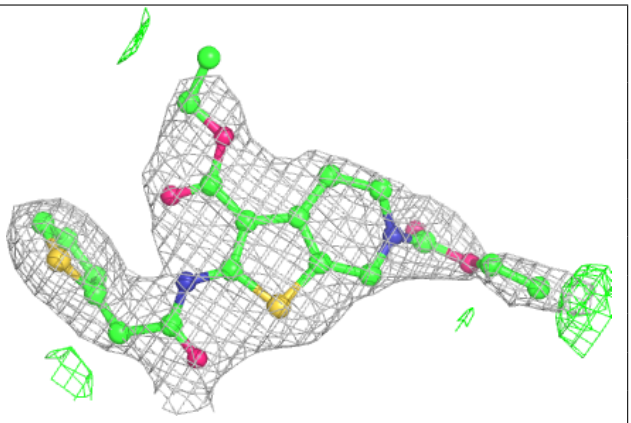


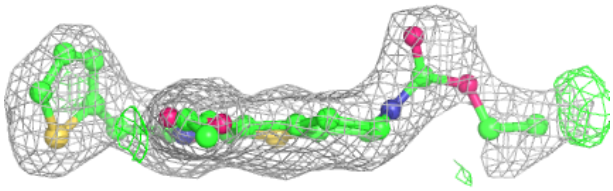


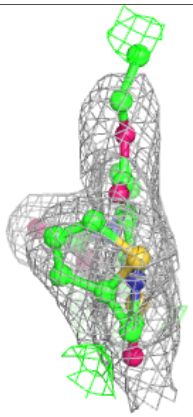


Electron density around J25 D 1:

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

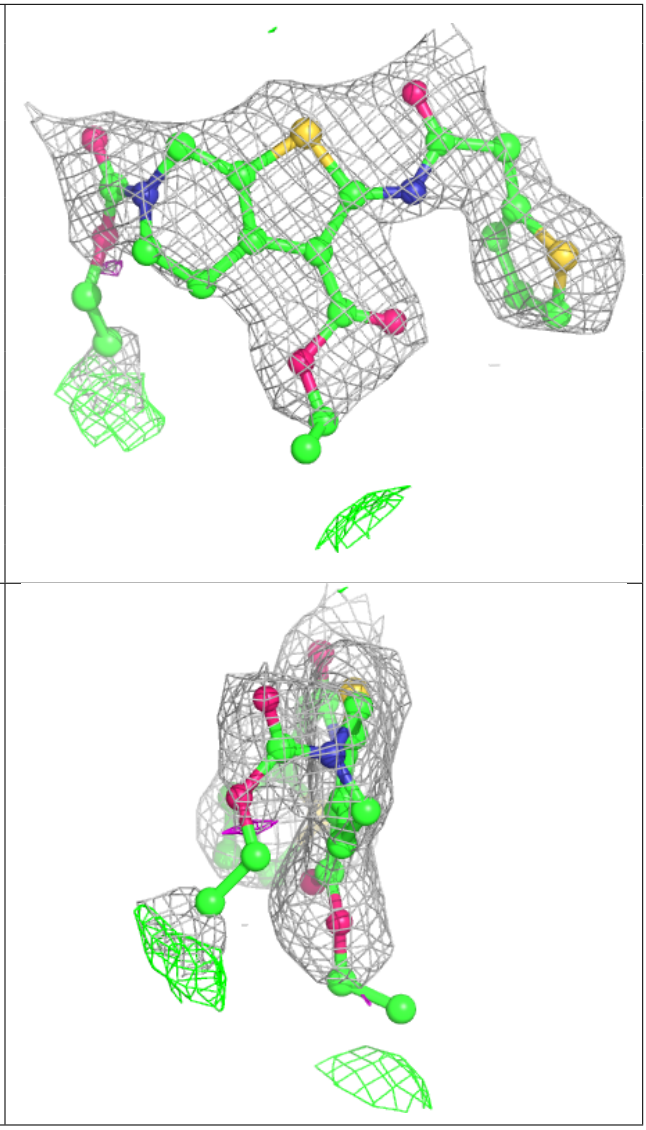






Electron density around J25 B 1:

$2mF_o$-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.