Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 08:22 PM EDT

PDB ID	:	3WSB
Title	:	The Tuberculosis Drug SQ109 Inhibits Trypanosoma cruzi Cell Proliferation and acts Synergistically with Posaconazole
Authors	:	Shang, N.; Li, Q.; Huang, C.H.; Oldfield, E.; Guo, R.T.
Deposited on	:	2014-03-05
Resolution	:	2.40 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:

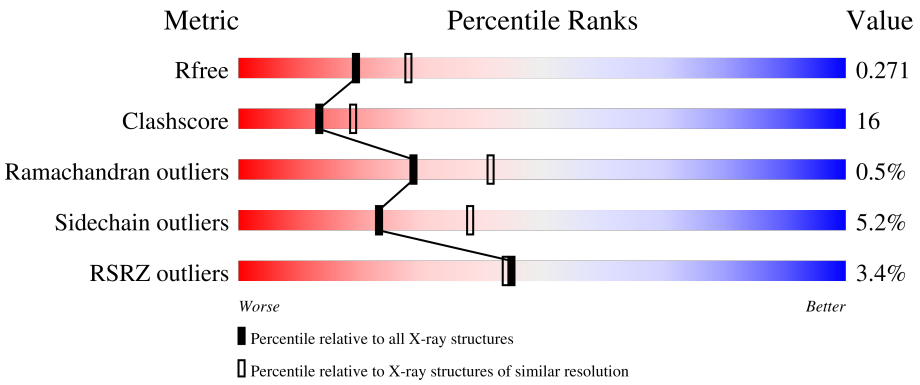
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	365	% 65% 26% • 7%
1	B	365	2% 66% 25% • 7%
1	C	365	4% 64% 28% • 7%
1	D	365	5% 56% 34% • 7%

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
2	FPS	D	401	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11630 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 Farnesyltransferase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2751	1745	473	511	22	0	0	0
1	B	341	2751	1745	473	511	22	0	0	0
1	C	341	2751	1745	473	511	22	0	0	0
1	D	341	2752	1745	473	512	22	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	expression tag	UNP Q4CWB4
A	5	GLY	-	expression tag	UNP Q4CWB4
A	6	SER	-	expression tag	UNP Q4CWB4
A	7	SER	-	expression tag	UNP Q4CWB4
A	8	HIS	-	expression tag	UNP Q4CWB4
A	9	HIS	-	expression tag	UNP Q4CWB4
A	10	HIS	-	expression tag	UNP Q4CWB4
A	11	HIS	-	expression tag	UNP Q4CWB4
A	12	HIS	-	expression tag	UNP Q4CWB4
A	13	HIS	-	expression tag	UNP Q4CWB4
A	14	SER	-	expression tag	UNP Q4CWB4
A	15	SER	-	expression tag	UNP Q4CWB4
A	16	GLY	-	expression tag	UNP Q4CWB4
A	17	LEU	-	expression tag	UNP Q4CWB4
A	18	VAL	-	expression tag	UNP Q4CWB4
A	19	PRO	-	expression tag	UNP Q4CWB4
A	20	ARG	-	expression tag	UNP Q4CWB4
A	21	GLY	-	expression tag	UNP Q4CWB4
A	22	SER	-	expression tag	UNP Q4CWB4
A	23	HIS	-	expression tag	UNP Q4CWB4
A	24	MET	-	expression tag	UNP Q4CWB4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	82	GLU	ASP	engineered mutation	UNP Q4CWB4
B	4	MET	-	expression tag	UNP Q4CWB4
B	5	GLY	-	expression tag	UNP Q4CWB4
B	6	SER	-	expression tag	UNP Q4CWB4
B	7	SER	-	expression tag	UNP Q4CWB4
B	8	HIS	-	expression tag	UNP Q4CWB4
B	9	HIS	-	expression tag	UNP Q4CWB4
B	10	HIS	-	expression tag	UNP Q4CWB4
B	11	HIS	-	expression tag	UNP Q4CWB4
B	12	HIS	-	expression tag	UNP Q4CWB4
B	13	HIS	-	expression tag	UNP Q4CWB4
B	14	SER	-	expression tag	UNP Q4CWB4
B	15	SER	-	expression tag	UNP Q4CWB4
B	16	GLY	-	expression tag	UNP Q4CWB4
B	17	LEU	-	expression tag	UNP Q4CWB4
B	18	VAL	-	expression tag	UNP Q4CWB4
B	19	PRO	-	expression tag	UNP Q4CWB4
B	20	ARG	-	expression tag	UNP Q4CWB4
B	21	GLY	-	expression tag	UNP Q4CWB4
B	22	SER	-	expression tag	UNP Q4CWB4
B	23	HIS	-	expression tag	UNP Q4CWB4
B	24	MET	-	expression tag	UNP Q4CWB4
B	82	GLU	ASP	engineered mutation	UNP Q4CWB4
C	4	MET	-	expression tag	UNP Q4CWB4
C	5	GLY	-	expression tag	UNP Q4CWB4
C	6	SER	-	expression tag	UNP Q4CWB4
C	7	SER	-	expression tag	UNP Q4CWB4
C	8	HIS	-	expression tag	UNP Q4CWB4
C	9	HIS	-	expression tag	UNP Q4CWB4
C	10	HIS	-	expression tag	UNP Q4CWB4
C	11	HIS	-	expression tag	UNP Q4CWB4
C	12	HIS	-	expression tag	UNP Q4CWB4
C	13	HIS	-	expression tag	UNP Q4CWB4
C	14	SER	-	expression tag	UNP Q4CWB4
C	15	SER	-	expression tag	UNP Q4CWB4
C	16	GLY	-	expression tag	UNP Q4CWB4
C	17	LEU	-	expression tag	UNP Q4CWB4
C	18	VAL	-	expression tag	UNP Q4CWB4
C	19	PRO	-	expression tag	UNP Q4CWB4
C	20	ARG	-	expression tag	UNP Q4CWB4
C	21	GLY	-	expression tag	UNP Q4CWB4
C	22	SER	-	expression tag	UNP Q4CWB4

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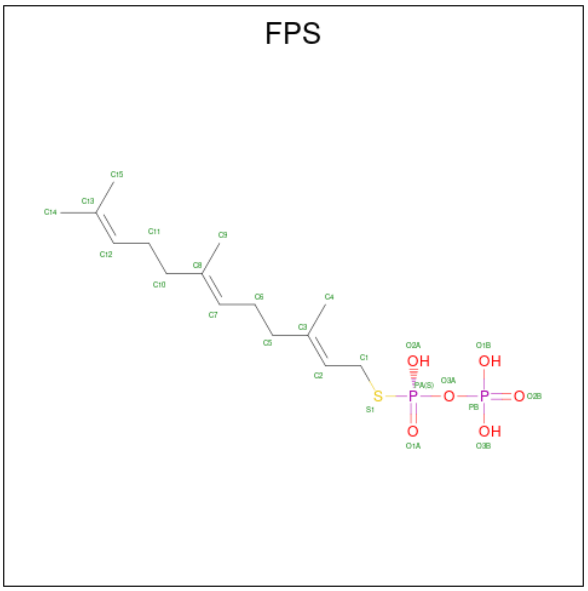
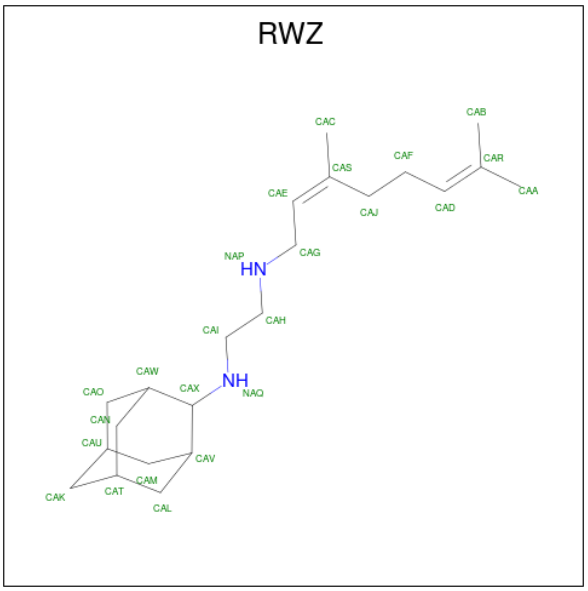
Chain	Residue	Modelled	Actual	Comment	Reference
C	23	HIS	-	expression tag	UNP Q4CWB4
C	24	MET	-	expression tag	UNP Q4CWB4
C	82	GLU	ASP	engineered mutation	UNP Q4CWB4
D	4	MET	-	expression tag	UNP Q4CWB4
D	5	GLY	-	expression tag	UNP Q4CWB4
D	6	SER	-	expression tag	UNP Q4CWB4
D	7	SER	-	expression tag	UNP Q4CWB4
D	8	HIS	-	expression tag	UNP Q4CWB4
D	9	HIS	-	expression tag	UNP Q4CWB4
D	10	HIS	-	expression tag	UNP Q4CWB4
D	11	HIS	-	expression tag	UNP Q4CWB4
D	12	HIS	-	expression tag	UNP Q4CWB4
D	13	HIS	-	expression tag	UNP Q4CWB4
D	14	SER	-	expression tag	UNP Q4CWB4
D	15	SER	-	expression tag	UNP Q4CWB4
D	16	GLY	-	expression tag	UNP Q4CWB4
D	17	LEU	-	expression tag	UNP Q4CWB4
D	18	VAL	-	expression tag	UNP Q4CWB4
D	19	PRO	-	expression tag	UNP Q4CWB4
D	20	ARG	-	expression tag	UNP Q4CWB4
D	21	GLY	-	expression tag	UNP Q4CWB4
D	22	SER	-	expression tag	UNP Q4CWB4
D	23	HIS	-	expression tag	UNP Q4CWB4
D	24	MET	-	expression tag	UNP Q4CWB4
D	82	GLU	ASP	engineered mutation	UNP Q4CWB4

- Molecule 2 is S-[(2E,6E)-3,7,11-TRIMETHYLDODECA-2,6,10-TRIENYL] TRIHYDROGEN THIODIPHOSPHATE (three-letter code: FPS) (formula: $C_{15}H_{28}O_6P_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	O	P	S		
2	A	1	24	15	6	2	1	0	0
			Total	C	O	P	S		
2	B	1	24	15	6	2	1	0	0
			Total	C	O	P	S		
2	C	1	24	15	6	2	1	0	0
			Total	C	O	P	S		
2	D	1	24	15	6	2	1	0	0

- Molecule 3 is N-[(2Z)-3,7-dimethylocta-2,6-dien-1-yl]-N'-[(1R,3S,5R,7R)-tricyclo[3.3.1.1 3,7]dec-2-yl]ethane-1,2-diamine (three-letter code: RWZ) (formula: $C_{22}H_{38}N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	A	1	24	22	2	0	0
3	B	1	24	22	2	0	0
3	C	1	24	22	2	0	0
3	D	1	24	22	2	0	0

- Molecule 4 is water.

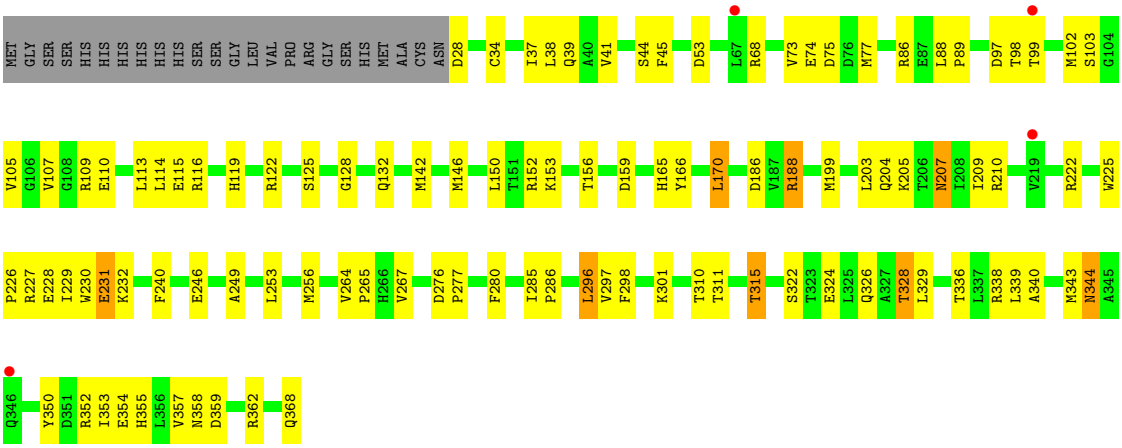
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	134	134	134	0	0
4	B	132	132	132	0	0
4	C	99	99	99	0	0
4	D	68	68	68	0	0

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.

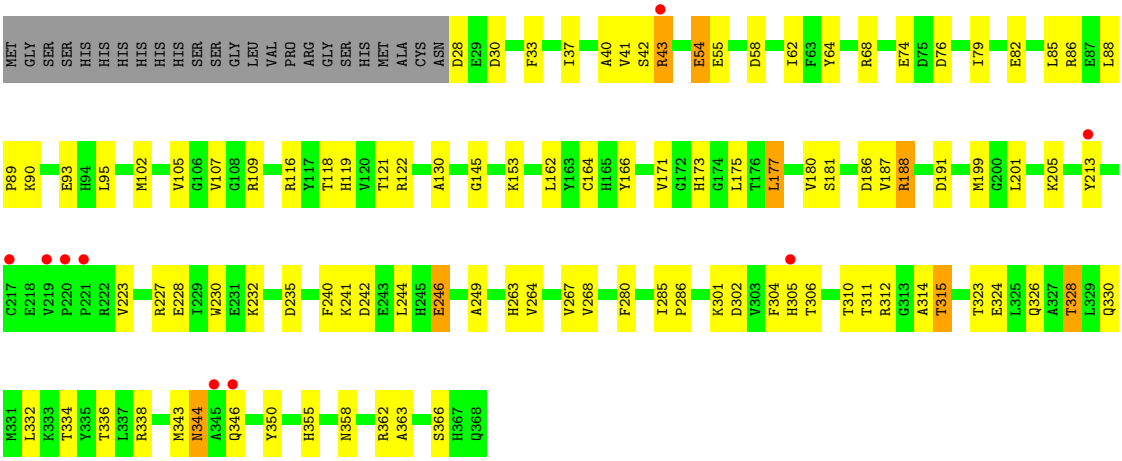
• Molecule 1: Farnesyltransferase, putative

Chain A:



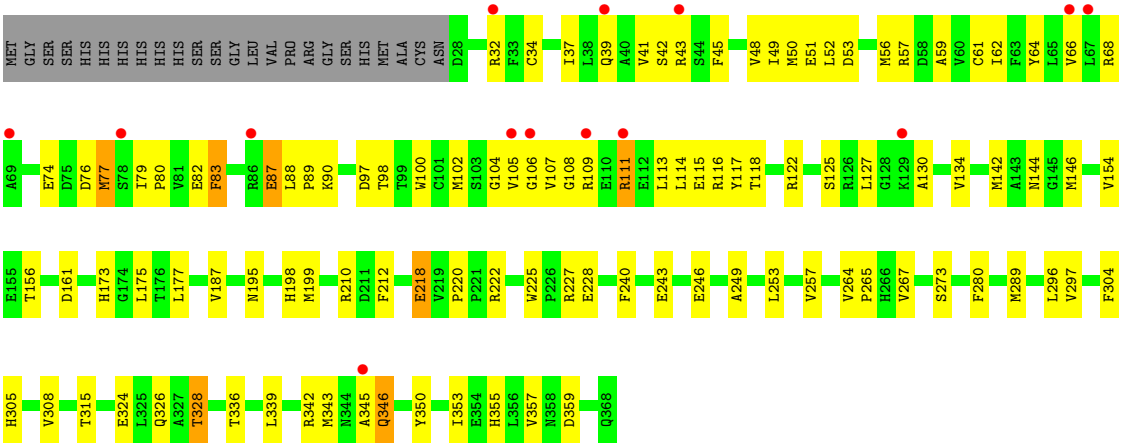
• Molecule 1: Farnesyltransferase, putative

Chain B:



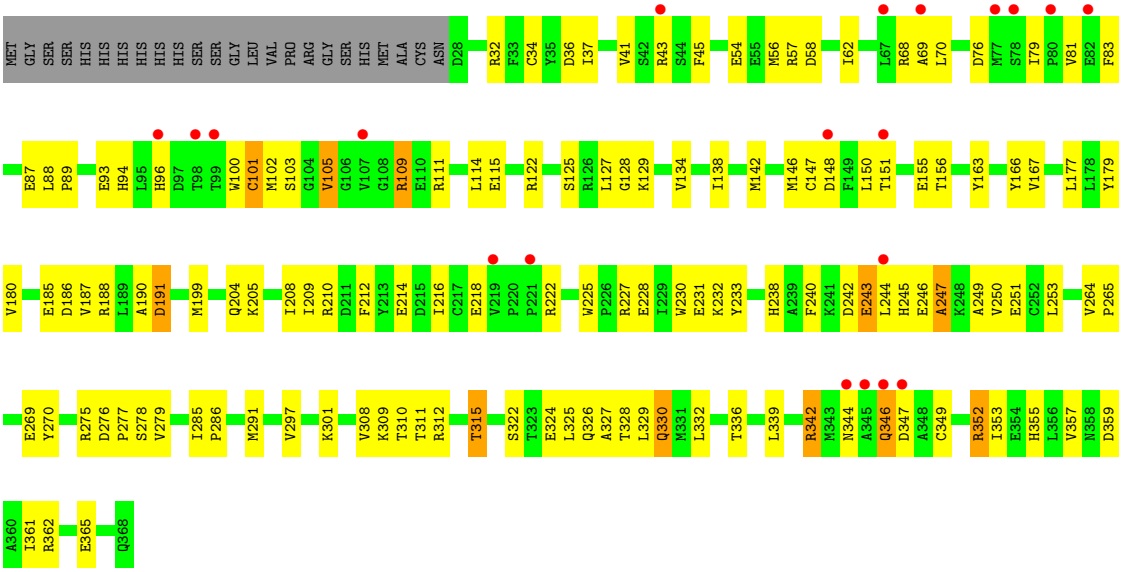
• Molecule 1: Farnesyltransferase, putative

Chain C:



- Molecule 1: Farnesyltransferase, putative

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	79.36Å 130.57Å 144.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.90 – 2.40 24.84 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (24.90-2.40) 91.7 (24.84-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.277 0.211 , 0.271	Depositor DCC
R_{free} test set	2761 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11630	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: RWZ, FPS

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	0/2809	0.58	0/3806
1	B	0.38	0/2809	0.59	0/3806
1	C	0.35	0/2809	0.58	0/3806
1	D	0.34	0/2810	0.55	0/3806
All	All	0.37	0/11237	0.57	0/15224

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	2751	0	2698	80	0
1	B	2751	0	2698	80	0
1	C	2751	0	2698	87	0
1	D	2752	0	2698	109	0
2	A	24	0	25	1	0
2	B	24	0	25	4	0
2	C	24	0	25	3	0
2	D	24	0	25	4	0
3	A	24	0	38	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	38	4	0
3	C	24	0	38	2	0
3	D	24	0	38	4	0
4	A	134	0	0	0	1
4	B	132	0	0	4	0
4	C	99	0	0	0	1
4	D	68	0	0	3	0
All	All	11630	0	11044	360	1

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 16.

All (360) 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:D:62:ILE:HG13	1:D:127:LEU:HD11	1.46	0.96
1:C:83:PHE:HE2	1:C:87:GLU:HG3	1.35	0.90
1:B:118:THR:HG22	1:B:122:ARG:HH21	1.38	0.88
1:B:344:ASN:HD22	1:B:346:GLN:HG3	1.38	0.86
1:C:106:GLY:O	1:C:111:ARG:HG2	1.74	0.86
1:D:186:ASP:OD1	1:D:188:ARG:HG2	1.76	0.86
1:A:188:ARG:HE	1:A:188:ARG:HA	1.40	0.85
1:C:79:ILE:HD11	1:C:105:VAL:HG21	1.57	0.85
1:D:103:SER:HA	1:D:115:GLU:HG2	1.58	0.85
1:C:80:PRO:HG2	1:C:83:PHE:HB2	1.58	0.84
1:B:118:THR:CG2	1:B:122:ARG:HH21	1.91	0.84
1:D:322:SER:HA	1:D:328:THR:HG22	1.62	0.82
1:D:243:GLU:HB2	1:D:246:GLU:HG3	1.62	0.81
1:C:343:MET:CE	1:C:350:TYR:HA	2.11	0.80
1:B:186:ASP:OD2	1:B:188:ARG:HB2	1.82	0.78
1:C:77:MET:HG2	1:C:220:PRO:HD2	1.65	0.78
1:B:33:PHE:O	1:B:37:ILE:HG22	1.82	0.78
1:C:118:THR:O	1:C:122:ARG:HG2	1.86	0.76
1:C:62:ILE:HD12	1:C:127:LEU:HD11	1.68	0.76
1:D:88:LEU:HB2	1:D:89:PRO:HD3	1.68	0.74
1:A:232:LYS:HD3	1:C:355:HIS:HB2	1.70	0.74
1:C:343:MET:HE2	1:C:350:TYR:HA	1.70	0.73
1:D:58:ASP:O	1:D:62:ILE:HG12	1.89	0.73
1:D:291:MET:SD	1:D:336:THR:HG22	2.30	0.71
1:D:81:VAL:HG13	1:D:150:LEU:HD22	1.72	0.71
1:D:227:ARG:HA	1:D:230:TRP:NE1	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ARG:HH21	1:A:119:HIS:HE1	1.35	0.71
1:C:79:ILE:HD11	1:C:105:VAL:CG2	2.21	0.71
1:B:343:MET:CE	1:B:350:TYR:HA	2.21	0.70
1:B:344:ASN:ND2	1:B:346:GLN:HE21	1.90	0.70
1:D:312:ARG:HA	1:D:315:THR:HG23	1.73	0.70
1:C:45:PHE:HB2	2:C:401:FPS:H11	1.72	0.70
1:B:228:GLU:O	1:B:232:LYS:HE3	1.91	0.69
1:A:344:ASN:C	1:A:344:ASN:HD22	1.95	0.69
1:B:324:GLU:O	1:B:328:THR:HG23	1.92	0.69
1:C:37:ILE:O	1:C:41:VAL:HG23	1.93	0.69
1:C:218:GLU:HG2	1:C:222:ARG:HH11	1.57	0.69
1:C:80:PRO:HG2	1:C:83:PHE:CB	2.23	0.68
1:B:130:ALA:HB1	1:B:181:SER:OG	1.94	0.68
1:C:98:THR:O	1:C:118:THR:HG23	1.95	0.67
1:C:42:SER:HB2	1:C:64:TYR:OH	1.94	0.67
1:C:218:GLU:HG2	1:C:222:ARG:NH1	2.10	0.66
1:C:83:PHE:CE2	1:C:87:GLU:HG3	2.25	0.66
1:D:83:PHE:O	1:D:87:GLU:HG2	1.96	0.65
1:D:264:VAL:HB	1:D:265:PRO:HD3	1.77	0.65
1:A:77:MET:HG2	1:A:222:ARG:NH2	2.10	0.65
1:D:186:ASP:CG	1:D:188:ARG:HG2	2.17	0.65
1:B:187:VAL:HG23	1:B:188:ARG:HE	1.60	0.65
1:C:343:MET:HE1	1:C:350:TYR:HA	1.79	0.64
1:C:79:ILE:HG23	1:C:83:PHE:HD1	1.63	0.63
1:D:214:GLU:HB2	4:D:557:HOH:O	1.98	0.63
1:C:343:MET:CE	1:C:353:ILE:HB	2.29	0.63
1:B:41:VAL:HG13	1:B:68:ARG:NH1	2.13	0.63
1:D:332:LEU:O	1:D:336:THR:HG23	1.98	0.63
1:B:246:GLU:OE1	1:B:301:LYS:HD2	1.98	0.63
1:C:111:ARG:HG2	1:C:111:ARG:HH11	1.64	0.63
1:A:102:MET:HE2	1:A:105:VAL:HB	1.80	0.63
1:B:344:ASN:ND2	1:B:346:GLN:HG3	2.13	0.63
1:D:155:GLU:CD	1:D:227:ARG:HE	2.02	0.63
1:B:343:MET:HE1	1:B:350:TYR:HA	1.81	0.62
1:A:225:TRP:HA	1:A:256:MET:HE1	1.81	0.62
1:B:41:VAL:CG1	1:B:68:ARG:NH1	2.61	0.62
1:C:76:ASP:OD2	1:C:105:VAL:HG13	2.00	0.62
1:D:180:VAL:HG21	1:D:190:ALA:HB2	1.81	0.62
1:D:243:GLU:HB2	1:D:246:GLU:CG	2.30	0.61
1:B:118:THR:HG22	1:B:122:ARG:NH2	2.10	0.61
1:D:142:MET:O	1:D:146:MET:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ARG:HG2	4:B:613:HOH:O	2.00	0.61
1:D:34:CYS:O	1:D:37:ILE:HG22	1.99	0.61
1:A:355:HIS:CD2	1:C:346:GLN:HB3	2.35	0.61
1:A:34:CYS:O	1:A:37:ILE:HG22	2.00	0.61
1:A:88:LEU:HB2	1:A:89:PRO:HD3	1.83	0.61
1:D:129:LYS:HD3	1:D:129:LYS:C	2.20	0.61
1:C:264:VAL:HB	1:C:265:PRO:HD3	1.82	0.61
1:B:363:ALA:O	1:B:366:SER:HB3	2.00	0.60
1:D:45:PHE:HB2	2:D:401:FPS:H11	1.82	0.60
1:B:118:THR:O	1:B:122:ARG:HB2	2.01	0.60
1:A:362:ARG:NH1	1:A:362:ARG:HG3	2.16	0.60
1:B:358:ASN:HB3	1:B:362:ARG:NH2	2.16	0.60
1:D:109:ARG:HH11	1:D:109:ARG:HG3	1.66	0.60
1:D:155:GLU:O	1:D:228:GLU:N	2.33	0.60
1:A:362:ARG:HG3	1:A:362:ARG:HH11	1.67	0.59
1:D:129:LYS:HD3	1:D:129:LYS:O	2.03	0.59
1:C:199:MET:SD	1:C:267:VAL:HG13	2.42	0.59
1:D:352:ARG:O	1:D:352:ARG:HD3	2.03	0.59
1:C:41:VAL:HG12	1:C:68:ARG:NH1	2.17	0.59
1:A:103:SER:HA	1:A:115:GLU:HG2	1.84	0.59
1:A:227:ARG:HA	1:A:230:TRP:CE2	2.37	0.59
1:C:122:ARG:NH1	1:C:122:ARG:HG3	2.18	0.58
1:A:343:MET:CE	1:A:350:TYR:HA	2.33	0.58
1:C:142:MET:O	1:C:146:MET:HG3	2.03	0.58
1:B:28:ASP:N	4:B:598:HOH:O	2.36	0.58
1:A:165:HIS:CE1	1:A:170:LEU:HD13	2.38	0.58
1:A:204:GLN:OE1	3:A:502:RWZ:HAX	2.03	0.58
1:D:179:TYR:CE1	1:D:279:VAL:HG13	2.38	0.58
1:D:188:ARG:HA	1:D:191:ASP:OD2	2.04	0.58
1:C:88:LEU:HB2	1:C:89:PRO:HD3	1.86	0.58
1:C:37:ILE:HD13	1:C:113:LEU:HD13	1.86	0.58
1:D:156:THR:HA	1:D:228:GLU:HB2	1.85	0.57
1:C:111:ARG:O	1:C:115:GLU:HG3	2.05	0.57
1:D:243:GLU:CB	1:D:246:GLU:HG3	2.34	0.57
1:D:326:GLN:O	1:D:330:GLN:HG2	2.05	0.57
1:B:344:ASN:HD22	1:B:346:GLN:CG	2.12	0.57
1:B:227:ARG:HA	1:B:230:TRP:NE1	2.20	0.57
1:D:43:ARG:HG2	1:D:43:ARG:HH21	1.70	0.57
1:B:242:ASP:C	1:B:244:LEU:H	2.07	0.56
1:D:109:ARG:HG3	1:D:109:ARG:NH1	2.20	0.56
1:D:111:ARG:O	1:D:115:GLU:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:LYS:O	1:D:209:ILE:HG13	2.05	0.56
1:D:344:ASN:HB2	1:D:346:GLN:HG3	1.87	0.56
1:C:122:ARG:HG3	1:C:122:ARG:HH11	1.69	0.56
1:D:163:TYR:CZ	1:D:167:VAL:HG21	2.41	0.56
1:C:80:PRO:O	1:C:83:PHE:HB3	2.05	0.56
1:B:332:LEU:O	1:B:336:THR:HG23	2.05	0.56
1:A:280:PHE:CZ	1:A:328:THR:HG21	2.41	0.56
1:B:358:ASN:O	1:B:362:ARG:HG3	2.05	0.56
1:D:253:LEU:HD21	1:D:297:VAL:O	2.07	0.55
1:D:352:ARG:HG3	1:D:352:ARG:HH11	1.70	0.55
1:A:102:MET:CE	1:A:114:LEU:HD13	2.37	0.55
1:A:344:ASN:C	1:A:344:ASN:ND2	2.60	0.55
1:C:343:MET:HE1	1:C:353:ILE:HB	1.88	0.55
1:A:74:GLU:O	1:A:74:GLU:HG2	2.07	0.55
1:B:311:THR:O	1:B:315:THR:HG22	2.06	0.55
1:B:326:GLN:O	1:B:330:GLN:HG3	2.08	0.55
1:C:130:ALA:O	1:C:134:VAL:HG23	2.07	0.55
1:B:42:SER:HB2	1:B:64:TYR:OH	2.06	0.54
1:D:227:ARG:HA	1:D:230:TRP:CE2	2.42	0.54
1:B:40:ALA:HA	1:B:43:ARG:NH2	2.22	0.54
1:C:82:GLU:CD	1:C:82:GLU:H	2.09	0.54
1:A:188:ARG:HA	1:A:188:ARG:NE	2.16	0.54
1:B:40:ALA:HB1	1:B:109:ARG:HD3	1.89	0.54
1:C:336:THR:HG22	1:C:357:VAL:HG13	1.89	0.54
1:A:156:THR:HA	1:A:228:GLU:HB2	1.90	0.54
1:B:173:HIS:O	1:B:177:LEU:HD22	2.08	0.54
1:C:339:LEU:C	1:C:339:LEU:HD23	2.28	0.54
1:D:342:ARG:HG3	1:D:342:ARG:HH11	1.72	0.54
1:C:342:ARG:HG2	1:C:342:ARG:HH11	1.72	0.53
1:C:52:LEU:O	1:C:57:ARG:HD3	2.08	0.53
1:B:102:MET:CE	1:B:105:VAL:HG21	2.38	0.53
1:D:180:VAL:HG13	1:D:187:VAL:HA	1.90	0.53
1:C:97:ASP:OD2	1:C:100:TRP:HB2	2.09	0.53
1:C:280:PHE:CE1	1:C:328:THR:HG21	2.45	0.53
1:A:352:ARG:HA	1:C:345:ALA:HB1	1.90	0.52
1:A:116:ARG:HH21	1:A:119:HIS:CE1	2.23	0.52
1:B:240:PHE:CD1	1:B:249:ALA:HB2	2.45	0.52
1:D:100:TRP:O	1:D:101:CYS:HB3	2.10	0.52
1:C:173:HIS:O	1:C:177:LEU:HG	2.10	0.52
1:D:361:ILE:O	1:D:365:GLU:HG3	2.10	0.52
1:A:226:PRO:HG2	1:A:229:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ALA:HB3	4:B:556:HOH:O	2.09	0.52
1:D:179:TYR:CZ	1:D:279:VAL:HG13	2.45	0.51
1:B:249:ALA:HB1	1:B:304:PHE:CZ	2.46	0.51
1:B:118:THR:HG22	1:B:122:ARG:HE	1.75	0.51
1:C:243:GLU:O	1:C:246:GLU:HB2	2.10	0.51
1:A:227:ARG:O	1:A:231:GLU:HB3	2.11	0.51
1:C:210:ARG:HD2	1:C:210:ARG:O	2.10	0.51
1:A:102:MET:HE2	1:A:114:LEU:HD13	1.91	0.51
1:B:302:ASP:HA	1:B:305:HIS:CE1	2.46	0.51
1:B:145:GLY:HA3	1:B:166:TYR:CD1	2.46	0.50
1:B:344:ASN:ND2	1:B:346:GLN:NE2	2.57	0.50
2:B:401:FPS:H61	3:B:402:RWZ:HAB	1.94	0.50
1:C:62:ILE:O	1:C:66:VAL:HG23	2.09	0.50
1:A:44:SER:HB2	2:A:501:FPS:O2B	2.12	0.50
1:A:280:PHE:CE1	1:A:328:THR:HG21	2.46	0.50
1:C:32:ARG:NH1	1:C:32:ARG:HB2	2.27	0.50
1:C:80:PRO:HB2	1:C:82:GLU:HG2	1.94	0.50
1:B:86:ARG:O	1:B:90:LYS:HD3	2.10	0.50
1:B:264:VAL:O	1:B:268:VAL:HG13	2.12	0.50
1:D:242:ASP:OD2	1:D:244:LEU:HB3	2.12	0.50
1:C:122:ARG:O	1:C:125:SER:OG	2.19	0.50
1:C:156:THR:HB	1:C:228:GLU:OE1	2.11	0.50
1:D:227:ARG:O	1:D:231:GLU:HB3	2.12	0.50
1:D:54:GLU:HA	1:D:57:ARG:HB3	1.94	0.49
1:B:280:PHE:CE1	1:B:328:THR:HG21	2.47	0.49
1:A:264:VAL:HB	1:A:265:PRO:HD3	1.94	0.49
1:D:339:LEU:HD23	1:D:339:LEU:C	2.33	0.49
1:B:242:ASP:C	1:B:244:LEU:N	2.65	0.49
1:B:199:MET:SD	1:B:267:VAL:HG13	2.53	0.49
1:D:122:ARG:O	1:D:125:SER:OG	2.30	0.49
1:C:102:MET:HB3	1:C:114:LEU:HB3	1.95	0.48
1:D:352:ARG:HD3	1:D:352:ARG:C	2.33	0.48
1:D:212:PHE:CZ	1:D:216:ILE:HD12	2.48	0.48
1:C:253:LEU:O	1:C:257:VAL:HG23	2.13	0.48
1:A:205:LYS:O	1:A:209:ILE:HG13	2.14	0.48
1:B:223:VAL:HG13	1:B:223:VAL:O	2.12	0.48
1:D:150:LEU:HD23	1:D:150:LEU:O	2.13	0.48
1:D:353:ILE:O	1:D:357:VAL:HG23	2.13	0.48
1:D:142:MET:HG3	1:D:166:TYR:O	2.13	0.48
1:B:90:LYS:O	1:B:93:GLU:HB2	2.13	0.48
1:C:43:ARG:HH21	1:C:43:ARG:HG3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:HIS:C	1:D:96:HIS:H	2.17	0.48
1:D:240:PHE:CD1	1:D:249:ALA:HA	2.48	0.48
1:A:186:ASP:OD2	1:A:188:ARG:HB2	2.14	0.47
1:B:188:ARG:HG3	1:B:191:ASP:OD2	2.13	0.47
1:C:113:LEU:O	1:C:117:TYR:N	2.46	0.47
1:D:185:GLU:OE1	1:D:275:ARG:HG2	2.14	0.47
1:B:227:ARG:HA	1:B:230:TRP:CE2	2.49	0.47
1:C:345:ALA:HA	1:C:350:TYR:CD1	2.49	0.47
1:A:343:MET:HE1	1:A:350:TYR:HA	1.95	0.47
1:C:253:LEU:HD21	1:C:297:VAL:O	2.14	0.47
1:B:175:LEU:HD12	2:B:401:FPS:H112	1.97	0.47
1:B:263:HIS:O	1:B:267:VAL:HG23	2.14	0.47
1:D:199:MET:HG3	2:D:401:FPS:H153	1.95	0.47
1:D:240:PHE:CE1	1:D:249:ALA:HA	2.49	0.47
1:D:246:GLU:OE2	1:D:301:LYS:HD2	2.14	0.47
1:A:340:ALA:O	1:A:343:MET:HG2	2.14	0.47
1:B:343:MET:HE2	1:B:350:TYR:HA	1.97	0.47
1:B:312:ARG:HA	1:B:315:THR:CG2	2.45	0.46
1:B:95:LEU:O	1:B:121:THR:HG23	2.14	0.46
1:C:280:PHE:HE1	1:C:328:THR:HG21	1.80	0.46
1:C:104:GLY:O	1:C:105:VAL:HG23	2.15	0.46
1:A:116:ARG:NH2	1:A:119:HIS:HE1	2.10	0.46
1:A:285:ILE:HB	1:A:286:PRO:HD3	1.96	0.46
1:A:329:LEU:HD23	1:A:368:GLN:HG2	1.95	0.46
1:A:336:THR:HG22	1:A:357:VAL:HG13	1.98	0.46
1:C:175:LEU:HD12	2:C:401:FPS:H112	1.98	0.46
1:A:156:THR:HB	1:A:228:GLU:OE1	2.15	0.46
1:A:343:MET:HE1	1:A:353:ILE:HB	1.98	0.46
1:D:285:ILE:HB	1:D:286:PRO:HD3	1.98	0.46
1:A:253:LEU:HD21	1:A:297:VAL:O	2.16	0.46
1:A:152:ARG:O	1:A:153:LYS:HD2	2.16	0.46
1:D:243:GLU:CA	1:D:246:GLU:HG3	2.46	0.46
1:B:54:GLU:HB2	1:B:55:GLU:H	1.62	0.46
1:D:352:ARG:NH1	4:D:506:HOH:O	2.49	0.46
1:A:199:MET:SD	1:A:267:VAL:HG13	2.55	0.45
1:A:210:ARG:C	1:A:210:ARG:HD2	2.37	0.45
1:A:41:VAL:CG1	1:A:68:ARG:CZ	2.95	0.45
1:B:249:ALA:HB1	1:B:304:PHE:CE2	2.51	0.45
1:A:98:THR:C	1:A:99:THR:HG23	2.37	0.45
1:C:87:GLU:O	1:C:90:LYS:HG2	2.17	0.45
1:B:162:LEU:HG	1:B:166:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:THR:O	1:B:338:ARG:HG3	2.17	0.45
1:A:166:TYR:HA	1:A:170:LEU:HD22	1.98	0.45
1:D:204:GLN:HE21	1:D:208:ILE:HD11	1.81	0.45
1:D:312:ARG:HA	1:D:315:THR:CG2	2.45	0.45
3:D:402:RWZ:HAF	3:D:402:RWZ:HAC	1.64	0.45
1:A:226:PRO:HG2	1:A:229:ILE:CG1	2.47	0.45
1:C:118:THR:HG22	1:C:122:ARG:NE	2.32	0.45
1:D:344:ASN:HB2	1:D:346:GLN:CG	2.47	0.45
1:B:344:ASN:HD21	1:B:346:GLN:HE21	1.64	0.45
1:D:246:GLU:O	1:D:247:ALA:C	2.55	0.45
1:C:49:ILE:HD11	1:C:61:CYS:HB2	1.99	0.45
1:C:116:ARG:C	1:C:118:THR:N	2.70	0.45
1:A:210:ARG:HD2	1:A:210:ARG:O	2.17	0.44
1:D:311:THR:O	1:D:315:THR:HG22	2.17	0.44
1:D:344:ASN:N	1:D:347:ASP:OD2	2.45	0.44
1:D:134:VAL:O	1:D:138:ILE:HG12	2.17	0.44
1:B:82:GLU:CD	1:B:82:GLU:H	2.21	0.44
1:D:76:ASP:OD1	1:D:79:ILE:HG23	2.17	0.44
1:A:355:HIS:NE2	1:C:346:GLN:HB3	2.33	0.44
1:C:212:PHE:HB2	1:C:225:TRP:CZ2	2.52	0.44
1:A:228:GLU:O	1:A:232:LYS:NZ	2.40	0.44
1:B:164:CYS:HB3	1:B:201:LEU:HG	1.98	0.44
1:A:362:ARG:HH11	1:A:362:ARG:CG	2.30	0.44
3:A:502:RWZ:HAFA	3:A:502:RWZ:HAB	1.77	0.44
1:B:88:LEU:HB2	1:B:89:PRO:HD3	1.98	0.44
2:B:401:FPS:H62	3:B:402:RWZ:HAMA	2.00	0.44
1:D:352:ARG:O	1:D:355:HIS:HB3	2.18	0.44
1:C:43:ARG:HH21	1:C:43:ARG:CG	2.31	0.43
1:C:227:ARG:NE	1:D:244:LEU:HD21	2.32	0.43
1:D:70:LEU:HD12	1:D:88:LEU:HD22	1.99	0.43
1:D:102:MET:HB3	1:D:105:VAL:HG21	2.00	0.43
1:D:309:LYS:HG2	1:D:310:THR:N	2.33	0.43
1:A:97:ASP:C	1:A:98:THR:O	2.54	0.43
1:B:180:VAL:HG13	1:B:187:VAL:HA	2.00	0.43
1:D:339:LEU:O	1:D:342:ARG:HB2	2.17	0.43
1:B:302:ASP:HB3	1:B:306:THR:CG2	2.47	0.43
1:D:222:ARG:HG3	1:D:222:ARG:HH11	1.84	0.43
1:A:227:ARG:HA	1:A:230:TRP:NE1	2.33	0.43
1:B:41:VAL:HG13	1:B:68:ARG:CZ	2.47	0.43
1:D:243:GLU:C	1:D:245:HIS:N	2.69	0.43
1:B:280:PHE:CZ	1:B:328:THR:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ARG:HG3	1:D:222:ARG:NH1	2.32	0.43
1:D:325:LEU:O	1:D:329:LEU:HG	2.17	0.43
1:A:324:GLU:O	1:A:328:THR:HG23	2.19	0.43
1:C:342:ARG:HG2	1:C:342:ARG:NH1	2.32	0.43
1:D:177:LEU:HD23	1:D:177:LEU:HA	1.89	0.43
1:D:270:TYR:CZ	2:D:401:FPS:H151	2.54	0.43
1:D:276:ASP:OD1	1:D:278:SER:HB2	2.18	0.43
1:A:122:ARG:O	1:A:125:SER:HB3	2.18	0.43
1:D:79:ILE:HD12	1:D:83:PHE:HD2	1.84	0.43
1:D:250:VAL:O	1:D:253:LEU:HB3	2.19	0.43
1:D:330:GLN:HG2	1:D:330:GLN:H	1.54	0.43
1:A:73:VAL:HG22	1:A:102:MET:CE	2.49	0.43
1:B:171:VAL:HB	2:B:401:FPS:H92	2.01	0.43
1:B:344:ASN:OD1	1:B:344:ASN:N	2.51	0.43
1:A:73:VAL:HG22	1:A:102:MET:HE3	2.01	0.42
1:A:156:THR:OG1	1:A:159:ASP:CG	2.57	0.42
1:A:338:ARG:HD2	1:A:338:ARG:HA	1.87	0.42
1:C:48:VAL:O	1:C:51:GLU:HB2	2.19	0.42
3:C:402:RWZ:HAC	3:C:402:RWZ:HAF	1.71	0.42
1:D:167:VAL:HG13	3:D:402:RWZ:HAI	2.00	0.42
1:A:38:LEU:HD11	1:A:45:PHE:HD2	1.84	0.42
1:A:146:MET:O	1:A:150:LEU:HG	2.19	0.42
1:B:76:ASP:HB3	1:B:79:ILE:HD12	2.00	0.42
1:A:311:THR:O	1:A:315:THR:HG23	2.19	0.42
3:B:402:RWZ:HAB	3:B:402:RWZ:HAFA	1.81	0.42
1:C:64:TYR:OH	1:C:68:ARG:NH1	2.52	0.42
1:A:246:GLU:CD	1:A:301:LYS:HD2	2.39	0.42
1:A:354:GLU:O	1:A:358:ASN:ND2	2.52	0.42
3:A:502:RWZ:HAC	3:A:502:RWZ:HAF	1.77	0.42
1:D:225:TRP:CD1	1:D:225:TRP:N	2.87	0.42
1:D:242:ASP:OD2	1:D:244:LEU:CB	2.68	0.42
1:A:170:LEU:HD12	1:A:170:LEU:HA	1.90	0.42
1:C:83:PHE:C	1:C:83:PHE:CD2	2.92	0.42
1:A:296:LEU:HD22	1:A:310:THR:HG22	2.01	0.42
1:B:285:ILE:HB	1:B:286:PRO:HD3	2.02	0.42
1:C:195:ASN:O	1:C:198:HIS:HB2	2.19	0.42
1:C:89:PRO:HB3	1:C:144:ASN:HD21	1.85	0.42
1:C:108:GLY:O	1:C:111:ARG:HB2	2.19	0.42
1:D:79:ILE:HD12	1:D:83:PHE:CD2	2.55	0.42
1:D:339:LEU:HD23	1:D:339:LEU:O	2.19	0.42
1:A:298:PHE:HZ	1:A:343:MET:HE3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ASP:O	1:B:62:ILE:HG12	2.20	0.42
1:B:312:ARG:O	1:B:315:THR:HG23	2.20	0.42
1:C:289:MET:HB3	1:C:289:MET:HE2	1.94	0.42
1:A:324:GLU:OE1	1:A:326:GLN:HB2	2.20	0.42
1:B:310:THR:OG1	1:B:314:ALA:HB3	2.20	0.42
1:C:240:PHE:CE1	1:C:249:ALA:HA	2.55	0.42
1:D:233:TYR:CE1	1:D:251:GLU:HG2	2.55	0.42
1:A:110:GLU:O	1:A:113:LEU:HB3	2.20	0.41
1:C:324:GLU:OE1	1:C:326:GLN:HB2	2.20	0.41
1:D:102:MET:HB3	1:D:105:VAL:CG2	2.49	0.41
1:A:339:LEU:C	1:A:339:LEU:HD23	2.40	0.41
1:B:30:ASP:OD2	1:B:122:ARG:HD2	2.20	0.41
1:B:116:ARG:HH21	1:B:119:HIS:HE1	1.67	0.41
1:C:225:TRP:CD1	1:C:225:TRP:N	2.87	0.41
1:D:69:ALA:HB1	1:D:114:LEU:HD21	2.01	0.41
2:D:401:FPS:H41	3:D:402:RWZ:HAB	2.03	0.41
1:A:142:MET:HG3	1:A:166:TYR:O	2.19	0.41
1:A:240:PHE:CE1	1:A:249:ALA:HA	2.55	0.41
1:A:203:LEU:O	1:A:207:ASN:HB2	2.21	0.41
1:D:187:VAL:O	1:D:187:VAL:HG22	2.21	0.41
1:C:56:MET:O	1:C:59:ALA:HB3	2.19	0.41
1:D:297:VAL:HG12	1:D:308:VAL:HB	2.03	0.41
1:C:249:ALA:HB1	1:C:304:PHE:CE2	2.55	0.41
1:B:213:TYR:HE1	1:B:241:LYS:HD2	1.84	0.41
1:C:210:ARG:HD3	1:C:308:VAL:O	2.21	0.41
1:D:41:VAL:HG13	1:D:68:ARG:CZ	2.51	0.41
1:D:186:ASP:OD1	1:D:187:VAL:N	2.54	0.41
1:D:210:ARG:HD2	1:D:210:ARG:O	2.20	0.41
1:D:276:ASP:HA	1:D:277:PRO:HD3	1.90	0.41
1:C:154:VAL:O	1:C:154:VAL:HG12	2.20	0.40
1:D:324:GLU:OE1	1:D:327:ALA:HB2	2.21	0.40
1:A:128:GLY:O	1:A:132:GLN:HG3	2.21	0.40
1:A:329:LEU:HD23	1:A:368:GLN:CG	2.51	0.40
2:C:401:FPS:H41	3:C:402:RWZ:HAB	2.03	0.40
1:A:285:ILE:HG12	1:A:322:SER:HB2	2.03	0.40
1:B:205:LYS:HD3	4:B:513:HOH:O	2.21	0.40
1:C:105:VAL:N	1:C:111:ARG:CZ	2.84	0.40
1:D:147:CYS:O	1:D:148:ASP:C	2.60	0.40
1:D:216:ILE:HD11	1:D:238:HIS:HA	2.04	0.40
1:A:86:ARG:CZ	1:B:355:HIS:HB3	2.51	0.40
1:B:323:THR:O	1:B:323:THR:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:LEU:O	1:D:128:GLY:C	2.57	0.40
1:D:167:VAL:CG1	3:D:402:RWZ:HAI	2.51	0.40
1:A:276:ASP:HA	1:A:277:PRO:HD3	1.79	0.40
3:B:402:RWZ:HAF	3:B:402:RWZ:HAC	1.84	0.40
1:C:34:CYS:O	1:C:37:ILE:HG22	2.21	0.40
1:D:269:GLU:HG3	4:D:526:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:722:HOH:O	4:C:596:HOH:O[3_544]	2.10	0.10

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	339/365 (93%)	324 (96%)	15 (4%)	0	100	100
1	B	339/365 (93%)	318 (94%)	21 (6%)	0	100	100
1	C	339/365 (93%)	314 (93%)	22 (6%)	3 (1%)	17	25
1	D	339/365 (93%)	307 (91%)	28 (8%)	4 (1%)	13	19
All	All	1356/1460 (93%)	1263 (93%)	86 (6%)	7 (0%)	29	41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	349	CYS
1	C	305	HIS
1	D	191	ASP
1	D	101	CYS

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Mol	Chain	Res	Type
1	D	247	ALA
1	C	107	VAL
1	C	187	VAL

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	298/318 (94%)	283 (95%)	15 (5%)	24	40
1	B	298/318 (94%)	285 (96%)	13 (4%)	28	45
1	C	298/318 (94%)	281 (94%)	17 (6%)	20	33
1	D	298/318 (94%)	281 (94%)	17 (6%)	20	33
All	All	1192/1272 (94%)	1130 (95%)	62 (5%)	23	38

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	39	GLN
1	A	53	ASP
1	A	75	ASP
1	A	107	VAL
1	A	109	ARG
1	A	170	LEU
1	A	188	ARG
1	A	207	ASN
1	A	231	GLU
1	A	296	LEU
1	A	315	THR
1	A	328	THR
1	A	344	ASN
1	A	359	ASP
1	B	43	ARG
1	B	54	GLU
1	B	74	GLU

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Mol	Chain	Res	Type
1	B	85	LEU
1	B	107	VAL
1	B	153	LYS
1	B	177	LEU
1	B	188	ARG
1	B	235	ASP
1	B	246	GLU
1	B	315	THR
1	B	328	THR
1	B	344	ASN
1	C	39	GLN
1	C	50	MET
1	C	53	ASP
1	C	74	GLU
1	C	77	MET
1	C	83	PHE
1	C	87	GLU
1	C	109	ARG
1	C	111	ARG
1	C	161	ASP
1	C	218	GLU
1	C	273	SER
1	C	296	LEU
1	C	315	THR
1	C	328	THR
1	C	346	GLN
1	C	359	ASP
1	D	32	ARG
1	D	36	ASP
1	D	56	MET
1	D	93	GLU
1	D	105	VAL
1	D	109	ARG
1	D	151	THR
1	D	218	GLU
1	D	232	LYS
1	D	243	GLU
1	D	315	THR
1	D	330	GLN
1	D	342	ARG
1	D	346	GLN
1	D	352	ARG

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Mol	Chain	Res	Type
1	D	359	ASP
1	D	362	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	94	HIS
1	A	119	HIS
1	A	144	ASN
1	A	245	HIS
1	A	266	HIS
1	A	320	HIS
1	A	344	ASN
1	A	358	ASN
1	B	119	HIS
1	B	144	ASN
1	B	305	HIS
1	B	320	HIS
1	B	330	GLN
1	B	344	ASN
1	C	144	ASN
1	D	144	ASN
1	D	204	GLN
1	D	266	HIS
1	D	320	HIS
1	D	358	ASN

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)

8 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	$\#\|Z\| > 2$
3	RWZ	D	402	-	25,26,26	1.87	3 (12%)	31,35,35	1.49	4 (12%)
2	FPS	C	401	-	20,23,23	1.33	2 (10%)	24,31,31	1.48	5 (20%)
2	FPS	B	401	-	20,23,23	1.29	2 (10%)	24,31,31	1.54	5 (20%)
3	RWZ	B	402	-	25,26,26	1.85	2 (8%)	31,35,35	1.51	4 (12%)
3	RWZ	C	402	-	25,26,26	1.85	3 (12%)	31,35,35	1.48	4 (12%)
3	RWZ	A	502	-	25,26,26	1.89	2 (8%)	31,35,35	1.47	5 (16%)
2	FPS	A	501	-	20,23,23	1.33	2 (10%)	24,31,31	1.56	6 (25%)
2	FPS	D	401	-	20,23,23	1.33	2 (10%)	24,31,31	1.56	6 (25%)

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
3	RWZ	D	402	-	-	8/15/43/43	0/4/3/3
2	FPS	C	401	-	-	7/19/25/25	-
2	FPS	B	401	-	-	7/19/25/25	-
3	RWZ	B	402	-	-	8/15/43/43	0/4/3/3
3	RWZ	C	402	-	-	6/15/43/43	0/4/3/3
3	RWZ	A	502	-	-	8/15/43/43	0/4/3/3
2	FPS	A	501	-	-	6/19/25/25	-
2	FPS	D	401	-	-	6/19/25/25	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	RWZ	CAX-NAQ	-8.05	1.33	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	RWZ	CAX-NAQ	-7.92	1.34	1.47
3	D	402	RWZ	CAX-NAQ	-7.83	1.34	1.47
3	C	402	RWZ	CAX-NAQ	-7.69	1.34	1.47
2	C	401	FPS	PA-O1A	3.39	1.54	1.46
2	D	401	FPS	PA-O1A	3.35	1.54	1.46
2	A	501	FPS	PA-O1A	3.34	1.53	1.46
2	B	401	FPS	PA-O1A	3.06	1.53	1.46
3	D	402	RWZ	CAE-CAS	2.61	1.39	1.33
3	A	502	RWZ	CAE-CAS	2.52	1.38	1.33
3	C	402	RWZ	CAE-CAS	2.50	1.38	1.33
3	B	402	RWZ	CAE-CAS	2.36	1.38	1.33
3	C	402	RWZ	CAD-CAR	2.22	1.39	1.32
2	A	501	FPS	PB-O2B	2.18	1.57	1.50
2	C	401	FPS	PB-O2B	2.13	1.57	1.50
3	D	402	RWZ	CAD-CAR	2.09	1.38	1.32
2	B	401	FPS	PB-O2B	2.09	1.57	1.50
2	D	401	FPS	PB-O2B	2.08	1.56	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	RWZ	CAC-CAS-CAJ	4.59	123.19	115.23
3	D	402	RWZ	CAI-NAQ-CAX	4.35	120.02	114.03
3	C	402	RWZ	CAI-NAQ-CAX	4.21	119.82	114.03
3	C	402	RWZ	CAC-CAS-CAJ	4.20	122.52	115.23
3	A	502	RWZ	CAG-NAP-CAH	4.18	121.32	112.85
3	D	402	RWZ	CAC-CAS-CAJ	4.15	122.43	115.23
3	A	502	RWZ	CAI-NAQ-CAX	4.07	119.63	114.03
3	D	402	RWZ	CAG-NAP-CAH	4.06	121.09	112.85
3	C	402	RWZ	CAG-NAP-CAH	4.01	120.99	112.85
3	B	402	RWZ	CAG-NAP-CAH	3.98	120.93	112.85
3	B	402	RWZ	CAI-NAQ-CAX	3.91	119.41	114.03
3	A	502	RWZ	CAC-CAS-CAJ	3.76	121.75	115.23
2	D	401	FPS	C9-C8-C10	3.10	120.61	115.23
2	B	401	FPS	C4-C3-C5	2.96	120.37	115.23
2	A	501	FPS	C4-C3-C5	2.95	120.35	115.23
2	C	401	FPS	C9-C8-C10	2.94	120.34	115.23
2	A	501	FPS	C9-C8-C10	2.91	120.27	115.23
2	D	401	FPS	C10-C8-C7	-2.86	114.75	121.17
2	B	401	FPS	C9-C8-C10	2.82	120.13	115.23
2	C	401	FPS	C4-C3-C5	2.75	120.00	115.23
2	A	501	FPS	C10-C8-C7	-2.75	115.00	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	FPS	C4-C3-C5	2.73	119.97	115.23
2	B	401	FPS	C10-C8-C7	-2.72	115.07	121.17
2	C	401	FPS	C10-C8-C7	-2.56	115.43	121.17
2	D	401	FPS	O1B-PB-O3A	2.40	112.69	104.64
3	A	502	RWZ	CAH-CAI-NAQ	-2.38	107.18	111.06
2	C	401	FPS	O1B-PB-O3A	2.36	112.55	104.64
2	B	401	FPS	C5-C3-C2	-2.33	115.94	121.17
2	A	501	FPS	O1B-PB-O3A	2.31	112.39	104.64
2	B	401	FPS	O1B-PB-O3A	2.23	112.11	104.64
2	D	401	FPS	C15-C13-C14	2.20	119.64	114.59
2	A	501	FPS	C15-C13-C14	2.18	119.61	114.59
2	A	501	FPS	C5-C3-C2	-2.16	116.33	121.17
2	D	401	FPS	C5-C3-C2	-2.15	116.33	121.17
3	A	502	RWZ	CAB-CAR-CAA	2.11	119.44	114.59
3	C	402	RWZ	CAH-CAI-NAQ	-2.09	107.65	111.06
3	D	402	RWZ	CAH-CAI-NAQ	-2.08	107.66	111.06
2	C	401	FPS	C15-C13-C14	2.06	119.32	114.59
3	B	402	RWZ	CAH-CAI-NAQ	-2.03	107.75	111.06

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FPS	C2-C3-C5-C6
2	A	501	FPS	C4-C3-C5-C6
2	B	401	FPS	PA-O3A-PB-O3B
3	A	502	RWZ	CAF-CAJ-CAS-CAC
3	A	502	RWZ	CAF-CAJ-CAS-CAE
3	B	402	RWZ	CAF-CAJ-CAS-CAC
3	B	402	RWZ	CAF-CAJ-CAS-CAE
3	D	402	RWZ	CAF-CAJ-CAS-CAC
3	D	402	RWZ	CAF-CAJ-CAS-CAE
2	A	501	FPS	C8-C10-C11-C12
2	D	401	FPS	C8-C10-C11-C12
3	A	502	RWZ	CAD-CAF-CAJ-CAS
3	B	402	RWZ	CAD-CAF-CAJ-CAS
3	C	402	RWZ	CAD-CAF-CAJ-CAS
3	D	402	RWZ	CAD-CAF-CAJ-CAS
3	A	502	RWZ	NAP-CAH-CAI-NAQ
3	D	402	RWZ	NAP-CAH-CAI-NAQ
2	D	401	FPS	C4-C3-C5-C6
3	C	402	RWZ	CAF-CAJ-CAS-CAC

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Mol	Chain	Res	Type	Atoms
3	C	402	RWZ	CAF-CAJ-CAS-CAE
2	B	401	FPS	C8-C10-C11-C12
2	C	401	FPS	C8-C10-C11-C12
3	B	402	RWZ	NAP-CAH-CAI-NAQ
2	B	401	FPS	C4-C3-C5-C6
2	C	401	FPS	C4-C3-C5-C6
2	B	401	FPS	C2-C3-C5-C6
2	D	401	FPS	C2-C3-C5-C6
3	C	402	RWZ	CAE-CAG-NAP-CAH
3	D	402	RWZ	CAI-CAH-NAP-CAG
2	C	401	FPS	C2-C3-C5-C6
3	C	402	RWZ	CAI-CAH-NAP-CAG
2	A	501	FPS	C11-C10-C8-C9
3	B	402	RWZ	CAI-CAH-NAP-CAG
3	A	502	RWZ	CAI-CAH-NAP-CAG
2	D	401	FPS	C11-C10-C8-C9
2	A	501	FPS	C11-C10-C8-C7
2	C	401	FPS	C11-C10-C8-C9
2	D	401	FPS	C11-C10-C8-C7
3	A	502	RWZ	CAV-CAX-NAQ-CAI
3	A	502	RWZ	CAW-CAX-NAQ-CAI
3	B	402	RWZ	CAV-CAX-NAQ-CAI
3	B	402	RWZ	CAW-CAX-NAQ-CAI
3	D	402	RWZ	CAV-CAX-NAQ-CAI
3	D	402	RWZ	CAW-CAX-NAQ-CAI
2	B	401	FPS	C11-C10-C8-C9
2	C	401	FPS	C11-C10-C8-C7
3	B	402	RWZ	CAE-CAG-NAP-CAH
2	B	401	FPS	C11-C10-C8-C7
2	D	401	FPS	PB-O3A-PA-O2A
3	C	402	RWZ	NAP-CAH-CAI-NAQ
2	B	401	FPS	PA-O3A-PB-O1B
3	A	502	RWZ	CAE-CAG-NAP-CAH
3	D	402	RWZ	CAE-CAG-NAP-CAH
2	C	401	FPS	PB-O3A-PA-O1A
2	A	501	FPS	PB-O3A-PA-O2A
2	C	401	FPS	PB-O3A-PA-O2A

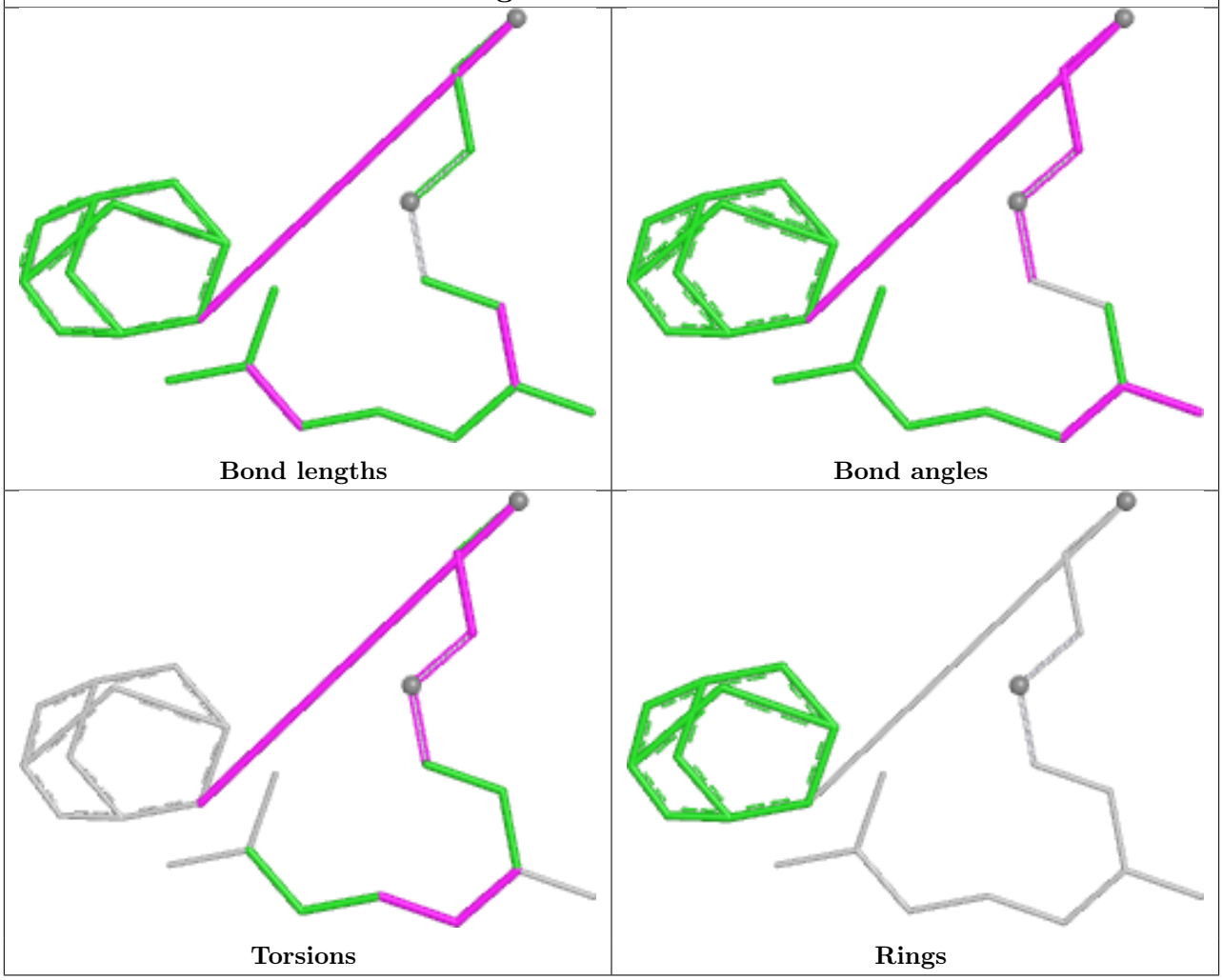
There are no ring outliers.

8 monomers are involved in 21 short contacts:

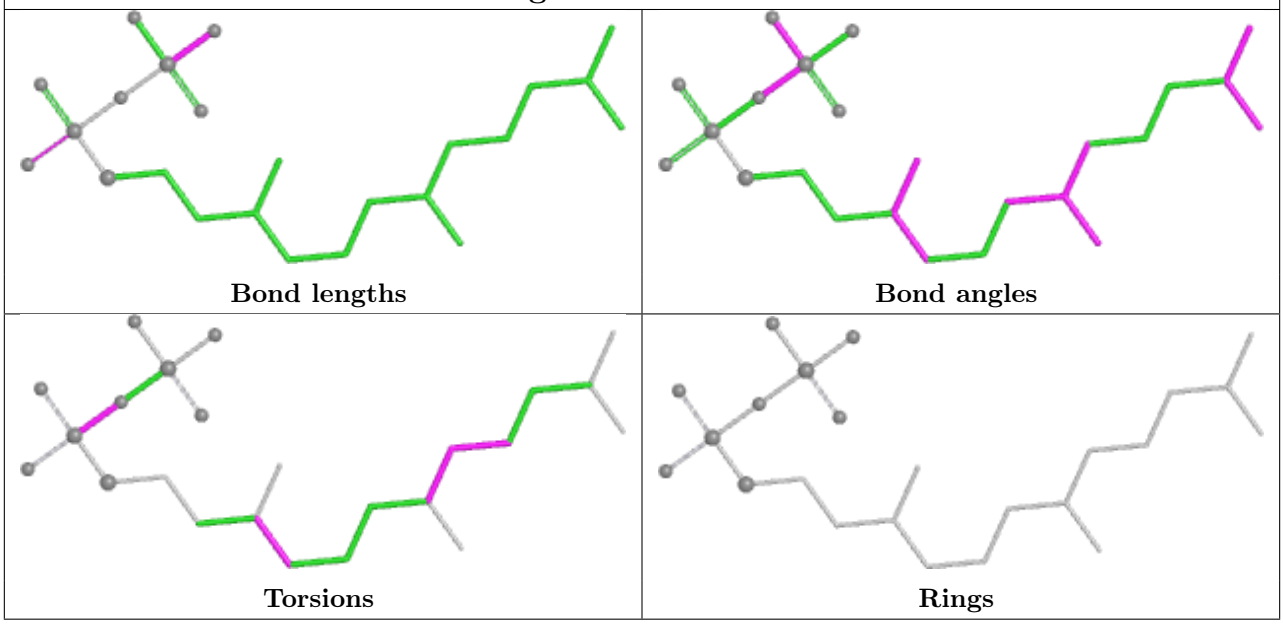
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	RWZ	4	0
2	C	401	FPS	3	0
2	B	401	FPS	4	0
3	B	402	RWZ	4	0
3	C	402	RWZ	2	0
3	A	502	RWZ	3	0
2	A	501	FPS	1	0
2	D	401	FPS	4	0

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.

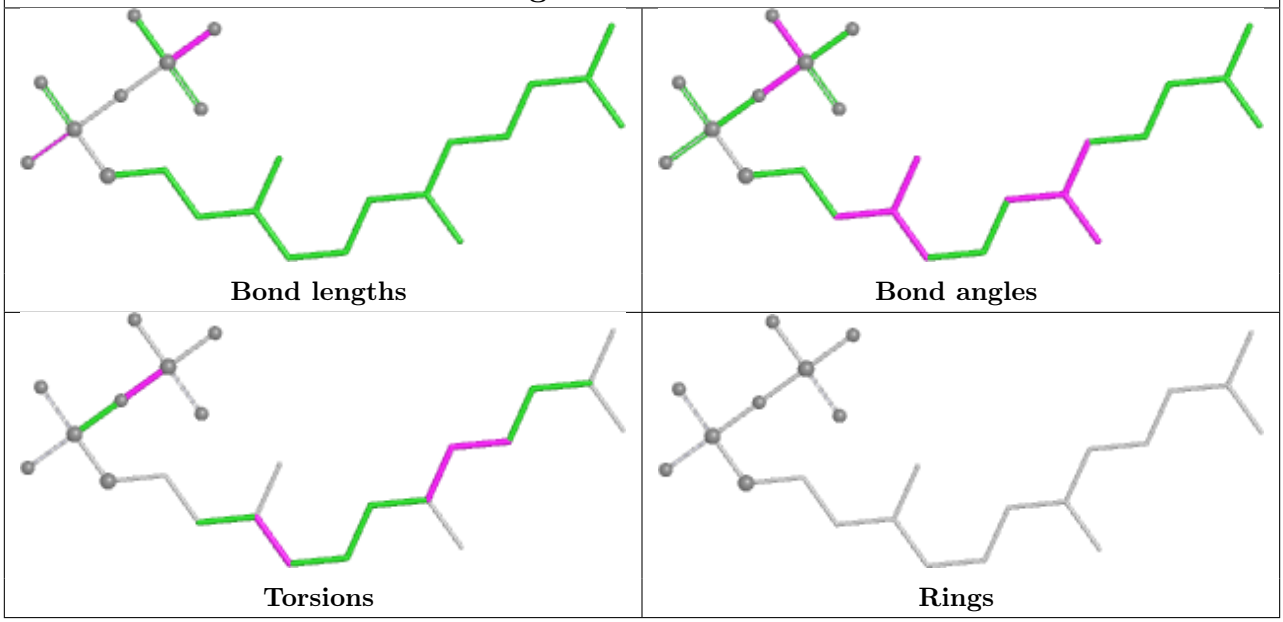
Ligand RWZ D 402



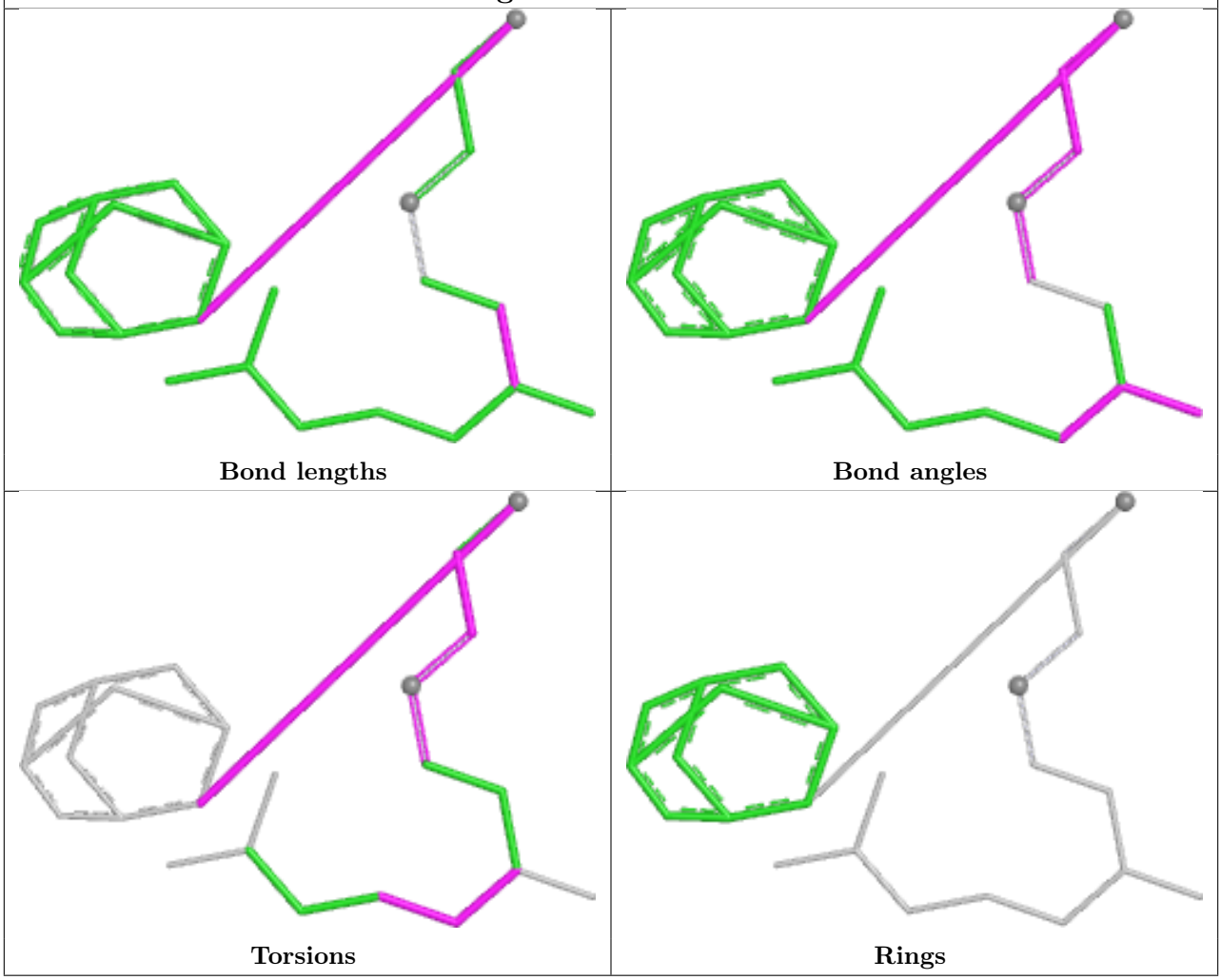
Ligand FPS C 401



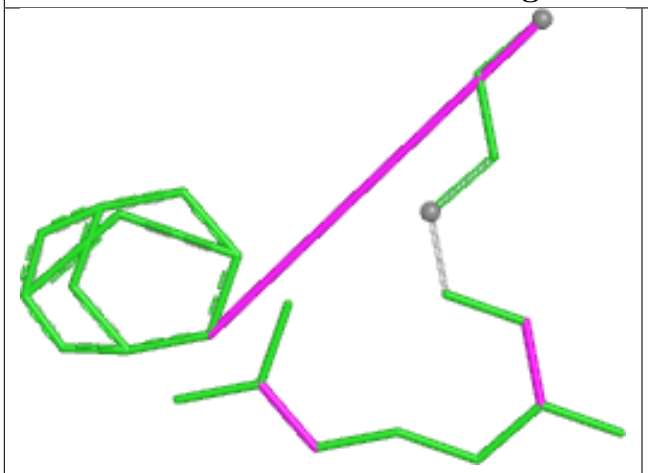
Ligand FPS B 401



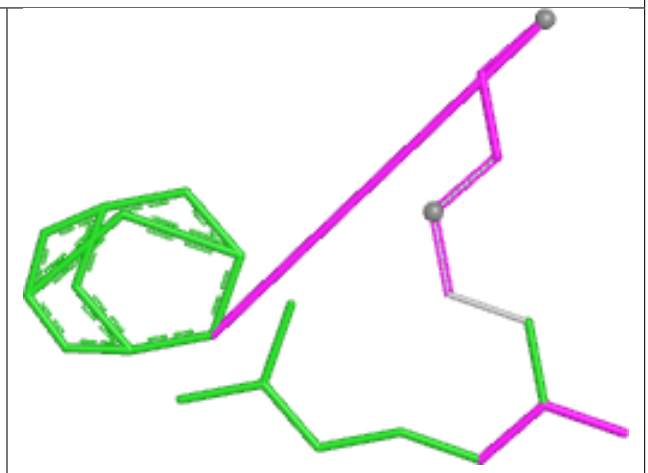
Ligand RWZ B 402



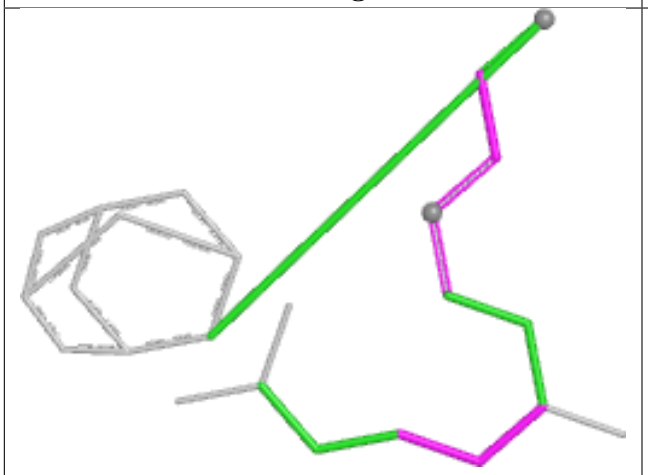
Ligand RWZ C 402



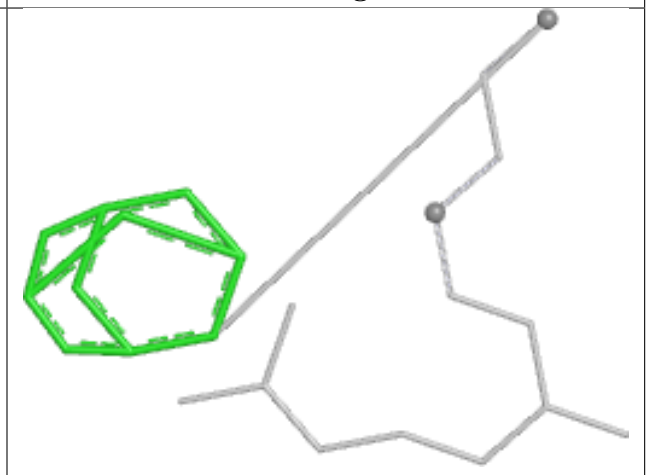
Bond lengths



Bond angles

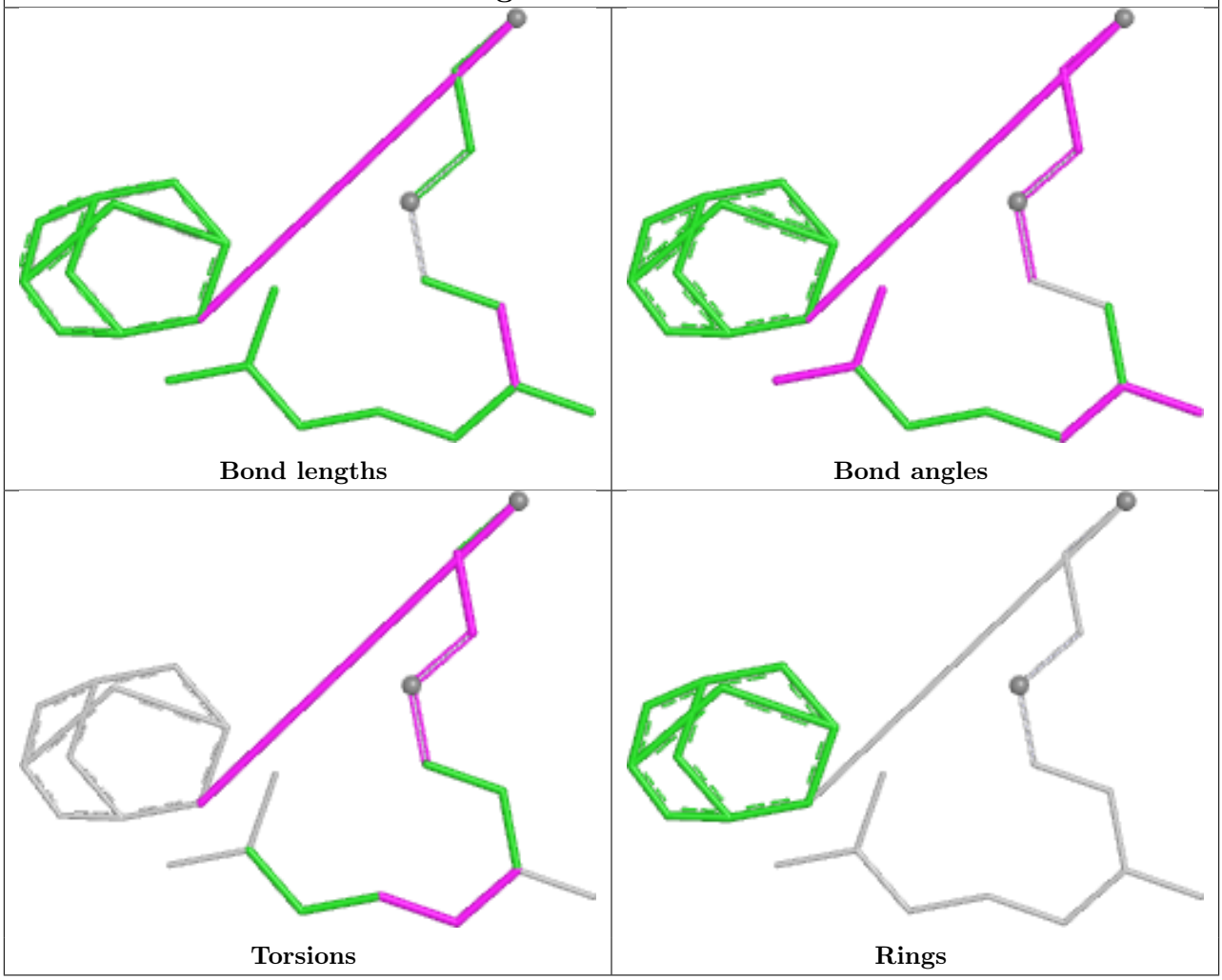


Torsions

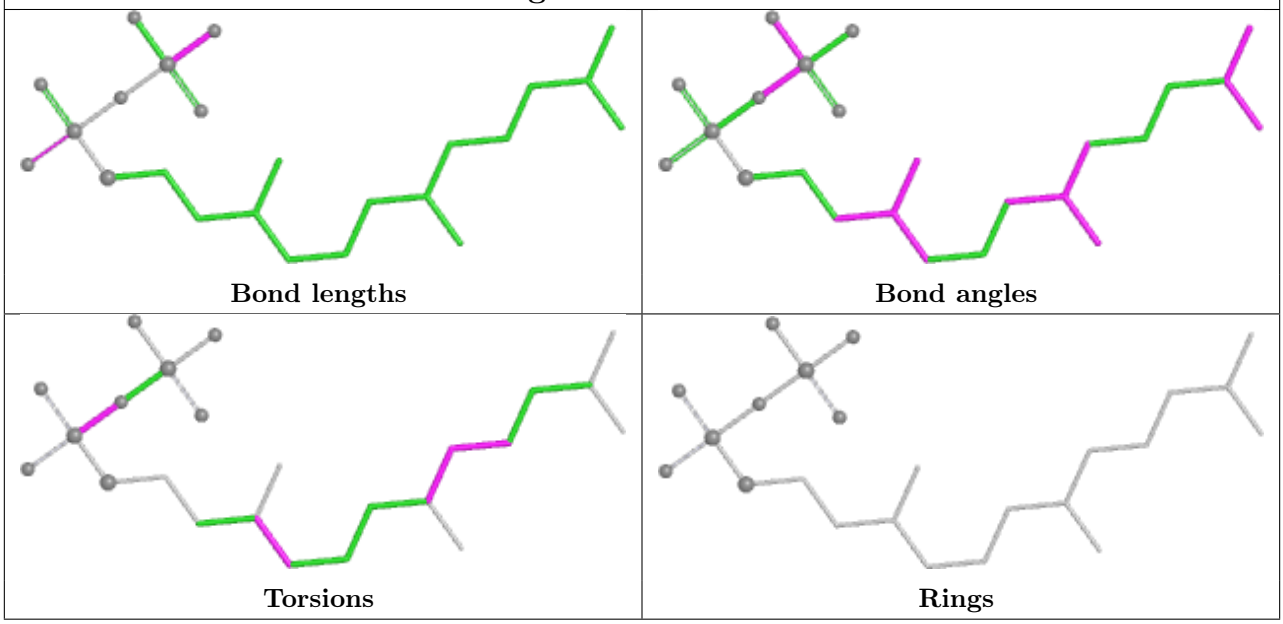


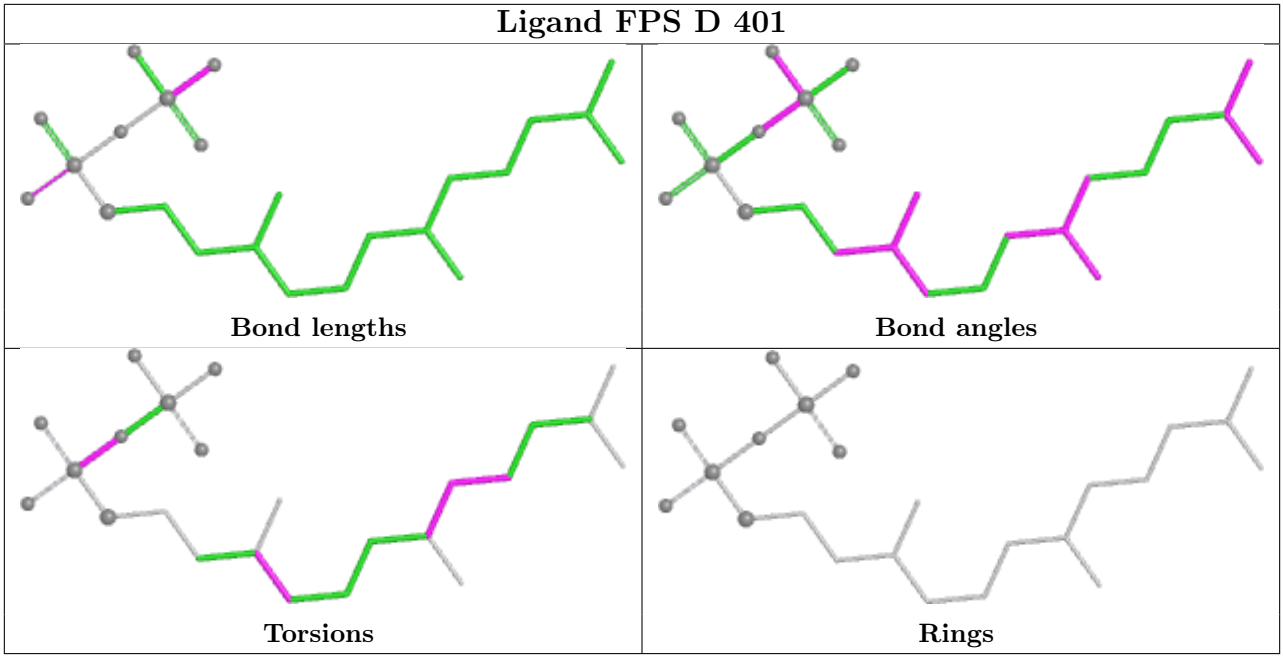
Rings

Ligand RWZ A 502



Ligand FPS A 501





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	341/365 (93%)	-0.09	4 (1%)	79	77	24, 44, 63, 80	0
1	B	341/365 (93%)	0.02	9 (2%)	56	54	20, 44, 75, 86	0
1	C	341/365 (93%)	0.18	14 (4%)	37	36	26, 51, 88, 97	0
1	D	341/365 (93%)	0.37	20 (5%)	22	21	27, 59, 90, 105	0
All	All	1364/1460 (93%)	0.12	47 (3%)	45	44	20, 49, 85, 105	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	346	GLN	4.5
1	D	346	GLN	4.0
1	B	43	ARG	3.9
1	C	345	ALA	3.7
1	B	213	TYR	3.7
1	B	346	GLN	3.6
1	C	43	ARG	3.6
1	D	78	SER	3.5
1	D	151	THR	3.4
1	A	219	VAL	3.1
1	C	86	ARG	3.1
1	D	244	LEU	3.0
1	A	99	THR	2.9
1	D	345	ALA	2.9
1	C	32	ARG	2.9
1	D	43	ARG	2.9
1	D	82	GLU	2.8
1	C	105	VAL	2.8
1	C	67	LEU	2.8
1	D	80	PRO	2.7
1	D	344	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	219	VAL	2.7
1	C	69	ALA	2.6
1	C	106	GLY	2.6
1	A	67	LEU	2.6
1	C	78	SER	2.6
1	B	220	PRO	2.5
1	D	77	MET	2.5
1	D	219	VAL	2.5
1	C	109	ARG	2.4
1	C	66	VAL	2.4
1	D	221	PRO	2.3
1	D	69	ALA	2.3
1	D	107	VAL	2.3
1	D	98	THR	2.2
1	C	39	GLN	2.2
1	C	129	LYS	2.2
1	D	99	THR	2.2
1	D	347	ASP	2.2
1	C	111	ARG	2.2
1	B	305	HIS	2.1
1	D	67	LEU	2.1
1	D	148	ASP	2.1
1	B	217	CYS	2.0
1	B	345	ALA	2.0
1	D	96	HIS	2.0
1	B	221	PRO	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)

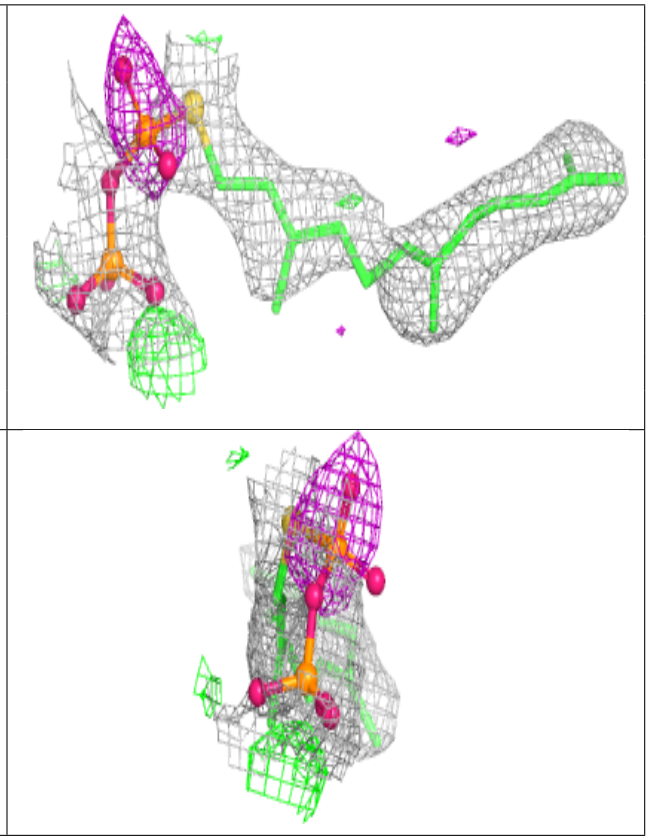
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FPS	B	401	24/24	0.55	0.40	45,90,119,119	0
2	FPS	D	401	24/24	0.58	0.42	64,102,126,126	0
2	FPS	C	401	24/24	0.61	0.39	79,107,123,124	0
2	FPS	A	501	24/24	0.64	0.37	48,81,111,112	0
3	RWZ	C	402	24/24	0.75	0.38	80,93,98,99	0
3	RWZ	B	402	24/24	0.86	0.27	57,72,74,74	0
3	RWZ	D	402	24/24	0.87	0.30	65,78,80,81	0
3	RWZ	A	502	24/24	0.88	0.29	56,58,61,63	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.

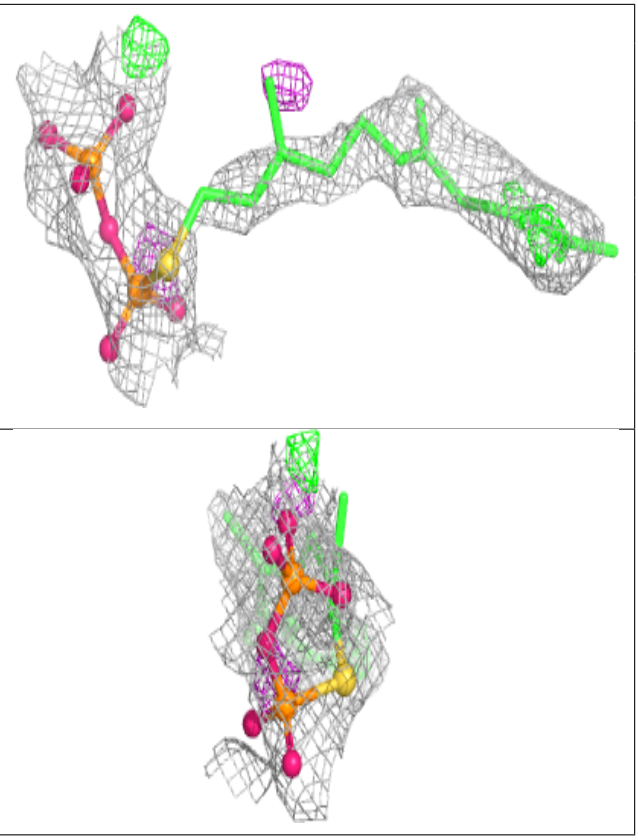
Electron density around FPS B 401:

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



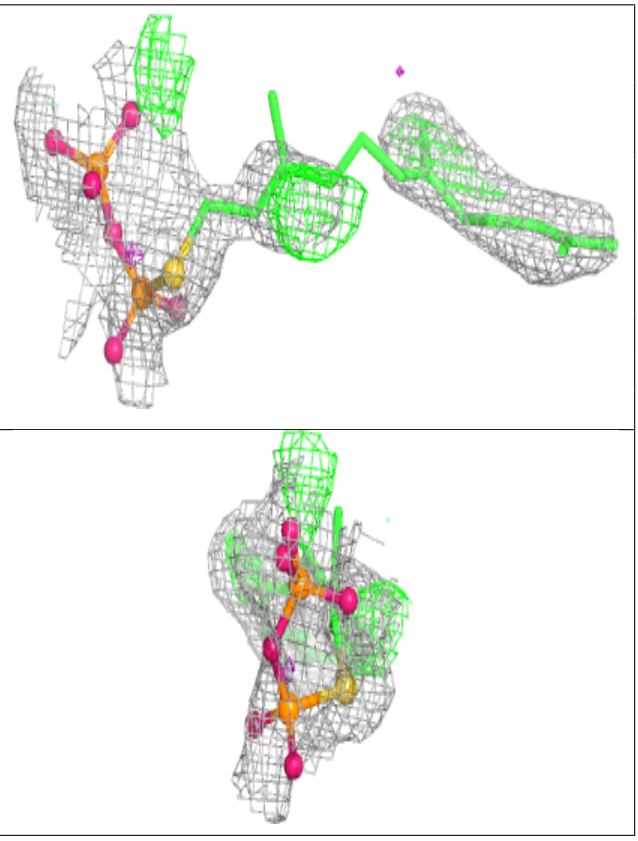
Electron density around FPS D 401:

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



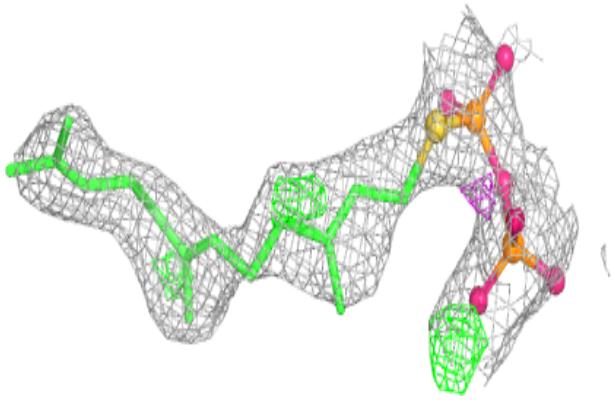
Electron density around FPS C 401:

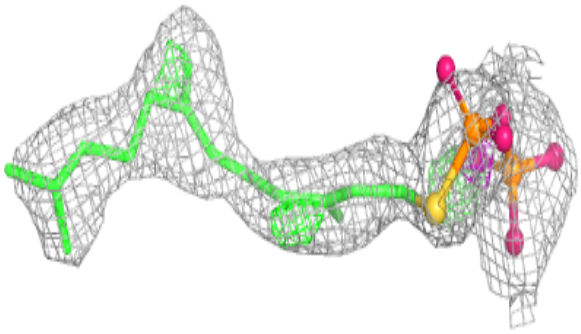
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

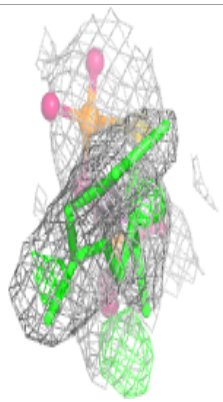


Electron density around FPS A 501:

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

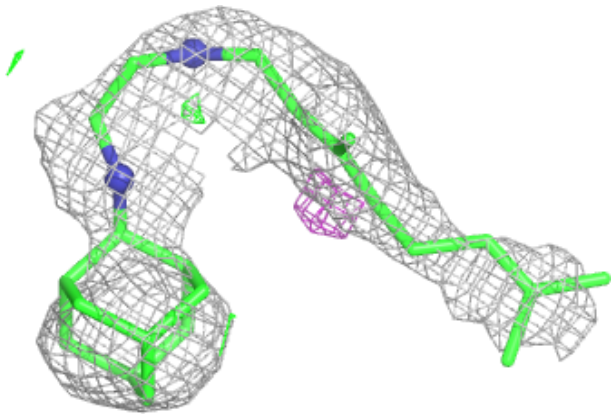


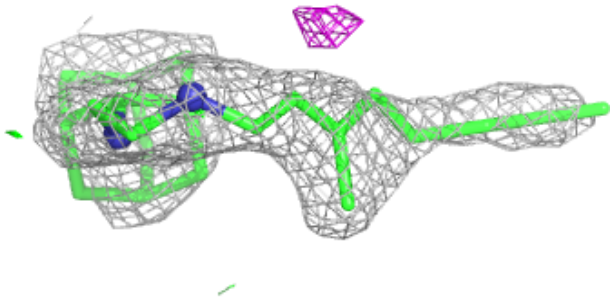


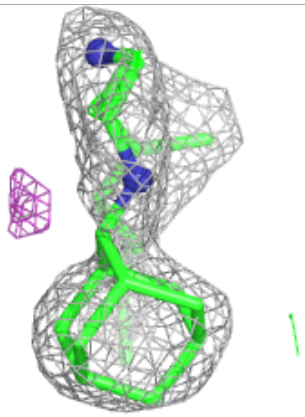


Electron density around RWZ C 402:

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

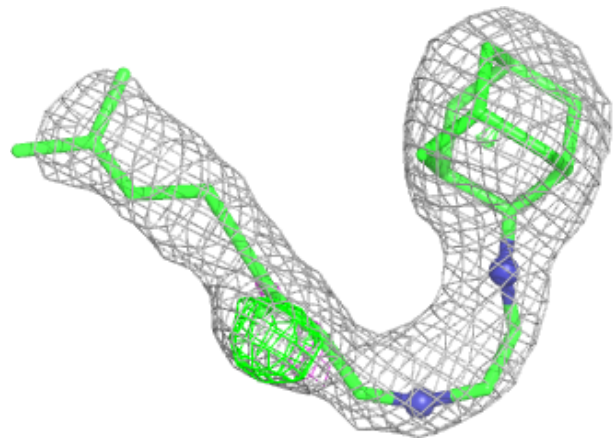


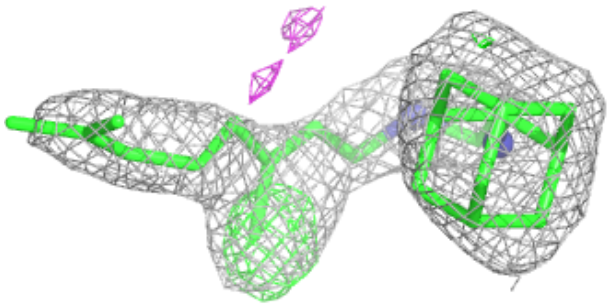


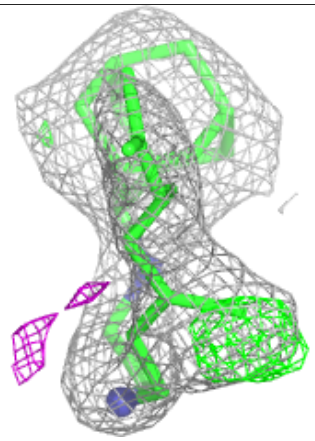


Electron density around RWZ B 402:

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







Electron density around RWZ D 402:

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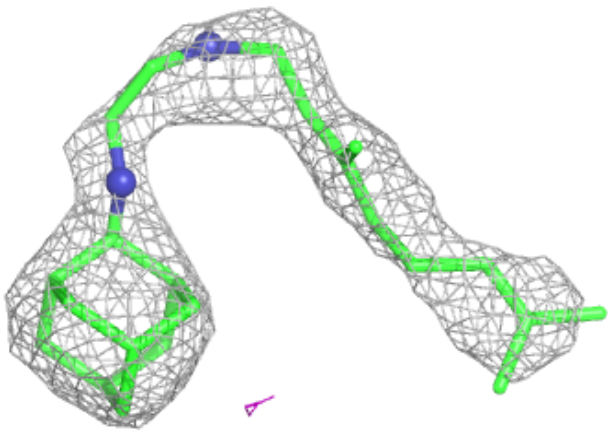
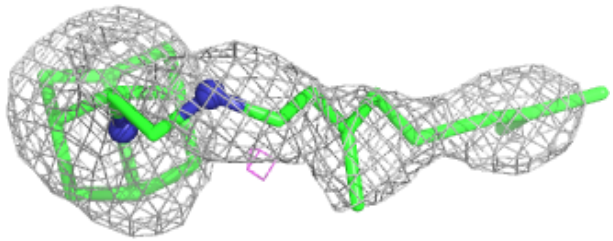
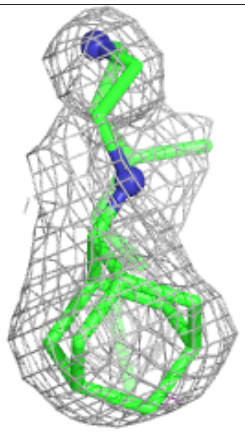
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

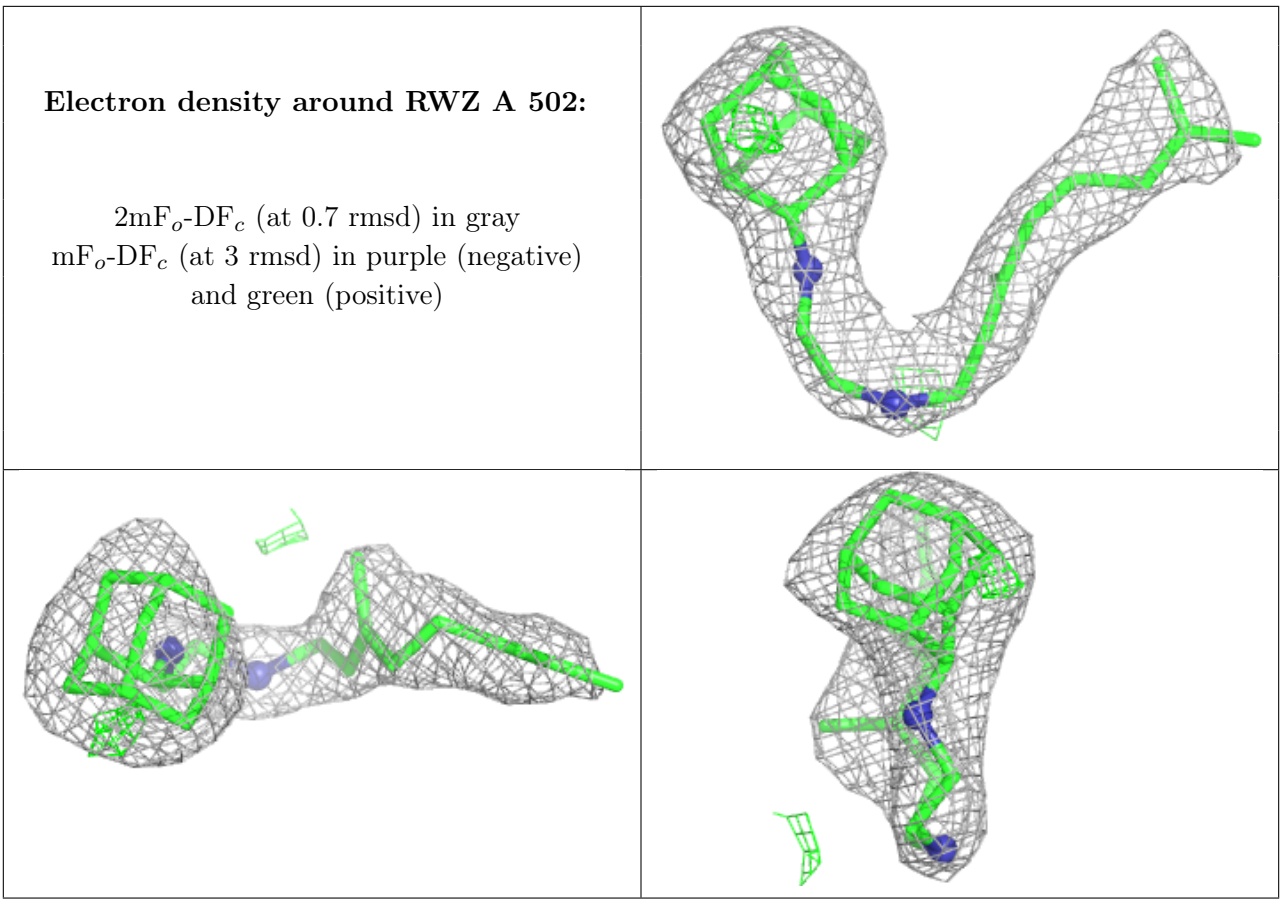






Electron density around RWZ A 502:

$2mF_o$-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.