



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:43 PM UTC

PDB ID : 3WSB / pdb_00003wsb
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

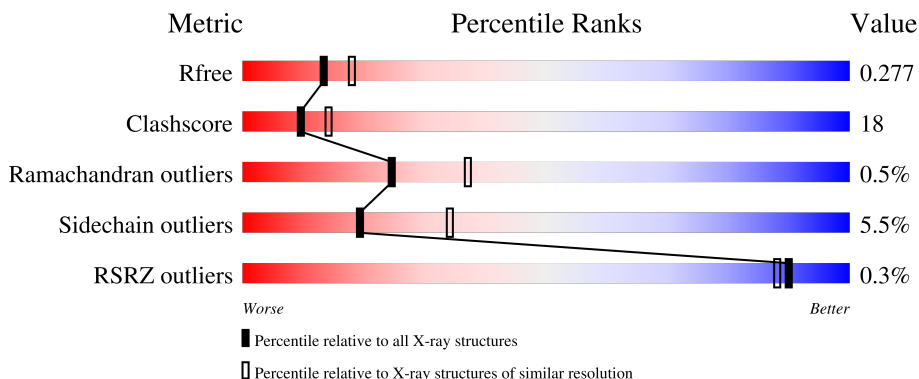
1 Overall quality at a glance

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	 62% 27% • 7%
1	B	365	 62% 28% • 7%
1	C	365	 61% 28% • 7%
1	D	365	 54% 36% • 7%

2 Entry composition

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
1	A	341	Total	C	N	O	S	0	0	0
			2751	1745	473	511	22			
1	B	341	Total	C	N	O	S	0	0	0
			2751	1745	473	511	22			
1	C	341	Total	C	N	O	S	0	0	0
			2751	1745	473	511	22			
1	D	341	Total	C	N	O	S	0	0	0
			2752	1745	473	512	22			

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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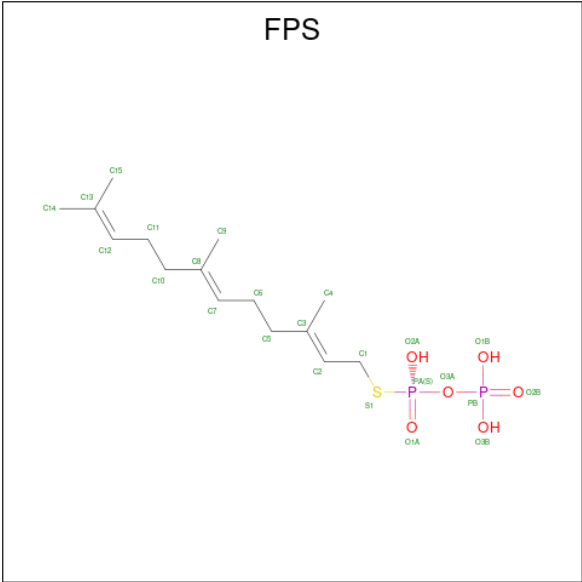
Chain	Residue	Modelled	Actual	Comment	Reference
A	82	GLU	ASP	engineered mutation	UNP Q4CWB4
B	4	MET	-	expression tag	UNP Q4CWB4
B	5	GLY	-	expression tag	UNP Q4CWB4
B	6	SER	-	expression tag	UNP Q4CWB4
B	7	SER	-	expression tag	UNP Q4CWB4
B	8	HIS	-	expression tag	UNP Q4CWB4
B	9	HIS	-	expression tag	UNP 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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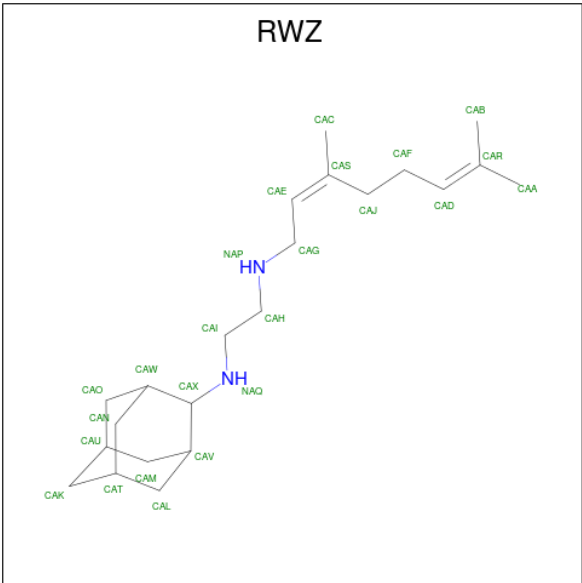
Chain	Residue	Modelled	Actual	Comment	Reference
C	23	HIS	-	expression tag	UNP Q4CWB4
C	24	MET	-	expression tag	UNP Q4CWB4
C	82	GLU	ASP	engineered mutation	UNP Q4CWB4
D	4	MET	-	expression tag	UNP Q4CWB4
D	5	GLY	-	expression tag	UNP Q4CWB4
D	6	SER	-	expression tag	UNP Q4CWB4
D	7	SER	-	expression tag	UNP 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] TRIHYDRO-GEN THIODIPHOSPHATE (CCD ID: FPS) (formula: C₁₅H₂₈O₆P₂S).



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

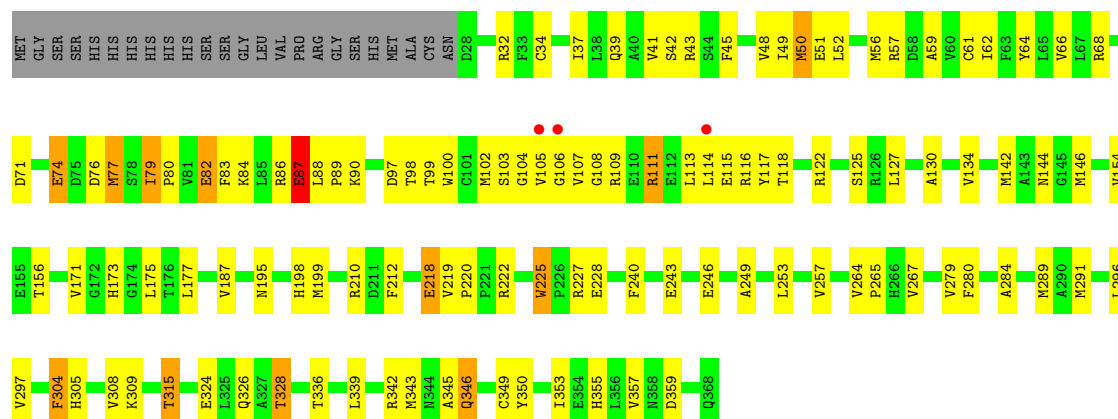
- Molecule 3 is N-[(2Z)-3,7-dimethylocta-2,6-dien-1-yl]-N'-[(1R,3S,5R,7R)-tricyclo[3.3.1.1 3,7]dec-2-yl]ethane-1,2-diamine (CCD ID: RWZ) (formula: C₂₂H₃₈N₂).



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

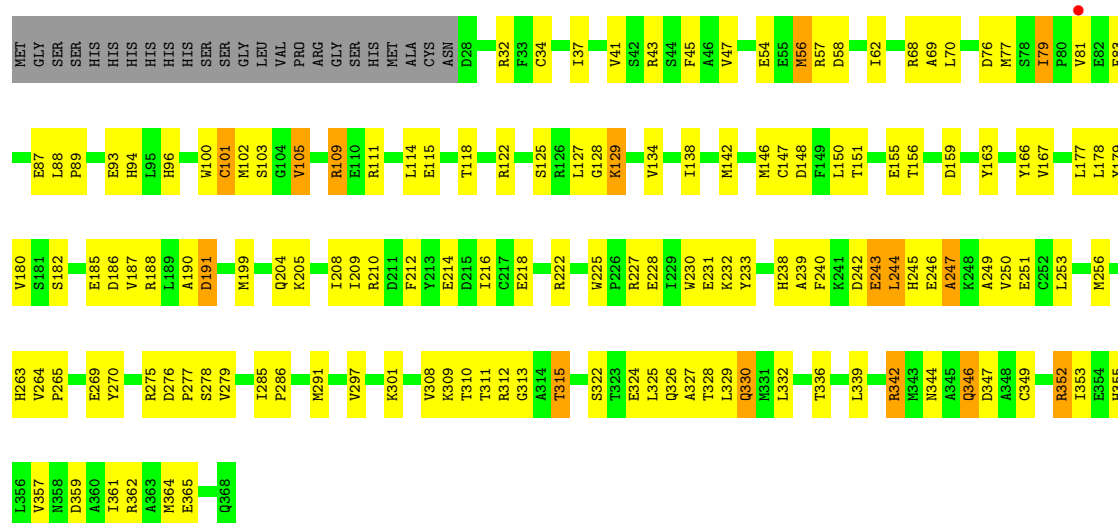
- Molecule 4 is water.

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



• Molecule 1: Farnesyltransferase, putative

Chain D: 54% 36% 7%



4 Data and refinement statistics

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 24.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (24.90-2.40) 91.6 (24.90-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.277 0.215 , 0.277	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)	0.33 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: FPS, RWZ

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	0.49	1/2809 (0.0%)	0.94	12/3806 (0.3%)
1	B	0.46	0/2809	0.93	9/3806 (0.2%)
1	C	0.42	0/2809	0.90	7/3806 (0.2%)
1	D	0.41	0/2810	0.89	7/3806 (0.2%)
All	All	0.44	1/11237 (0.0%)	0.92	35/15224 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	VAL	CA-CB	5.10	1.56	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	GLU	N-CA-C	-9.49	101.47	113.23
1	D	244	LEU	N-CA-C	-8.01	102.60	112.38
1	A	103	SER	N-CA-C	7.85	123.03	113.38
1	A	150	LEU	N-CA-C	-7.75	103.96	113.41
1	B	41	VAL	N-CA-C	7.44	119.47	111.58
1	D	263	HIS	N-CA-C	6.46	119.32	111.82
1	B	325	LEU	N-CA-C	6.45	118.89	111.02
1	C	171	VAL	N-CA-C	-6.41	104.08	110.62
1	C	103	SER	N-CA-C	6.28	120.77	111.04
1	B	53	ASP	N-CA-C	6.21	124.03	110.80
1	D	79	ILE	CA-C-N	6.14	126.09	119.76
1	D	79	ILE	C-N-CA	6.14	126.09	119.76
1	D	159	ASP	N-CA-C	-6.10	104.55	111.07
1	B	103	SER	N-CA-C	6.02	122.49	114.12
1	A	98	THR	N-CA-C	-5.92	102.69	110.33
1	B	127	LEU	N-CA-C	5.87	117.48	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	LEU	N-CA-C	-5.86	106.29	113.50
1	A	276	ASP	CA-C-N	5.80	125.49	119.05
1	A	276	ASP	C-N-CA	5.80	125.49	119.05
1	B	284	ALA	N-CA-C	5.67	118.66	111.69
1	C	304	PHE	N-CA-C	5.60	119.20	112.93
1	D	313	GLY	N-CA-C	-5.57	106.04	112.50
1	C	87	GLU	N-CA-C	5.54	117.39	111.36
1	C	225	TRP	CA-C-N	5.38	125.14	119.76
1	C	225	TRP	C-N-CA	5.38	125.14	119.76
1	B	110	GLU	N-CA-C	-5.32	105.65	111.82
1	A	235	ASP	N-CA-C	-5.29	106.99	113.50
1	A	225	TRP	N-CA-C	-5.25	101.92	109.48
1	A	353	ILE	N-CA-C	5.23	115.44	110.42
1	A	320	HIS	N-CA-C	5.23	116.98	111.28
1	C	284	ALA	N-CA-C	5.20	117.02	111.36
1	A	321	TYR	N-CA-C	5.12	119.58	113.23
1	A	325	LEU	N-CA-C	5.07	119.68	111.37
1	B	310	THR	N-CA-C	-5.04	103.06	110.52
1	D	47	VAL	N-CA-C	-5.03	106.89	111.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	87	0
1	B	2751	0	2698	87	0
1	C	2751	0	2698	99	0
1	D	2752	0	2698	119	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
3	B	24	0	38	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	396	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 18.

All (396) 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:C:343:MET:HE2	1:C:350:TYR:HA	1.28	1.16
1:C:343:MET:HE1	1:C:353:ILE:HB	1.39	1.05
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:A:73:VAL:HG22	1:A:102:MET:HE1	1.58	0.86
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:A:102:MET:HE2	1:A:114:LEU:HD13	1.58	0.83
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:B:186:ASP:OD2	1:B:188:ARG:HB2	1.82	0.78
1:C:343:MET:CE	1:C:350:TYR:HA	2.11	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:A:102:MET:HE3	1:A:105:VAL:HB	1.67	0.76
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:A:344:ASN:C	1:A:344:ASN:HD22	1.95	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:MET:HE2	1:B:350:TYR:HA	1.71	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
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:D:186:ASP:CG	1:D:188:ARG:HG2	2.17	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:D:77:MET:HE2	1:D:77:MET:HA	1.75	0.68
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:D:155:GLU:CD	1:D:227:ARG:HE	2.02	0.67
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:56:MET:HE1	1:C:279:VAL:HG22	1.76	0.66
1:C:218:GLU:HG2	1:C:222:ARG:NH1	2.10	0.66
1:D:129:LYS:HD3	1:D:129:LYS:C	2.20	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:B:187:VAL:HG23	1:B:188:ARG:HE	1.60	0.65
1:B:56:MET:HE1	1:B:179:TYR:HA	1.80	0.64
1:A:102:MET:HE3	1:A:105:VAL:CB	2.29	0.63
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:A:225:TRP:CG	1:A:256:MET:HE2	2.33	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:B:344:ASN:ND2	1:B:346:GLN:HG3	2.13	0.63
1:B:41:VAL:CG1	1:B:68:ARG:NH1	2.61	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:343:MET:HE2	1:A:350:TYR:HA	1.81	0.61
1:B:242:ASP:C	1:B:244:LEU:H	2.07	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:B:336:THR:HG21	1:B:364:MET:HE1	1.82	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:73:VAL:CG2	1:A:102:MET:HE1	2.32	0.59
1:A:362:ARG:HG3	1:A:362:ARG:HH11	1.67	0.59
1:C:339:LEU:C	1:C:339:LEU:HD23	2.28	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:D:239:ALA:HB1	1:D:245:HIS:HD1	1.67	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: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:C:82:GLU:CD	1:C:82:GLU:H	2.09	0.58
1:A:343:MET:CE	1:A:350:TYR:HA	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ILE:HD13	1:C:113:LEU:HD13	1.86	0.58
1:C:122:ARG:O	1:C:125:SER:OG	2.19	0.57
1:D:156:THR:HA	1:D:228:GLU:HB2	1.85	0.57
1:D:264:VAL:HG21	1:D:291:MET:HE1	1.85	0.57
1:A:264:VAL:CG2	1:A:291:MET:HE1	2.34	0.57
1:A:56:MET:HE1	1:A:179:TYR:HA	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: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
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:344:ASN:C	1:A:344:ASN:ND2	2.60	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:C:289:MET:HE1	1:C:315:THR:HG22	1.87	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: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:102:MET:HE3	1:B:105:VAL:HG21	1.89	0.54
1:B:173:HIS:O	1:B:177:LEU:HD22	2.08	0.54
1:B:264:VAL:HG21	1:B:291:MET:HE1	1.88	0.54
1:D:342:ARG:HG3	1:D:342:ARG:HH11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:339:LEU:HD23	1:D:339:LEU:C	2.33	0.53
1:A:343:MET:HE1	1:A:353:ILE:HB	1.88	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:B:242:ASP:C	1:B:244:LEU:N	2.65	0.53
1:C:280:PHE:CE1	1:C:328:THR:HG21	2.45	0.53
1:D:352:ARG:HD3	1:D:352:ARG:C	2.33	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:D:225:TRP:CG	1:D:256:MET:HE2	2.44	0.52
1:D:94:HIS:C	1:D:96:HIS:H	2.17	0.52
1:B:73:VAL:HG22	1:B:102:MET:HE1	1.90	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
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:D:336:THR:HG21	1:D:364:MET:HE1	1.90	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: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:D:264:VAL:CG2	1:D:291:MET:HE1	2.42	0.50
1:A:44:SER:HB2	2:A:501:FPS:O2B	2.12	0.50
1:A:210:ARG:C	1:A:210:ARG:HD2	2.37	0.50
1:A:98:THR:C	1:A:99:THR:HG23	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:246:GLU:O	1:D:247:ALA:C	2.55	0.49
1:A:264:VAL:HG22	1:A:291:MET:HE1	1.94	0.49
1:A:264:VAL:HB	1:A:265:PRO:HD3	1.94	0.49
1:B:82:GLU:CD	1:B:82:GLU:H	2.21	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:243:GLU:C	1:D:245:HIS:N	2.69	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:C:116:ARG:C	1:C:118:THR:N	2.70	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
1:D:240:PHE:CD1	1:D:249:ALA:HA	2.48	0.48
1:D:56:MET:HE1	1:D:178:LEU:C	2.38	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:A:264:VAL:HG21	1:A:291:MET:HE1	1.95	0.47
1:C:264:VAL:HG21	1:C:291:MET:HE1	1.96	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:156:THR:OG1	1:A:159:ASP:CG	2.57	0.47
1:C:77:MET:HE3	1:C:77:MET:HA	1.96	0.47
1:C:253:LEU:HD21	1:C:297:VAL:O	2.14	0.47
1:A:246:GLU:CD	1:A:301:LYS:HD2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:102:MET:CE	1:A:114:LEU:HD13	2.37	0.47
1:C:74:GLU:OE2	1:C:146:MET:HE2	2.15	0.47
1:A:340:ALA:O	1:A:343:MET:HG2	2.14	0.47
1:A:97:ASP:C	1:A:98:THR:O	2.54	0.46
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: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:A:339:LEU:C	1:A:339:LEU:HD23	2.40	0.46
1:C:116:ARG:C	1:C:118:THR:H	2.23	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: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: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
1:B:334:THR:O	1:B:338:ARG:HG3	2.17	0.45
1:D:56:MET:HE2	1:D:182:SER:HB3	1.99	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:D:94:HIS:C	1:D:96:HIS:N	2.75	0.45
1:D:147:CYS:O	1:D:148:ASP:C	2.60	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:127:LEU:O	1:D:128:GLY:C	2.57	0.45
1:D:344:ASN:HB2	1:D:346:GLN:CG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:ASN:HD21	1:B:346:GLN:HE21	1.64	0.45
1:C:49:ILE:HD11	1:C:61:CYS:HB2	1.99	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: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:B:164:CYS:HB3	1:B:201:LEU:HG	1.98	0.44
1:C:289:MET:HE1	1:C:315:THR:CG2	2.47	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:C:83:PHE:C	1:C:83:PHE:CD2	2.92	0.44
1:C:105:VAL:C	1:C:111:ARG:NH1	2.76	0.44
1:B:64:TYR:C	1:B:64:TYR:CD2	2.96	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:B:74:GLU:OE2	1:B:146:MET:HE2	2.18	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:B:280:PHE:CZ	1:B:328:THR:HG21	2.53	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:50:MET:HE3	1:C:57:ARG:CZ	2.50	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:C:343:MET:CE	1:C:353:ILE:HB	2.29	0.42
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: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:71:ASP:HA	1:C:146:MET:HE1	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:CYS:O	1:C:350:TYR:C	2.63	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:102:MET:HE3	1:A:105:VAL:CG2	2.50	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:D:56:MET:HE3	1:D:179:TYR:HA	2.01	0.41
1:A:56:MET:HE3	1:A:182:SER:HB3	2.02	0.41
1:A:203:LEU:O	1:A:207:ASN:HB2	2.21	0.41
1:C:104:GLY:C	1:C:105:VAL:HG23	2.46	0.41
1:C:50:MET:HE3	1:C:57:ARG:NE	2.36	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:102:MET:HE3	1:B:105:VAL:CG2	2.51	0.40
1:B:205:LYS:HD3	4:B:513:HOH:O	2.21	0.40
1:C:84:LYS:C	1:C:86:ARG:N	2.79	0.40
1:C:105:VAL:N	1:C:111:ARG:CZ	2.84	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:A:228:GLU:O	1:A:232:LYS:NZ	2.40	0.40
1:A:349:CYS:O	1:A:350:TYR:C	2.64	0.40
1:B:323:THR:O	1:B:323:THR:HG22	2.21	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%)	14	22
1	D	339/365 (93%)	307 (91%)	28 (8%)	4 (1%)	10	16
All	All	1356/1460 (93%)	1263 (93%)	86 (6%)	7 (0%)	24	37

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
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%)	22	38
1	B	298/318 (94%)	283 (95%)	15 (5%)	22	38
1	C	298/318 (94%)	280 (94%)	18 (6%)	17	31
1	D	298/318 (94%)	280 (94%)	18 (6%)	17	31
All	All	1192/1272 (94%)	1126 (94%)	66 (6%)	19	34

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	39	GLN
1	A	75	ASP
1	A	82	GLU
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	54	GLU
1	B	74	GLU
1	B	85	LEU
1	B	102	MET
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	268	VAL
1	B	315	THR
1	B	328	THR
1	B	344	ASN
1	B	354	GLU
1	C	39	GLN

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Mol	Chain	Res	Type
1	C	50	MET
1	C	74	GLU
1	C	77	MET
1	C	79	ILE
1	C	82	GLU
1	C	87	GLU
1	C	99	THR
1	C	109	ARG
1	C	111	ARG
1	C	218	GLU
1	C	219	VAL
1	C	296	LEU
1	C	309	LYS
1	C	315	THR
1	C	328	THR
1	C	346	GLN
1	C	359	ASP
1	D	32	ARG
1	D	56	MET
1	D	93	GLU
1	D	105	VAL
1	D	109	ARG
1	D	118	THR
1	D	129	LYS
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
1	D	359	ASP
1	D	362	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	94	HIS
1	A	119	HIS

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Mol	Chain	Res	Type
1	A	144	ASN
1	A	245	HIS
1	A	266	HIS
1	A	320	HIS
1	A	326	GLN
1	A	344	ASN
1	A	346	GLN
1	A	358	ASN
1	A	368	GLN
1	B	119	HIS
1	B	144	ASN
1	B	245	HIS
1	B	287	GLN
1	B	305	HIS
1	B	330	GLN
1	B	344	ASN
1	B	368	GLN
1	C	39	GLN
1	C	144	ASN
1	C	204	GLN
1	C	207	ASN
1	C	355	HIS
1	C	368	GLN
1	D	94	HIS
1	D	144	ASN
1	D	204	GLN
1	D	266	HIS
1	D	299	ASN
1	D	320	HIS
1	D	346	GLN
1	D	358	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	C	402	-	25,26,26	1.85	3 (12%)	31,35,35	1.48	4 (12%)
3	RWZ	B	402	-	25,26,26	1.85	2 (8%)	31,35,35	1.51	4 (12%)
2	FPS	D	401	-	20,23,23	1.33	2 (10%)	24,31,31	1.56	6 (25%)
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	B	401	-	20,23,23	1.29	2 (10%)	24,31,31	1.54	5 (20%)
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%)

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

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
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(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FPS	C10-C8-C7	-2.75	115.00	121.17
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

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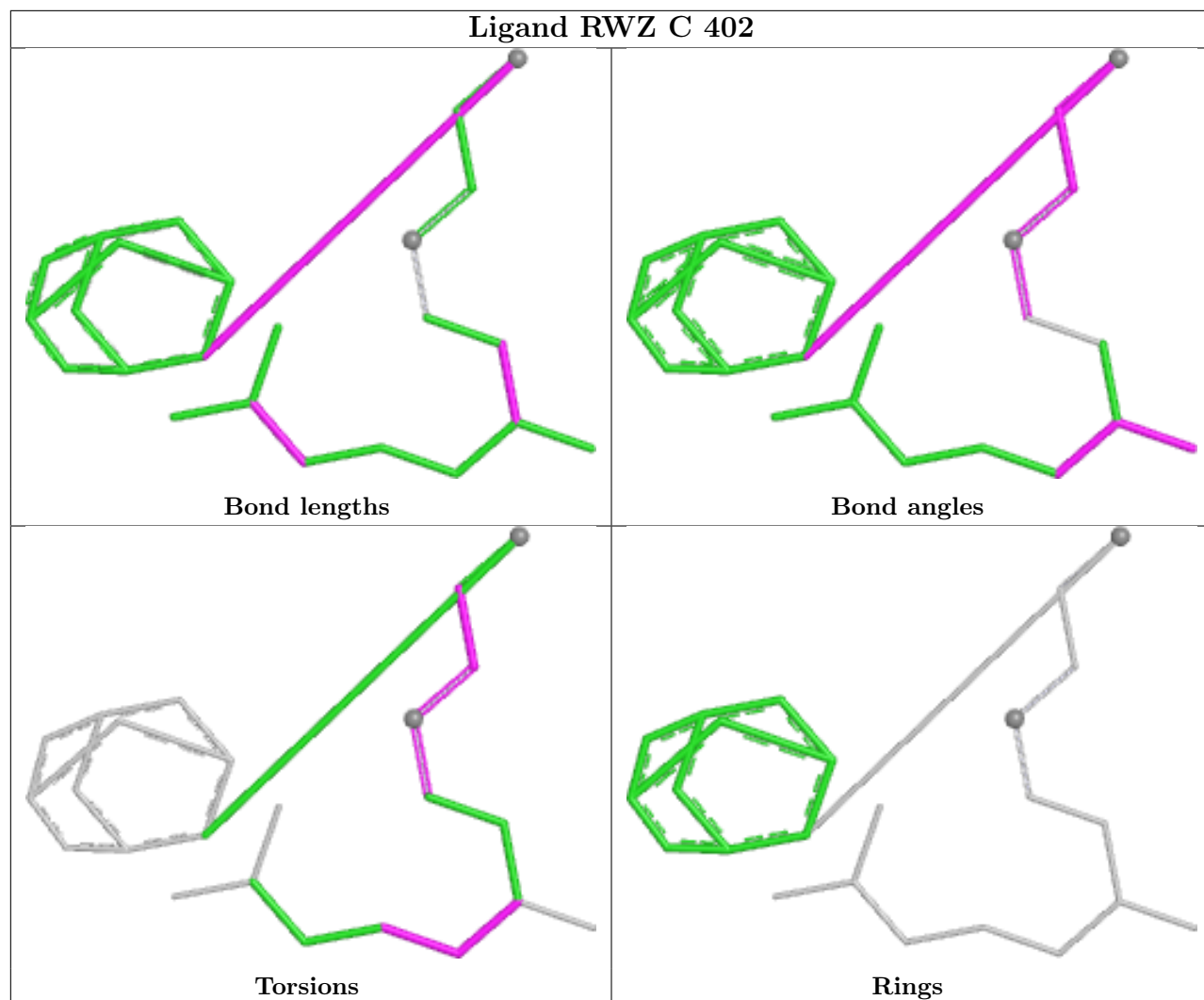
Mol	Chain	Res	Type	Atoms
3	C	402	RWZ	CAF-CAJ-CAS-CAC
3	C	402	RWZ	CAF-CAJ-CAS-CAE
2	B	401	FPS	C8-C10-C11-C12
2	C	401	FPS	C8-C10-C11-C12
3	B	402	RWZ	NAP-CAH-CAI-NAQ
2	B	401	FPS	C4-C3-C5-C6
2	C	401	FPS	C4-C3-C5-C6
2	B	401	FPS	C2-C3-C5-C6
2	D	401	FPS	C2-C3-C5-C6
3	C	402	RWZ	CAE-CAG-NAP-CAH
3	D	402	RWZ	CAI-CAH-NAP-CAG
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

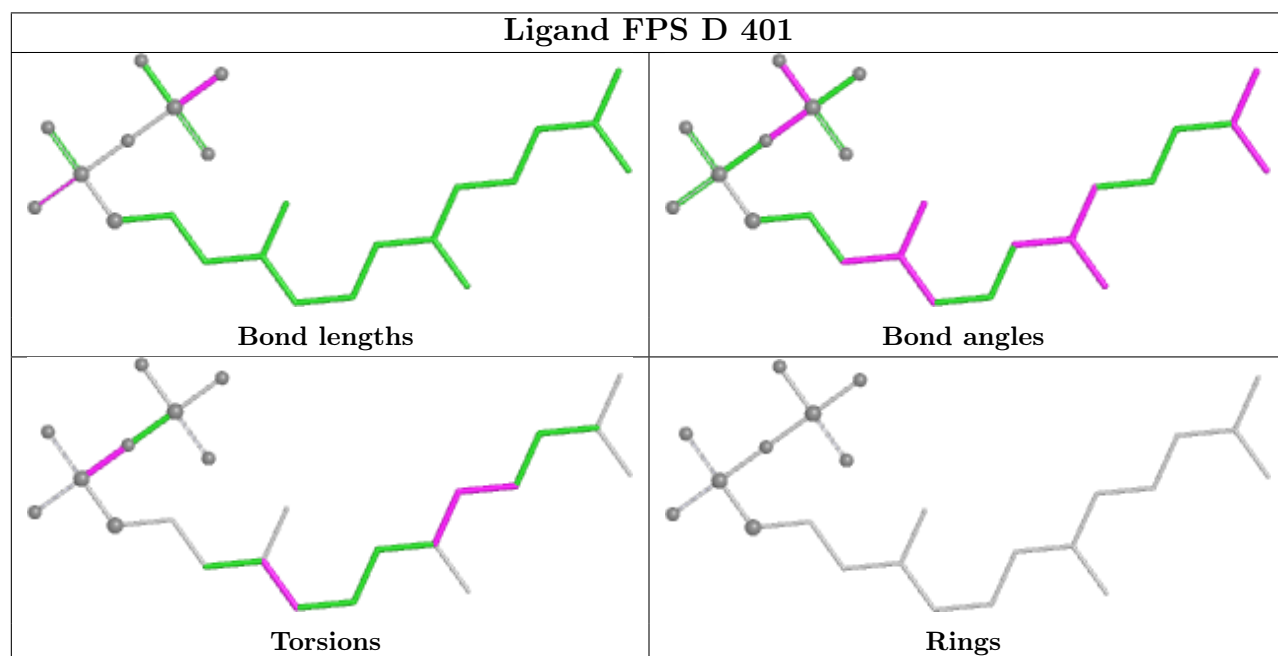
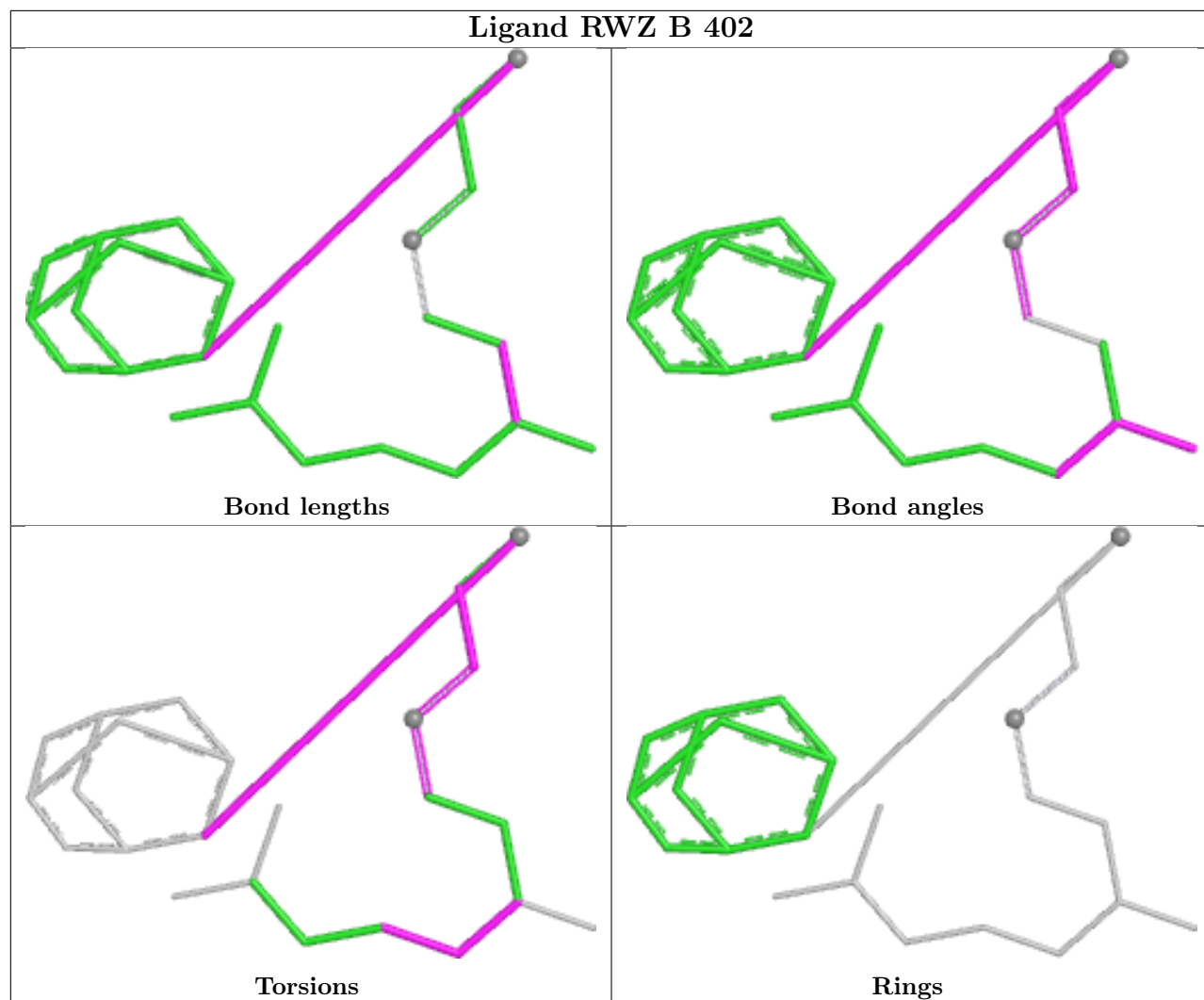
There are no ring outliers.

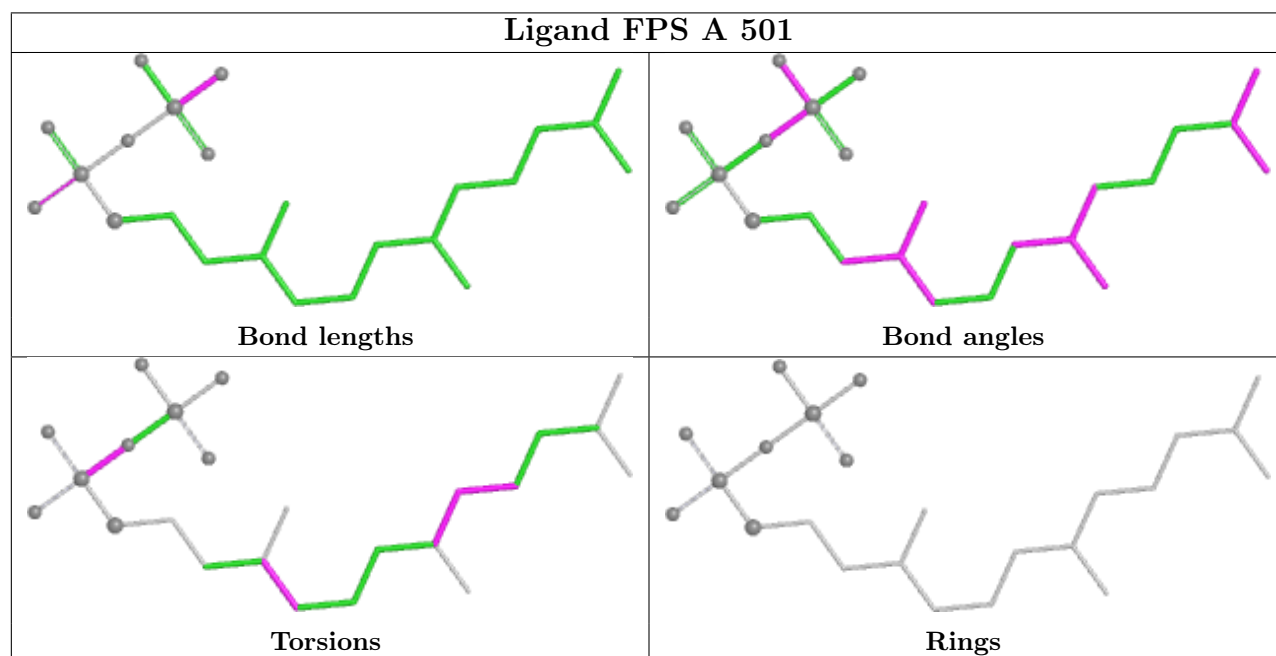
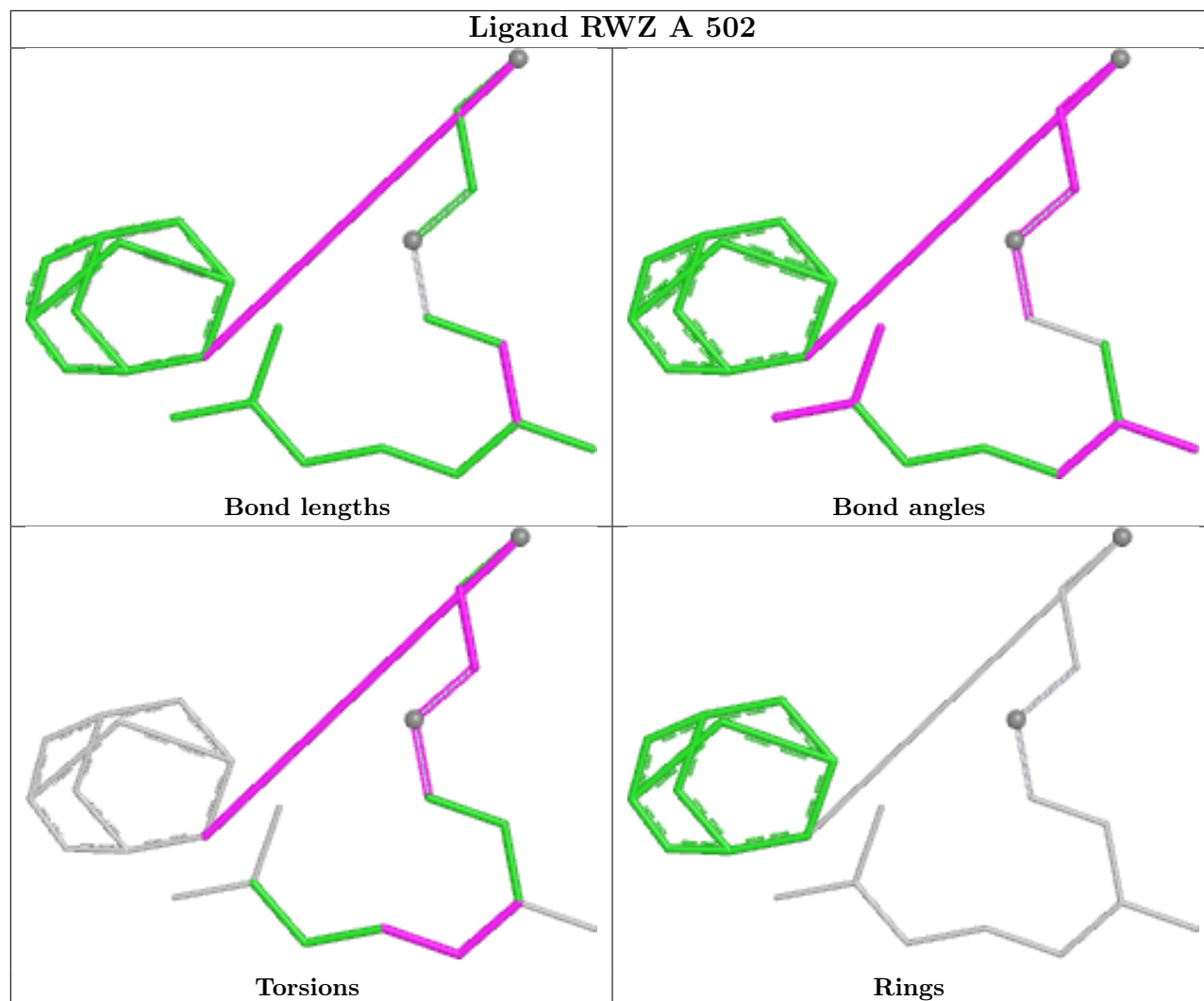
8 monomers are involved in 21 short contacts:

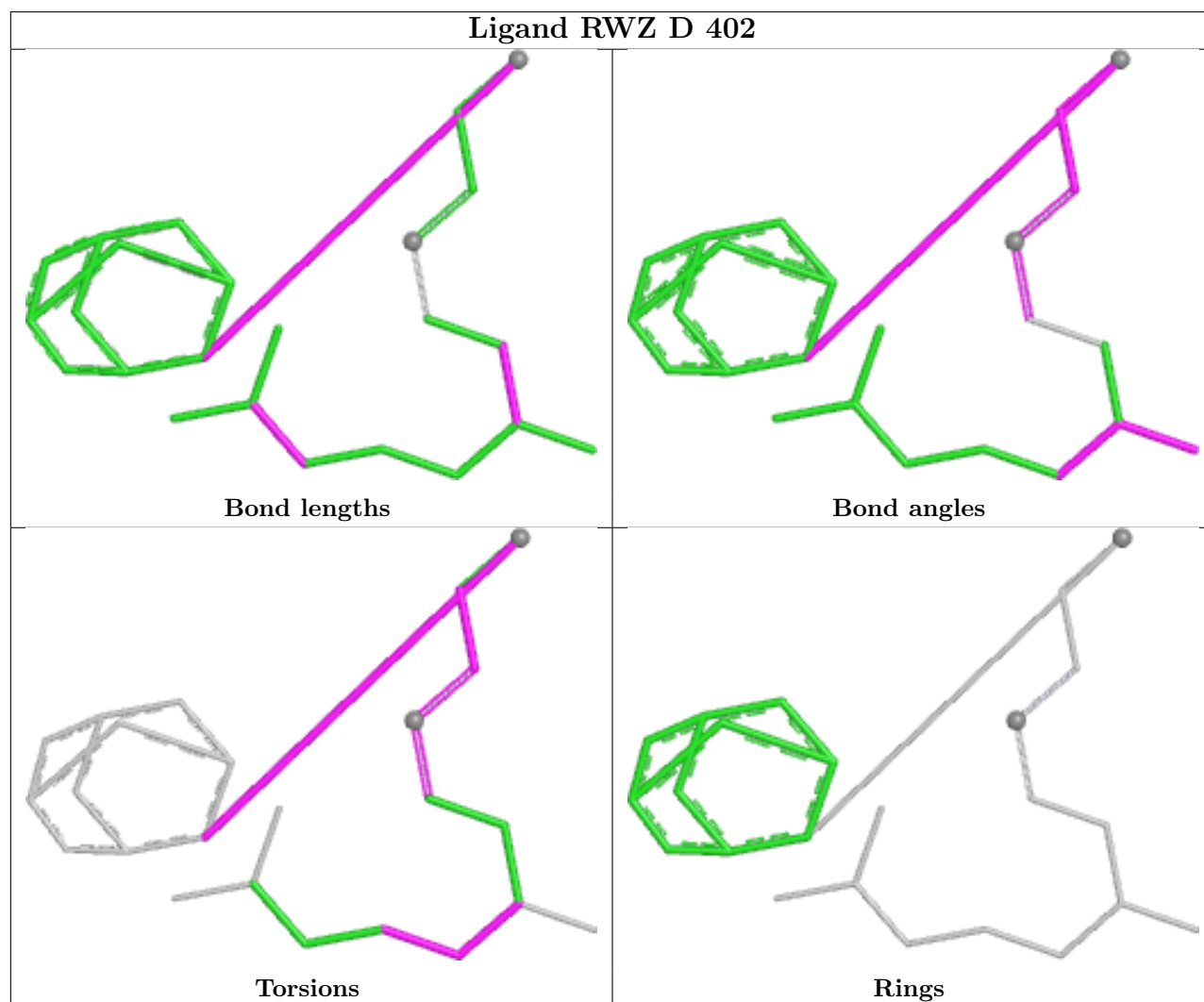
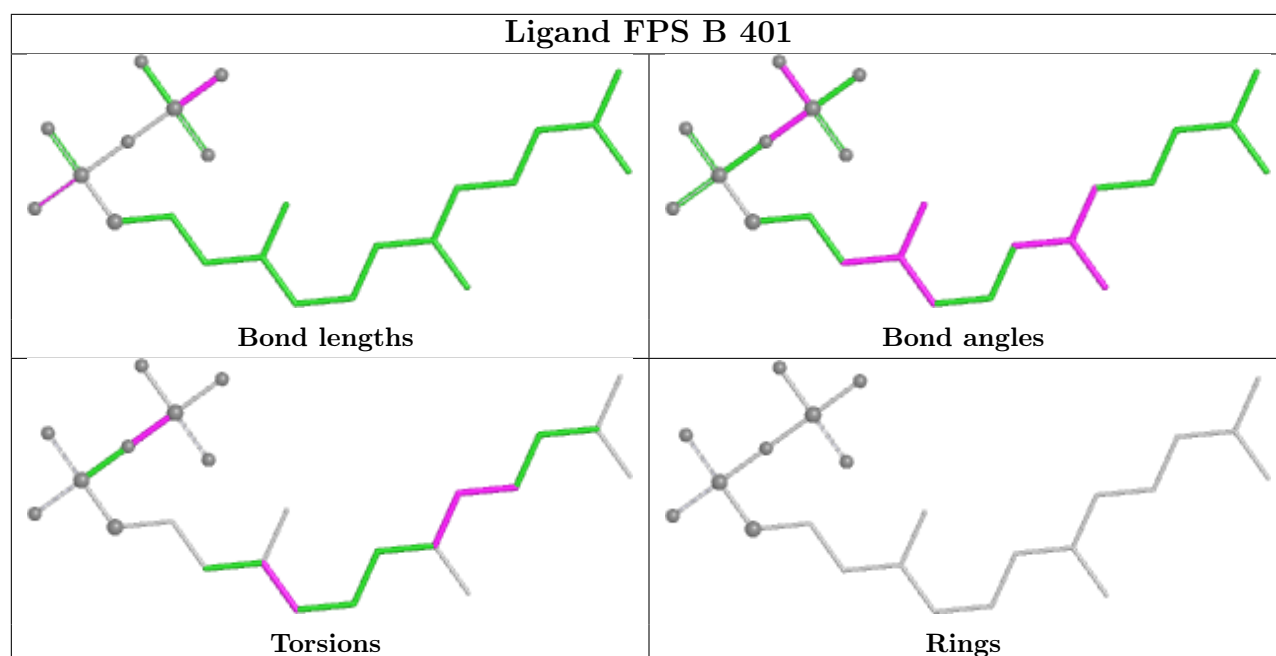
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	RWZ	2	0
3	B	402	RWZ	4	0
2	D	401	FPS	4	0
3	A	502	RWZ	3	0
2	A	501	FPS	1	0
2	B	401	FPS	4	0
3	D	402	RWZ	4	0
2	C	401	FPS	3	0

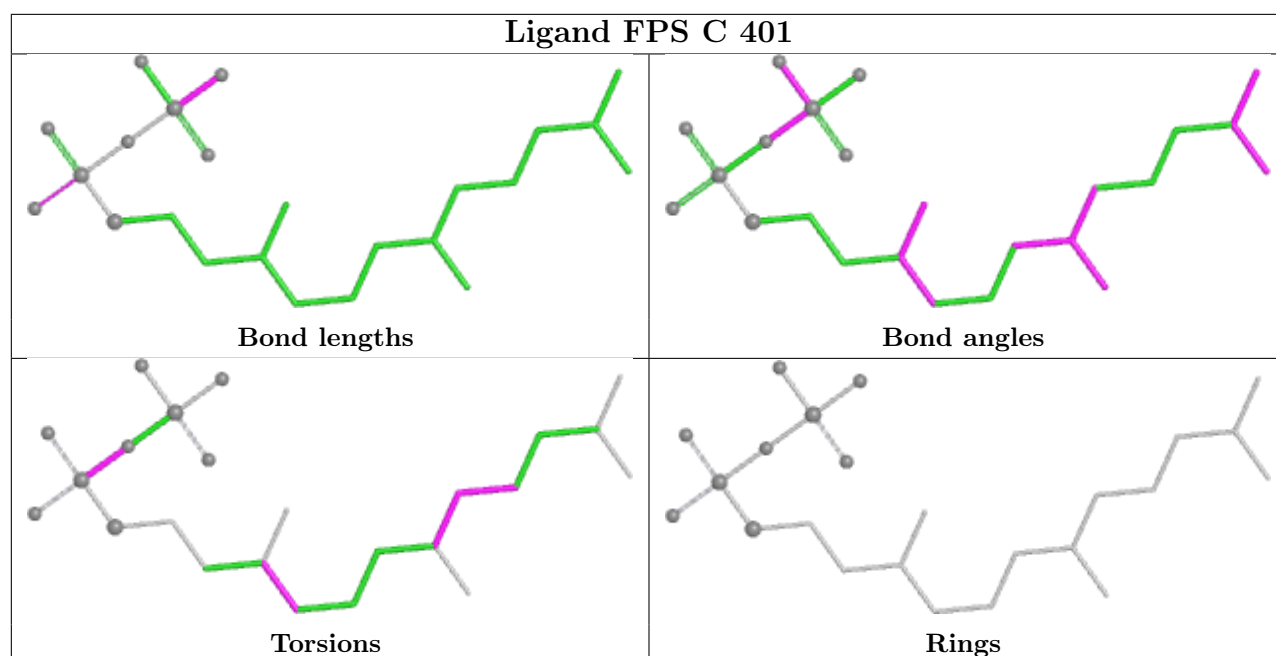
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.











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%)	-0.26	0	100 100	24, 44, 63, 80	0
1	B	341/365 (93%)	-0.21	0	100 100	20, 44, 75, 86	0
1	C	341/365 (93%)	-0.05	3 (0%)	81 78	26, 51, 88, 97	0
1	D	341/365 (93%)	0.13	1 (0%)	90 88	27, 59, 90, 105	0
All	All	1364/1460 (93%)	-0.10	4 (0%)	90 88	20, 49, 85, 105	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	105	VAL	2.8
1	D	81	VAL	2.4
1	C	114	LEU	2.1
1	C	106	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

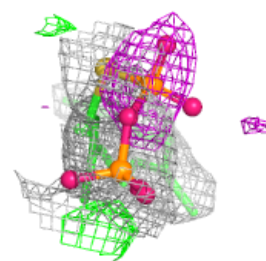
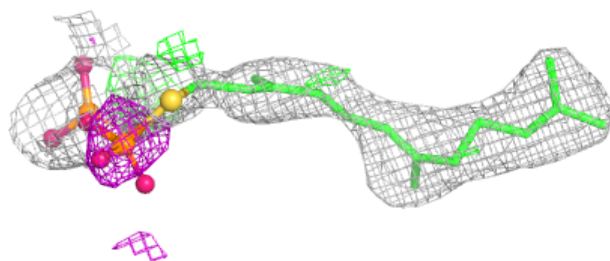
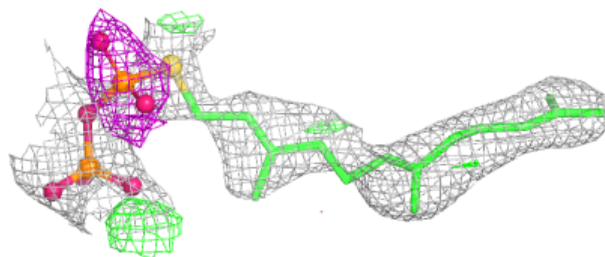
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FPS	B	401	24/24	0.76	0.19	45,90,119,119	0
2	FPS	C	401	24/24	0.78	0.19	79,107,123,124	0
2	FPS	A	501	24/24	0.80	0.15	48,81,111,112	0
2	FPS	D	401	24/24	0.80	0.18	64,102,126,126	0
3	RWZ	C	402	24/24	0.85	0.20	80,93,98,99	0
3	RWZ	B	402	24/24	0.86	0.16	57,72,74,74	0
3	RWZ	A	502	24/24	0.90	0.14	56,58,61,63	0
3	RWZ	D	402	24/24	0.90	0.16	65,78,80,81	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.

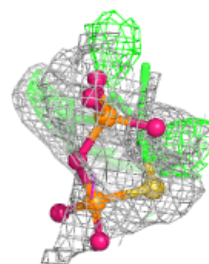
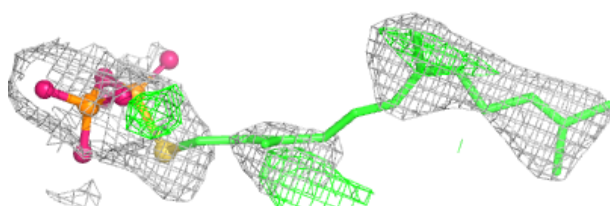
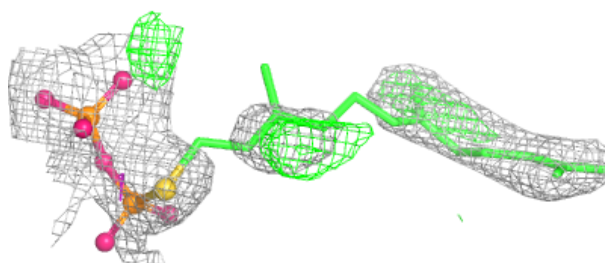
Electron density around FPS B 401:

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

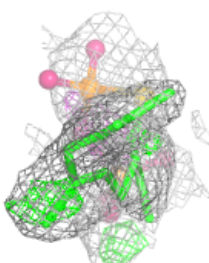
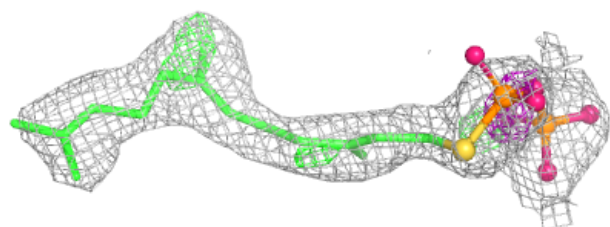
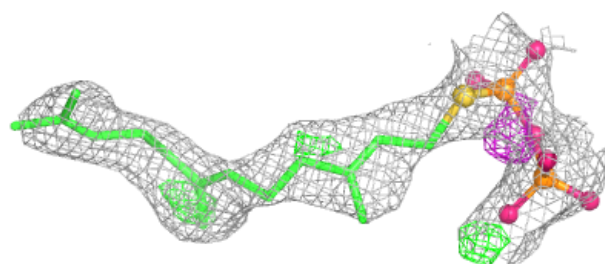


Electron density around FPS C 401:

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

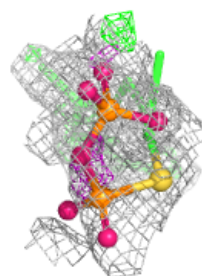
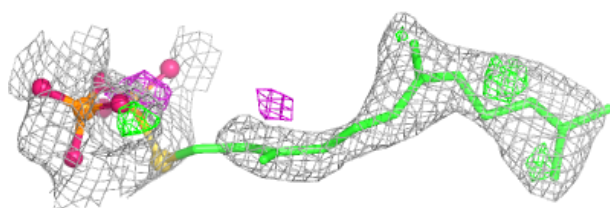
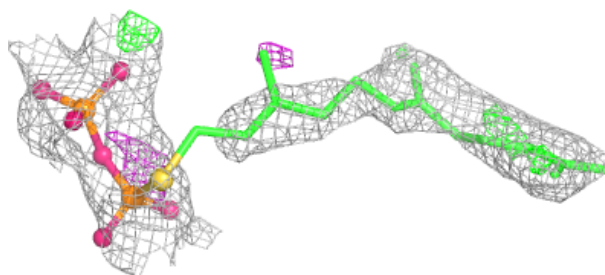
**Electron density around FPS A 501:**

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

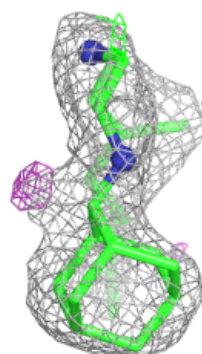
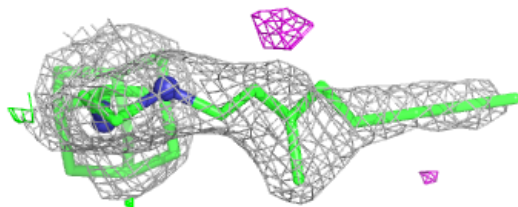
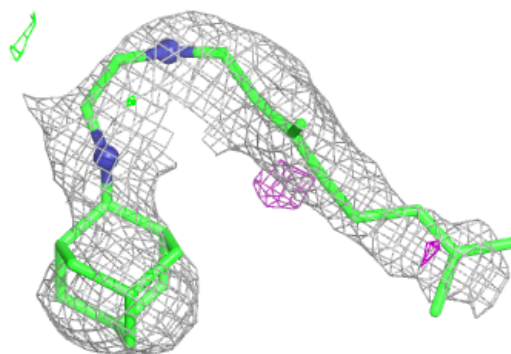


Electron density around FPS D 401:

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

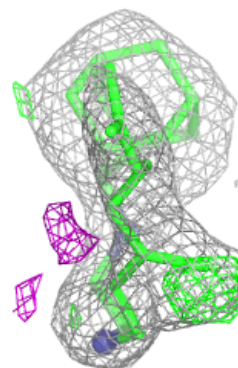
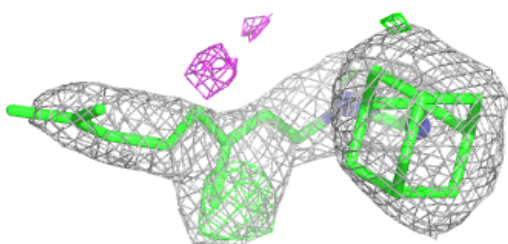
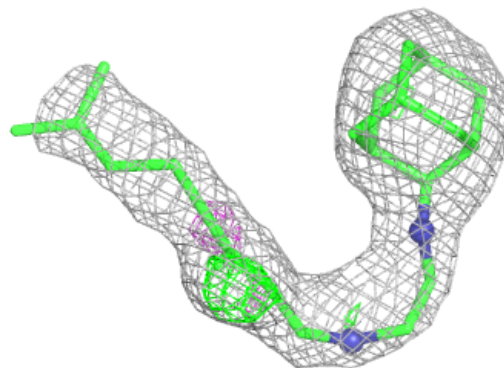
**Electron density around RWZ C 402:**

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

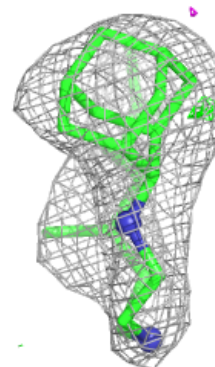
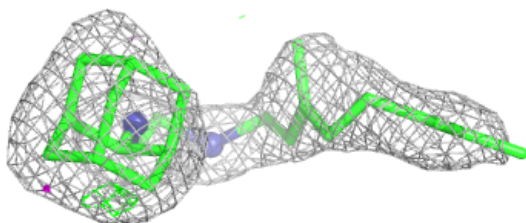
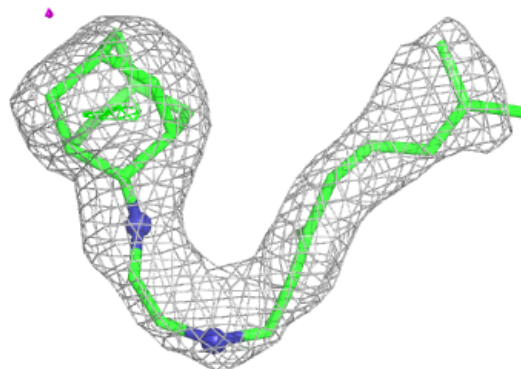


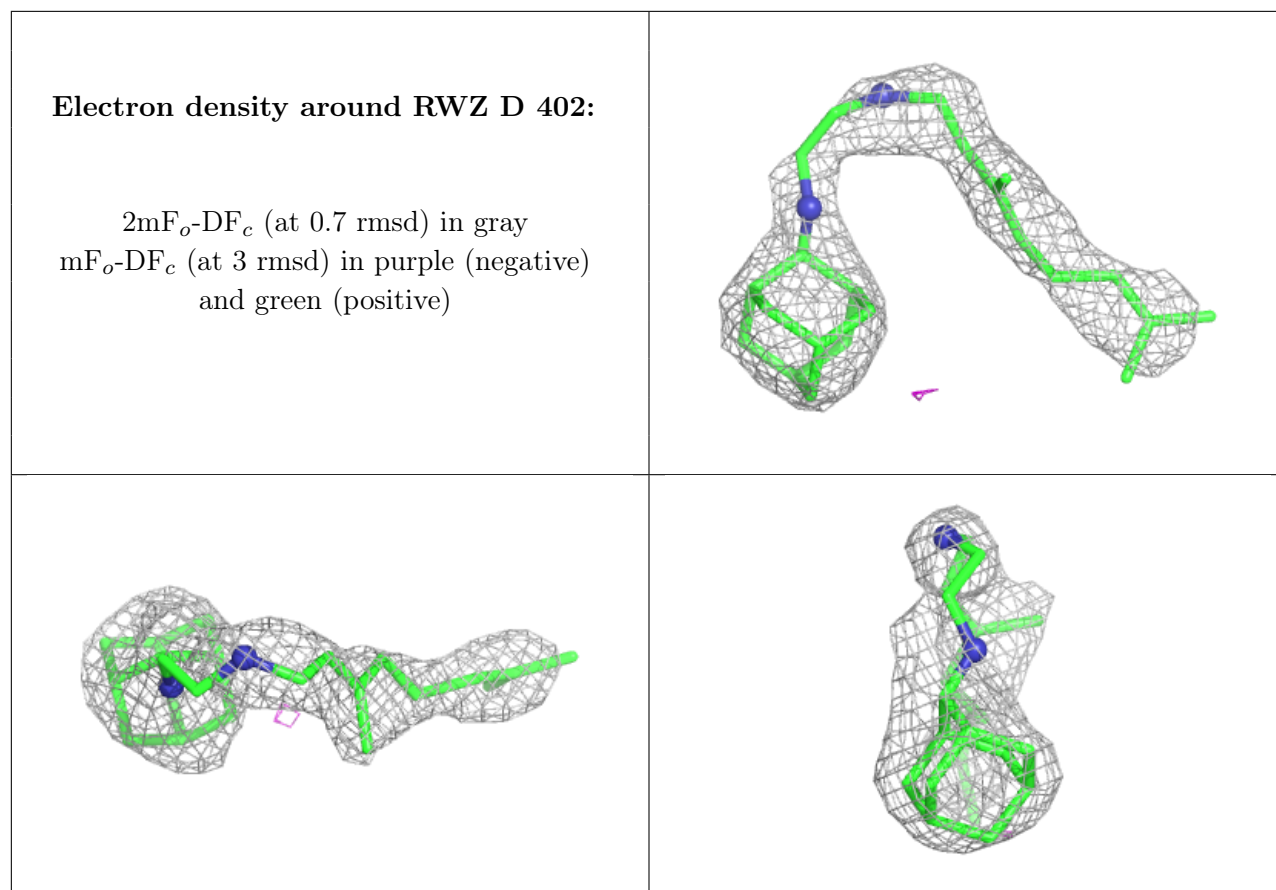
Electron density around RWZ B 402:

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

**Electron density around RWZ 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 ⓘ

There are no such residues in this entry.