



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:59 AM UTC

PDB ID : 6FVJ / pdb_00006fvj
Title : TesA a major thioesterase from Mycobacterium tuberculosis
Authors : Cambillau, C.; Nguyen, V.S.; Canaan, S.
Deposited on : 2018-03-03
Resolution : 2.60 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

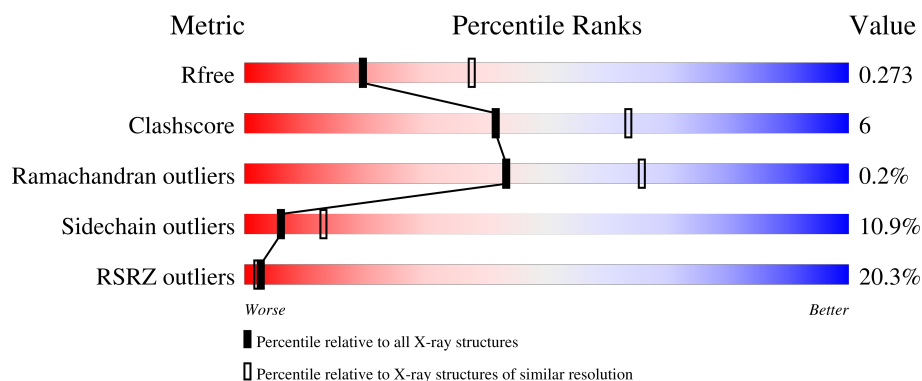
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	261	10% 65% 14% • 20%
1	B	261	7% 68% 11% • 19%
1	C	261	10% 64% 11% • • 21%
1	D	261	7% 70% 13% • 15%
1	E	261	14% 64% 15% • 18%

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Mol	Chain	Length	Quality of chain
1	F	261	15% 65% 12% • 20%
1	G	261	28% 62% 14% •• 21%
1	H	261	39% 57% 18% • 21%

2 Entry composition

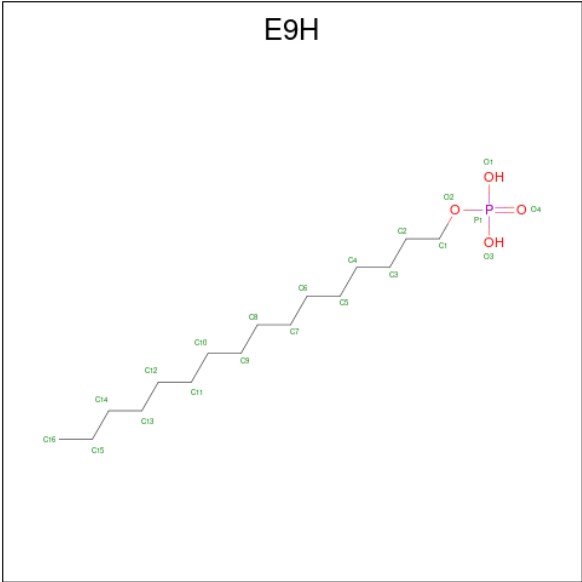
There are 5 unique types of molecules in this entry. The entry contains 13549 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thioesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1598	1029	268	293	8			
1	B	212	Total	C	N	O	S	0	0	0
			1628	1038	278	303	9			
1	C	205	Total	C	N	O	S	0	0	0
			1590	1023	261	297	9			
1	D	223	Total	C	N	O	S	0	0	0
			1696	1085	286	317	8			
1	E	213	Total	C	N	O	S	0	0	0
			1651	1063	274	305	9			
1	F	208	Total	C	N	O	S	0	0	0
			1616	1033	273	301	9			
1	G	206	Total	C	N	O	S	0	0	0
			1577	1015	263	291	8			
1	H	205	Total	C	N	O	S	0	0	0
			1579	1010	267	293	9			

- Molecule 2 is hexadecyl dihydrogen phosphate (CCD ID: E9H) (formula: C₁₆H₃₅O₄P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			7	3	3	1		
2	B	1	Total	C	O	P	0	0
			5	2	2	1		
2	C	1	Total	C	O	P	0	0
			8	4	3	1		
2	D	1	Total	C	O	P	0	0
			8	4	3	1		
2	E	1	Total	C	O	P	0	0
			6	2	3	1		
2	F	1	Total	C	O	P	0	0
			5	1	3	1		
2	G	1	Total	C	O	P	0	0
			5	1	3	1		
2	H	1	Total	C	O	P	0	0
			6	2	3	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0

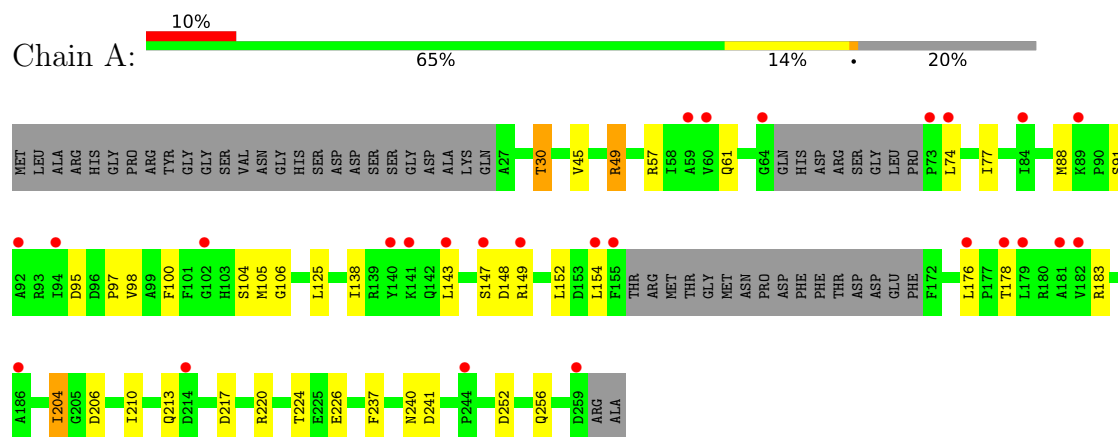
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	69	Total O 69 69	0	0
5	B	72	Total O 72 72	0	0
5	C	72	Total O 72 72	0	0
5	D	83	Total O 83 83	0	0
5	E	49	Total O 49 49	0	0
5	F	49	Total O 49 49	0	0
5	G	36	Total O 36 36	0	0
5	H	36	Total O 36 36	0	0

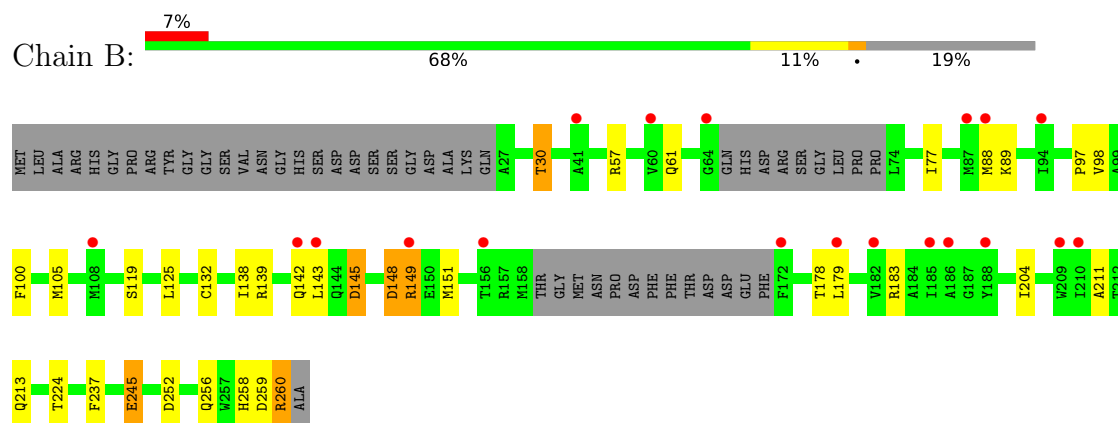
3 Residue-property plots [i](#)

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.

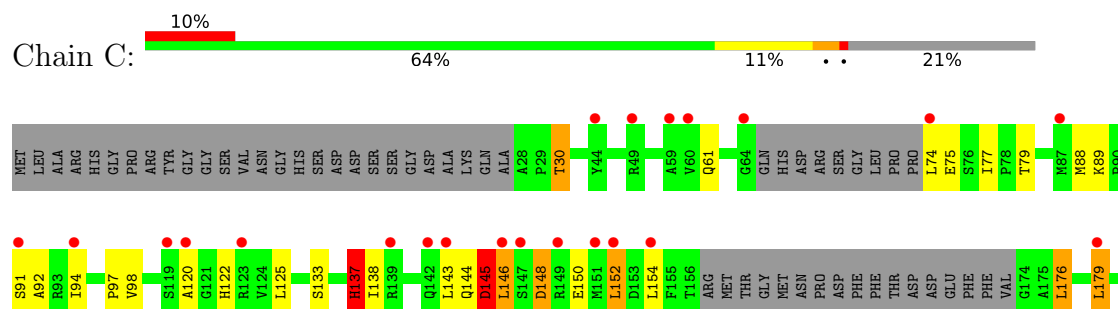
• Molecule 1: Thioesterase

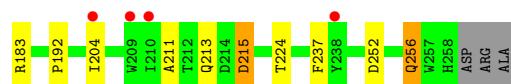


• Molecule 1: Thioesterase

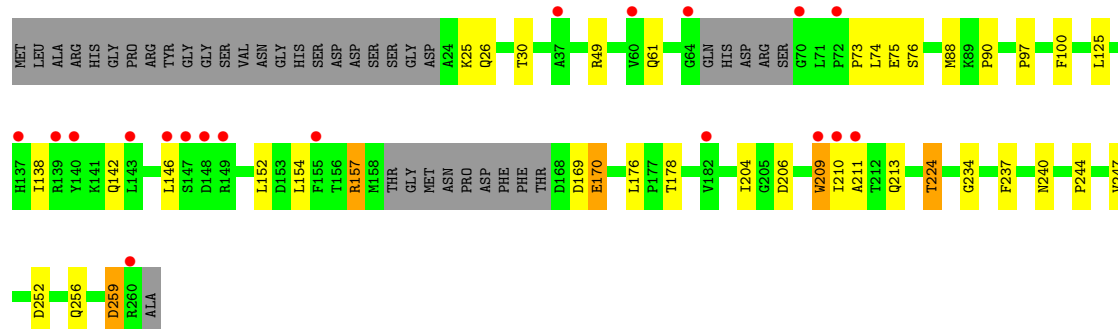


• Molecule 1: Thioesterase

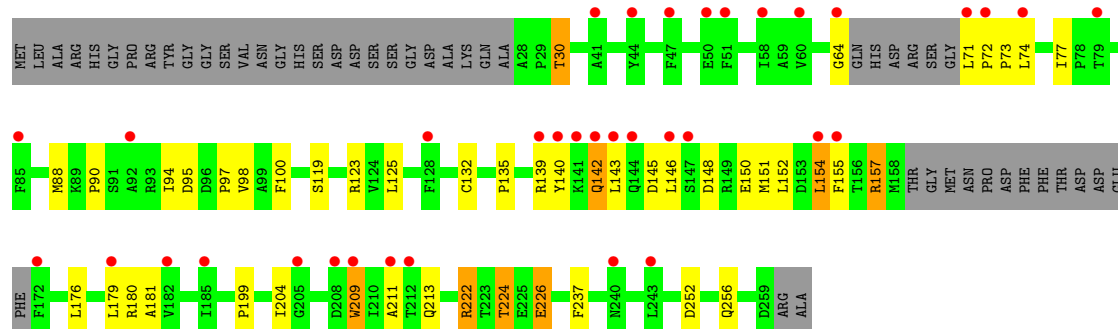




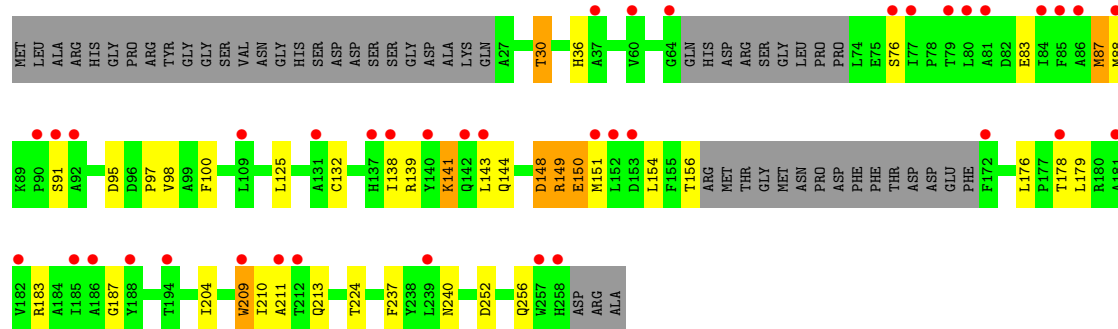
• Molecule 1: Thioesterase



• Molecule 1: Thioesterase

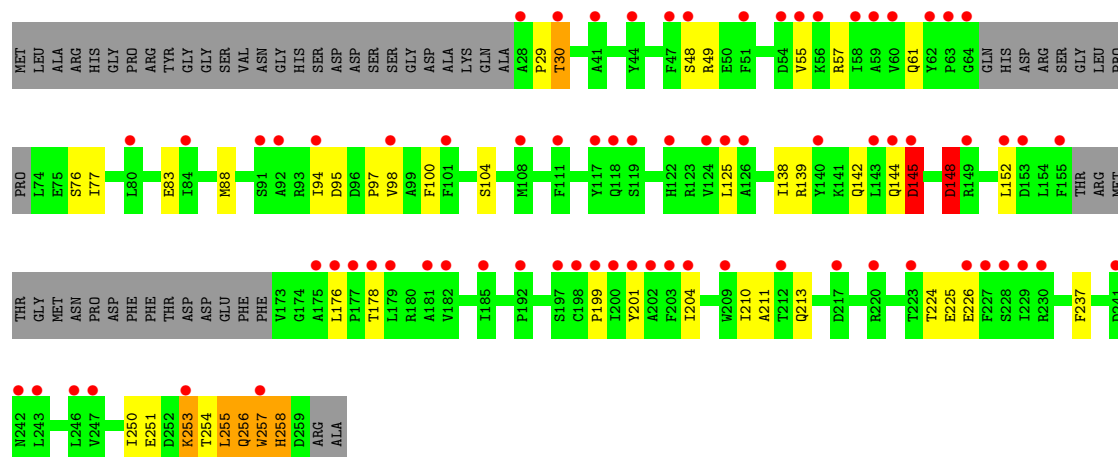


• Molecule 1: Thioesterase

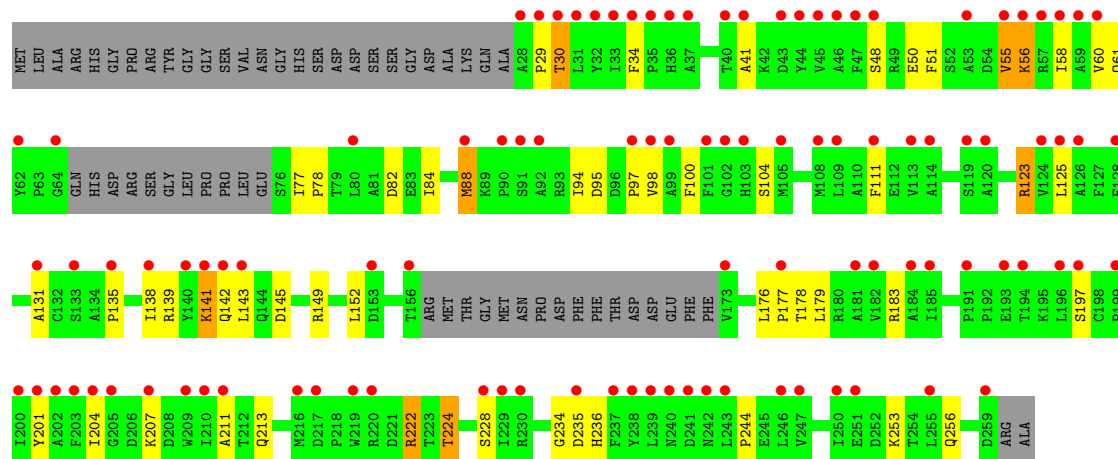


• Molecule 1: Thioesterase





• Molecule 1: Thioesterase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	79.07Å 224.58Å 222.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.83 – 2.60 43.83 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.83-2.60) 99.8 (43.83-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.236 , 0.259 0.250 , 0.273	Depositor DCC
R_{free} test set	3056 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 96.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13549	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1067e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: E9H, MPD, CA

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	0.78	1/1643 (0.1%)	1.30	6/2238 (0.3%)
1	B	0.79	1/1672 (0.1%)	1.35	6/2274 (0.3%)
1	C	0.78	1/1634 (0.1%)	1.36	9/2223 (0.4%)
1	D	0.78	0/1741	1.32	9/2370 (0.4%)
1	E	0.79	2/1698 (0.1%)	1.34	9/2311 (0.4%)
1	F	0.79	0/1660	1.32	6/2256 (0.3%)
1	G	0.77	1/1621 (0.1%)	1.35	13/2208 (0.6%)
1	H	0.83	1/1622 (0.1%)	1.47	7/2206 (0.3%)
All	All	0.79	7/13291 (0.1%)	1.35	65/18086 (0.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	77	ILE	CA-CB	6.22	1.57	1.54
1	B	77	ILE	CA-CB	6.20	1.57	1.54
1	A	77	ILE	CA-CB	5.68	1.57	1.54
1	E	77	ILE	CA-CB	5.61	1.57	1.54
1	H	77	ILE	CA-CB	5.45	1.57	1.54
1	C	77	ILE	CA-CB	5.33	1.57	1.54
1	E	77	ILE	CA-C	5.12	1.57	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	104	SER	CA-CB-OG	28.21	167.51	111.10
1	G	104	SER	CA-CB-OG	7.71	126.52	111.10
1	B	145	ASP	CA-CB-CG	7.57	120.17	112.60
1	G	257	TRP	CA-C-N	7.17	132.61	122.72
1	G	257	TRP	C-N-CA	7.17	132.61	122.72
1	C	215	ASP	CA-CB-CG	7.05	119.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	235	ASP	CA-CB-CG	6.72	119.32	112.60
1	B	259	ASP	CA-CB-CG	6.43	119.03	112.60
1	E	142	GLN	CA-C-N	6.34	128.68	120.44
1	E	142	GLN	C-N-CA	6.34	128.68	120.44
1	D	169	ASP	CB-CA-C	-6.15	109.47	116.54
1	F	148	ASP	CA-CB-CG	6.14	118.74	112.60
1	F	139	ARG	N-CA-C	6.02	117.64	111.14
1	A	104	SER	CA-CB-OG	5.99	123.07	111.10
1	C	148	ASP	CA-CB-CG	5.99	118.59	112.60
1	H	51	PHE	N-CA-C	-5.94	100.16	109.25
1	E	140	TYR	CA-C-N	5.93	130.99	122.21
1	E	140	TYR	C-N-CA	5.93	130.99	122.21
1	H	224	THR	N-CA-C	-5.82	100.81	109.94
1	G	148	ASP	CA-CB-CG	5.75	118.34	112.60
1	C	237	PHE	CA-C-N	5.59	128.33	120.28
1	C	237	PHE	C-N-CA	5.59	128.33	120.28
1	C	137	HIS	CA-C-N	5.59	132.03	121.97
1	C	137	HIS	C-N-CA	5.59	132.03	121.97
1	E	72	PRO	N-CA-C	5.55	117.48	110.70
1	C	145	ASP	CA-CB-CG	-5.43	107.17	112.60
1	G	237	PHE	CA-C-N	5.41	128.07	120.28
1	G	237	PHE	C-N-CA	5.41	128.07	120.28
1	G	225	GLU	CA-C-N	5.41	129.43	120.94
1	G	225	GLU	C-N-CA	5.41	129.43	120.94
1	E	237	PHE	CA-C-N	5.41	128.06	120.28
1	E	237	PHE	C-N-CA	5.41	128.06	120.28
1	B	237	PHE	CA-C-N	5.37	128.01	120.28
1	B	237	PHE	C-N-CA	5.37	128.01	120.28
1	G	250	ILE	CA-C-N	5.34	128.21	120.79
1	G	250	ILE	C-N-CA	5.34	128.21	120.79
1	G	76	SER	CA-C-N	5.30	124.57	120.33
1	G	76	SER	C-N-CA	5.30	124.57	120.33
1	D	170	GLU	CA-C-N	5.27	131.60	121.54
1	D	170	GLU	C-N-CA	5.27	131.60	121.54
1	D	237	PHE	CA-C-N	5.26	127.85	120.28
1	D	237	PHE	C-N-CA	5.26	127.85	120.28
1	C	145	ASP	CA-C-N	5.21	127.69	120.29
1	C	145	ASP	C-N-CA	5.21	127.69	120.29
1	B	148	ASP	N-CA-C	-5.17	106.73	112.57
1	A	237	PHE	CA-C-N	5.14	127.68	120.28
1	A	237	PHE	C-N-CA	5.14	127.68	120.28
1	G	145	ASP	CA-CB-CG	5.12	117.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	48	SER	CA-C-N	5.12	127.66	120.28
1	H	48	SER	C-N-CA	5.12	127.66	120.28
1	D	206	ASP	CA-CB-CG	5.12	117.72	112.60
1	D	224	THR	N-CA-C	-5.11	107.05	113.28
1	D	76	SER	CA-C-N	5.08	124.39	120.33
1	D	76	SER	C-N-CA	5.08	124.39	120.33
1	F	237	PHE	CA-C-N	5.08	127.59	120.28
1	F	237	PHE	C-N-CA	5.08	127.59	120.28
1	A	106	GLY	CA-C-N	5.07	125.57	120.00
1	A	106	GLY	C-N-CA	5.07	125.57	120.00
1	E	148	ASP	N-CA-C	5.06	116.79	111.28
1	H	234	GLY	N-CA-C	5.03	117.41	110.56
1	F	76	SER	CA-C-N	5.03	124.35	120.33
1	F	76	SER	C-N-CA	5.03	124.35	120.33
1	E	224	THR	N-CA-C	-5.01	107.02	113.23
1	A	206	ASP	CA-CB-CG	5.00	117.60	112.60
1	B	258	HIS	N-CA-C	-5.00	103.08	110.48

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	1598	0	1503	17	0
1	B	1628	0	1510	20	0
1	C	1590	0	1504	28	0
1	D	1696	0	1582	16	0
1	E	1651	0	1560	23	0
1	F	1616	0	1524	20	0
1	G	1577	0	1476	22	0
1	H	1579	0	1484	29	0
2	A	7	0	0	0	0
2	B	5	0	0	0	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	6	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	6	0	0	0	0
3	A	16	0	28	2	0
3	B	16	0	28	1	0
3	C	16	0	28	1	0
3	D	16	0	28	2	0
3	E	8	0	14	2	0
3	F	16	0	28	6	0
3	G	8	0	14	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	69	0	0	1	0
5	B	72	0	0	2	0
5	C	72	0	0	0	0
5	D	83	0	0	0	0
5	E	49	0	0	0	0
5	F	49	0	0	1	0
5	G	36	0	0	4	0
5	H	36	0	0	0	0
All	All	13549	0	12311	163	0

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

All (163) 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:145:ASP:OD2	1:C:148:ASP:CB	1.74	1.35
1:C:145:ASP:OD2	1:C:148:ASP:HB2	1.09	1.26
1:H:50:GLU:OE2	1:H:244:PRO:HA	1.62	1.00
1:H:149:ARG:NH1	1:H:183:ARG:HB2	1.77	0.97
1:G:55:VAL:HA	5:G:401:HOH:O	1.64	0.95
1:C:146:LEU:HD21	1:C:176:LEU:HD21	1.48	0.95
1:H:149:ARG:HH12	1:H:183:ARG:HB2	1.37	0.90
1:F:138:ILE:HG23	3:F:302:MPD:H13	1.54	0.90
1:E:64:GLY:HA3	1:E:73:PRO:HD3	1.51	0.89
1:C:152:LEU:HD22	1:C:179:LEU:HD21	1.53	0.89
1:C:145:ASP:CG	1:C:148:ASP:HB2	1.98	0.89
1:E:199:PRO:HB3	1:E:226:GLU:HG2	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:LEU:HB2	1:C:79:THR:HG21	1.61	0.82
1:D:26:GLN:NE2	1:D:259:ASP:HA	1.94	0.82
1:C:146:LEU:HD23	1:C:176:LEU:HD11	1.64	0.78
1:C:145:ASP:OD2	1:C:148:ASP:HB3	1.80	0.78
1:G:255:LEU:HD12	1:G:258:HIS:HE1	1.49	0.76
1:A:149:ARG:HH22	1:A:183:ARG:HB2	1.54	0.73
1:E:150:GLU:HB3	1:E:179:LEU:HD22	1.71	0.73
1:F:36:HIS:HD2	5:F:403:HOH:O	1.72	0.72
1:G:88:MET:HE1	1:G:100:PHE:HE1	1.55	0.71
1:H:149:ARG:HH12	1:H:183:ARG:CB	2.05	0.69
1:E:64:GLY:CA	1:E:73:PRO:HD3	2.22	0.68
1:G:125:LEU:HD22	1:G:256:GLN:HE22	1.58	0.67
1:G:258:HIS:H	1:G:258:HIS:CD2	2.10	0.67
1:B:256:GLN:O	1:B:260:ARG:HG3	1.95	0.67
1:H:135:PRO:HB2	1:H:222:ARG:NH1	2.09	0.66
1:A:226:GLU:HB3	1:E:226:GLU:HB2	1.79	0.65
1:G:145:ASP:HB3	1:G:148:ASP:HB2	1.78	0.64
1:C:148:ASP:C	1:C:150:GLU:H	2.05	0.64
1:E:209:TRP:HE3	1:E:209:TRP:H	1.45	0.64
1:A:240:ASN:HB3	1:D:49:ARG:HD2	1.80	0.63
1:C:133:SER:H	3:C:303:MPD:H13	1.64	0.63
1:E:71:LEU:HD21	1:E:181:ALA:CB	2.28	0.63
1:F:209:TRP:HE3	1:F:209:TRP:H	1.45	0.63
1:H:29:PRO:HG2	1:H:55:VAL:HG13	1.81	0.62
1:H:201:TYR:CE1	1:H:253:LYS:HD2	2.35	0.62
1:H:149:ARG:NH1	1:H:183:ARG:HE	1.98	0.61
1:C:152:LEU:CD2	1:C:179:LEU:HD21	2.29	0.61
1:A:204:ILE:HG12	5:A:501:HOH:O	2.01	0.60
1:H:34:PHE:CZ	1:H:84:ILE:HG21	2.36	0.60
1:A:256:GLN:HE22	1:E:256:GLN:HE22	1.50	0.60
1:F:138:ILE:HG23	3:F:302:MPD:C1	2.30	0.59
1:D:209:TRP:HE3	1:D:209:TRP:H	1.46	0.59
1:B:143:LEU:HA	1:B:183:ARG:HG3	1.85	0.59
1:C:146:LEU:CD2	1:C:176:LEU:HD21	2.30	0.58
1:H:88:MET:HE1	1:H:100:PHE:HE1	1.67	0.58
1:E:132:CYS:HA	3:E:302:MPD:HM3	1.85	0.58
1:H:135:PRO:HB2	1:H:222:ARG:HH11	1.68	0.57
1:F:210:ILE:HG22	3:F:302:MPD:H32	1.86	0.57
1:D:210:ILE:HG22	3:D:302:MPD:H12	1.85	0.57
1:H:149:ARG:NH1	1:H:183:ARG:NE	2.53	0.56
1:D:240:ASN:HD21	3:D:303:MPD:H32	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:LEU:HD13	1:C:179:LEU:HD11	1.88	0.56
1:D:88:MET:HE1	1:D:100:PHE:HE2	1.72	0.55
1:G:201:TYR:CZ	1:G:253:LYS:HG3	2.41	0.55
1:E:64:GLY:HA3	1:E:73:PRO:CD	2.29	0.55
1:D:26:GLN:HE22	1:D:259:ASP:HA	1.68	0.54
1:E:88:MET:HE1	1:E:100:PHE:HE2	1.71	0.54
1:G:254:THR:HB	1:G:255:LEU:HD23	1.90	0.54
1:F:88:MET:HE1	1:F:100:PHE:HE2	1.71	0.54
1:H:149:ARG:HD2	1:H:179:LEU:HG	1.88	0.54
1:C:137:HIS:CE1	1:C:192:PRO:HG3	2.42	0.54
1:A:240:ASN:HD21	3:A:403:MPD:H32	1.73	0.54
1:H:149:ARG:HH12	1:H:183:ARG:CG	2.21	0.54
1:H:88:MET:HE1	1:H:100:PHE:CE1	2.42	0.53
1:A:210:ILE:HG22	3:A:402:MPD:HM1	1.91	0.53
1:E:155:PHE:O	1:E:155:PHE:HD1	1.92	0.53
1:G:125:LEU:HD13	1:G:254:THR:O	2.09	0.53
1:G:48:SER:OG	1:G:57:ARG:HD2	2.08	0.52
1:B:252:ASP:O	1:B:256:GLN:HB2	2.09	0.52
1:C:92:ALA:HB1	1:C:122:HIS:CE1	2.44	0.52
1:F:138:ILE:O	1:F:141:LYS:HG2	2.10	0.52
1:A:61:GLN:HB3	1:C:61:GLN:HB3	1.91	0.52
1:A:88:MET:HE1	1:A:100:PHE:HE2	1.75	0.52
1:E:143:LEU:H	1:E:143:LEU:HD12	1.74	0.52
1:E:135:PRO:HD2	1:E:222:ARG:HD3	1.93	0.51
1:H:176:LEU:N	1:H:177:PRO:HD2	2.26	0.51
1:A:241:ASP:O	1:B:89:LYS:HD3	2.10	0.51
1:B:88:MET:HE1	1:B:100:PHE:HE2	1.75	0.51
1:H:30:THR:HG23	1:H:98:VAL:HG12	1.93	0.50
1:C:145:ASP:OD2	1:C:148:ASP:CG	2.51	0.50
1:G:29:PRO:HG2	5:G:401:HOH:O	2.10	0.50
1:A:45:VAL:HG11	1:D:244:PRO:HB3	1.94	0.49
1:G:29:PRO:HD2	5:G:401:HOH:O	2.12	0.49
1:G:210:ILE:HG22	3:G:302:MPD:HM1	1.95	0.49
1:B:204:ILE:HD11	1:B:211:ALA:O	2.13	0.49
1:B:149:ARG:HD2	1:B:179:LEU:HB3	1.95	0.49
1:H:197:SER:HA	1:H:224:THR:CG2	2.43	0.48
1:F:210:ILE:O	3:F:302:MPD:H11	2.12	0.48
1:G:255:LEU:HD12	1:G:258:HIS:CE1	2.38	0.48
1:A:57:ARG:H	1:C:91:SER:HB2	1.79	0.48
1:H:34:PHE:HZ	1:H:84:ILE:HG21	1.78	0.48
1:F:149:ARG:HH12	1:F:183:ARG:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:123:ARG:HA	1:H:123:ARG:HE	1.78	0.47
1:E:90:PRO:HB3	1:G:57:ARG:NH2	2.30	0.47
1:B:30:THR:HG22	5:B:534:HOH:O	2.14	0.46
1:B:132:CYS:HA	3:B:402:MPD:H13	1.97	0.46
1:C:89:LYS:HE2	1:C:120:ALA:HB1	1.97	0.46
1:F:149:ARG:NH1	1:F:183:ARG:HB2	2.31	0.46
1:E:157:ARG:HA	1:E:157:ARG:HD3	1.68	0.46
1:F:132:CYS:HA	3:F:302:MPD:H4	1.96	0.46
1:C:74:LEU:HD21	1:D:234:GLY:HA2	1.97	0.46
1:G:204:ILE:HD11	1:G:211:ALA:O	2.16	0.46
1:B:30:THR:HG23	1:B:98:VAL:HG12	1.98	0.45
1:B:57:ARG:CZ	1:D:90:PRO:HB3	2.45	0.45
1:D:204:ILE:HD11	1:D:211:ALA:O	2.16	0.45
1:F:83:GLU:O	1:F:87:MET:HG2	2.16	0.45
1:H:131:ALA:O	1:H:236:HIS:HE1	1.98	0.45
1:C:204:ILE:HD11	1:C:211:ALA:O	2.16	0.45
1:F:144:GLN:HG3	1:F:187:GLY:HA3	1.99	0.45
1:A:30:THR:HG23	1:A:98:VAL:HG12	1.99	0.45
1:B:149:ARG:HD3	1:B:179:LEU:HD22	1.97	0.45
1:H:41:ALA:HB2	1:H:61:GLN:NE2	2.32	0.45
1:D:157:ARG:HD3	1:D:157:ARG:HA	1.33	0.45
1:G:29:PRO:CD	5:G:401:HOH:O	2.65	0.45
1:B:149:ARG:HH21	1:B:183:ARG:HB2	1.81	0.45
1:E:139:ARG:H	3:E:302:MPD:H51	1.82	0.45
1:G:253:LYS:O	1:G:253:LYS:HD3	2.17	0.45
1:H:84:ILE:O	1:H:88:MET:HB2	2.17	0.45
1:B:149:ARG:CB	1:B:149:ARG:HH11	2.30	0.44
1:G:97:PRO:HB2	1:G:125:LEU:HD11	1.98	0.44
1:G:199:PRO:HB3	1:G:226:GLU:HB3	2.00	0.44
1:B:61:GLN:HB3	1:D:61:GLN:HB3	1.97	0.44
1:H:97:PRO:HB2	1:H:125:LEU:HD11	1.98	0.44
1:A:49:ARG:HH21	1:D:247:VAL:HG12	1.81	0.44
1:F:204:ILE:HD11	1:F:211:ALA:O	2.17	0.44
1:A:97:PRO:HB2	1:A:125:LEU:HD11	2.00	0.44
1:B:256:GLN:HG3	1:B:260:ARG:NH2	2.33	0.44
1:C:146:LEU:HD12	1:C:183:ARG:HH22	1.83	0.44
1:G:30:THR:HG23	1:G:98:VAL:HG12	1.99	0.43
1:B:245:GLU:H	1:B:245:GLU:CD	2.26	0.43
1:F:30:THR:HG23	1:F:98:VAL:HG12	1.99	0.43
1:E:204:ILE:HD11	1:E:211:ALA:O	2.18	0.43
1:E:252:ASP:O	1:E:256:GLN:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:56:LYS:HE3	1:H:56:LYS:HB2	1.79	0.43
1:G:201:TYR:OH	1:G:253:LYS:HD2	2.18	0.43
1:E:30:THR:HG23	1:E:98:VAL:HG12	2.00	0.43
1:E:154:LEU:HD13	1:E:179:LEU:HD11	2.01	0.43
1:H:204:ILE:HD11	1:H:211:ALA:O	2.19	0.43
1:A:252:ASP:O	1:A:256:GLN:HB2	2.19	0.42
1:B:149:ARG:HH11	1:B:149:ARG:HB2	1.84	0.42
1:E:176:LEU:HD21	1:E:180:ARG:HE	1.83	0.42
1:C:30:THR:HG23	1:C:98:VAL:HG12	2.01	0.42
1:C:148:ASP:C	1:C:150:GLU:N	2.73	0.42
1:B:97:PRO:HB2	1:B:125:LEU:HD11	2.01	0.42
1:C:137:HIS:NE2	1:C:192:PRO:HG3	2.35	0.42
1:F:150:GLU:O	1:F:154:LEU:N	2.53	0.42
1:H:88:MET:HE2	1:H:88:MET:HB3	1.85	0.42
1:H:111:PHE:CZ	1:H:222:ARG:HD3	2.55	0.42
1:H:78:PRO:O	1:H:82:ASP:OD1	2.38	0.41
1:C:92:ALA:HB1	1:C:122:HIS:HE1	1.85	0.41
1:F:240:ASN:HD21	3:F:303:MPD:H32	1.86	0.41
1:F:252:ASP:O	1:F:256:GLN:HB2	2.20	0.41
1:F:149:ARG:NH1	1:F:179:LEU:O	2.54	0.41
1:A:217:ASP:HB3	1:A:220:ARG:NH1	2.36	0.41
1:B:151:MET:HB3	5:B:501:HOH:O	2.21	0.41
1:C:97:PRO:HB2	1:C:125:LEU:HD11	2.01	0.41
1:C:252:ASP:O	1:C:256:GLN:HB2	2.20	0.41
1:F:97:PRO:HB2	1:F:125:LEU:HD11	2.01	0.41
1:E:97:PRO:HB2	1:E:125:LEU:HD11	2.01	0.41
1:D:97:PRO:HB2	1:D:125:LEU:HD11	2.02	0.40
1:D:252:ASP:O	1:D:256:GLN:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	203/261 (78%)	194 (96%)	9 (4%)	0	100	100
1	B	206/261 (79%)	199 (97%)	7 (3%)	0	100	100
1	C	199/261 (76%)	190 (96%)	8 (4%)	1 (0%)	24	46
1	D	217/261 (83%)	199 (92%)	16 (7%)	2 (1%)	14	30
1	E	207/261 (79%)	198 (96%)	9 (4%)	0	100	100
1	F	202/261 (77%)	190 (94%)	12 (6%)	0	100	100
1	G	200/261 (77%)	191 (96%)	9 (4%)	0	100	100
1	H	199/261 (76%)	186 (94%)	12 (6%)	1 (0%)	24	46
All	All	1633/2088 (78%)	1547 (95%)	82 (5%)	4 (0%)	43	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	138	ILE
1	H	141	LYS
1	D	170	GLU
1	D	73	PRO

5.3.2 Protein sidechains ⓘ

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	160/216 (74%)	143 (89%)	17 (11%)	6	14
1	B	162/216 (75%)	148 (91%)	14 (9%)	10	22
1	C	164/216 (76%)	147 (90%)	17 (10%)	7	14
1	D	169/216 (78%)	153 (90%)	16 (10%)	8	18
1	E	169/216 (78%)	151 (89%)	18 (11%)	6	14
1	F	165/216 (76%)	149 (90%)	16 (10%)	8	17
1	G	158/216 (73%)	135 (85%)	23 (15%)	3	6
1	H	160/216 (74%)	138 (86%)	22 (14%)	3	7
All	All	1307/1728 (76%)	1164 (89%)	143 (11%)	6	13

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	49	ARG
1	A	74	LEU
1	A	91	SER
1	A	95	ASP
1	A	105	MET
1	A	138	ILE
1	A	143	LEU
1	A	147	SER
1	A	148	ASP
1	A	152	LEU
1	A	154	LEU
1	A	176	LEU
1	A	178	THR
1	A	204	ILE
1	A	213	GLN
1	A	224	THR
1	B	30	THR
1	B	105	MET
1	B	119	SER
1	B	138	ILE
1	B	139	ARG
1	B	142	GLN
1	B	145	ASP
1	B	148	ASP
1	B	149	ARG
1	B	178	THR
1	B	213	GLN
1	B	224	THR
1	B	245	GLU
1	B	260	ARG
1	C	30	THR
1	C	75	GLU
1	C	88	MET
1	C	94	ILE
1	C	137	HIS
1	C	143	LEU
1	C	144	GLN
1	C	145	ASP
1	C	146	LEU
1	C	152	LEU
1	C	154	LEU

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Mol	Chain	Res	Type
1	C	176	LEU
1	C	179	LEU
1	C	213	GLN
1	C	215	ASP
1	C	224	THR
1	C	256	GLN
1	D	25	LYS
1	D	30	THR
1	D	74	LEU
1	D	75	GLU
1	D	138	ILE
1	D	142	GLN
1	D	146	LEU
1	D	152	LEU
1	D	154	LEU
1	D	157	ARG
1	D	176	LEU
1	D	178	THR
1	D	209	TRP
1	D	213	GLN
1	D	224	THR
1	D	259	ASP
1	E	30	THR
1	E	74	LEU
1	E	94	ILE
1	E	95	ASP
1	E	119	SER
1	E	123	ARG
1	E	142	GLN
1	E	145	ASP
1	E	146	LEU
1	E	151	MET
1	E	152	LEU
1	E	154	LEU
1	E	157	ARG
1	E	209	TRP
1	E	213	GLN
1	E	222	ARG
1	E	224	THR
1	E	226	GLU
1	F	30	THR
1	F	87	MET

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Mol	Chain	Res	Type
1	F	91	SER
1	F	95	ASP
1	F	141	LYS
1	F	143	LEU
1	F	148	ASP
1	F	149	ARG
1	F	150	GLU
1	F	151	MET
1	F	156	THR
1	F	176	LEU
1	F	178	THR
1	F	209	TRP
1	F	213	GLN
1	F	224	THR
1	G	30	THR
1	G	49	ARG
1	G	61	GLN
1	G	83	GLU
1	G	94	ILE
1	G	95	ASP
1	G	138	ILE
1	G	139	ARG
1	G	142	GLN
1	G	144	GLN
1	G	145	ASP
1	G	148	ASP
1	G	152	LEU
1	G	176	LEU
1	G	178	THR
1	G	213	GLN
1	G	224	THR
1	G	251	GLU
1	G	253	LYS
1	G	255	LEU
1	G	256	GLN
1	G	257	TRP
1	G	258	HIS
1	H	30	THR
1	H	55	VAL
1	H	56	LYS
1	H	58	ILE
1	H	60	VAL

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Mol	Chain	Res	Type
1	H	88	MET
1	H	94	ILE
1	H	95	ASP
1	H	123	ARG
1	H	138	ILE
1	H	139	ARG
1	H	141	LYS
1	H	142	GLN
1	H	143	LEU
1	H	145	ASP
1	H	152	LEU
1	H	178	THR
1	H	207	LYS
1	H	213	GLN
1	H	222	ARG
1	H	228	SER
1	H	256	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	137	HIS
1	A	256	GLN
1	B	61	GLN
1	B	142	GLN
1	C	61	GLN
1	D	26	GLN
1	D	61	GLN
1	D	137	HIS
1	D	142	GLN
1	D	240	ASN
1	E	61	GLN
1	E	122	HIS
1	E	137	HIS
1	F	61	GLN
1	F	137	HIS
1	G	61	GLN
1	G	122	HIS
1	G	137	HIS
1	G	256	GLN
1	G	258	HIS

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Mol	Chain	Res	Type
1	H	61	GLN
1	H	142	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	E9H	H	301	1	2,5,20	0.64	0	1,5,22	0.32	0
2	E9H	C	301	1	4,7,20	0.35	0	3,7,22	0.31	0
3	MPD	A	402	-	7,7,7	0.39	0	9,10,10	0.46	0
2	E9H	E	301	1	2,5,20	0.63	0	1,5,22	0.32	0
3	MPD	B	403	-	7,7,7	0.64	0	9,10,10	0.55	0
3	MPD	C	304	-	7,7,7	0.74	0	9,10,10	0.64	0
3	MPD	D	302	-	7,7,7	0.35	0	9,10,10	0.33	0
3	MPD	C	303	-	7,7,7	0.52	0	9,10,10	0.39	0
2	E9H	A	401	1	3,6,20	0.42	0	2,6,22	0.27	0
3	MPD	A	403	-	7,7,7	0.55	0	9,10,10	0.29	0
3	MPD	D	303	-	7,7,7	0.52	0	9,10,10	0.33	0
3	MPD	F	303	-	7,7,7	0.45	0	9,10,10	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MPD	G	302	-	7,7,7	0.42	0	9,10,10	0.40	0
2	E9H	B	401	1	1,4,20	0.83	0	1,3,22	0.19	0
2	E9H	D	301	1	4,7,20	0.36	0	3,7,22	0.38	0
3	MPD	B	402	-	7,7,7	0.56	0	9,10,10	0.36	0
3	MPD	E	302	-	7,7,7	0.56	0	9,10,10	0.62	0
2	E9H	F	301	1	1,4,20	0.20	0	0,4,22	-	-
2	E9H	G	301	1	1,4,20	0.19	0	0,4,22	-	-
3	MPD	F	302	-	7,7,7	0.39	0	9,10,10	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	E9H	H	301	1	-	0/1/3/18	-
2	E9H	C	301	1	-	1/3/5/18	-
3	MPD	A	402	-	-	4/5/5/5	-
2	E9H	E	301	1	-	0/1/3/18	-
3	MPD	B	403	-	-	0/5/5/5	-
3	MPD	C	304	-	-	4/5/5/5	-
3	MPD	D	302	-	-	2/5/5/5	-
3	MPD	C	303	-	-	1/5/5/5	-
2	E9H	A	401	1	-	1/2/4/18	-
3	MPD	A	403	-	-	1/5/5/5	-
3	MPD	D	303	-	-	2/5/5/5	-
3	MPD	F	303	-	-	1/5/5/5	-
3	MPD	G	302	-	-	5/5/5/5	-
2	E9H	B	401	1	-	0/0/2/18	-
2	E9H	D	301	1	-	2/3/5/18	-
3	MPD	B	402	-	-	1/5/5/5	-
3	MPD	E	302	-	-	3/5/5/5	-
2	E9H	F	301	1	-	0/0/2/18	-
2	E9H	G	301	1	-	0/0/2/18	-
3	MPD	F	302	-	-	4/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	304	MPD	C1-C2-C3-C4
3	C	304	MPD	C2-C3-C4-O4
3	C	304	MPD	C2-C3-C4-C5
3	F	302	MPD	C2-C3-C4-C5
3	G	302	MPD	C2-C3-C4-O4
2	C	301	E9H	O2-C1-C2-C3
2	D	301	E9H	O2-C1-C2-C3
2	D	301	E9H	C1-C2-C3-C4
2	A	401	E9H	O2-C1-C2-C3
3	B	402	MPD	O2-C2-C3-C4
3	F	303	MPD	O2-C2-C3-C4
3	A	402	MPD	C2-C3-C4-O4
3	C	304	MPD	CM-C2-C3-C4
3	F	302	MPD	C1-C2-C3-C4
3	F	302	MPD	CM-C2-C3-C4
3	A	402	MPD	C2-C3-C4-C5
3	E	302	MPD	C2-C3-C4-C5
3	G	302	MPD	C2-C3-C4-C5
3	A	402	MPD	O2-C2-C3-C4
3	C	303	MPD	O2-C2-C3-C4
3	D	303	MPD	O2-C2-C3-C4
3	F	302	MPD	O2-C2-C3-C4
3	G	302	MPD	O2-C2-C3-C4
3	A	402	MPD	C1-C2-C3-C4
3	A	403	MPD	C1-C2-C3-C4
3	D	302	MPD	C1-C2-C3-C4
3	D	302	MPD	CM-C2-C3-C4
3	D	303	MPD	CM-C2-C3-C4
3	E	302	MPD	C1-C2-C3-C4
3	E	302	MPD	CM-C2-C3-C4
3	G	302	MPD	C1-C2-C3-C4
3	G	302	MPD	CM-C2-C3-C4

There are no ring outliers.

10 monomers are involved in 15 short contacts:

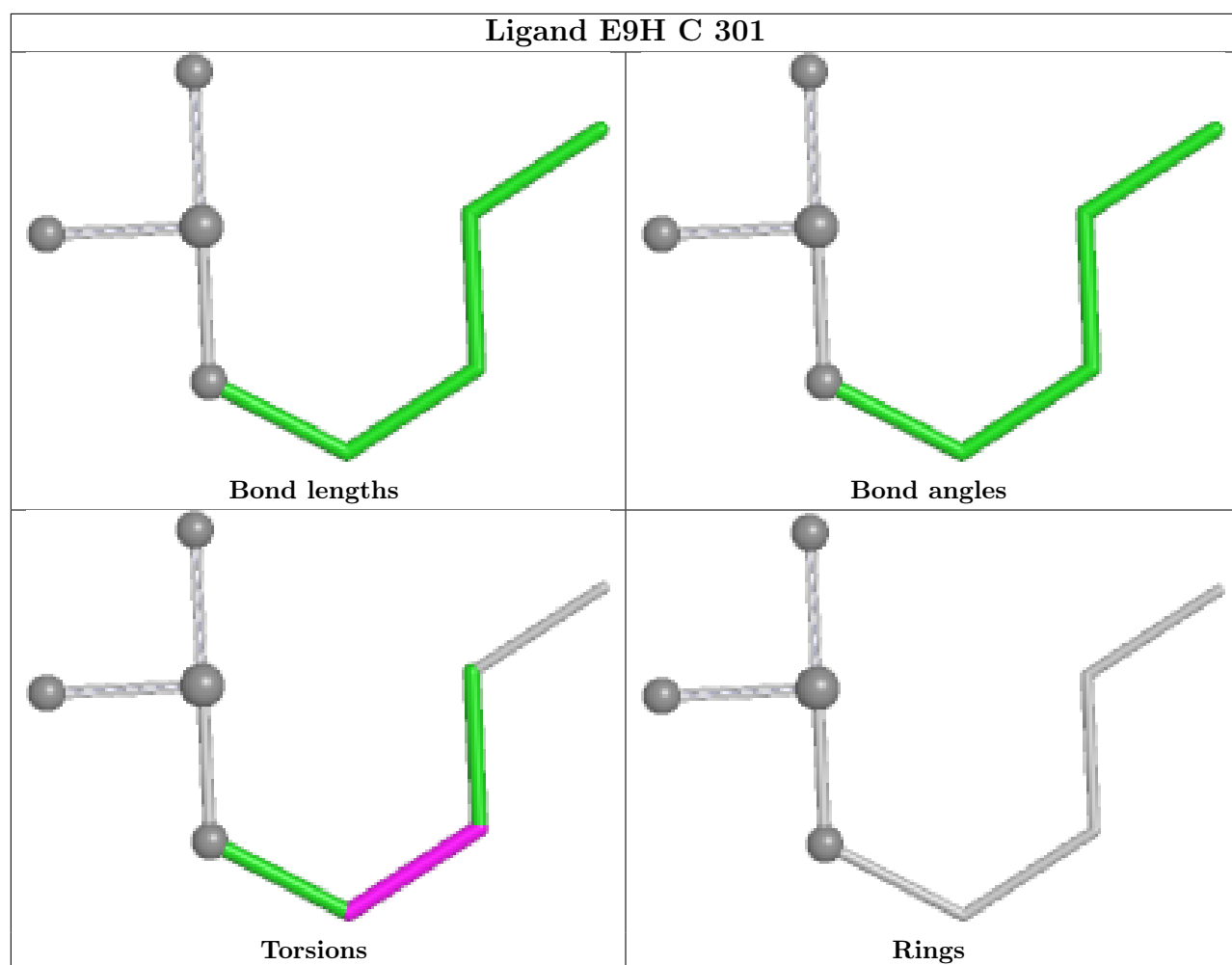
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	MPD	1	0
3	D	302	MPD	1	0
3	C	303	MPD	1	0
3	A	403	MPD	1	0

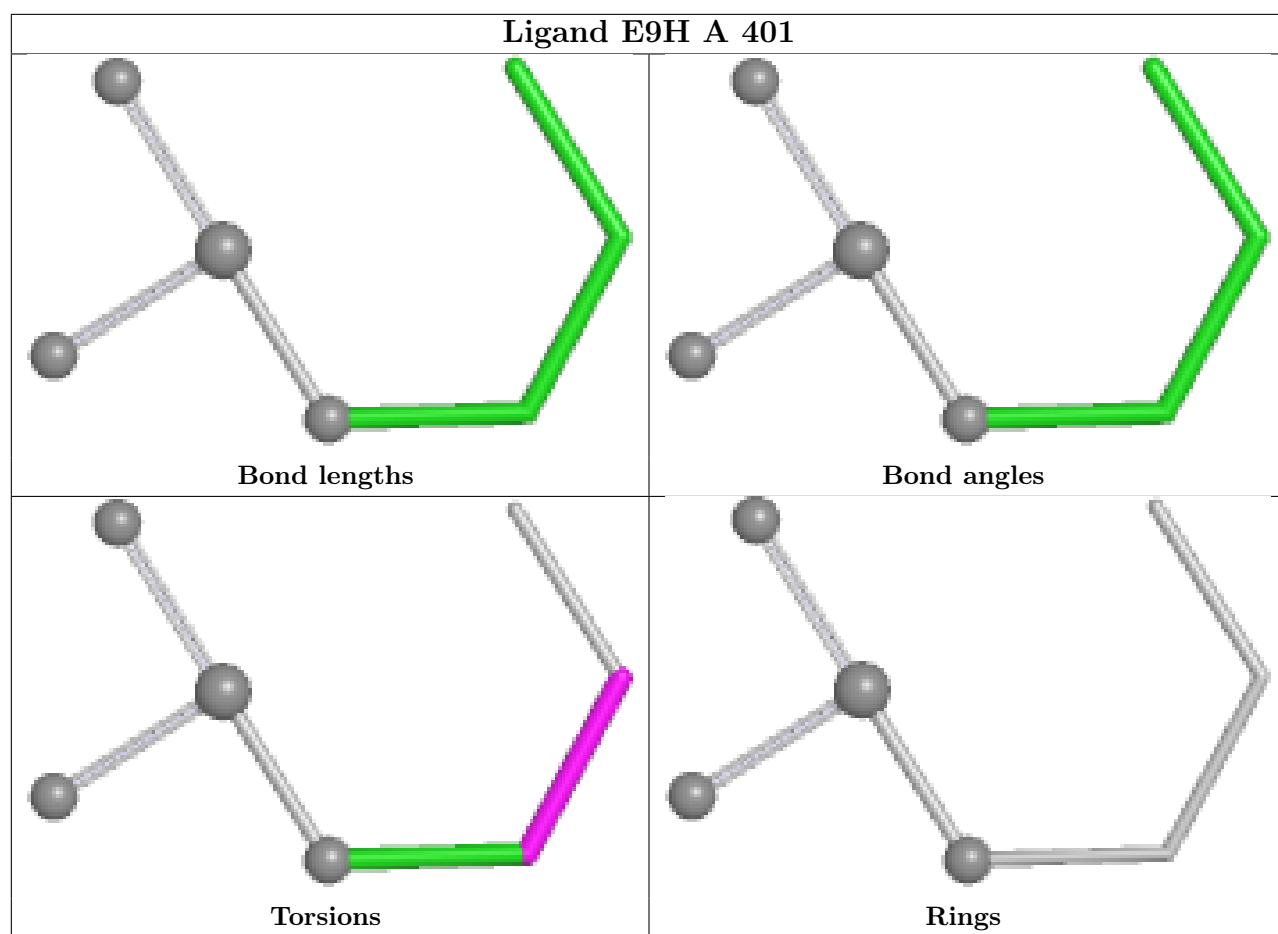
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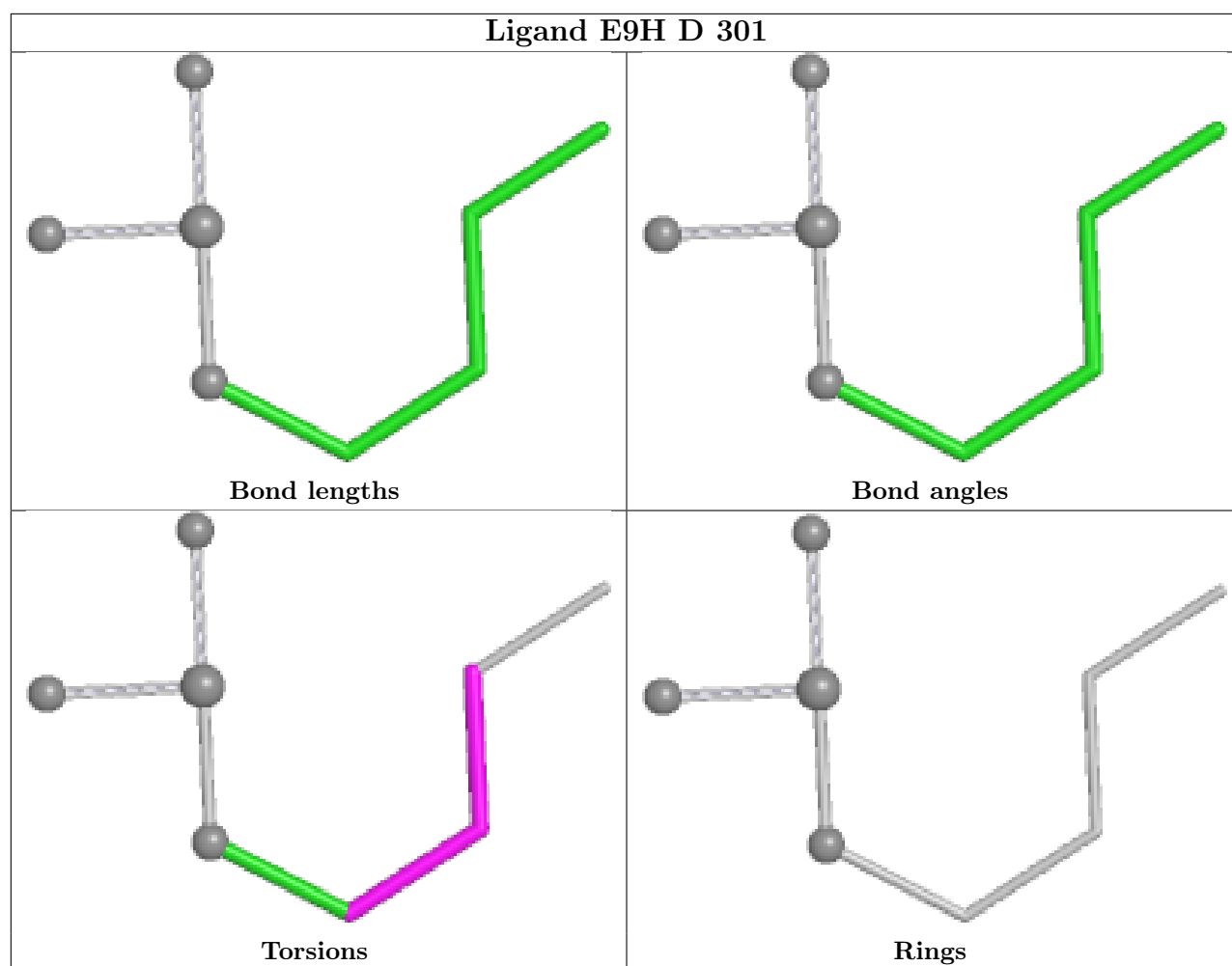
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	303	MPD	1	0
3	F	303	MPD	1	0
3	G	302	MPD	1	0
3	B	402	MPD	1	0
3	E	302	MPD	2	0
3	F	302	MPD	5	0

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

6.1 Protein, DNA and RNA chains

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	209/261 (80%)	0.77	26 (12%) 8 6	41, 65, 157, 216	0
1	B	212/261 (81%)	0.65	19 (8%) 15 11	41, 60, 160, 195	0
1	C	205/261 (78%)	0.78	26 (12%) 8 6	43, 67, 149, 190	0
1	D	223/261 (85%)	0.62	19 (8%) 16 13	37, 55, 149, 193	0
1	E	213/261 (81%)	1.06	36 (16%) 4 3	45, 84, 145, 155	0
1	F	208/261 (79%)	1.23	39 (18%) 3 2	55, 83, 136, 149	0
1	G	206/261 (78%)	1.85	74 (35%) 1 1	72, 110, 163, 247	0
1	H	205/261 (78%)	2.13	103 (50%) 0 0	80, 107, 144, 165	0
All	All	1681/2088 (80%)	1.13	342 (20%) 3 2	37, 80, 149, 247	0

All (342) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	204	ILE	6.7
1	G	47	PHE	5.8
1	G	181	ALA	5.8
1	B	149	ARG	5.8
1	H	41	ALA	5.7
1	H	44	TYR	5.7
1	H	181	ALA	5.6
1	F	182	VAL	5.4
1	G	98	VAL	5.3
1	H	239	LEU	5.1
1	D	209	TRP	5.0
1	G	153	ASP	5.0
1	D	210	ILE	4.8
1	H	182	VAL	4.7
1	G	44	TYR	4.7
1	B	142	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
1	G	182	VAL	4.6
1	G	149	ARG	4.6
1	G	155	PHE	4.5
1	H	47	PHE	4.3
1	H	125	LEU	4.3
1	F	181	ALA	4.3
1	A	186	ALA	4.3
1	G	178	THR	4.3
1	H	33	ILE	4.2
1	H	60	VAL	4.2
1	F	137	HIS	4.2
1	H	126	ALA	4.1
1	H	120	ALA	4.1
1	E	182	VAL	4.1
1	E	154	LEU	4.0
1	H	246	LEU	4.0
1	H	124	VAL	4.0
1	H	58	ILE	4.0
1	H	238	TYR	4.0
1	C	143	LEU	3.9
1	H	108	MET	3.9
1	D	72	PRO	3.9
1	F	77	ILE	3.9
1	G	175	ALA	3.9
1	H	45	VAL	3.9
1	H	250	ILE	3.8
1	H	200	ILE	3.8
1	B	186	ALA	3.7
1	H	184	ALA	3.7
1	H	199	PRO	3.7
1	G	229	ILE	3.7
1	G	41	ALA	3.7
1	G	55	VAL	3.7
1	B	179	LEU	3.7
1	G	28	ALA	3.7
1	H	203	PHE	3.7
1	F	86	ALA	3.6
1	H	59	ALA	3.6
1	H	99	ALA	3.6
1	G	179	LEU	3.6
1	F	209	TRP	3.6
1	G	92	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	85	PHE	3.6
1	F	188	TYR	3.6
1	G	203	PHE	3.6
1	C	91	SER	3.6
1	F	91	SER	3.6
1	G	80	LEU	3.6
1	H	119	SER	3.5
1	F	153	ASP	3.5
1	H	101	PHE	3.5
1	C	120	ALA	3.5
1	G	246	LEU	3.5
1	B	182	VAL	3.5
1	G	201	TYR	3.4
1	C	74	LEU	3.4
1	H	205	GLY	3.4
1	H	88	MET	3.4
1	G	119	SER	3.4
1	F	212	THR	3.4
1	C	64	GLY	3.4
1	G	209	TRP	3.3
1	E	79	THR	3.3
1	H	193	GLU	3.3
1	H	131	ALA	3.3
1	C	139	ARG	3.3
1	E	146	LEU	3.3
1	E	41	ALA	3.3
1	H	242	ASN	3.3
1	D	147	SER	3.3
1	E	179	LEU	3.3
1	F	37	ALA	3.3
1	F	131	ALA	3.3
1	H	55	VAL	3.3
1	A	149	ARG	3.2
1	H	209	TRP	3.2
1	G	117	TYR	3.2
1	F	81	ALA	3.2
1	E	47	PHE	3.2
1	E	64	GLY	3.2
1	E	147	SER	3.2
1	G	91	SER	3.2
1	H	229	ILE	3.2
1	F	92	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	28	ALA	3.1
1	C	119	SER	3.1
1	F	60	VAL	3.1
1	H	173	VAL	3.1
1	H	243	LEU	3.1
1	E	140	TYR	3.1
1	G	108	MET	3.1
1	H	201	TYR	3.1
1	H	237	PHE	3.1
1	H	133	SER	3.1
1	F	90	PRO	3.1
1	G	59	ALA	3.1
1	H	185	ILE	3.1
1	H	247	VAL	3.1
1	H	48	SER	3.1
1	F	80	LEU	3.0
1	G	200	ILE	3.0
1	G	199	PRO	3.0
1	A	214	ASP	3.0
1	B	88	MET	3.0
1	B	94	ILE	3.0
1	D	70	GLY	3.0
1	G	64	GLY	3.0
1	H	34	PHE	3.0
1	H	31	LEU	3.0
1	G	124	VAL	3.0
1	E	143	LEU	2.9
1	G	143	LEU	2.9
1	A	140	TYR	2.9
1	C	44	TYR	2.9
1	A	143	LEU	2.9
1	H	202	ALA	2.9
1	H	219	TRP	2.9
1	G	126	ALA	2.9
1	H	46	ALA	2.9
1	H	92	ALA	2.9
1	G	30	THR	2.9
1	B	60	VAL	2.9
1	G	60	VAL	2.9
1	G	125	LEU	2.9
1	C	149	ARG	2.8
1	H	220	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	185	ILE	2.8
1	A	182	VAL	2.8
1	H	142	GLN	2.8
1	G	185	ILE	2.8
1	C	146	LEU	2.8
1	A	181	ALA	2.8
1	D	60	VAL	2.8
1	A	73	PRO	2.8
1	A	94	ILE	2.8
1	H	109	LEU	2.8
1	H	153	ASP	2.8
1	C	238	TYR	2.8
1	H	251	GLU	2.8
1	C	147	SER	2.8
1	H	255	LEU	2.8
1	E	208	ASP	2.8
1	F	211	ALA	2.8
1	E	44	TYR	2.8
1	E	58	ILE	2.7
1	F	152	LEU	2.7
1	G	228	SER	2.7
1	G	242	ASN	2.7
1	H	30	THR	2.7
1	H	194	THR	2.7
1	H	32	TYR	2.7
1	F	84	ILE	2.7
1	A	60	VAL	2.7
1	B	156	THR	2.7
1	E	211	ALA	2.7
1	G	177	PRO	2.7
1	G	54	ASP	2.7
1	G	176	LEU	2.7
1	H	103	HIS	2.7
1	D	260	ARG	2.7
1	E	205	GLY	2.7
1	E	92	ALA	2.7
1	H	141	LYS	2.7
1	E	142	GLN	2.6
1	H	143	LEU	2.6
1	H	57	ARG	2.6
1	H	191	PRO	2.6
1	G	58	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	143	LEU	2.6
1	G	122	HIS	2.6
1	A	59	ALA	2.6
1	A	155	PHE	2.6
1	G	48	SER	2.6
1	H	37	ALA	2.6
1	H	210	ILE	2.6
1	E	71	LEU	2.6
1	D	149	ARG	2.6
1	H	36	HIS	2.6
1	F	88	MET	2.6
1	F	109	LEU	2.6
1	H	35	PRO	2.6
1	H	240	ASN	2.6
1	E	128	PHE	2.5
1	G	198	CYS	2.5
1	H	40	THR	2.5
1	A	154	LEU	2.5
1	H	62	TYR	2.5
1	G	247	VAL	2.5
1	C	59	ALA	2.5
1	H	228	SER	2.5
1	C	49	ARG	2.5
1	G	94	ILE	2.5
1	H	111	PHE	2.5
1	C	152	LEU	2.5
1	E	243	LEU	2.5
1	A	92	ALA	2.5
1	F	172	PHE	2.5
1	H	128	PHE	2.5
1	C	154	LEU	2.4
1	G	145	ASP	2.4
1	G	241	ASP	2.4
1	B	64	GLY	2.4
1	C	151	MET	2.4
1	G	144	GLN	2.4
1	D	155	PHE	2.4
1	G	63	PRO	2.4
1	H	98	VAL	2.4
1	G	51	PHE	2.4
1	B	143	LEU	2.4
1	F	79	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	243	LEU	2.4
1	H	56	LYS	2.4
1	H	177	PRO	2.4
1	G	230	ARG	2.4
1	B	172	PHE	2.4
1	G	101	PHE	2.4
1	E	50	GLU	2.3
1	B	87	MET	2.3
1	E	209	TRP	2.3
1	F	64	GLY	2.3
1	C	60	VAL	2.3
1	C	179	LEU	2.3
1	D	137	HIS	2.3
1	H	156	THR	2.3
1	B	108	MET	2.3
1	G	253	LYS	2.3
1	B	209	TRP	2.3
1	H	230	ARG	2.3
1	F	178	THR	2.3
1	H	140	TYR	2.3
1	A	147	SER	2.3
1	G	220	ARG	2.3
1	E	144	GLN	2.3
1	E	74	LEU	2.3
1	F	239	LEU	2.3
1	D	211	ALA	2.3
1	F	186	ALA	2.3
1	F	194	THR	2.3
1	G	140	TYR	2.3
1	E	72	PRO	2.3
1	E	139	ARG	2.3
1	H	217	ASP	2.3
1	C	209	TRP	2.3
1	H	64	GLY	2.3
1	E	51	PHE	2.3
1	B	210	ILE	2.2
1	H	53	ALA	2.2
1	B	188	TYR	2.2
1	E	240	ASN	2.2
1	C	123	ARG	2.2
1	A	64	GLY	2.2
1	A	176	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	141	LYS	2.2
1	G	56	LYS	2.2
1	F	140	TYR	2.2
1	H	259	ASP	2.2
1	A	179	LEU	2.2
1	A	84	ILE	2.2
1	E	155	PHE	2.2
1	H	138	ILE	2.2
1	H	216	MET	2.2
1	B	41	ALA	2.2
1	D	37	ALA	2.2
1	G	118	GLN	2.2
1	D	64	GLY	2.2
1	D	146	LEU	2.2
1	H	235	ASP	2.2
1	D	182	VAL	2.2
1	C	94	ILE	2.2
1	E	185	ILE	2.2
1	G	202	ALA	2.2
1	H	114	ALA	2.2
1	G	226	GLU	2.2
1	A	89	LYS	2.2
1	F	151	MET	2.2
1	H	105	MET	2.2
1	C	204	ILE	2.2
1	G	204	ILE	2.2
1	E	172	PHE	2.2
1	H	90	PRO	2.1
1	H	97	PRO	2.1
1	H	135	PRO	2.1
1	C	142	GLN	2.1
1	A	259	ASP	2.1
1	E	60	VAL	2.1
1	F	76	SER	2.1
1	G	84	ILE	2.1
1	G	197	SER	2.1
1	H	91	SER	2.1
1	A	178	THR	2.1
1	G	192	PRO	2.1
1	H	80	LEU	2.1
1	H	196	LEU	2.1
1	B	185	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	210	ILE	2.1
1	D	148	ASP	2.1
1	G	217	ASP	2.1
1	G	257	TRP	2.1
1	E	212	THR	2.1
1	A	141	LYS	2.1
1	H	207	LYS	2.1
1	C	87	MET	2.1
1	E	85	PHE	2.1
1	H	43	ASP	2.1
1	H	241	ASP	2.1
1	H	211	ALA	2.1
1	A	102	GLY	2.1
1	H	102	GLY	2.1
1	G	62	TYR	2.1
1	G	111	PHE	2.1
1	F	257	TRP	2.0
1	G	223	THR	2.0
1	A	244	PRO	2.0
1	H	29	PRO	2.0
1	F	142	GLN	2.0
1	F	258	HIS	2.0
1	D	140	TYR	2.0
1	G	227	PHE	2.0
1	H	197	SER	2.0
1	G	212	THR	2.0
1	A	74	LEU	2.0
1	F	143	LEU	2.0
1	G	152	LEU	2.0
1	F	138	ILE	2.0
1	D	139	ARG	2.0
1	H	113	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

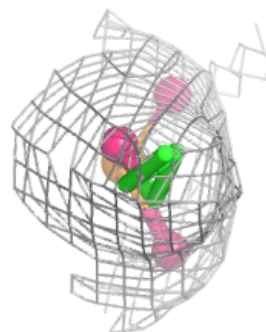
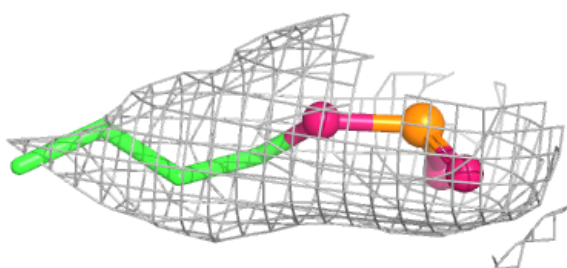
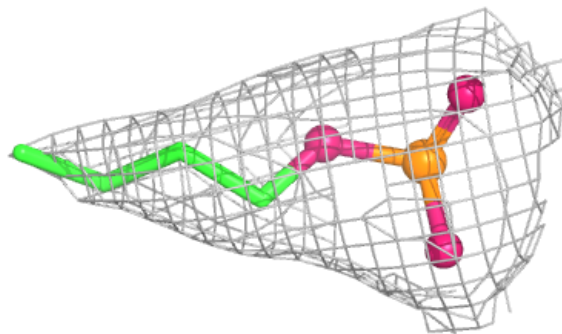
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MPD	C	304	8/8	0.78	0.17	83,85,85,86	0
3	MPD	D	302	8/8	0.82	0.26	86,87,88,89	0
3	MPD	F	303	8/8	0.83	0.14	89,90,91,91	0
3	MPD	F	302	8/8	0.84	0.17	107,108,108,109	0
3	MPD	B	402	8/8	0.86	0.16	73,75,77,78	0
3	MPD	G	302	8/8	0.86	0.17	84,85,88,88	0
2	E9H	H	301	6/21	0.87	0.15	95,96,100,100	0
3	MPD	D	303	8/8	0.88	0.14	80,82,83,83	0
3	MPD	C	303	8/8	0.89	0.19	69,70,72,72	0
4	CA	C	302	1/1	0.89	0.09	125,125,125,125	0
3	MPD	E	302	8/8	0.90	0.15	94,96,97,97	0
3	MPD	A	403	8/8	0.91	0.14	71,73,74,75	0
3	MPD	A	402	8/8	0.91	0.20	85,85,86,88	0
3	MPD	B	403	8/8	0.91	0.13	84,84,85,85	0
2	E9H	F	301	5/21	0.92	0.11	67,69,70,70	0
4	CA	A	404	1/1	0.94	0.10	72,72,72,72	0
2	E9H	B	401	5/21	0.94	0.11	52,54,56,57	0
2	E9H	G	301	5/21	0.95	0.09	81,81,81,81	0
2	E9H	C	301	8/21	0.95	0.10	56,59,66,67	0
2	E9H	E	301	6/21	0.97	0.10	63,63,68,69	0
2	E9H	A	401	7/21	0.97	0.09	50,52,55,55	0
2	E9H	D	301	8/21	0.97	0.09	44,51,57,58	0

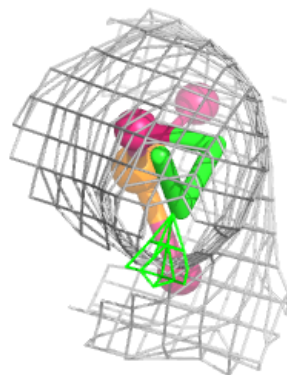
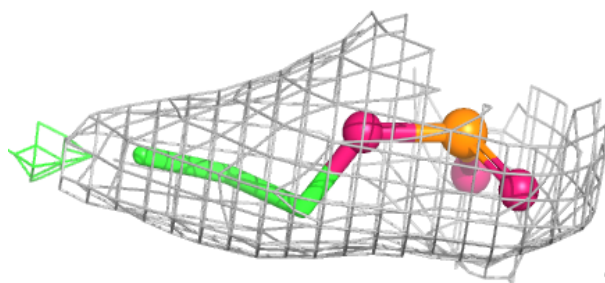
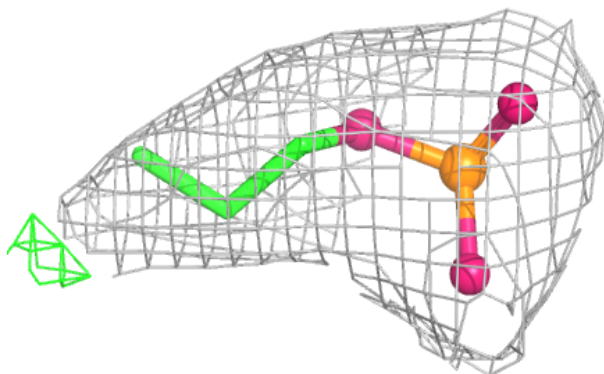
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around E9H C 301:

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

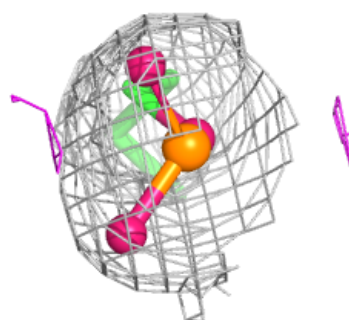
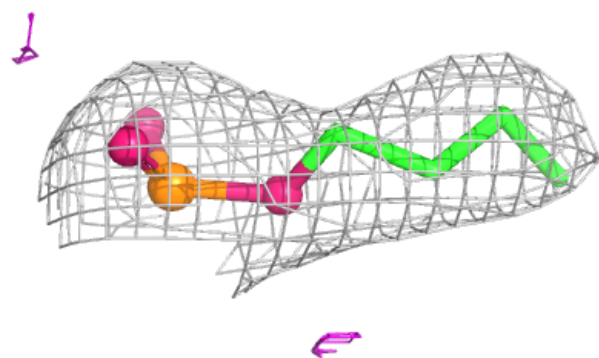
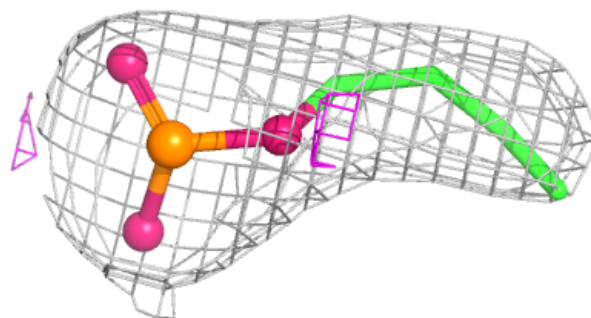
**Electron density around E9H A 401:**

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



Electron density around E9H D 301:

$2mF_o-DF_c$ (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.