Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 07:46 PM EDT

PDB ID	:	6FVJ
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 (i) symbol.

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

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

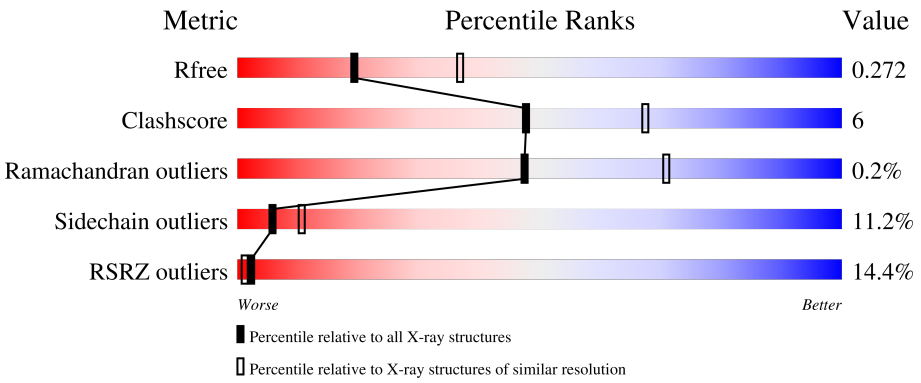
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	6% 68% 10% • 20%
1	B	261	8% 70% 9% • 19%
1	C	261	5% 64% 11% • 21%
1	D	261	8% 73% 11% • 15%
1	E	261	8% 66% 13% • 18%

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Mol	Chain	Length	Quality of chain
1	F	261	8% 67% 10% • 20%
1	G	261	21% 64% 12% • 21%
1	H	261	29% 59% 16% • 21%

2 Entry composition (i)

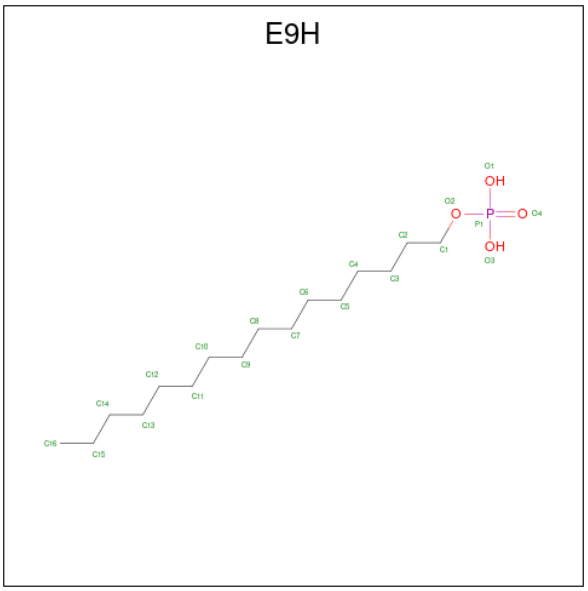
There are 5 unique types of molecules in this entry. The entry contains 13549 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

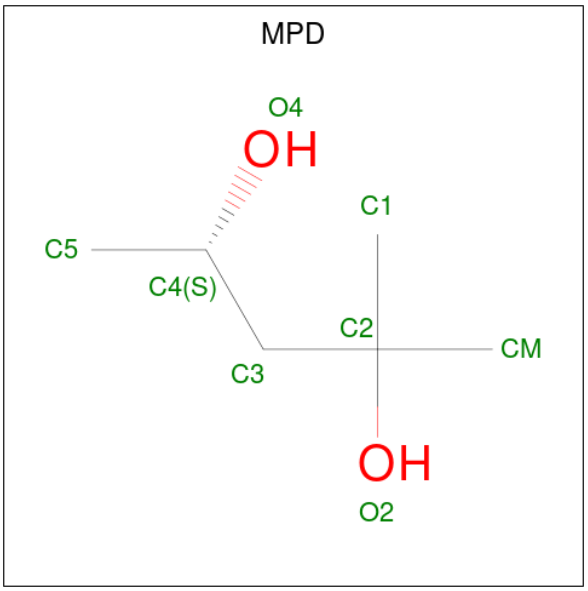
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	209	1598	1029	268	293	8	0	0	0
1	B	212	1628	1038	278	303	9	0	0	0
1	C	205	1590	1023	261	297	9	0	0	0
1	D	223	1696	1085	286	317	8	0	0	0
1	E	213	1651	1063	274	305	9	0	0	0
1	F	208	1616	1033	273	301	9	0	0	0
1	G	206	1577	1015	263	291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

- Molecule 2 is hexadecyl dihydrogen phosphate (three-letter code: E9H) (formula: $C_{16}H_{35}O_4P$).



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

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is water.

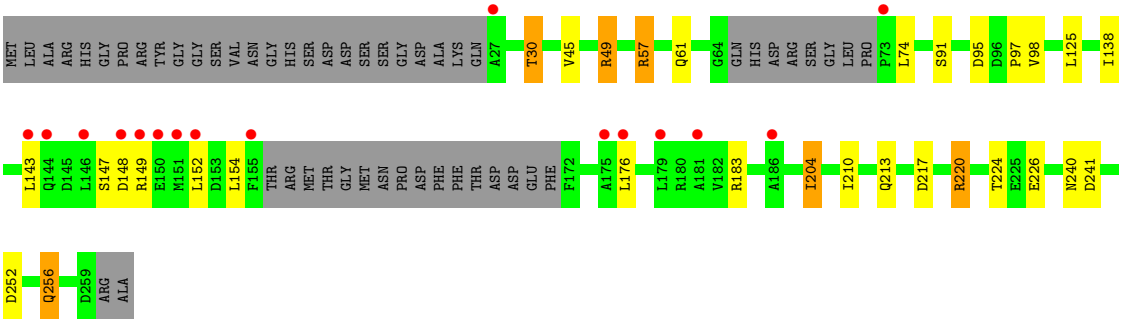
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	69	69	69	0	0
			Total	O		
5	B	72	72	72	0	0
			Total	O		
5	C	72	72	72	0	0
			Total	O		
5	D	83	83	83	0	0
			Total	O		
5	E	49	49	49	0	0
			Total	O		
5	F	49	49	49	0	0
			Total	O		
5	G	36	36	36	0	0
			Total	O		
5	H	36	36	36	0	0

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.

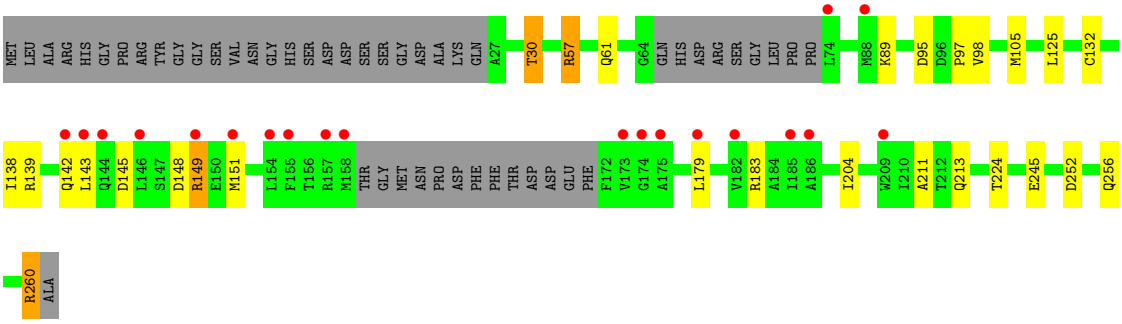
- Molecule 1: Thioesterase

Chain A:



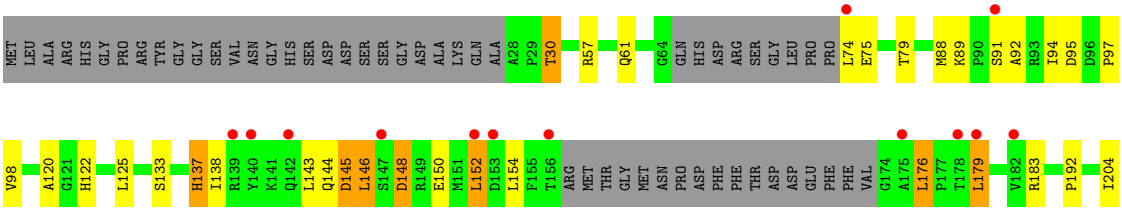
- Molecule 1: Thioesterase

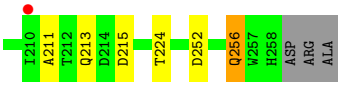
Chain B:



- Molecule 1: Thioesterase

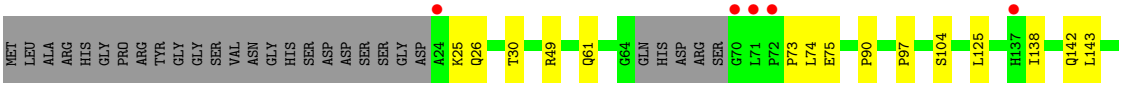
Chain C:

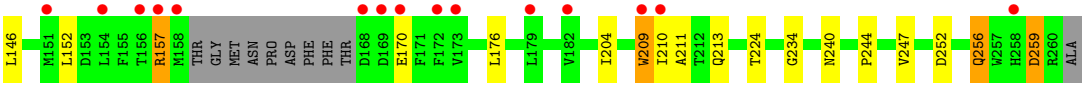




• Molecule 1: Thioesterase

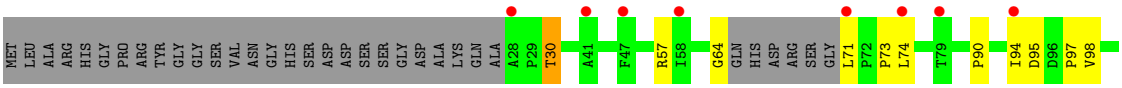
Chain D:

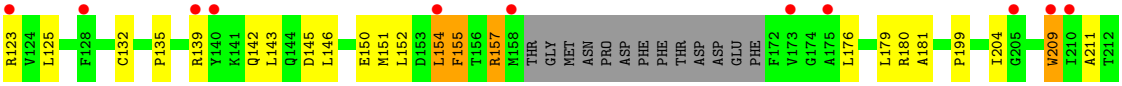




• Molecule 1: Thioesterase

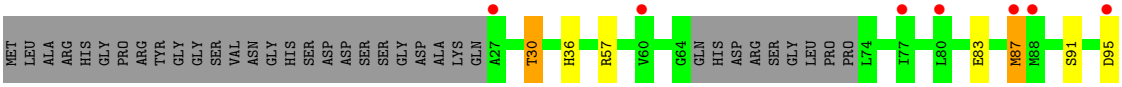
Chain E:

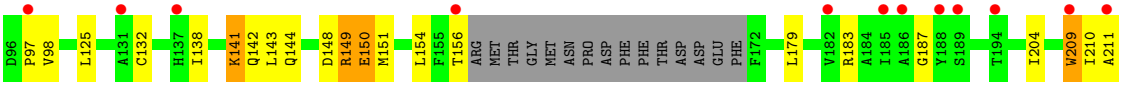




• Molecule 1: Thioesterase

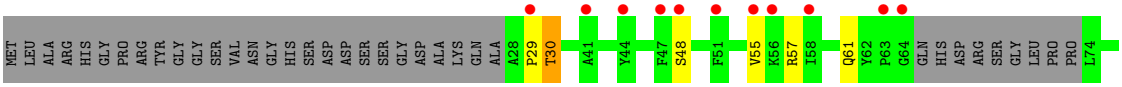
Chain F:

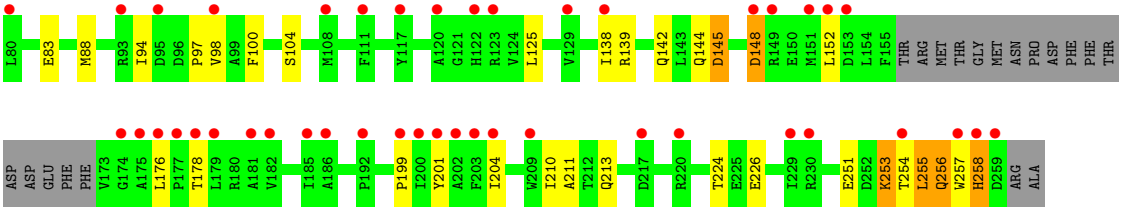




• Molecule 1: Thioesterase

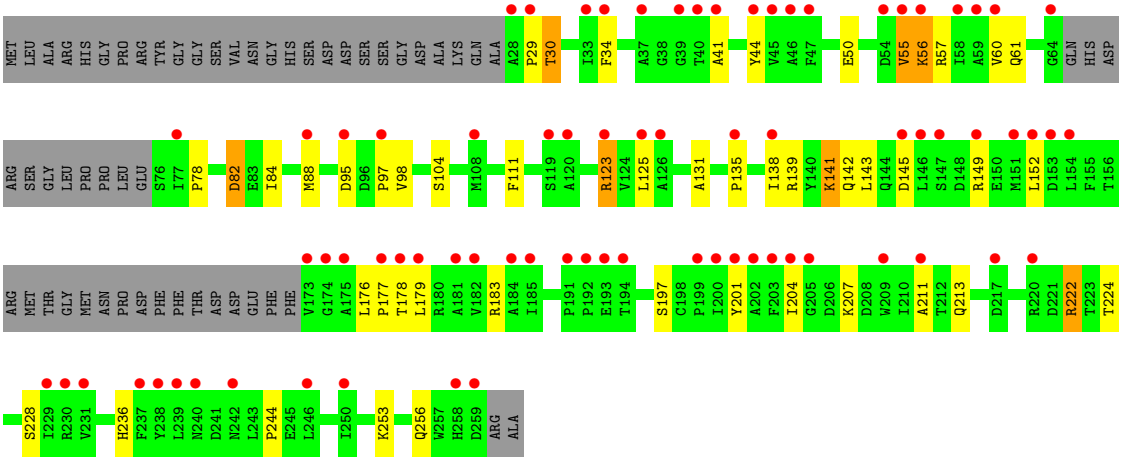
Chain G:





- Molecule 1: Thioesterase

Chain H:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.85 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.236 , 0.259 0.250 , 0.272	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)	0.30 , 69.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	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.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.43	0/1643	0.63	0/2238
1	B	0.44	0/1672	0.64	0/2274
1	C	0.43	0/1634	0.65	0/2223
1	D	0.45	1/1741 (0.1%)	0.64	0/2370
1	E	0.43	0/1698	0.64	0/2311
1	F	0.43	0/1660	0.64	0/2256
1	G	0.41	0/1621	0.65	1/2208 (0.0%)
1	H	0.47	0/1622	0.81	1/2206 (0.0%)
All	All	0.44	1/13291 (0.0%)	0.66	2/18086 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	104	SER	CB-OG	-5.24	1.35	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	104	SER	CA-CB-OG	20.86	167.51	111.20
1	G	104	SER	CA-CB-OG	5.67	126.52	111.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1598	0	1503	16	0
1	B	1628	0	1510	18	0
1	C	1590	0	1504	28	0
1	D	1696	0	1582	15	0
1	E	1651	0	1560	22	0
1	F	1616	0	1524	19	0
1	G	1577	0	1476	22	0
1	H	1579	0	1484	26	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
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	154	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 (154) 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:E:199:PRO:HB3	1:E:226:GLU:HG2	1.58	0.84
1:C:145:ASP:CG	1:C:148:ASP:HB2	1.98	0.84
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:132:CYS:HA	3:E:302:MPD:HM3	1.85	0.58
1:C:148:ASP:C	1:C:150:GLU:H	2.05	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:G:88:MET:HE1	1:G:100:PHE:HE1	1.69	0.56
1:D:240:ASN:HD21	3:D:303:MPD:H32	1.70	0.56
1:C:152:LEU:HD13	1:C:179:LEU:HD11	1.88	0.56
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:G:254:THR:HB	1:G:255:LEU:HD23	1.90	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: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: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:H:30:THR:HG23	1:H:98:VAL:HG12	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:145:ASP:OD2	1:C:148:ASP:CG	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:111:PHE:CZ	1:H:222:ARG:HD3	2.55	0.42
1:C:148:ASP:C	1:C:150:GLU:N	2.73	0.41
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%)	29	52
1	D	217/261 (83%)	199 (92%)	16 (7%)	2 (1%)	17	35
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%)	29	52
All	All	1633/2088 (78%)	1547 (95%)	82 (5%)	4 (0%)	47	71

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 (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	160/216 (74%)	142 (89%)	18 (11%)	6	10
1	B	162/216 (75%)	148 (91%)	14 (9%)	10	20
1	C	164/216 (76%)	144 (88%)	20 (12%)	5	9
1	D	169/216 (78%)	153 (90%)	16 (10%)	8	16
1	E	169/216 (78%)	150 (89%)	19 (11%)	6	10
1	F	165/216 (76%)	148 (90%)	17 (10%)	7	13
1	G	158/216 (73%)	137 (87%)	21 (13%)	4	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	160/216 (74%)	138 (86%)	22 (14%)	3 6
All	All	1307/1728 (76%)	1160 (89%)	147 (11%)	6 10

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	49	ARG
1	A	57	ARG
1	A	74	LEU
1	A	91	SER
1	A	95	ASP
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	204	ILE
1	A	213	GLN
1	A	220	ARG
1	A	224	THR
1	A	256	GLN
1	B	30	THR
1	B	57	ARG
1	B	95	ASP
1	B	105	MET
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	213	GLN
1	B	224	THR
1	B	245	GLU
1	B	260	ARG
1	C	30	THR
1	C	57	ARG
1	C	75	GLU
1	C	88	MET

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Mol	Chain	Res	Type
1	C	94	ILE
1	C	95	ASP
1	C	137	HIS
1	C	143	LEU
1	C	144	GLN
1	C	145	ASP
1	C	146	LEU
1	C	148	ASP
1	C	152	LEU
1	C	154	LEU
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	143	LEU
1	D	146	LEU
1	D	152	LEU
1	D	157	ARG
1	D	176	LEU
1	D	209	TRP
1	D	213	GLN
1	D	224	THR
1	D	256	GLN
1	D	259	ASP
1	E	30	THR
1	E	57	ARG
1	E	74	LEU
1	E	94	ILE
1	E	95	ASP
1	E	123	ARG
1	E	142	GLN
1	E	145	ASP
1	E	146	LEU
1	E	151	MET

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Mol	Chain	Res	Type
1	E	152	LEU
1	E	154	LEU
1	E	155	PHE
1	E	157	ARG
1	E	209	TRP
1	E	213	GLN
1	E	222	ARG
1	E	224	THR
1	E	256	GLN
1	F	30	THR
1	F	57	ARG
1	F	87	MET
1	F	91	SER
1	F	95	ASP
1	F	141	LYS
1	F	142	GLN
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	209	TRP
1	F	213	GLN
1	F	224	THR
1	F	256	GLN
1	G	30	THR
1	G	61	GLN
1	G	83	GLU
1	G	94	ILE
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

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Mol	Chain	Res	Type
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	44	TYR
1	H	55	VAL
1	H	56	LYS
1	H	57	ARG
1	H	60	VAL
1	H	82	ASP
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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	142	GLN
1	D	26	GLN
1	D	142	GLN
1	D	240	ASN
1	E	256	GLN
1	G	256	GLN
1	G	258	HIS
1	H	61	GLN
1	H	142	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	$\#\|Z\| > 2$
3	MPD	A	403	-	7,7,7	0.63	0	9,10,10	0.30	0
2	E9H	G	301	1	1,4,20	0.20	0	0,4,22	-	-
3	MPD	C	303	-	7,7,7	0.60	0	9,10,10	0.40	0
3	MPD	E	302	-	7,7,7	0.64	0	9,10,10	0.58	0
2	E9H	H	301	1	2,5,20	0.83	0	1,5,22	0.34	0
3	MPD	F	302	-	7,7,7	0.47	0	9,10,10	0.49	0
3	MPD	B	403	-	7,7,7	0.71	0	9,10,10	0.52	0
3	MPD	D	302	-	7,7,7	0.41	0	9,10,10	0.29	0
3	MPD	C	304	-	7,7,7	0.84	0	9,10,10	0.61	0
3	MPD	A	402	-	7,7,7	0.46	0	9,10,10	0.41	0
2	E9H	B	401	1	2,4,20	0.68	0	1,3,22	0.27	0
2	E9H	F	301	1	1,4,20	0.21	0	0,4,22	-	-
3	MPD	B	402	-	7,7,7	0.64	0	9,10,10	0.37	0
3	MPD	F	303	-	7,7,7	0.52	0	9,10,10	0.38	0
2	E9H	D	301	1	4,7,20	0.47	0	3,7,22	0.35	0
3	MPD	G	302	-	7,7,7	0.50	0	9,10,10	0.35	0
2	E9H	E	301	1	2,5,20	0.78	0	1,5,22	0.34	0
2	E9H	C	301	1	4,7,20	0.43	0	3,7,22	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MPD	D	303	-	7,7,7	0.60	0	9,10,10	0.34	0
2	E9H	A	401	1	3,6,20	0.56	0	2,6,22	0.33	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
3	MPD	A	403	-	-	0/5/5/5	-
2	E9H	G	301	1	-	0/0/2/18	-
3	MPD	C	303	-	-	0/5/5/5	-
3	MPD	E	302	-	-	2/5/5/5	-
2	E9H	H	301	1	-	0/1/3/18	-
3	MPD	F	302	-	-	3/5/5/5	-
3	MPD	B	403	-	-	1/5/5/5	-
3	MPD	D	302	-	-	0/5/5/5	-
3	MPD	C	304	-	-	4/5/5/5	-
3	MPD	A	402	-	-	3/5/5/5	-
2	E9H	B	401	1	-	0/0/2/18	-
2	E9H	F	301	1	-	0/0/2/18	-
3	MPD	B	402	-	-	0/5/5/5	-
3	MPD	F	303	-	-	0/5/5/5	-
2	E9H	D	301	1	-	2/3/5/18	-
3	MPD	G	302	-	-	3/5/5/5	-
2	E9H	E	301	1	-	0/1/3/18	-
2	E9H	C	301	1	-	1/3/5/18	-
3	MPD	D	303	-	-	1/5/5/5	-
2	E9H	A	401	1	-	1/2/4/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	E9H	O2-C1-C2-C3
3	C	304	MPD	C1-C2-C3-C4
3	C	304	MPD	C2-C3-C4-O4

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

There are no ring outliers.

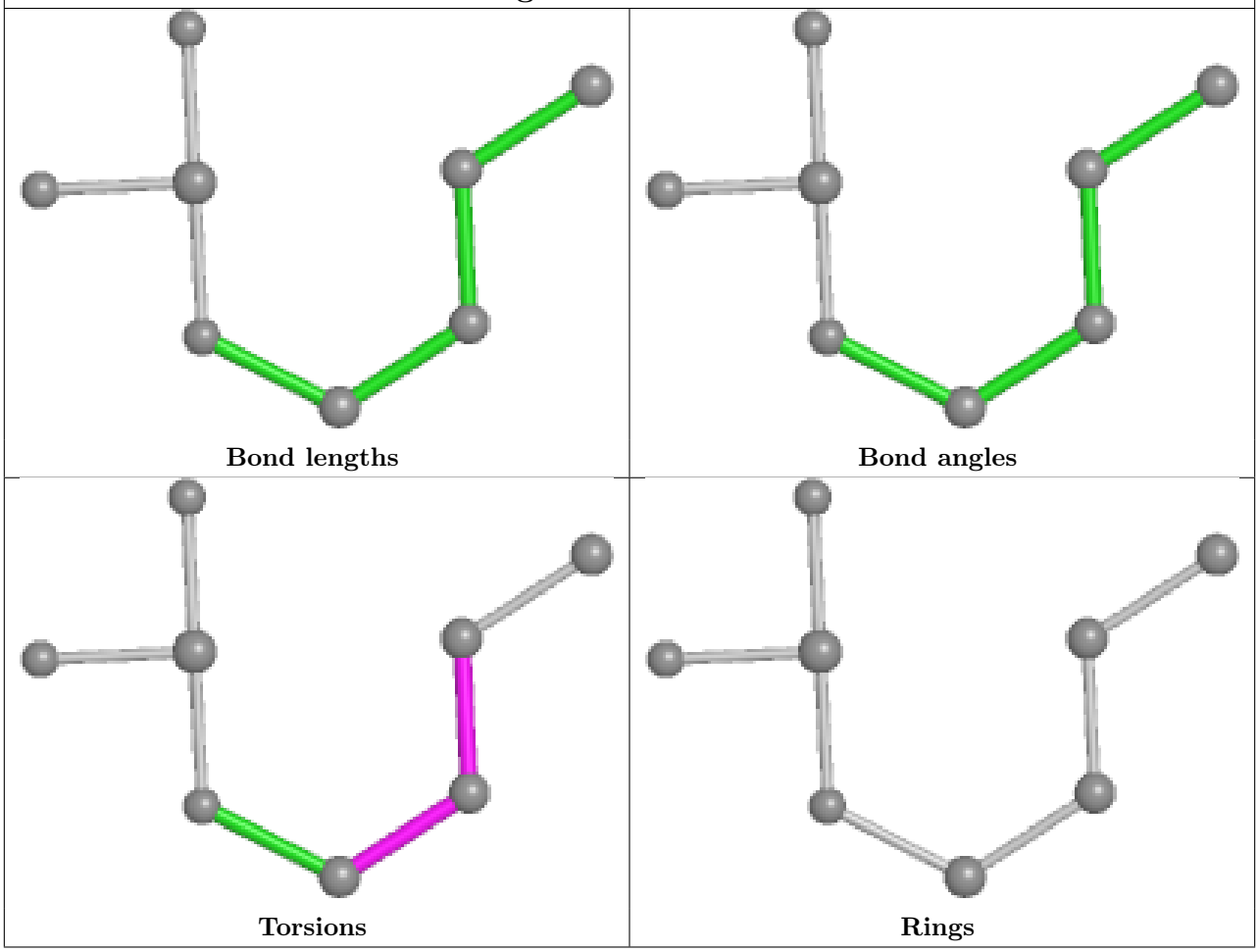
10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	MPD	1	0
3	C	303	MPD	1	0
3	E	302	MPD	2	0
3	F	302	MPD	5	0
3	D	302	MPD	1	0
3	A	402	MPD	1	0
3	B	402	MPD	1	0
3	F	303	MPD	1	0
3	G	302	MPD	1	0
3	D	303	MPD	1	0

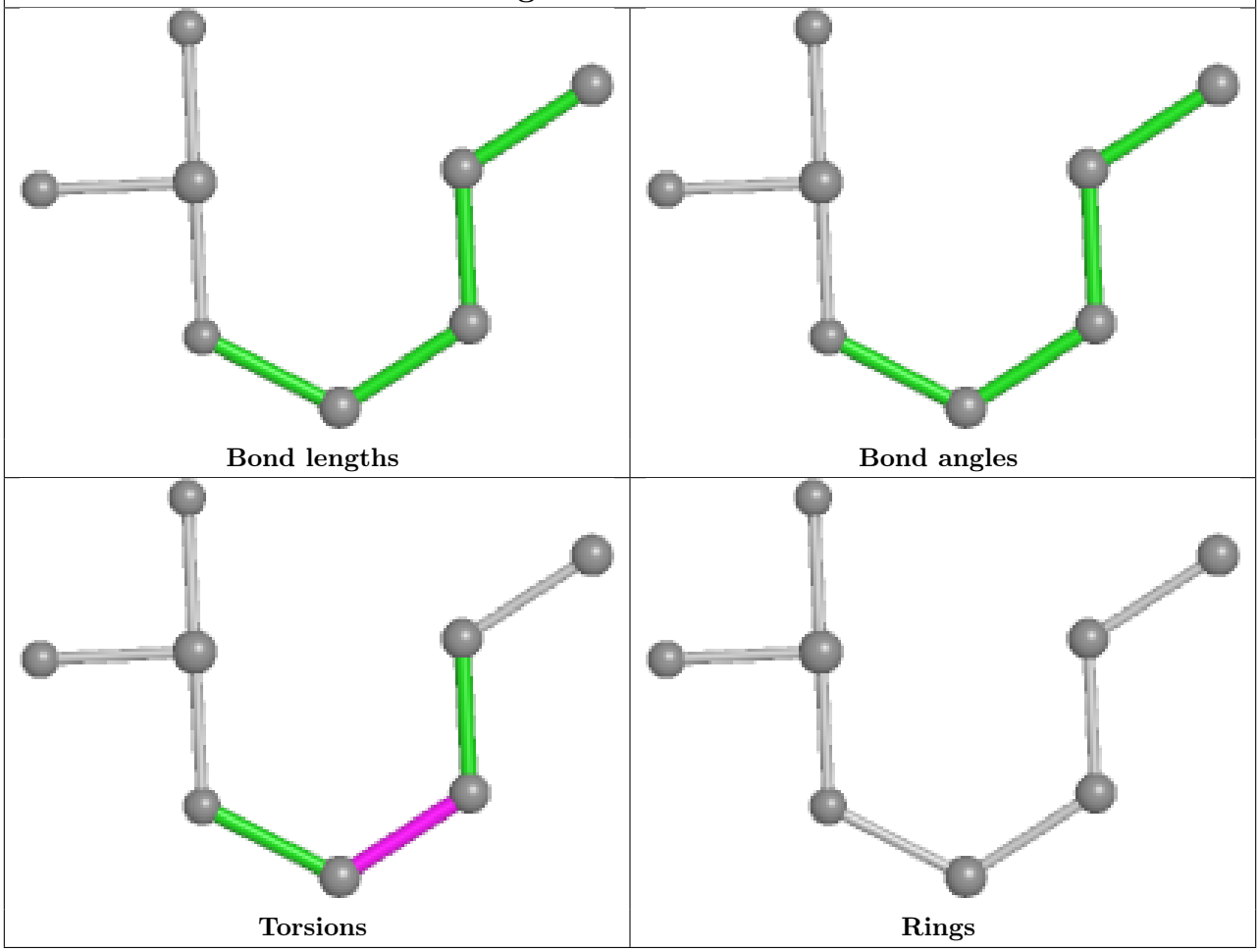
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

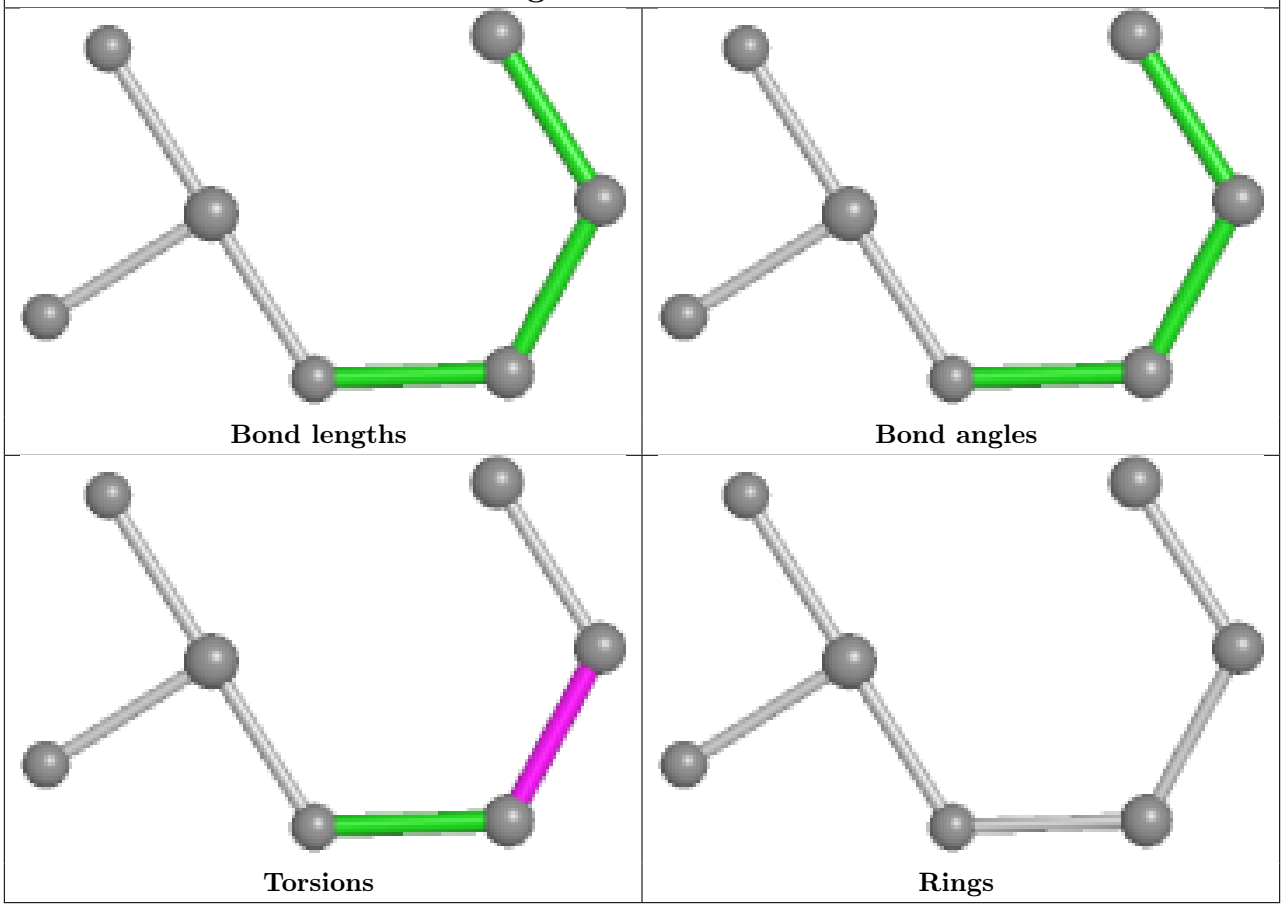
Ligand E9H D 301



Ligand E9H C 301



Ligand E9H A 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	209/261 (80%)	0.40	16 (7%)	13	10	41, 65, 157, 216	0
1	B	212/261 (81%)	0.44	20 (9%)	8	5	41, 60, 160, 195	0
1	C	205/261 (78%)	0.33	14 (6%)	17	12	43, 67, 149, 190	0
1	D	223/261 (85%)	0.40	20 (8%)	9	6	37, 55, 149, 193	0
1	E	213/261 (81%)	0.43	21 (9%)	7	5	45, 84, 145, 155	0
1	F	208/261 (79%)	0.60	21 (10%)	7	4	55, 83, 136, 149	0
1	G	206/261 (78%)	1.43	54 (26%)	0	0	72, 110, 163, 247	0
1	H	205/261 (78%)	1.80	76 (37%)	0	0	80, 107, 144, 165	0
All	All	1681/2088 (80%)	0.72	242 (14%)	2	1	37, 80, 149, 247	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	178	THR	9.5
1	G	175	ALA	9.3
1	H	204	ILE	9.1
1	G	149	ARG	7.7
1	H	181	ALA	7.6
1	H	177	PRO	7.2
1	G	179	LEU	7.1
1	D	172	PHE	7.1
1	G	181	ALA	7.0
1	H	125	LEU	6.9
1	B	151	MET	6.9
1	D	158	MET	6.8
1	A	150	GLU	6.7
1	G	55	VAL	6.6
1	H	242	ASN	6.6
1	H	146	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
1	H	173	VAL	6.0
1	C	156	THR	5.9
1	H	239	LEU	5.9
1	G	174	GLY	5.8
1	B	149	ARG	5.7
1	B	179	LEU	5.5
1	H	119	SER	5.4
1	H	120	ALA	5.4
1	B	154	LEU	5.4
1	H	179	LEU	5.3
1	B	146	LEU	5.3
1	G	98	VAL	5.2
1	H	41	ALA	5.2
1	G	123	ARG	5.2
1	H	149	ARG	5.1
1	C	74	LEU	5.1
1	A	148	ASP	5.1
1	C	152	LEU	5.1
1	H	154	LEU	5.0
1	G	185	ILE	5.0
1	F	137	HIS	5.0
1	F	188	TYR	5.0
1	H	175	ALA	4.9
1	G	259	ASP	4.8
1	H	55	VAL	4.7
1	C	147	SER	4.6
1	H	153	ASP	4.6
1	D	209	TRP	4.6
1	H	58	ILE	4.6
1	G	153	ASP	4.6
1	D	179	LEU	4.6
1	H	182	VAL	4.6
1	C	139	ARG	4.5
1	A	149	ARG	4.5
1	B	155	PHE	4.5
1	D	70	GLY	4.3
1	C	179	LEU	4.3
1	F	182	VAL	4.2
1	H	174	GLY	4.1
1	H	37	ALA	4.1
1	A	186	ALA	4.1
1	D	72	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	178	THR	4.0
1	H	108	MET	4.0
1	H	126	ALA	4.0
1	D	157	ARG	4.0
1	H	258	HIS	4.0
1	F	189	SER	4.0
1	G	257	TRP	4.0
1	F	209	TRP	3.9
1	H	44	TYR	3.9
1	C	153	ASP	3.9
1	H	185	ILE	3.9
1	H	184	ALA	3.9
1	G	182	VAL	3.8
1	D	169	ASP	3.8
1	H	201	TYR	3.8
1	G	192	PRO	3.8
1	H	259	ASP	3.8
1	A	179	LEU	3.8
1	E	154	LEU	3.8
1	H	147	SER	3.7
1	G	47	PHE	3.7
1	B	175	ALA	3.7
1	H	135	PRO	3.7
1	H	145	ASP	3.7
1	C	91	SER	3.6
1	B	173	VAL	3.6
1	A	175	ALA	3.6
1	H	64	GLY	3.5
1	G	258	HIS	3.5
1	E	158	MET	3.5
1	H	95	ASP	3.4
1	G	186	ALA	3.4
1	G	200	ILE	3.4
1	H	193	GLU	3.4
1	H	191	PRO	3.4
1	D	173	VAL	3.4
1	G	220	ARG	3.4
1	G	201	TYR	3.3
1	C	182	VAL	3.3
1	B	174	GLY	3.3
1	H	200	ILE	3.3
1	G	56	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	111	PHE	3.3
1	F	211	ALA	3.3
1	G	138	ILE	3.3
1	B	142	GLN	3.3
1	F	212	THR	3.2
1	G	117	TYR	3.2
1	G	108	MET	3.2
1	H	178	THR	3.2
1	G	152	LEU	3.2
1	D	151	MET	3.1
1	E	173	VAL	3.1
1	B	185	ILE	3.1
1	D	71	LEU	3.1
1	H	209	TRP	3.1
1	H	250	ILE	3.1
1	G	176	LEU	3.1
1	H	217	ASP	3.1
1	D	24	ALA	3.0
1	H	40	THR	3.0
1	E	258	HIS	3.0
1	F	186	ALA	3.0
1	G	44	TYR	3.0
1	C	140	TYR	2.9
1	G	120	ALA	2.9
1	H	47	PHE	2.9
1	D	210	ILE	2.9
1	G	122	HIS	2.9
1	H	231	VAL	2.9
1	G	199	PRO	2.9
1	H	28	ALA	2.9
1	H	203	PHE	2.9
1	G	64	GLY	2.8
1	H	39	GLY	2.8
1	G	95	ASP	2.8
1	H	238	TYR	2.8
1	G	229	ILE	2.8
1	F	88	MET	2.8
1	H	46	ALA	2.8
1	E	123	ARG	2.8
1	G	230	ARG	2.8
1	E	71	LEU	2.8
1	A	143	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	74	LEU	2.8
1	D	154	LEU	2.8
1	G	41	ALA	2.8
1	G	209	TRP	2.8
1	G	203	PHE	2.8
1	B	157	ARG	2.8
1	F	97	PRO	2.7
1	H	29	PRO	2.7
1	E	209	TRP	2.7
1	H	246	LEU	2.7
1	G	93	ARG	2.7
1	H	211	ALA	2.7
1	F	185	ILE	2.6
1	H	34	PHE	2.6
1	E	47	PHE	2.6
1	D	156	THR	2.6
1	E	139	ARG	2.6
1	G	129	VAL	2.6
1	G	204	ILE	2.6
1	H	60	VAL	2.6
1	F	77	ILE	2.6
1	F	95	ASP	2.5
1	E	28	ALA	2.5
1	B	186	ALA	2.5
1	F	27	ALA	2.5
1	H	152	LEU	2.5
1	H	123	ARG	2.5
1	C	142	GLN	2.5
1	E	58	ILE	2.5
1	H	88	MET	2.5
1	E	140	TYR	2.5
1	B	88	MET	2.4
1	D	170	GLU	2.4
1	C	175	ALA	2.4
1	C	210	ILE	2.4
1	B	182	VAL	2.4
1	F	87	MET	2.4
1	H	194	THR	2.4
1	H	237	PHE	2.4
1	B	158	MET	2.4
1	G	151	MET	2.4
1	H	54	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	230	ARG	2.4
1	A	176	LEU	2.4
1	G	217	ASP	2.4
1	H	151	MET	2.4
1	H	59	ALA	2.4
1	F	131	ALA	2.3
1	E	128	PHE	2.3
1	F	194	THR	2.3
1	E	210	ILE	2.3
1	F	60	VAL	2.3
1	G	29	PRO	2.3
1	H	202	ALA	2.3
1	A	151	MET	2.3
1	B	143	LEU	2.3
1	A	155	PHE	2.3
1	E	205	GLY	2.3
1	G	63	PRO	2.3
1	A	146	LEU	2.3
1	A	73	PRO	2.3
1	H	33	ILE	2.3
1	B	209	TRP	2.2
1	A	181	ALA	2.2
1	H	97	PRO	2.2
1	H	220	ARG	2.2
1	A	144	GLN	2.2
1	H	229	ILE	2.2
1	H	77	ILE	2.2
1	D	182	VAL	2.2
1	G	80	LEU	2.2
1	G	177	PRO	2.2
1	H	199	PRO	2.2
1	G	254	THR	2.2
1	D	168	ASP	2.2
1	E	175	ALA	2.2
1	G	58	ILE	2.1
1	B	144	GLN	2.1
1	H	45	VAL	2.1
1	D	258	HIS	2.1
1	E	41	ALA	2.1
1	G	48	SER	2.1
1	E	259	ASP	2.1
1	H	192	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	56	LYS	2.1
1	A	152	LEU	2.1
1	F	156	THR	2.1
1	E	74	LEU	2.1
1	G	202	ALA	2.1
1	E	79	THR	2.1
1	H	240	ASN	2.1
1	F	80	LEU	2.1
1	A	27	ALA	2.1
1	H	205	GLY	2.1
1	H	138	ILE	2.0
1	G	148	ASP	2.0
1	F	258	HIS	2.0
1	E	94	ILE	2.0
1	G	51	PHE	2.0
1	D	137	HIS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	C	302	1/1	0.79	0.15	125,125,125,125	0
3	MPD	D	302	8/8	0.81	0.56	86,87,88,89	0
3	MPD	C	304	8/8	0.83	0.30	83,85,85,86	0
3	MPD	F	302	8/8	0.84	0.37	107,108,108,109	0
3	MPD	F	303	8/8	0.86	0.30	89,90,91,91	0
3	MPD	D	303	8/8	0.89	0.22	80,82,83,83	0
3	MPD	B	402	8/8	0.90	0.26	73,75,77,78	0

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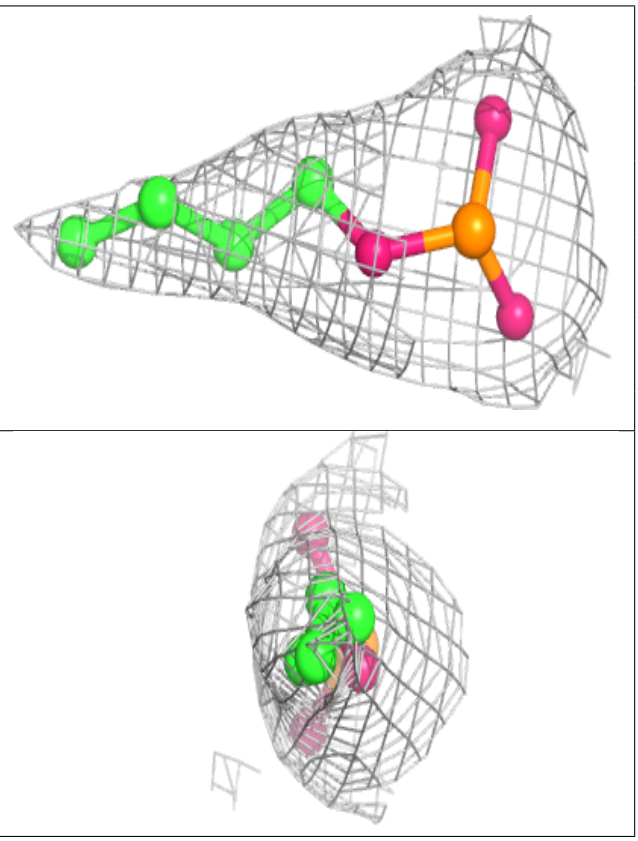
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MPD	A	403	8/8	0.90	0.28	71,73,74,75	0
3	MPD	E	302	8/8	0.90	0.46	94,96,97,97	0
2	E9H	H	301	6/21	0.91	0.20	95,96,100,100	0
3	MPD	G	302	8/8	0.93	0.27	84,85,88,88	0
3	MPD	C	303	8/8	0.93	0.27	69,70,72,72	0
3	MPD	B	403	8/8	0.94	0.23	84,84,85,85	0
4	CA	A	404	1/1	0.94	0.09	72,72,72,72	0
3	MPD	A	402	8/8	0.94	0.26	85,85,86,88	0
2	E9H	F	301	5/21	0.96	0.13	67,69,70,70	0
2	E9H	B	401	5/21	0.96	0.17	52,54,56,57	0
2	E9H	G	301	5/21	0.97	0.16	81,81,81,81	0
2	E9H	C	301	8/21	0.97	0.19	56,59,66,67	0
2	E9H	E	301	6/21	0.98	0.17	63,63,68,69	0
2	E9H	A	401	7/21	0.98	0.19	50,52,55,55	0
2	E9H	D	301	8/21	0.98	0.15	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.

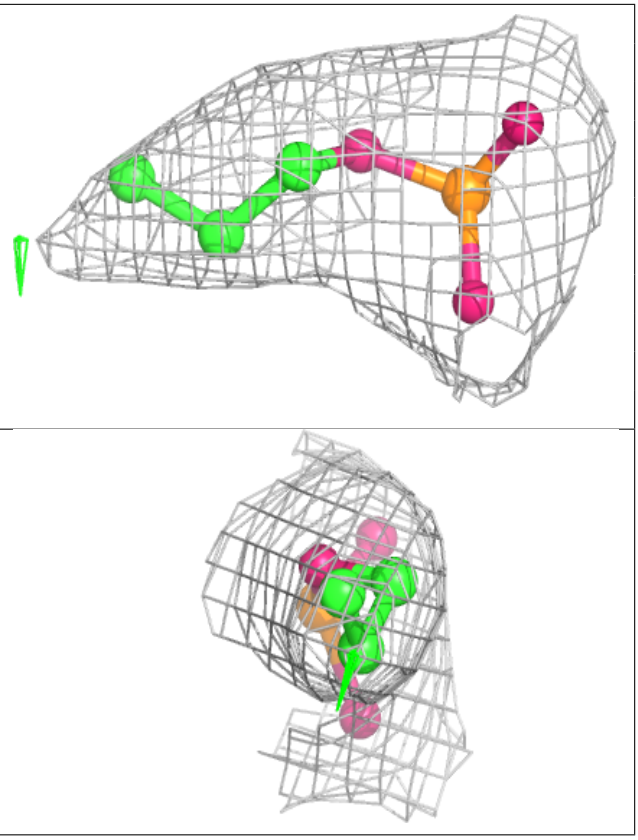
Electron density around E9H C 301:

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



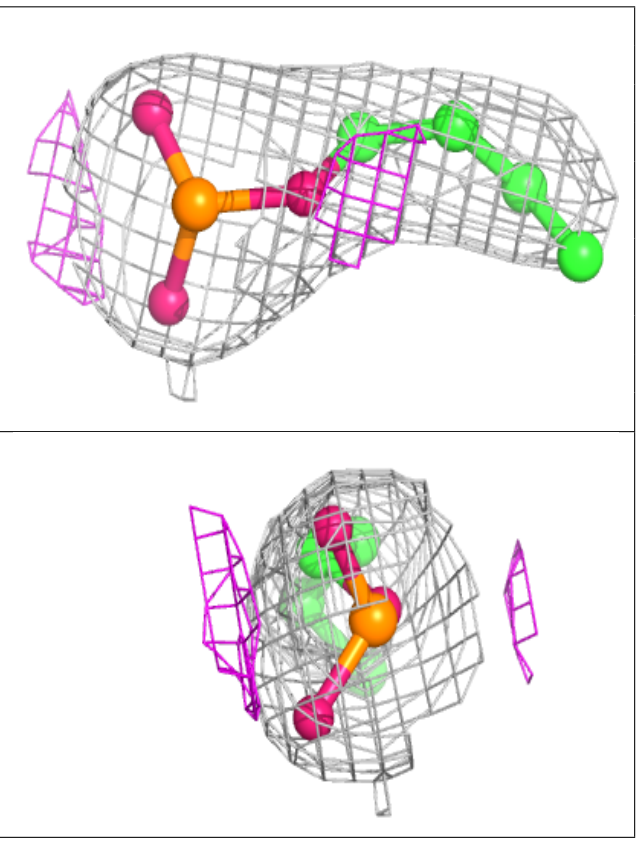
Electron density around E9H A 401:

$2mF_o$-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.