



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:21 AM UTC

PDB ID : 6TXL / pdb_00006txl
Title : Crystal structure of thermotoga maritima E65Q Ferritin
Authors : Wilk, P.; Grudnik, P.; Kumar, M.; Heddle, J.; Chakraborti, S.
Deposited on : 2020-01-14
Resolution : 2.10 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

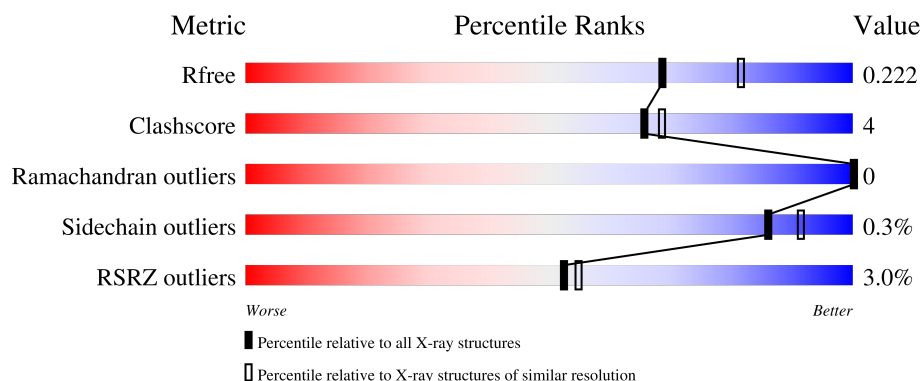
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	164	3% 90% 10%
1	B	164	% 92% 8%
1	C	164	4% 90% 10%
1	D	164	% 93% 7%
1	E	164	% 95% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	164	4% 89% 11%
1	G	164	4% 91% 9%
1	H	164	7% 85% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	F	202	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11921 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 Ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	2	0
			1379	882	225	266	6			
1	B	164	Total	C	N	O	S	0	7	0
			1413	905	233	269	6			
1	C	164	Total	C	N	O	S	0	4	0
			1391	890	226	269	6			
1	D	164	Total	C	N	O	S	0	3	0
			1387	888	229	264	6			
1	E	164	Total	C	N	O	S	0	5	0
			1396	894	229	267	6			
1	F	164	Total	C	N	O	S	0	3	0
			1385	886	226	267	6			
1	G	164	Total	C	N	O	S	0	2	0
			1382	884	227	265	6			
1	H	164	Total	C	N	O	S	0	6	0
			1404	899	233	266	6			

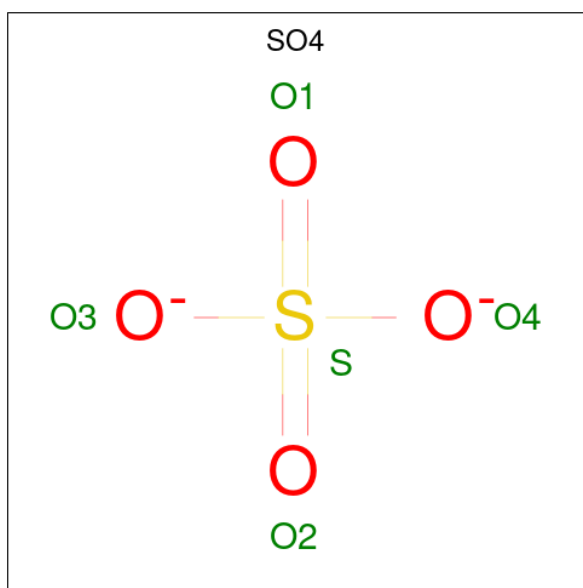
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	GLN	GLU	engineered mutation	UNP Q9X0L2
B	65	GLN	GLU	engineered mutation	UNP Q9X0L2
C	65	GLN	GLU	engineered mutation	UNP Q9X0L2
D	65	GLN	GLU	engineered mutation	UNP Q9X0L2
E	65	GLN	GLU	engineered mutation	UNP Q9X0L2
F	65	GLN	GLU	engineered mutation	UNP Q9X0L2
G	65	GLN	GLU	engineered mutation	UNP Q9X0L2
H	65	GLN	GLU	engineered mutation	UNP Q9X0L2

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0
2	G	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

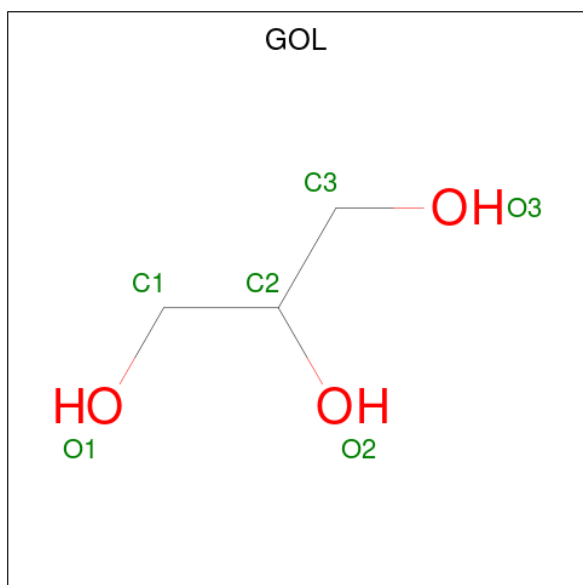
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



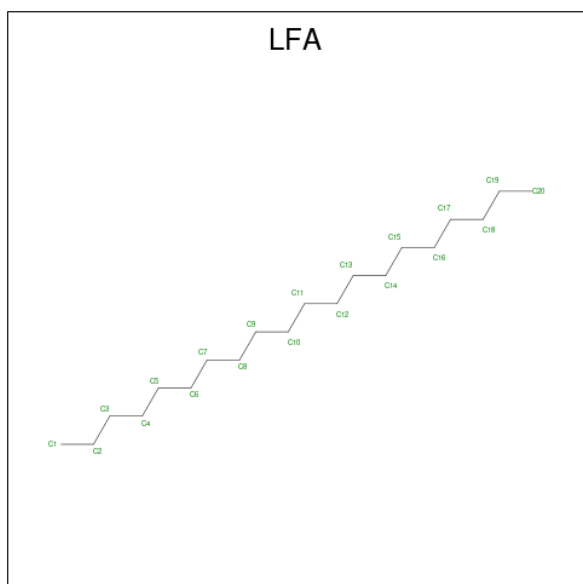
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0

- Molecule 5 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C 20 20	0	0
5	C	1	Total C 20 20	0	0
5	E	1	Total C 20 20	0	0
5	H	1	Total C 20 20	0	0

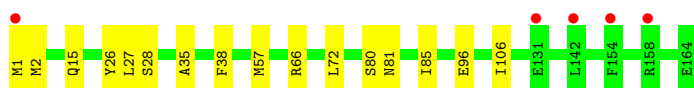
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	89	Total 89	O 89	0	0
6	B	91	Total 91	O 91	0	0
6	C	48	Total 48	O 48	0	0
6	D	68	Total 68	O 68	0	0
6	E	74	Total 74	O 74	0	0
6	F	56	Total 56	O 56	0	0
6	G	31	Total 31	O 31	0	0
6	H	14	Total 14	O 14	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.

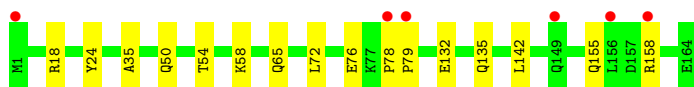
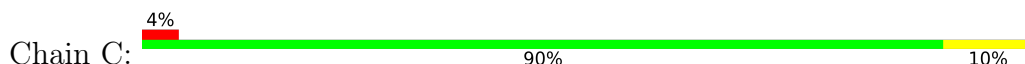
- Molecule 1: Ferritin



- Molecule 1: Ferritin



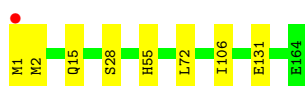
- Molecule 1: Ferritin



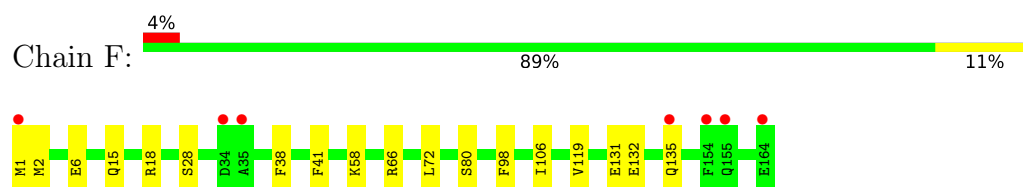
- Molecule 1: Ferritin



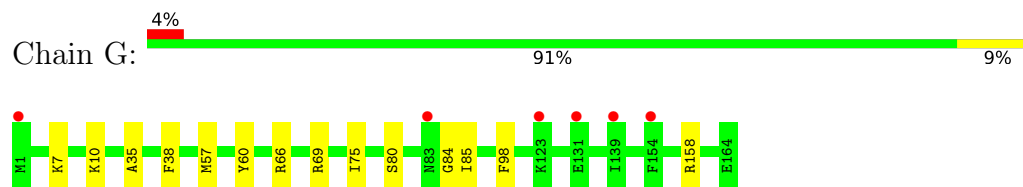
- Molecule 1: Ferritin



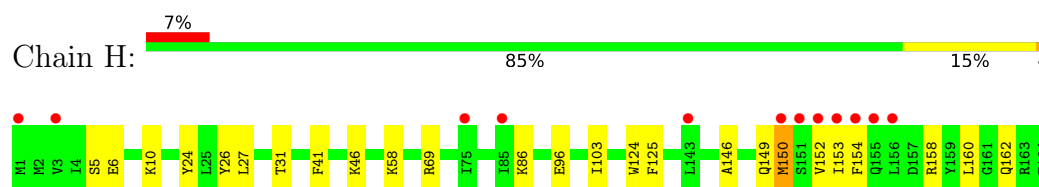
- Molecule 1: Ferritin



• Molecule 1: Ferritin



• Molecule 1: Ferritin



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	176.22Å 176.22Å 355.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.88 – 2.10 26.88 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (26.88-2.10) 88.8 (26.88-2.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.32 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.15.1_3469	Depositor
R, R_{free}	0.193 , 0.222 0.194 , 0.222	Depositor DCC
R_{free} test set	2100 reflections (1.70%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.6	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	0.96	EDS
Total number of atoms	11921	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, GOL, SO4, LFA

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	0.25	0/1414	0.38	0/1900
1	B	0.26	0/1460	0.40	0/1959
1	C	0.23	0/1431	0.40	0/1920
1	D	0.22	0/1425	0.40	0/1913
1	E	0.21	0/1440	0.35	0/1933
1	F	0.21	0/1423	0.37	0/1912
1	G	0.19	0/1414	0.34	0/1899
1	H	0.32	1/1451 (0.1%)	0.58	5/1947 (0.3%)
All	All	0.24	1/11458 (0.0%)	0.41	5/15383 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	150	MET	CB-CG	6.69	1.72	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	149	GLN	CA-C-N	-8.29	106.63	122.06
1	H	149	GLN	C-N-CA	-8.29	106.63	122.06
1	H	150	MET	CA-CB-CG	-6.34	101.41	114.10
1	H	86	LYS	CB-CG-CD	5.46	123.85	111.30
1	H	86	LYS	N-CA-CB	5.24	117.83	110.12

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	1379	0	1335	12	0
1	B	1413	0	1387	10	0
1	C	1391	0	1349	11	0
1	D	1387	0	1355	13	0
1	E	1396	0	1366	6	0
1	F	1385	0	1343	14	0
1	G	1382	0	1340	15	0
1	H	1404	0	1381	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	25	0	0	2	0
3	B	30	0	0	0	0
3	C	15	0	0	0	0
3	D	20	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	3	0
3	G	15	0	0	1	0
3	H	10	0	0	1	0
4	A	18	0	24	0	0
4	B	12	0	16	0	0
4	C	12	0	16	0	0
4	D	12	0	16	1	0
4	E	6	0	8	0	0
4	F	6	0	8	1	0
4	G	12	0	16	3	0
4	H	12	0	16	2	0
5	B	20	0	42	1	0
5	C	20	0	42	2	0
5	E	20	0	42	0	0
5	H	20	0	42	2	0
6	A	89	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	91	0	0	1	0
6	C	48	0	0	1	0
6	D	68	0	0	2	0
6	E	74	0	0	1	0
6	F	56	0	0	7	0
6	G	31	0	0	0	0
6	H	14	0	0	1	0
All	All	11921	0	11144	86	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 4.

All (86) 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:F:131[A]:GLU:OE2	6:F:301:HOH:O	1.97	0.81
1:D:66[B]:ARG:NH2	1:D:115:ASP:OD1	2.20	0.74
1:D:66[B]:ARG:HH21	1:D:117:ALA:HB3	1.55	0.71
1:H:46:LYS:HB3	5:H:205:LFA:H22	1.74	0.69
1:A:57:MET:HG3	5:B:207:LFA:H32	1.74	0.68
1:F:18:ARG:NH2	6:F:304:HOH:O	2.29	0.66
1:H:69[B]:ARG:NH1	6:H:301:HOH:O	2.25	0.64
3:F:202:SO4:O2	6:F:302:HOH:O	2.11	0.64
1:A:28:SER:HB2	1:B:72:LEU:HD12	1.81	0.63
1:B:50[A]:GLN:NE2	6:B:301:HOH:O	2.33	0.61
1:C:72:LEU:HD12	1:D:28:SER:HB2	1.83	0.60
1:G:75:ILE:HD11	1:H:24:TYR:CZ	2.35	0.60
1:B:141:ASP:OD2	1:B:145:LYS:NZ	2.35	0.59
1:A:1:MET:HE3	1:A:2:MET:H	1.70	0.57
1:D:50[A]:GLN:OE1	6:D:301:HOH:O	2.18	0.57
1:C:65:GLN:NE2	1:E:131[A]:GLU:OE2	2.33	0.54
1:G:158:ARG:HG3	1:G:158:ARG:HH11	1.73	0.54
1:G:57:MET:HE2	5:H:205:LFA:H21	1.89	0.54
1:D:3:VAL:O	1:D:66[B]:ARG:NH1	2.41	0.54
1:H:150:MET:HG2	1:H:153:ILE:HB	1.90	0.53
1:F:98:PHE:CZ	4:F:203:GOL:H12	2.43	0.53
1:F:132:GLU:O	1:F:135:GLN:HG2	2.10	0.52
1:G:98:PHE:HZ	4:G:203:GOL:H32	1.74	0.52
1:C:155:GLN:O	1:C:158:ARG:HG3	2.10	0.51
1:E:72:LEU:HD12	1:F:28:SER:HB2	1.93	0.51
3:F:202:SO4:O4	6:F:303:HOH:O	2.16	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:SER:HB2	4:H:204:GOL:H32	1.93	0.51
1:C:142:LEU:HD22	1:H:154:PHE:CZ	2.46	0.50
5:C:204:LFA:H192	1:D:57:MET:HE2	1.93	0.50
1:G:10:LYS:HD3	1:G:10:LYS:C	2.37	0.49
1:D:3:VAL:HG23	1:D:66[B]:ARG:HD2	1.95	0.49
1:A:35:ALA:HB2	1:B:69[B]:ARG:HG3	1.96	0.48
1:F:80:SER:N	3:F:204:SO4:O4	2.38	0.48
1:C:50[B]:GLN:NE2	5:C:204:LFA:H182	2.29	0.48
1:A:38:PHE:CE2	1:A:85:ILE:HD11	2.49	0.47
1:C:18:ARG:NH2	6:C:302:HOH:O	2.47	0.47
1:F:1:MET:N	6:F:305:HOH:O	2.45	0.47
1:G:98:PHE:CZ	4:G:203:GOL:H12	2.50	0.47
3:A:208:SO4:O2	6:A:301:HOH:O	2.20	0.47
1:C:35:ALA:HB2	1:D:69:ARG:HG3	1.97	0.47
1:E:55:HIS:HE1	6:E:311:HOH:O	1.98	0.46
1:A:81:ASN:OD1	1:B:69[B]:ARG:NH2	2.46	0.46
1:E:15:GLN:HB2	1:E:106:ILE:HD11	1.96	0.46
1:G:35:ALA:HB2	1:H:69[A]:ARG:HG3	1.97	0.46
1:D:18:ARG:NH1	4:D:203:GOL:O2	2.45	0.46
1:H:6:GLU:H	4:H:204:GOL:H11	1.80	0.46
1:A:72:LEU:HD12	1:B:28:SER:HB2	1.98	0.46
1:C:78:PRO:C	1:C:79:PRO:N	2.73	0.45
1:C:132:GLU:O	1:C:135[A]:GLN:HG2	2.16	0.45
1:F:15:GLN:HB2	1:F:106:ILE:HD11	2.00	0.44
1:H:158:ARG:O	1:H:162:GLN:HG2	2.17	0.44
1:D:18:ARG:NH2	6:D:305:HOH:O	2.51	0.44
1:H:146:ALA:HA	1:H:152:VAL:HG11	1.98	0.44
1:A:15:GLN:HB2	1:A:106:ILE:HD11	2.00	0.44
1:F:38:PHE:HB3	1:F:41:PHE:HD2	1.83	0.43
1:G:80:SER:N	3:G:205:SO4:O1	2.40	0.43
1:H:27:LEU:O	1:H:31:THR:HG23	2.19	0.43
1:B:66:ARG:HA	1:B:66:ARG:HD2	1.82	0.43
1:G:66:ARG:HA	1:G:66:ARG:HD2	1.82	0.43
1:H:41:PHE:CD1	1:H:160:LEU:HD12	2.54	0.43
1:F:66:ARG:HA	1:F:66:ARG:HD2	1.92	0.43
1:G:35:ALA:HB2	1:H:69[B]:ARG:HG3	2.00	0.43
1:A:80:SER:N	3:A:206:SO4:O3	2.47	0.43
1:D:141:ASP:OD1	1:D:145:LYS:NZ	2.51	0.42
1:A:26:TYR:OH	1:A:96:GLU:OE2	2.37	0.42
1:C:54:THR:O	1:C:58:LYS:HG3	2.18	0.42
1:G:7:LYS:HB2	1:G:7:LYS:HE2	1.80	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:PHE:CE2	1:G:85:ILE:HD11	2.55	0.42
1:H:26:TYR:OH	1:H:96:GLU:OE2	2.29	0.42
1:F:58:LYS:HD3	6:F:355:HOH:O	2.19	0.42
1:G:84:GLY:HA3	4:G:202:GOL:H12	1.99	0.42
1:C:24:TYR:CZ	1:D:75:ILE:HD11	2.55	0.42
1:B:132:GLU:O	1:B:135[B]:GLN:HG2	2.19	0.41
1:E:1:MET:HE3	1:E:2:MET:O	2.19	0.41
1:H:58:LYS:HE2	1:H:124:TRP:CZ3	2.56	0.41
1:D:66[A]:ARG:HA	1:D:66[A]:ARG:HD2	1.93	0.41
1:G:60:TYR:CE2	1:H:31:THR:HG22	2.56	0.41
1:F:2:MET:HE1	1:F:6:GLU:HG2	2.03	0.41
1:H:103:ILE:HD13	1:H:125:PHE:HB3	2.02	0.41
1:A:27:LEU:HG	1:B:72:LEU:HD11	2.03	0.40
1:B:15:GLN:HB2	1:B:106:ILE:HD11	2.03	0.40
1:E:28:SER:HB2	1:F:72:LEU:HD12	2.04	0.40
1:F:119:VAL:HG13	6:F:353:HOH:O	2.21	0.40
1:A:66:ARG:HA	1:A:66:ARG:HD2	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	164/164 (100%)	164 (100%)	0	0	100	100
1	B	169/164 (103%)	169 (100%)	0	0	100	100
1	C	164/164 (100%)	163 (99%)	1 (1%)	0	100	100
1	D	165/164 (101%)	164 (99%)	1 (1%)	0	100	100
1	E	167/164 (102%)	167 (100%)	0	0	100	100
1	F	165/164 (101%)	164 (99%)	1 (1%)	0	100	100
1	G	164/164 (100%)	163 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	168/164 (102%)	167 (99%)	1 (1%)	0	100	100
All	All	1326/1312 (101%)	1321 (100%)	5 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	146/144 (101%)	146 (100%)	0	100	100
1	B	151/144 (105%)	148 (98%)	3 (2%)	48	56
1	C	148/144 (103%)	146 (99%)	2 (1%)	59	67
1	D	147/144 (102%)	147 (100%)	0	100	100
1	E	149/144 (104%)	149 (100%)	0	100	100
1	F	147/144 (102%)	147 (100%)	0	100	100
1	G	146/144 (101%)	146 (100%)	0	100	100
1	H	150/144 (104%)	148 (99%)	2 (1%)	61	69
All	All	1184/1152 (103%)	1177 (99%)	7 (1%)	86	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	52	GLU
1	B	131[A]	GLU
1	B	131[B]	GLU
1	C	76[A]	GLU
1	C	76[B]	GLU
1	H	10[A]	LYS
1	H	10[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	B	65	GLN
1	B	129	GLN
1	D	65	GLN
1	D	101	GLN
1	E	129	GLN
1	F	101	GLN
1	G	129	GLN
1	H	55	HIS
1	H	129	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 8 are monoatomic - leaving 46 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	SO4	F	204	-	4,4,4	0.25	0	6,6,6	0.13	0
4	GOL	A	205	-	5,5,5	1.06	0	5,5,5	1.04	0
4	GOL	G	203	-	5,5,5	1.06	0	5,5,5	0.96	0
4	GOL	H	203	-	5,5,5	1.05	0	5,5,5	1.00	0
3	SO4	A	206	-	4,4,4	0.25	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	206	-	4,4,4	0.24	0	6,6,6	0.15	0
3	SO4	H	206	-	4,4,4	0.22	0	6,6,6	0.09	0
3	SO4	D	202	-	4,4,4	0.24	0	6,6,6	0.17	0
4	GOL	F	203	-	5,5,5	1.10	0	5,5,5	1.01	0
4	GOL	C	202	-	5,5,5	1.01	0	5,5,5	0.94	0
3	SO4	B	208	-	4,4,4	0.26	0	6,6,6	0.12	0
4	GOL	A	203	-	5,5,5	1.04	0	5,5,5	1.07	0
4	GOL	D	204	-	5,5,5	1.07	0	5,5,5	0.89	0
4	GOL	G	202	-	5,5,5	0.96	0	5,5,5	1.09	0
5	LFA	E	204	-	19,19,19	0.09	0	18,18,18	0.19	0
3	SO4	G	204	-	4,4,4	0.27	0	6,6,6	0.09	0
3	SO4	E	205	-	4,4,4	0.25	0	6,6,6	0.13	0
3	SO4	G	205	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	B	202	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	B	205	-	4,4,4	0.24	0	6,6,6	0.22	0
3	SO4	A	202	-	4,4,4	0.25	0	6,6,6	0.17	0
3	SO4	A	207	-	4,4,4	0.24	0	6,6,6	0.15	0
3	SO4	D	205	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	G	206	-	4,4,4	0.24	0	6,6,6	0.12	0
4	GOL	C	203	-	5,5,5	0.85	0	5,5,5	1.11	0
3	SO4	D	207	-	4,4,4	0.26	0	6,6,6	0.06	0
3	SO4	F	202	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	H	202	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	C	206	-	4,4,4	0.25	0	6,6,6	0.06	0
4	GOL	D	203	-	5,5,5	1.10	0	5,5,5	0.96	0
3	SO4	C	207	-	4,4,4	0.24	0	6,6,6	0.04	0
3	SO4	B	203	-	4,4,4	0.20	0	6,6,6	0.13	0
3	SO4	A	208	-	4,4,4	0.20	0	6,6,6	0.12	0
4	GOL	E	203	-	5,5,5	0.95	0	5,5,5	1.10	0
4	GOL	H	204	-	5,5,5	1.03	0	5,5,5	0.90	0
3	SO4	A	209	-	4,4,4	0.24	0	6,6,6	0.16	0
4	GOL	A	204	-	5,5,5	0.95	0	5,5,5	1.05	0
5	LFA	C	204	-	19,19,19	0.13	0	18,18,18	0.28	0
5	LFA	B	207	-	19,19,19	0.13	0	18,18,18	0.30	0
4	GOL	B	206	-	5,5,5	1.11	0	5,5,5	0.98	0
3	SO4	E	202	-	4,4,4	0.26	0	6,6,6	0.11	0
4	GOL	B	204	-	5,5,5	1.14	0	5,5,5	0.94	0
3	SO4	C	205	-	4,4,4	0.25	0	6,6,6	0.11	0
5	LFA	H	205	-	19,19,19	0.08	0	18,18,18	0.16	0
3	SO4	B	210	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	B	209	-	4,4,4	0.20	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	205	-	-	1/4/4/4	-
4	GOL	G	203	-	-	0/4/4/4	-
4	GOL	H	203	-	-	0/4/4/4	-
4	GOL	F	203	-	-	2/4/4/4	-
4	GOL	C	202	-	-	2/4/4/4	-
4	GOL	A	203	-	-	4/4/4/4	-
4	GOL	D	204	-	-	4/4/4/4	-
4	GOL	G	202	-	-	2/4/4/4	-
5	LFA	E	204	-	-	2/17/17/17	-
4	GOL	C	203	-	-	2/4/4/4	-
4	GOL	D	203	-	-	1/4/4/4	-
4	GOL	H	204	-	-	3/4/4/4	-
4	GOL	E	203	-	-	2/4/4/4	-
4	GOL	A	204	-	-	1/4/4/4	-
5	LFA	C	204	-	-	1/17/17/17	-
5	LFA	B	207	-	-	2/17/17/17	-
4	GOL	B	206	-	-	2/4/4/4	-
4	GOL	B	204	-	-	2/4/4/4	-
5	LFA	H	205	-	-	4/17/17/17	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	203	GOL	O1-C1-C2-C3
4	A	203	GOL	C1-C2-C3-O3
4	B	206	GOL	C1-C2-C3-O3
4	C	202	GOL	O1-C1-C2-C3
4	F	203	GOL	C1-C2-C3-O3
4	G	202	GOL	O1-C1-C2-C3
4	H	204	GOL	C1-C2-C3-O3
4	C	203	GOL	O1-C1-C2-C3
4	D	204	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	204	GOL	C1-C2-C3-O3
4	E	203	GOL	O1-C1-C2-C3
4	A	203	GOL	O1-C1-C2-O2
4	B	206	GOL	O2-C2-C3-O3
4	A	203	GOL	O2-C2-C3-O3
4	C	202	GOL	O1-C1-C2-O2
4	F	203	GOL	O2-C2-C3-O3
4	G	202	GOL	O1-C1-C2-O2
4	H	204	GOL	O2-C2-C3-O3
5	C	204	LFA	C11-C10-C9-C8
4	C	203	GOL	O1-C1-C2-O2
5	E	204	LFA	C10-C11-C12-C13
5	B	207	LFA	C9-C10-C11-C12
5	H	205	LFA	C13-C14-C15-C16
5	B	207	LFA	C12-C13-C14-C15
4	A	204	GOL	O2-C2-C3-O3
4	D	204	GOL	O1-C1-C2-O2
4	E	203	GOL	O1-C1-C2-O2
4	B	204	GOL	O1-C1-C2-C3
4	H	204	GOL	O1-C1-C2-C3
5	H	205	LFA	C11-C12-C13-C14
5	E	204	LFA	C11-C12-C13-C14
5	H	205	LFA	C12-C13-C14-C15
5	H	205	LFA	C10-C11-C12-C13
4	D	204	GOL	O2-C2-C3-O3
4	D	203	GOL	O2-C2-C3-O3
4	A	205	GOL	O2-C2-C3-O3
4	B	204	GOL	O1-C1-C2-O2

There are no ring outliers.

14 monomers are involved in 19 short contacts:

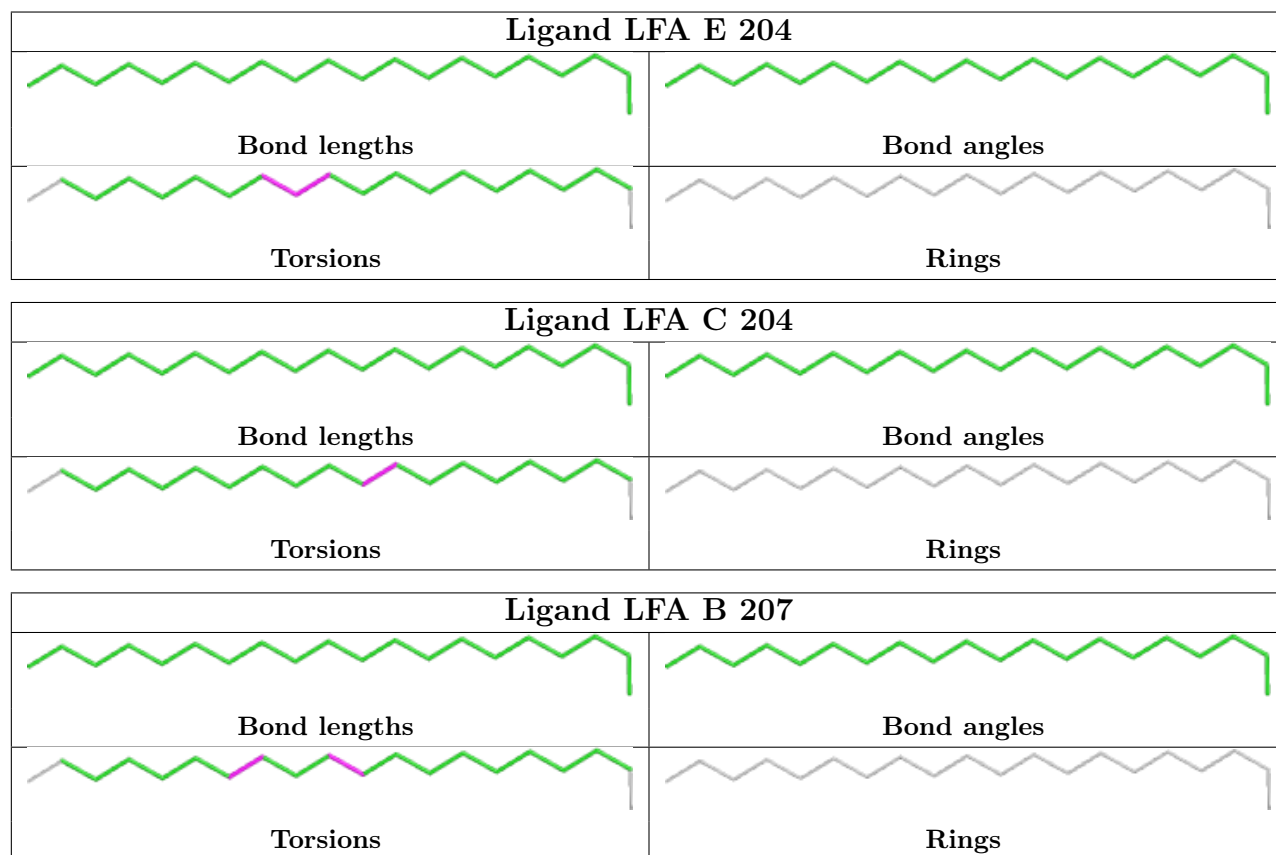
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	204	SO4	1	0
4	G	203	GOL	2	0
3	A	206	SO4	1	0
3	H	206	SO4	1	0
4	F	203	GOL	1	0
4	G	202	GOL	1	0
3	G	205	SO4	1	0
3	F	202	SO4	2	0
4	D	203	GOL	1	0

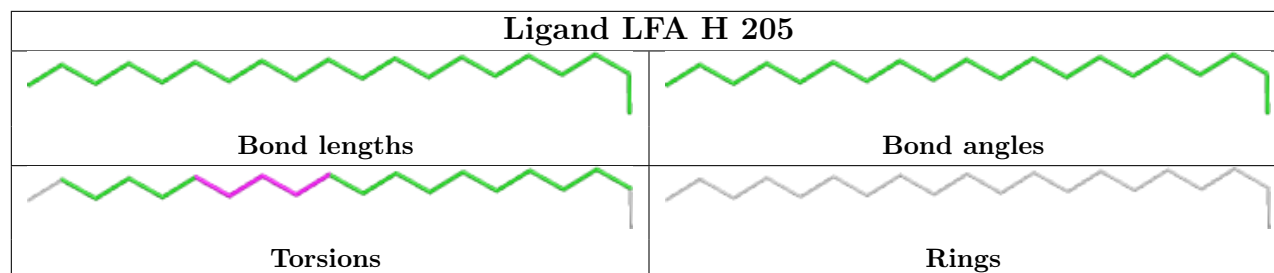
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	208	SO4	1	0
4	H	204	GOL	2	0
5	C	204	LFA	2	0
5	B	207	LFA	1	0
5	H	205	LFA	2	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	78:PRO	C	79:PRO	N	2.73

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	164/164 (100%)	0.17	5 (3%)	52	55	33, 56, 73, 113	2 (1%)
1	B	164/164 (100%)	0.10	1 (0%)	85	87	29, 54, 78, 114	7 (4%)
1	C	164/164 (100%)	0.32	6 (3%)	45	47	37, 64, 88, 111	4 (2%)
1	D	164/164 (100%)	0.27	1 (0%)	85	87	35, 61, 79, 115	3 (1%)
1	E	164/164 (100%)	0.16	1 (0%)	85	87	36, 59, 76, 116	5 (3%)
1	F	164/164 (100%)	0.40	7 (4%)	40	41	36, 64, 90, 105	3 (1%)
1	G	164/164 (100%)	0.55	6 (3%)	45	47	36, 69, 92, 122	2 (1%)
1	H	164/164 (100%)	0.76	12 (7%)	21	22	40, 74, 111, 131	6 (3%)
All	All	1312/1312 (100%)	0.34	39 (2%)	52	55	29, 63, 90, 131	32 (2%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	150	MET	6.5
1	H	153	ILE	4.7
1	C	1	MET	4.3
1	G	123[A]	LYS	3.7
1	A	1	MET	3.3
1	H	152	VAL	3.2
1	E	1	MET	3.1
1	H	3	VAL	3.0
1	H	1	MET	3.0
1	H	85	ILE	2.9
1	C	79	PRO	2.9
1	A	154	PHE	2.8
1	C	156	LEU	2.8
1	H	155[A]	GLN	2.7
1	B	1	MET	2.7
1	F	1	MET	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	151	SER	2.6
1	H	154	PHE	2.5
1	G	1	MET	2.5
1	F	164	GLU	2.4
1	A	142	LEU	2.4
1	H	143	LEU	2.4
1	G	139	ILE	2.4
1	A	131	GLU	2.3
1	G	154	PHE	2.2
1	F	35	ALA	2.2
1	C	78	PRO	2.2
1	G	83	ASN	2.2
1	F	154	PHE	2.1
1	G	131	GLU	2.1
1	H	156	LEU	2.1
1	D	83	ASN	2.1
1	C	149	GLN	2.1
1	F	135	GLN	2.1
1	F	155[A]	GLN	2.1
1	A	158	ARG	2.1
1	C	158	ARG	2.1
1	H	75	ILE	2.1
1	F	34	ASP	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 [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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	D	202	5/5	0.66	0.15	126,127,127,127	0
4	GOL	D	203	6/6	0.66	0.21	104,105,105,106	0
4	GOL	G	203	6/6	0.70	0.18	105,106,107,107	0
3	SO4	G	205	5/5	0.73	0.14	106,106,106,106	5
4	GOL	H	204	6/6	0.74	0.17	105,105,105,105	0
4	GOL	C	202	6/6	0.75	0.18	94,95,96,97	0
4	GOL	H	203	6/6	0.75	0.17	99,101,102,104	0
3	SO4	C	206	5/5	0.75	0.14	87,87,88,90	5
3	SO4	C	207	5/5	0.76	0.15	115,115,116,116	5
3	SO4	H	202	5/5	0.76	0.18	117,117,117,117	5
3	SO4	H	206	5/5	0.76	0.12	102,102,102,102	5
3	SO4	B	210	5/5	0.76	0.20	132,133,133,133	5
4	GOL	A	205	6/6	0.78	0.18	92,93,93,94	0
3	SO4	D	206	5/5	0.78	0.24	82,83,83,84	5
3	SO4	A	209	5/5	0.78	0.13	89,90,90,91	5
4	GOL	F	203	6/6	0.79	0.17	92,92,93,93	0
3	SO4	F	204	5/5	0.79	0.14	88,88,89,89	5
3	SO4	E	205	5/5	0.79	0.23	100,100,100,100	5
4	GOL	A	203	6/6	0.79	0.15	89,90,90,91	0
4	GOL	B	206	6/6	0.80	0.23	87,88,88,88	0
3	SO4	A	202	5/5	0.80	0.19	121,121,121,122	0
3	SO4	D	205	5/5	0.80	0.13	84,84,84,85	5
4	GOL	E	203	6/6	0.80	0.15	84,86,86,87	0
3	SO4	G	206	5/5	0.81	0.16	118,118,118,119	5
3	SO4	B	202	5/5	0.82	0.11	116,116,116,116	5
3	SO4	A	207	5/5	0.82	0.16	87,87,88,89	5
4	GOL	G	202	6/6	0.82	0.14	86,86,87,87	0
3	SO4	D	207	5/5	0.83	0.13	111,111,112,112	5
4	GOL	C	203	6/6	0.83	0.20	95,97,97,100	0
3	SO4	B	208	5/5	0.83	0.14	71,71,71,71	5
3	SO4	B	203	5/5	0.84	0.11	101,102,102,102	0
3	SO4	A	208	5/5	0.85	0.20	80,80,81,82	5
3	SO4	C	205	5/5	0.85	0.17	79,80,80,81	5
3	SO4	E	202	5/5	0.85	0.18	92,92,93,93	5
3	SO4	G	204	5/5	0.86	0.15	86,86,86,86	5
3	SO4	F	202	5/5	0.87	0.11	99,100,100,100	5
4	GOL	B	204	6/6	0.87	0.17	73,75,76,76	0
3	SO4	B	209	5/5	0.88	0.16	70,71,72,74	5
3	SO4	A	206	5/5	0.89	0.11	67,68,68,68	5
4	GOL	D	204	6/6	0.89	0.14	86,87,88,88	0
5	LFA	H	205	20/20	0.89	0.20	69,73,83,84	0

Continued on next page...

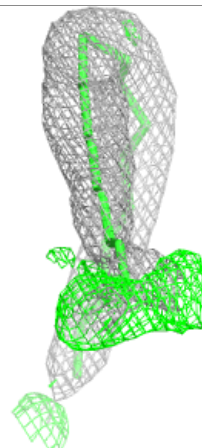
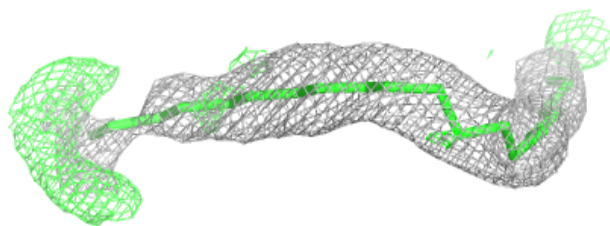
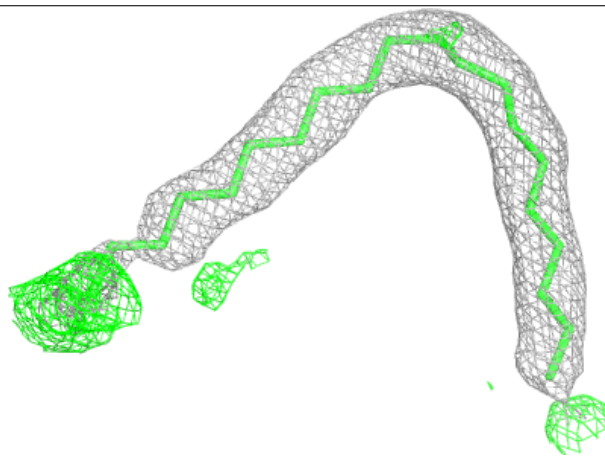
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	204	6/6	0.90	0.15	103,104,105,105	0
5	LFA	B	207	20/20	0.91	0.16	59,60,80,81	0
5	LFA	E	204	20/20	0.92	0.19	65,69,86,87	0
5	LFA	C	204	20/20	0.92	0.18	62,66,75,76	0
2	FE	F	201	1/1	0.93	0.10	62,62,62,62	1
2	FE	A	201	1/1	0.93	0.11	113,113,113,113	1
2	FE	G	201	1/1	0.94	0.12	88,88,88,88	0
2	FE	C	201	1/1	0.97	0.08	58,58,58,58	1
3	SO4	B	205	5/5	0.97	0.11	60,61,64,64	5
2	FE	E	201	1/1	0.97	0.05	48,48,48,48	1
2	FE	H	201	1/1	0.97	0.09	93,93,93,93	0
2	FE	D	201	1/1	0.98	0.07	59,59,59,59	1
2	FE	B	201	1/1	0.99	0.04	50,50,50,50	1

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.

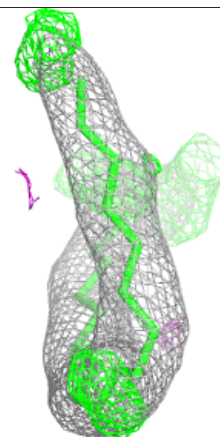
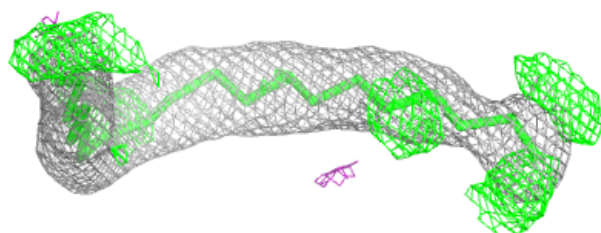
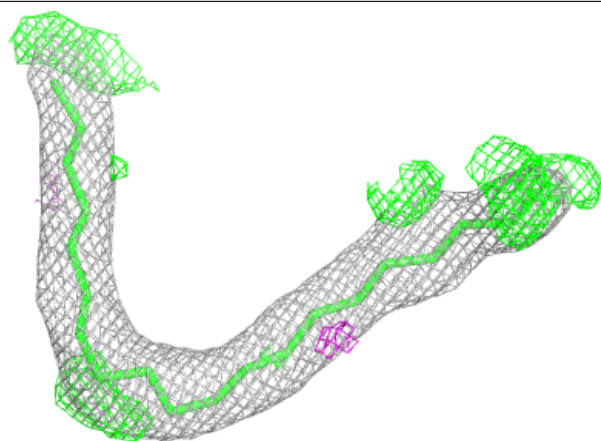
Electron density around LFA H 205:

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



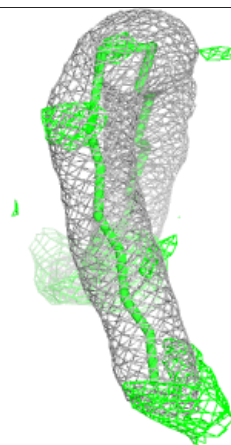
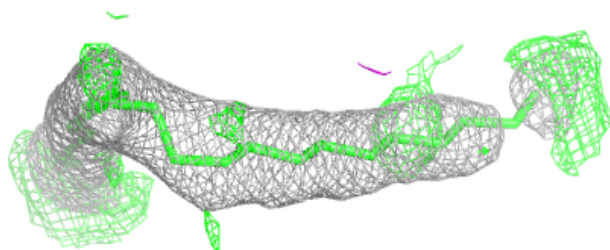
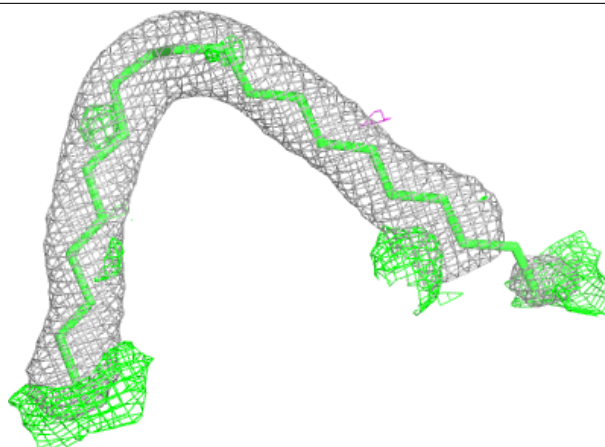
Electron density around LFA B 207:

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



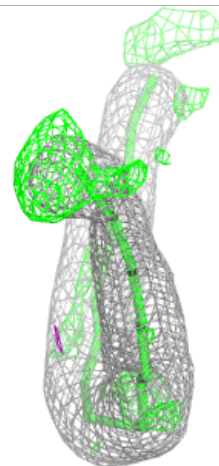
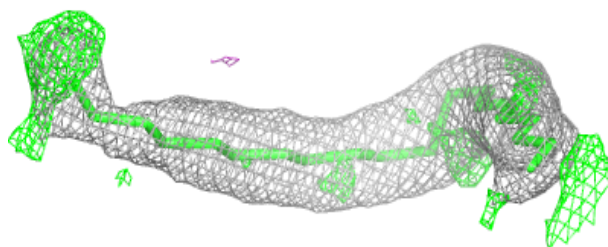
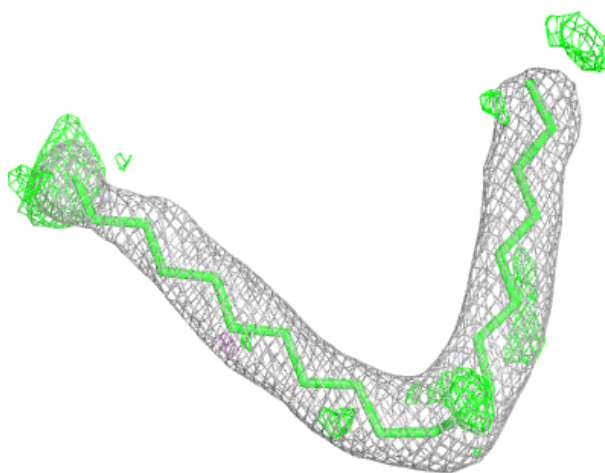
Electron density around LFA E 204:

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



Electron density around LFA C 204:

$2mF_o-DF_c$ (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.