



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:55 PM UTC

PDB ID : 6TCP / pdb_00006tcp
Title : Crystal structure of the omalizumab Fab Leu158Pro light chain mutant - crystal form II
Authors : Mitropoulou, A.N.; Ceska, T.; Beavil, A.J.; Henry, A.J.; McDonnell, J.M.; Sutton, B.J.; Davies, A.M.
Deposited on : 2019-11-06
Resolution : 2.50 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
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

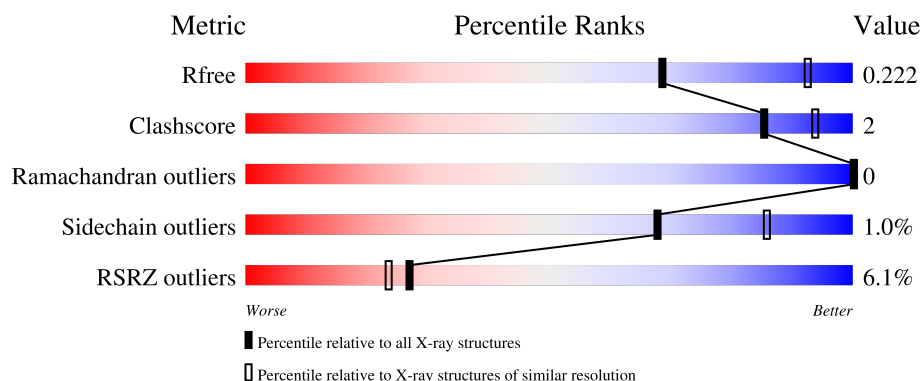
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	218	3% 95% .
1	C	218	6% 95% ..
1	E	218	6% 96% ..
1	L	218	4% 95% 5%
2	B	230	2% 87% 6% 6%

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Mol	Chain	Length	Quality of chain
2	D	230	9% 83% 10% 7%
2	F	230	11% 87% 7% 6%
2	H	230	7% 87% 6% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13271 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 Omalizumab Fab Leu158Pro light chain mutant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	217	Total	C	N	O	S	0	1	0
			1632	1023	266	338	5			
1	A	217	Total	C	N	O	S	0	1	0
			1630	1024	263	338	5			
1	C	216	Total	C	N	O	S	0	1	0
			1627	1017	268	336	6			
1	E	216	Total	C	N	O	S	0	1	0
			1626	1014	268	339	5			

- Molecule 2 is a protein called Omalizumab Fab Leu158Pro light chain mutant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1579	1006	262	306	5			
2	B	216	Total	C	N	O	S	0	2	1
			1604	1019	267	312	6			
2	D	214	Total	C	N	O	S	0	0	2
			1556	991	261	299	5			
2	F	217	Total	C	N	O	S	0	1	0
			1590	1012	267	306	5			

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



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			7	4	3		

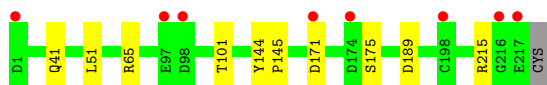
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	51	Total	O	0	0
			51	51		
6	H	28	Total	O	0	0
			28	28		
6	A	59	Total	O	0	0
			59	59		
6	B	49	Total	O	0	0
			49	49		
6	C	46	Total	O	0	0
			46	46		
6	D	14	Total	O	0	0
			14	14		
6	E	30	Total	O	0	0
			30	30		
6	F	22	Total	O	0	0
			22	22		

3 Residue-property plots

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: Omalizumab Fab Leu158Pro light chain mutant



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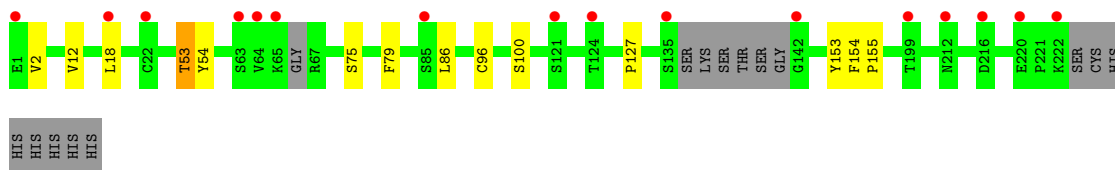
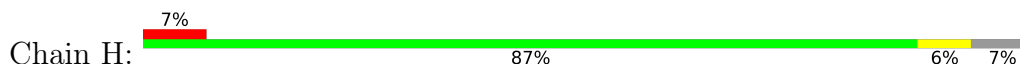
- Molecule 1: Omalizumab Fab Leu158Pro light chain mutant



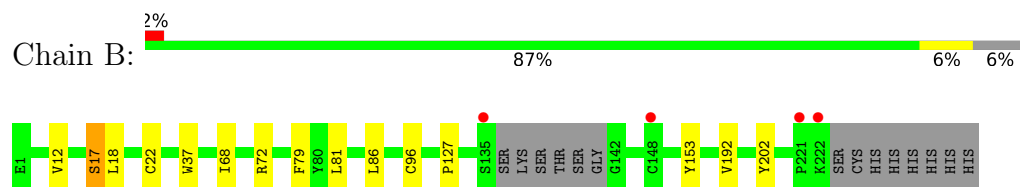
- Molecule 1: Omalizumab Fab Leu158Pro light chain mutant



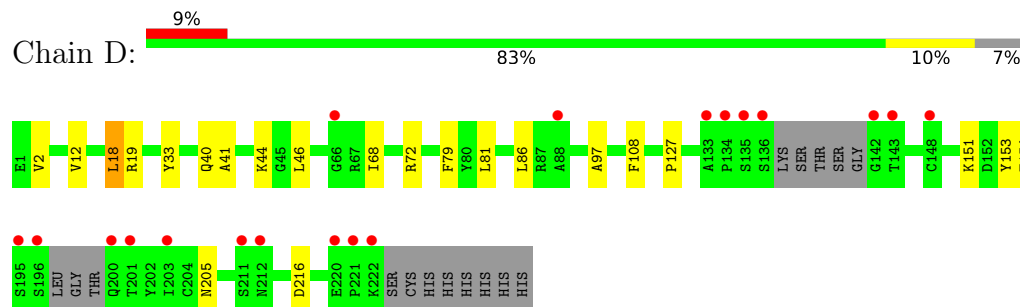
- Molecule 2: Omalizumab Fab Leu158Pro light chain mutant



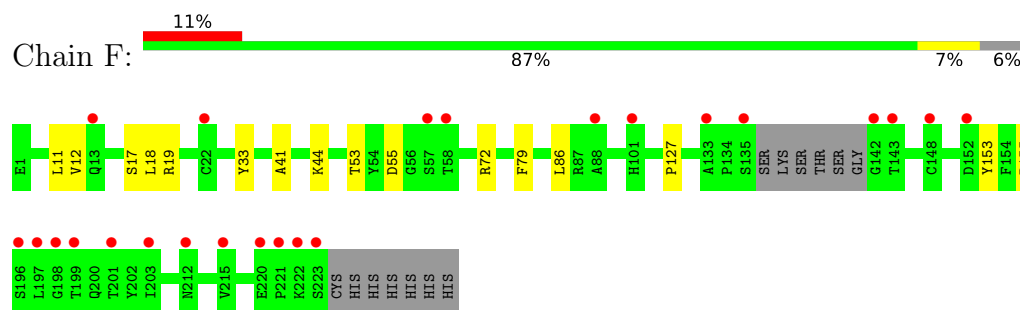
- Molecule 2: Omalizumab Fab Leu158Pro light chain mutant



- Molecule 2: Omalizumab Fab Leu158Pro light chain mutant



- Molecule 2: Omalizumab Fab Leu158Pro light chain mutant



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.11Å 162.04Å 164.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.02 – 2.50 81.02 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (81.02-2.50) 99.8 (81.02-2.50)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.212 , 0.239 0.220 , 0.222	Depositor DCC
R_{free} test set	3794 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13271	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.10	0/1668	0.29	0/2275
1	C	0.09	0/1668	0.29	0/2277
1	E	0.09	0/1666	0.28	0/2272
1	L	0.09	0/1672	0.30	0/2278
2	B	0.10	0/1654	0.30	0/2265
2	D	0.09	0/1599	0.29	0/2191
2	F	0.10	0/1637	0.29	0/2245
2	H	0.09	0/1622	0.29	0/2223
All	All	0.09	0/13186	0.29	0/18026

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1630	0	1496	6	0
1	C	1627	0	1504	4	0
1	E	1626	0	1507	3	0
1	L	1632	0	1512	6	0
2	B	1604	0	1516	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1556	0	1439	12	0
2	F	1590	0	1485	10	0
2	H	1579	0	1470	7	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	10	0	0	0	0
3	H	10	0	0	0	0
3	L	5	0	0	0	0
4	A	12	0	16	1	0
4	B	6	0	8	0	0
4	D	12	0	16	1	0
4	E	6	0	8	1	0
4	F	6	0	8	2	0
4	L	24	0	32	2	0
5	L	7	0	10	0	0
6	A	59	0	0	0	0
6	B	49	0	0	0	0
6	C	46	0	0	1	0
6	D	14	0	0	1	0
6	E	30	0	0	0	0
6	F	22	0	0	1	0
6	H	28	0	0	0	0
6	L	51	0	0	0	0
All	All	13271	0	12027	56	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 2.

All (56) 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)
2:D:33:TYR:H	4:D:302:GOL:H32	1.59	0.68
2:D:18:LEU:HD22	2:D:86:LEU:HD11	1.79	0.64
1:E:24:ARG:NE	1:E:74:ASP:OD1	2.29	0.63
1:L:65:ARG:HH22	4:L:303:GOL:H32	1.63	0.62
1:A:41:GLN:HB2	1:A:51:LEU:HD11	1.81	0.62
1:E:60:SER:HA	4:E:302:GOL:H12	1.84	0.60
1:A:215:ARG:HH12	4:A:302:GOL:H31	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:205:ASN:ND2	2:D:216:ASP:OD2	2.35	0.60
2:F:127:PRO:HB3	2:F:153:TYR:HB3	1.83	0.59
2:F:72:ARG:HA	2:F:79:PHE:HA	1.85	0.58
2:H:18:LEU:HB2	2:H:86:LEU:HD11	1.86	0.58
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.88	0.55
2:D:19:ARG:NH1	6:D:401:HOH:O	2.35	0.55
1:C:146:ARG:NH1	6:C:404:HOH:O	2.40	0.53
2:D:72:ARG:HA	2:D:79:PHE:HA	1.90	0.53
1:L:41:GLN:HB2	1:L:51:LEU:HD11	1.91	0.53
2:B:12:VAL:HG11	2:B:86:LEU:HD12	1.90	0.53
2:F:41:ALA:HB3	2:F:44:LYS:HB2	1.90	0.53
1:L:171:ASP:O	1:L:175:SER:N	2.38	0.52
2:B:72:ARG:HA	2:B:79:PHE:HA	1.91	0.52
1:E:41:GLN:HB2	1:E:51:LEU:HD11	1.91	0.52
1:C:23[B]:CYS:HB2	1:C:92:CYS:SG	2.49	0.51
2:B:22[B]:CYS:HB2	2:B:96:CYS:SG	2.51	0.50
2:F:33:TYR:H	4:F:302:GOL:H31	1.77	0.50
2:F:33:TYR:HA	4:F:302:GOL:H12	1.92	0.50
2:B:68:ILE:HD11	2:B:81:LEU:HD11	1.93	0.49
2:D:40:GLN:HB2	2:D:46:LEU:HD23	1.95	0.49
1:C:41:GLN:HB2	1:C:51:LEU:HD11	1.93	0.49
1:C:6:GLN:NE2	1:C:90:TYR:O	2.40	0.49
2:F:12:VAL:HG11	2:F:86:LEU:HD12	1.94	0.49
1:A:96:HIS:HD1	1:A:97:GLU:HG3	1.79	0.48
2:F:19:ARG:NH1	6:F:403:HOH:O	2.44	0.48
2:F:53:THR:OG1	2:F:55:ASP:OD1	2.32	0.47
2:F:18:LEU:HB3	2:F:86:LEU:HD11	1.97	0.47
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.97	0.47
1:L:215:ARG:HH22	4:L:302:GOL:H2	1.80	0.46
1:A:96:HIS:ND1	1:A:97:GLU:HG3	2.30	0.46
2:D:12:VAL:HG11	2:D:86:LEU:HD12	1.96	0.46
2:H:12:VAL:HG21	2:H:18:LEU:HD13	1.98	0.46
1:A:170:GLN:HE21	1:A:175:SER:HB3	1.79	0.46
1:L:189:ASP:OD2	2:B:17:SER:HB2	2.17	0.45
2:B:18:LEU:HB2	2:B:86:LEU:HD11	1.99	0.45
2:H:79:PHE:HZ	2:H:96:CYS:HB2	1.82	0.45
2:B:37:TRP:CE2	2:B:81:LEU:HB2	2.52	0.44
1:A:87:PHE:HB2	1:A:110:ILE:HD13	2.00	0.44
2:F:11:LEU:HB2	2:F:155:PRO:HG3	2.00	0.43
2:D:68:ILE:HD11	2:D:81:LEU:HD11	2.00	0.43
2:D:127:PRO:HB3	2:D:153:TYR:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:79:PHE:CZ	2:H:96:CYS:HB2	2.54	0.43
2:H:53:THR:HG22	2:H:54:TYR:H	1.84	0.42
2:D:97:ALA:HB1	2:D:108:PHE:HB3	2.02	0.41
2:H:154:PHE:HA	2:H:155:PRO:HA	1.82	0.41
2:D:154:PHE:HA	2:D:155:PRO:HA	1.85	0.41
2:D:41:ALA:HB3	2:D:44:LYS:HB2	2.02	0.41
1:L:144:TYR:CG	1:L:145:PRO:HA	2.57	0.40
2:B:192:VAL:HG11	2:B:202:TYR:CE1	2.56	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	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
1	C	215/218 (99%)	208 (97%)	7 (3%)	0	100	100
1	E	215/218 (99%)	209 (97%)	6 (3%)	0	100	100
1	L	216/218 (99%)	212 (98%)	4 (2%)	0	100	100
2	B	214/230 (93%)	207 (97%)	7 (3%)	0	100	100
2	D	208/230 (90%)	200 (96%)	8 (4%)	0	100	100
2	F	214/230 (93%)	208 (97%)	6 (3%)	0	100	100
2	H	209/230 (91%)	203 (97%)	6 (3%)	0	100	100
All	All	1707/1792 (95%)	1658 (97%)	49 (3%)	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	175/192 (91%)	175 (100%)	0	100	100
1	C	178/192 (93%)	177 (99%)	1 (1%)	78	91
1	E	180/192 (94%)	178 (99%)	2 (1%)	65	84
1	L	177/192 (92%)	176 (99%)	1 (1%)	78	91
2	B	173/194 (89%)	172 (99%)	1 (1%)	78	91
2	D	160/194 (82%)	157 (98%)	3 (2%)	50	76
2	F	167/194 (86%)	166 (99%)	1 (1%)	78	91
2	H	165/194 (85%)	161 (98%)	4 (2%)	43	70
All	All	1375/1544 (89%)	1362 (99%)	13 (1%)	68	87

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	101	THR
2	H	2	VAL
2	H	53	THR
2	H	75	SER
2	H	100	SER
2	B	17	SER
1	C	1	ASP
2	D	2	VAL
2	D	18	LEU
2	D	151	LYS
1	E	27	GLN
1	E	172	SER
2	F	17	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	13	GLN

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Mol	Chain	Res	Type
1	A	214	ASN
1	C	142	ASN
2	D	172	HIS
2	F	105	HIS

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](#)

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	L	302	-	5,5,5	0.37	0	5,5,5	0.38	0
4	GOL	D	302	-	5,5,5	0.37	0	5,5,5	0.31	0
5	PEG	L	305	-	6,6,6	0.83	0	5,5,5	0.27	0
3	SO4	H	302	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	L	301	-	4,4,4	0.24	0	6,6,6	0.07	0
4	GOL	A	302	-	5,5,5	0.37	0	5,5,5	0.32	0
3	SO4	F	301	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	A	301	-	4,4,4	0.23	0	6,6,6	0.07	0
4	GOL	F	302	-	5,5,5	0.36	0	5,5,5	0.32	0
4	GOL	B	302	-	5,5,5	0.39	0	5,5,5	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	303	-	5,5,5	0.37	0	5,5,5	0.33	0
3	SO4	C	301	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	H	301	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	E	301	-	4,4,4	0.23	0	6,6,6	0.08	0
4	GOL	E	302	-	5,5,5	0.35	0	5,5,5	0.34	0
4	GOL	L	303	-	5,5,5	0.38	0	5,5,5	0.25	0
3	SO4	C	302	-	4,4,4	0.23	0	6,6,6	0.09	0
4	GOL	A	303	-	5,5,5	0.38	0	5,5,5	0.29	0
4	GOL	L	304	-	5,5,5	0.36	0	5,5,5	0.26	0
3	SO4	D	301	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	F	303	-	4,4,4	0.23	0	6,6,6	0.07	0
4	GOL	L	306	-	5,5,5	0.39	0	5,5,5	0.30	0
3	SO4	B	301	-	4,4,4	0.25	0	6,6,6	0.07	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	302	-	-	2/4/4/4	-
4	GOL	D	303	-	-	0/4/4/4	-
4	GOL	F	302	-	-	2/4/4/4	-
4	GOL	B	302	-	-	2/4/4/4	-
4	GOL	E	302	-	-	4/4/4/4	-
4	GOL	L	303	-	-	4/4/4/4	-
4	GOL	A	303	-	-	2/4/4/4	-
4	GOL	L	306	-	-	4/4/4/4	-
4	GOL	L	302	-	-	0/4/4/4	-
4	GOL	D	302	-	-	2/4/4/4	-
4	GOL	L	304	-	-	4/4/4/4	-
5	PEG	L	305	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	303	GOL	O1-C1-C2-C3
4	L	304	GOL	O1-C1-C2-O2
4	L	304	GOL	O1-C1-C2-C3
4	L	306	GOL	O1-C1-C2-O2
4	L	306	GOL	O1-C1-C2-C3
4	A	302	GOL	O1-C1-C2-C3
4	A	303	GOL	O1-C1-C2-C3
4	B	302	GOL	O1-C1-C2-O2
4	E	302	GOL	C1-C2-C3-O3
4	E	302	GOL	O2-C2-C3-O3
4	F	302	GOL	O1-C1-C2-C3
4	L	303	GOL	C1-C2-C3-O3
4	L	304	GOL	C1-C2-C3-O3
4	B	302	GOL	O1-C1-C2-C3
4	D	302	GOL	O1-C1-C2-C3
4	E	302	GOL	O1-C1-C2-C3
4	L	303	GOL	O1-C1-C2-O2
4	A	303	GOL	O1-C1-C2-O2
4	F	302	GOL	O1-C1-C2-O2
5	L	305	PEG	O2-C3-C4-O4
4	A	302	GOL	O1-C1-C2-O2
4	E	302	GOL	O1-C1-C2-O2
4	L	303	GOL	O2-C2-C3-O3
4	L	304	GOL	O2-C2-C3-O3
4	D	302	GOL	O1-C1-C2-O2
5	L	305	PEG	C4-C3-O2-C2
4	L	306	GOL	O2-C2-C3-O3
4	L	306	GOL	C1-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	302	GOL	1	0
4	D	302	GOL	1	0
4	A	302	GOL	1	0
4	F	302	GOL	2	0
4	E	302	GOL	1	0
4	L	303	GOL	1	0

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	217/218 (99%)	0.40	6 (2%) 55 50	14, 30, 55, 71	1 (0%)
1	C	216/218 (99%)	0.55	13 (6%) 27 24	13, 33, 67, 80	1 (0%)
1	E	216/218 (99%)	0.62	12 (5%) 30 26	18, 37, 70, 101	1 (0%)
1	L	217/218 (99%)	0.32	8 (3%) 45 40	11, 27, 49, 70	1 (0%)
2	B	216/230 (93%)	0.41	4 (1%) 66 62	11, 32, 51, 80	2 (0%)
2	D	214/230 (93%)	0.91	21 (9%) 13 11	16, 40, 79, 100	0
2	F	217/230 (94%)	0.96	26 (11%) 9 7	19, 43, 75, 93	1 (0%)
2	H	215/230 (93%)	0.71	16 (7%) 20 18	16, 37, 58, 76	0
All	All	1728/1792 (96%)	0.61	106 (6%) 27 23	11, 35, 66, 101	7 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	223	SER	9.4
2	B	222	LYS	6.4
2	D	136	SER	5.3
1	A	217	GLU	5.2
2	H	135	SER	5.2
2	D	135	SER	5.1
2	F	199	THR	4.4
1	C	216	GLY	4.3
2	D	221	PRO	4.2
1	E	31	TYR	4.1
1	E	1	ASP	4.0
2	B	135	SER	4.0
2	H	222	LYS	3.9
2	D	212	ASN	3.9
2	F	220	GLU	3.7
2	H	1	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
2	H	85	SER	3.6
2	D	200	GLN	3.6
2	D	196	SER	3.5
1	E	216	GLY	3.5
1	C	127	GLU	3.5
1	C	188	ALA	3.5
2	F	142	GLY	3.5
1	C	131	SER	3.3
2	F	196	SER	3.3
1	L	174	ASP	3.3
2	F	166	ALA	3.3
2	D	203	ILE	3.2
2	D	166	ALA	3.2
2	D	142	GLY	3.2
2	F	222	LYS	3.2
2	H	22	CYS	3.2
1	E	34	ASP	3.1
1	E	198	CYS	3.1
2	F	158[A]	VAL	3.1
2	F	101	HIS	3.0
2	D	222	LYS	3.0
2	H	199	THR	2.9
2	D	148	CYS	2.9
2	F	148	CYS	2.9
1	E	127	GLU	2.9
1	A	1	ASP	2.9
1	C	31	TYR	2.9
1	L	216	GLY	2.9
1	L	198	CYS	2.9
2	F	88	ALA	2.9
1	A	31	TYR	2.9
1	C	130	LYS	2.8
1	C	198	CYS	2.8
1	L	98	ASP	2.8
2	D	195	SER	2.8
2	H	64	VAL	2.8
2	F	221	PRO	2.8
2	D	143	THR	2.8
2	F	212	ASN	2.7
2	F	135	SER	2.7
2	D	194	SER	2.7
1	L	217	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	198	GLY	2.6
2	D	88	ALA	2.6
1	C	189	ASP	2.6
1	E	32	ASP	2.6
2	F	201	THR	2.6
2	H	65	LYS	2.6
2	D	66	GLY	2.6
2	D	220	GLU	2.6
2	F	58	THR	2.6
1	A	207	SER	2.5
1	C	133	THR	2.5
1	L	1	ASP	2.5
2	D	134	PRO	2.4
1	A	216	GLY	2.4
2	F	197	LEU	2.4
2	F	143	THR	2.4
2	H	121	SER	2.4
1	L	171	ASP	2.4
2	F	152	ASP	2.4
1	C	187	LYS	2.4
2	D	201	THR	2.3
2	F	215	VAL	2.3
2	D	133	ALA	2.3
2	F	13	GLN	2.3
1	E	30	ASP	2.3
2	H	212	ASN	2.2
1	E	133	THR	2.2
1	E	132	GLY	2.2
2	H	124	THR	2.2
1	C	81	SER	2.2
1	C	60	SER	2.1
1	E	98	ASP	2.1
2	F	133	ALA	2.1
1	A	133	THR	2.1
2	H	18	LEU	2.1
2	H	220	GLU	2.1
1	E	156	ASN	2.1
1	C	155	ASP	2.1
2	H	63	SER	2.1
2	F	22	CYS	2.1
2	F	57	SER	2.1
2	B	221	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	203	ILE	2.1
2	D	211	SER	2.1
2	H	142	GLY	2.0
2	H	216	ASP	2.0
2	B	148	CYS	2.0
1	L	97	GLU	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	E	302	6/6	0.65	0.26	57,58,59,59	0
3	SO4	F	303	5/5	0.70	0.21	102,102,102,102	0
4	GOL	L	303	6/6	0.72	0.23	50,52,52,52	0
4	GOL	L	302	6/6	0.72	0.15	55,56,56,56	0
4	GOL	A	302	6/6	0.75	0.15	56,56,56,56	0
4	GOL	F	302	6/6	0.75	0.21	58,58,59,59	0
4	GOL	B	302	6/6	0.76	0.22	55,55,55,56	0
5	PEG	L	305	7/7	0.77	0.24	58,58,59,60	0
4	GOL	D	303	6/6	0.78	0.19	62,63,63,63	0
4	GOL	L	304	6/6	0.83	0.19	55,55,55,55	0
4	GOL	L	306	6/6	0.83	0.26	61,61,61,62	0
4	GOL	A	303	6/6	0.84	0.21	64,64,65,65	0
3	SO4	C	302	5/5	0.84	0.16	70,70,70,70	0
3	SO4	E	301	5/5	0.84	0.15	81,81,82,82	0
3	SO4	L	301	5/5	0.86	0.18	72,72,72,72	0
4	GOL	D	302	6/6	0.86	0.16	53,53,54,54	0
3	SO4	F	301	5/5	0.87	0.16	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	301	5/5	0.87	0.17	70,70,70,70	0
3	SO4	H	302	5/5	0.90	0.16	59,59,60,60	0
3	SO4	D	301	5/5	0.92	0.14	63,64,64,64	0
3	SO4	C	301	5/5	0.95	0.13	46,46,46,46	0
3	SO4	H	301	5/5	0.95	0.08	41,41,42,42	0
3	SO4	B	301	5/5	0.97	0.09	30,31,32,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.