



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 12:22 AM UTC

PDB ID : 3QPQ / pdb_00003qpq
Title : Crystal structure of ANTI-TLR3 antibody C1068 FAB
Authors : Luo, J.; Obmolova, G.; Teplyakov, A.; Gilliland, G.L.
Deposited on : 2011-02-14
Resolution : 1.90 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

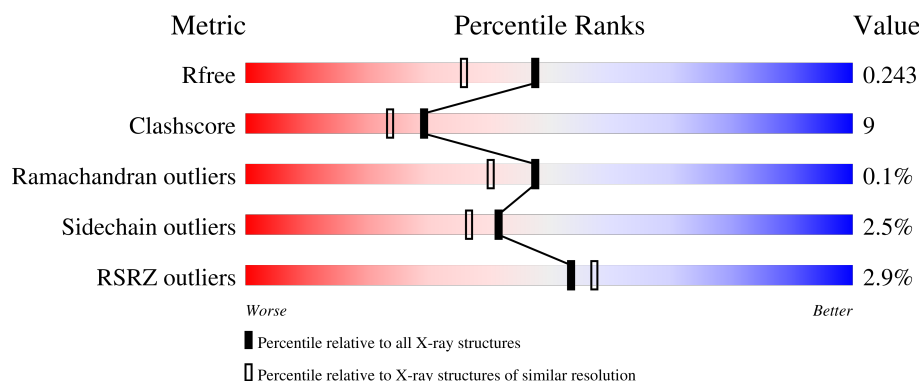
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	C	215	2% 86% 13% .
1	E	215	89% 11%
1	I	215	% 85% 14% .
1	L	215	2% 87% 13% .
2	D	223	5% 86% 11% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	223	4% 77% 21% ..
2	H	223	2% 87% 10% .
2	J	223	5% 82% 14% ..

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	GOL	L	216	-	-	X	-
4	SO4	L	219	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15233 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 C1068 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	6	0
			1691	1059	282	343	7			
1	E	215	Total	C	N	O	S	0	5	0
			1682	1054	280	341	7			
1	C	215	Total	C	N	O	S	0	4	0
			1677	1052	279	339	7			
1	I	215	Total	C	N	O	S	0	3	0
			1672	1049	279	337	7			

- Molecule 2 is a protein called C1068 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	2	0
			1652	1049	275	321	7			
2	F	221	Total	C	N	O	S	0	4	0
			1710	1085	289	329	7			
2	D	219	Total	C	N	O	S	0	2	0
			1682	1067	284	324	7			
2	J	217	Total	C	N	O	S	0	1	0
			1659	1053	278	321	7			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



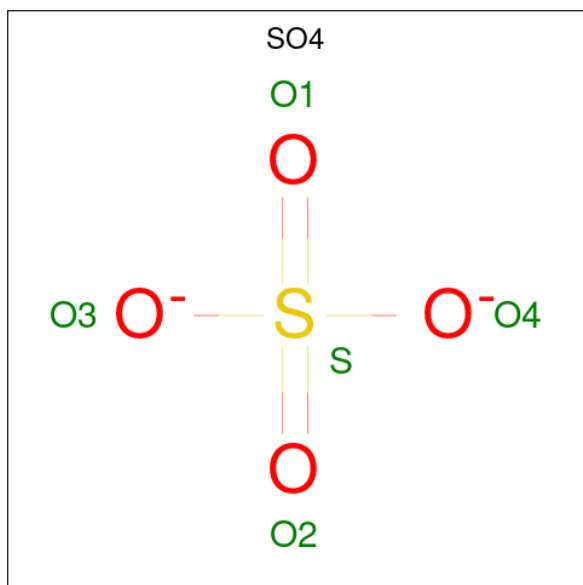
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	J	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	228	Total	O	0	0
			228	228		
5	H	222	Total	O	0	0
			222	222		
5	E	229	Total	O	0	0
			229	229		
5	F	189	Total	O	0	0
			189	189		
5	C	229	Total	O	0	0
			229	229		

Continued on next page...

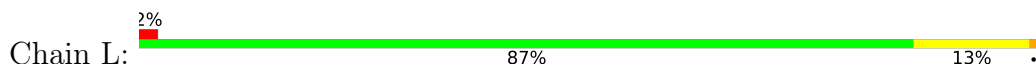
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	223	Total 223	O 223	0	0
5	I	184	Total 184	O 184	0	0
5	J	197	Total 197	O 197	0	0

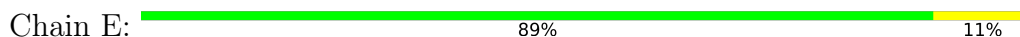
3 Residue-property plots [i](#)

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.

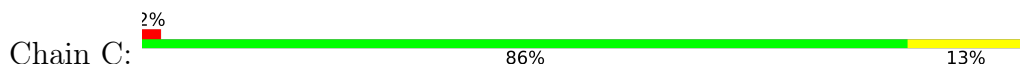
- Molecule 1: C1068 light chain



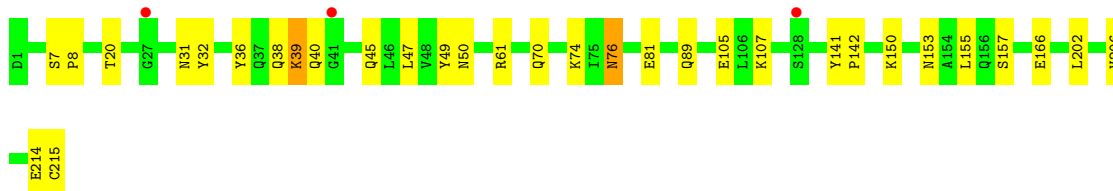
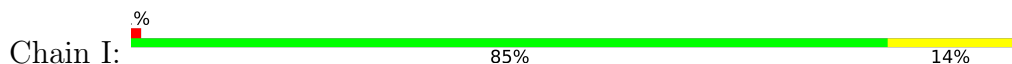
- Molecule 1: C1068 light chain



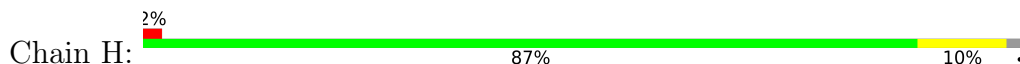
- Molecule 1: C1068 light chain



- Molecule 1: C1068 light chain

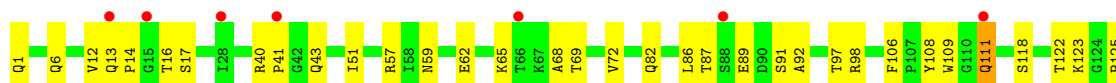
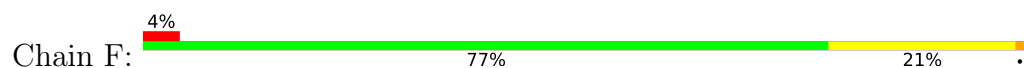


- Molecule 2: C1068 heavy chain

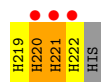
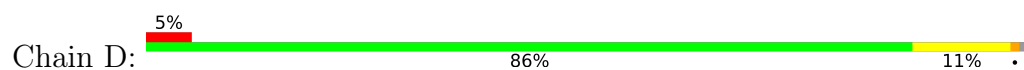




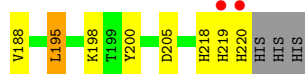
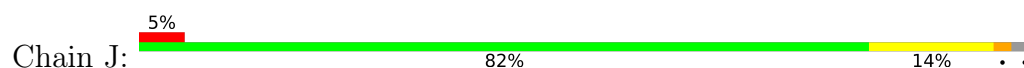
- Molecule 2: C1068 heavy chain



- Molecule 2: C1068 heavy chain



- Molecule 2: C1068 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.48Å 136.94Å 83.25Å 90.00° 114.95° 90.00°	Depositor
Resolution (Å)	44.55 – 1.90 44.55 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.2 (44.55-1.90) 89.2 (44.55-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_601), CNX	Depositor
R, R_{free}	0.201 , 0.256 0.188 , 0.243	Depositor DCC
R_{free} test set	5917 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15233	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 35.31 % 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 5.9489e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PCA, 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	C	0.44	0/1727	0.75	0/2342
1	E	0.44	0/1735	0.74	1/2352 (0.0%)
1	I	0.42	0/1719	0.73	0/2331
1	L	0.48	0/1744	0.74	0/2365
2	D	0.43	0/1726	0.75	0/2359
2	F	0.40	0/1761	0.74	0/2406
2	H	0.44	0/1693	0.76	0/2314
2	J	0.42	0/1698	0.77	0/2321
All	All	0.43	0/13803	0.75	1/18790 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	96	PHE	N-CA-C	-5.22	103.14	110.50

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	C	1677	0	1622	29	0
1	E	1682	0	1626	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1672	0	1618	19	0
1	L	1691	0	1634	22	0
2	D	1682	0	1648	27	0
2	F	1710	0	1679	47	0
2	H	1652	0	1627	26	0
2	J	1659	0	1629	41	0
3	C	36	0	48	6	0
3	D	6	0	8	1	0
3	E	6	0	8	2	0
3	F	6	0	8	0	0
3	I	12	0	16	3	0
3	J	18	0	24	7	0
3	L	18	0	24	6	0
4	L	5	0	0	3	0
5	C	229	0	0	5	1
5	D	223	0	0	4	0
5	E	229	0	0	4	0
5	F	189	0	0	7	0
5	H	222	0	0	6	1
5	I	184	0	0	4	0
5	J	197	0	0	6	1
5	L	228	0	0	9	1
All	All	15233	0	13219	229	2

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 9.

All (229) 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)
3:I:216:GOL:H31	5:I:484:HOH:O	1.46	1.15
3:L:216:GOL:H2	5:L:526:HOH:O	0.95	1.12
2:H:97[B]:THR:HG21	2:H:106:PHE:HB3	1.45	0.99
2:J:97[B]:THR:HG21	2:J:106:PHE:HB3	1.47	0.95
2:D:221:HIS:O	2:D:222:HIS:HB2	1.68	0.93
2:H:199:THR:HG23	5:H:514:HOH:O	1.67	0.93
2:H:55:ASN:HD21	2:H:57:ARG:HH11	1.17	0.91
2:F:6:GLN:H	2:F:111:GLN:HE22	1.18	0.91
2:J:46:GLU:OE1	5:J:417:HOH:O	1.93	0.86
1:L:92:TRP:O	5:L:312:HOH:O	1.93	0.85
2:D:219:HIS:O	2:D:220:HIS:HB2	1.73	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:97[A]:THR:HG21	2:F:106:PHE:HB3	1.57	0.84
1:I:38:GLN:HE22	2:J:39:GLN:HE22	1.26	0.83
1:L:38:GLN:HE22	2:H:39:GLN:HE22	1.28	0.81
1:L:200[A]:GLN:OE1	5:L:442:HOH:O	1.99	0.80
2:D:221:HIS:O	2:D:222:HIS:CB	2.29	0.80
2:D:219:HIS:HD2	2:D:220:HIS:HD2	1.26	0.80
2:F:13:GLN:O	2:F:16:THR:HG22	1.80	0.80
2:D:219:HIS:HD2	2:D:220:HIS:CD2	2.00	0.79
1:L:94:THR:OG1	5:L:451:HOH:O	2.00	0.78
3:E:216:GOL:O3	5:E:512:HOH:O	2.02	0.77
3:L:216:GOL:C2	5:L:526:HOH:O	1.70	0.76
2:F:219:HIS:HD2	2:F:221:HIS:H	1.34	0.76
2:F:189:THR:OG1	5:F:424:HOH:O	2.03	0.76
2:F:206:HIS:HB3	2:F:211:THR:HG23	1.67	0.76
2:F:57:ARG:HH11	2:F:59:ASN:HD21	1.31	0.76
1:C:74:LYS:HE2	1:C:76:ASN:HD21	1.51	0.75
2:J:57:ARG:HH21	2:J:57:ARG:CG	1.99	0.75
1:L:199:HIS:CD2	1:L:201:GLY:H	2.05	0.75
1:C:199:HIS:CD2	1:C:201:GLY:H	2.05	0.73
2:D:219:HIS:CD2	2:D:220:HIS:HD2	2.06	0.73
2:H:97[B]:THR:HG21	2:H:106:PHE:CB	2.17	0.73
1:E:80:PRO:HA	1:E:106:LEU:HG	1.70	0.73
2:F:123:LYS:NZ	5:F:427:HOH:O	2.20	0.73
1:C:38:GLN:HE22	2:D:39:GLN:HE22	1.36	0.72
2:H:7:PRO:HD3	5:H:444:HOH:O	1.88	0.72
4:L:219:SO4:O2	2:H:46:GLU:HG3	1.89	0.72
2:J:57:ARG:HH21	2:J:57:ARG:HG2	1.56	0.71
2:H:199:THR:HG22	5:H:522:HOH:O	1.89	0.71
1:C:66:GLU:O	3:C:219:GOL:H32	1.90	0.71
2:F:97[A]:THR:HG23	2:F:108:TYR:O	1.91	0.70
2:J:218:HIS:ND1	5:J:497:HOH:O	2.22	0.70
2:F:157:THR:CG2	2:F:205:ASP:HB3	2.21	0.70
2:D:129:PRO:HD3	2:D:215:LYS:HE2	1.74	0.70
2:H:97[B]:THR:HG23	2:H:108:TYR:O	1.92	0.70
2:F:209:SER:OG	2:F:211:THR:HG22	1.93	0.69
1:C:123:ASP:OD1	5:C:409:HOH:O	2.10	0.69
1:E:76:ASN:HB3	5:E:515:HOH:O	1.92	0.69
2:H:59:ASN:ND2	5:H:500:HOH:O	2.18	0.68
2:F:125:PRO:HD2	2:F:211:THR:HG21	1.74	0.68
2:J:220:HIS:H	3:J:226:GOL:H11	1.59	0.68
1:I:74:LYS:NZ	5:I:363:HOH:O	2.26	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148[B]:GLN:CG	1:E:155:LEU:HD12	2.24	0.67
1:L:199:HIS:HD2	1:L:201:GLY:H	1.42	0.67
2:F:206:HIS:HB3	2:F:211:THR:CG2	2.24	0.67
2:D:207:LYS:HB2	2:D:208:PRO:HD3	1.73	0.67
1:E:146:LYS:HD3	1:E:148[A]:GLN:HG3	1.75	0.67
2:J:97[B]:THR:CG2	2:J:106:PHE:HB3	2.23	0.66
2:H:97[B]:THR:CG2	2:H:106:PHE:HB3	2.21	0.66
2:J:97[B]:THR:HG21	2:J:106:PHE:CB	2.25	0.65
1:C:31:ASN:HD22	1:C:31:ASN:H	1.45	0.65
1:I:215:CYS:HB2	3:I:217:GOL:H31	1.78	0.65
1:C:199:HIS:HD2	1:C:201:GLY:H	1.43	0.64
1:L:81:GLU:HG2	5:L:525:HOH:O	1.97	0.64
1:C:66:GLU:HG3	3:C:219:GOL:H11	1.79	0.64
2:F:62:GLU:HA	2:F:65:LYS:HG2	1.79	0.64
2:J:31:THR:OG1	5:J:486:HOH:O	2.15	0.64
1:C:156:GLN:HE21	1:C:159:ASN:HD21	1.43	0.64
2:J:195:LEU:HD11	2:J:219:HIS:HB3	1.80	0.64
4:L:219:SO4:O2	2:H:46:GLU:HA	1.98	0.64
1:C:60:SER:O	5:C:393:HOH:O	2.14	0.63
1:E:150:LYS:HE3	1:E:155:LEU:HD11	1.79	0.63
2:H:97[B]:THR:HG21	2:H:106:PHE:CG	2.34	0.63
1:C:103:LYS:HB2	5:C:507:HOH:O	1.99	0.63
1:C:74:LYS:HE2	1:C:76:ASN:ND2	2.14	0.62
2:F:157:THR:HG22	2:F:205:ASP:HB3	1.81	0.62
1:C:215:CYS:O	3:C:217:GOL:H32	2.01	0.61
2:D:63:LYS:HD3	2:D:63:LYS:N	2.15	0.60
1:C:40:GLN:HB3	5:C:493:HOH:O	2.02	0.60
2:J:97[B]:THR:HG23	2:J:108:TYR:O	2.01	0.60
2:F:153:PRO:O	2:F:206:HIS:HE1	1.85	0.60
2:F:111:GLN:CD	2:F:111:GLN:H	2.08	0.59
1:L:98:PHE:HD2	4:L:219:SO4:O4	1.86	0.59
2:J:57:ARG:CG	2:J:57:ARG:NH2	2.64	0.59
2:F:57:ARG:NH1	2:F:59:ASN:HD21	1.99	0.59
2:F:219:HIS:CD2	2:F:221:HIS:HB2	2.38	0.59
2:F:51:ILE:HD13	2:F:72:VAL:HG13	1.83	0.58
2:D:61:ASN:OD1	2:D:63:LYS:HE2	2.02	0.58
1:C:120:PRO:O	2:D:222:HIS:CE1	2.56	0.58
3:L:217:GOL:H32	5:L:343:HOH:O	2.04	0.58
2:F:40:ARG:HD2	5:F:393:HOH:O	2.04	0.58
2:J:43:GLN:HG2	5:J:436:HOH:O	2.05	0.57
2:H:216:ARG:CZ	2:H:218:HIS:HD2	2.18	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:133:CYS:O	2:H:134:SER:C	2.47	0.56
2:H:55:ASN:ND2	2:H:57:ARG:HH11	1.96	0.56
1:I:214:GLU:HG3	2:J:133:CYS:SG	2.46	0.56
2:F:111:GLN:H	2:F:111:GLN:NE2	2.04	0.56
1:C:142:PRO:O	1:C:199:HIS:HE1	1.89	0.56
2:D:55:ASN:HD21	2:D:57:ARG:HH11	1.54	0.56
2:F:57:ARG:HH11	2:F:59:ASN:ND2	2.02	0.55
1:C:202:LEU:HD13	1:C:206[A]:VAL:HG12	1.88	0.55
1:E:148[B]:GLN:HG2	1:E:155:LEU:HD12	1.88	0.55
2:F:69:THR:HG23	5:F:407:HOH:O	2.05	0.55
2:H:157:THR:HG21	5:H:495:HOH:O	2.04	0.55
1:I:150:LYS:HG2	1:I:155[B]:LEU:HD23	1.89	0.55
1:L:40:GLN:HG3	1:L:166:GLU:OE1	2.07	0.55
2:J:219:HIS:CD2	2:J:219:HIS:H	2.25	0.54
2:F:40:ARG:HG2	2:F:40:ARG:HH11	1.73	0.54
2:F:12:VAL:HG21	2:F:86:LEU:HD13	1.88	0.54
3:L:216:GOL:C1	5:L:526:HOH:O	2.27	0.54
2:F:65:LYS:O	5:F:468:HOH:O	2.19	0.53
2:H:216:ARG:CZ	2:H:218:HIS:CD2	2.91	0.53
3:E:216:GOL:C3	5:E:512:HOH:O	2.55	0.53
2:D:131:ALA:H	2:D:222:HIS:CE1	2.26	0.53
2:D:170:HIS:CD2	3:D:224:GOL:H11	2.44	0.53
2:F:41:PRO:O	2:F:43:GLN:HG2	2.08	0.53
1:E:141:TYR:CG	1:E:142:PRO:HA	2.44	0.53
1:C:31:ASN:HD22	1:C:31:ASN:N	2.03	0.53
2:J:62:GLU:HA	2:J:65:LYS:HE3	1.91	0.53
1:L:122:SER:OG	1:L:124[A]:GLU:HG2	2.09	0.52
2:F:206:HIS:HD2	2:F:209:SER:OG	1.92	0.52
2:D:12:VAL:HG21	2:D:86:LEU:HD13	1.91	0.52
3:I:216:GOL:C3	5:I:484:HOH:O	2.27	0.52
2:J:184:LEU:C	2:J:184:LEU:HD23	2.34	0.52
2:F:157:THR:HG23	5:F:354:HOH:O	2.08	0.52
2:D:80:TYR:OH	5:D:421:HOH:O	2.19	0.51
2:F:125:PRO:HB3	2:F:151:TYR:HB3	1.91	0.51
1:I:141:TYR:CG	1:I:142:PRO:HA	2.46	0.51
2:F:151:TYR:CE1	2:F:156[B]:VAL:HG23	2.45	0.51
2:H:55:ASN:HD21	2:H:57:ARG:NH1	1.98	0.50
2:F:97[A]:THR:CG2	2:F:108:TYR:O	2.59	0.50
2:J:198:LYS:HE2	2:J:200:TYR:CE2	2.47	0.50
1:E:150:LYS:HE3	1:E:155:LEU:CD1	2.41	0.50
1:C:189:LYS:HE3	3:C:218:GOL:H2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:GLU:O	1:C:127:LYS:HG2	2.13	0.49
2:J:97[B]:THR:HG22	2:J:98:ARG:H	1.78	0.49
1:I:61:ARG:HB2	1:I:76:ASN:O	2.11	0.49
1:E:143:ARG:CZ	1:E:164:VAL:HG21	2.42	0.49
1:C:189:LYS:HG2	3:C:218:GOL:H2	1.95	0.49
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.94	0.49
2:J:97[B]:THR:HG21	2:J:106:PHE:CG	2.48	0.49
2:F:219:HIS:HD2	2:F:221:HIS:N	2.07	0.48
1:C:54:LEU:HD11	1:C:60:SER:HA	1.94	0.48
1:C:120:PRO:HG2	2:D:222:HIS:ND1	2.28	0.48
2:J:218:HIS:HB3	3:J:226:GOL:H2	1.95	0.48
1:L:31:ASN:HD22	1:L:31:ASN:H	1.61	0.48
2:H:216:ARG:HG2	2:H:218:HIS:NE2	2.28	0.48
1:E:150:LYS:HG2	1:E:155:LEU:HD13	1.95	0.48
2:D:99:VAL:HA	2:D:105:THR:O	2.13	0.48
2:F:40:ARG:HG2	2:F:40:ARG:NH1	2.28	0.47
1:C:189:LYS:HE3	3:C:218:GOL:C2	2.44	0.47
3:L:217:GOL:O1	2:H:170:HIS:HD2	1.97	0.47
1:E:141:TYR:CD2	1:E:142:PRO:HA	2.49	0.47
1:E:184:LYS:NZ	5:E:468:HOH:O	2.34	0.47
2:F:184:LEU:HD12	2:F:184:LEU:C	2.39	0.47
1:I:153:ASN:HB2	5:I:440:HOH:O	2.15	0.47
2:J:219:HIS:CD2	2:J:219:HIS:N	2.80	0.47
1:L:24:ARG:NH1	1:L:70:GLN:HE21	2.13	0.46
1:C:156:GLN:NE2	1:C:159:ASN:HD21	2.12	0.46
2:J:97[B]:THR:HG22	2:J:98:ARG:N	2.31	0.46
2:J:171:THR:O	3:J:224:GOL:H12	2.16	0.46
2:F:219:HIS:CD2	2:F:221:HIS:H	2.23	0.46
1:I:7:SER:HB2	1:I:8:PRO:HA	1.98	0.46
2:J:47:TRP:HZ2	2:J:50:GLU:HB3	1.81	0.46
2:J:111:GLN:O	2:J:111:GLN:HG2	2.09	0.46
2:J:97[B]:THR:CG2	2:J:108:TYR:O	2.64	0.45
2:J:171:THR:H	3:J:224:GOL:H12	1.82	0.45
2:F:87:THR:OG1	2:F:89:GLU:HB2	2.16	0.45
2:J:62:GLU:O	2:J:65:LYS:HG3	2.17	0.45
2:D:154:GLU:OE1	5:D:393:HOH:O	2.20	0.45
2:J:205:ASP:HB2	5:J:418:HOH:O	2.15	0.45
1:E:148[B]:GLN:CD	1:E:155:LEU:HD12	2.42	0.45
1:I:31:ASN:O	1:I:50:ASN:HA	2.17	0.45
1:I:39:LYS:NZ	1:I:81:GLU:O	2.50	0.44
1:I:49:TYR:CE1	3:J:225:GOL:H31	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:57:ARG:NH2	5:J:308:HOH:O	2.28	0.44
2:F:16:THR:HG23	2:F:17:SER:N	2.33	0.43
1:I:20:THR:OG1	1:I:74:LYS:HE3	2.18	0.43
2:J:171:THR:H	3:J:224:GOL:C1	2.31	0.43
2:J:220:HIS:HB3	3:J:226:GOL:O1	2.18	0.43
1:L:38:GLN:NE2	2:H:39:GLN:HE22	2.07	0.43
1:L:142:PRO:O	1:L:199:HIS:HE1	2.01	0.43
2:H:97[B]:THR:HG22	2:H:98:ARG:N	2.33	0.43
2:D:111:GLN:HG2	5:D:446:HOH:O	2.18	0.43
1:E:66:GLU:HG3	1:E:71:TYR:CE1	2.53	0.43
3:L:216:GOL:H11	5:L:526:HOH:O	2.04	0.43
1:I:36:TYR:HE2	1:I:89:GLN:HE21	1.67	0.43
1:I:40:GLN:HG3	1:I:166:GLU:OE1	2.19	0.43
2:J:27:TYR:CZ	2:J:98:ARG:HD2	2.54	0.43
1:L:40:GLN:HG3	1:L:166:GLU:CD	2.43	0.42
2:F:68:ALA:HA	2:F:82:GLN:O	2.19	0.42
1:L:31:ASN:HD22	1:L:31:ASN:N	2.15	0.42
1:L:107:LYS:HA	1:L:141:TYR:OH	2.19	0.42
2:F:14:PRO:HD3	2:F:118:SER:C	2.44	0.42
2:D:27:TYR:CZ	2:D:98:ARG:HD2	2.54	0.42
1:I:202:LEU:HD13	1:I:206:VAL:HG23	2.00	0.42
1:L:8:PRO:HG2	1:L:11:LEU:HG	2.00	0.42
2:J:169:VAL:HG22	2:J:188:VAL:HG12	2.02	0.42
2:H:216:ARG:NH2	2:H:218:HIS:HD2	2.18	0.42
2:F:91:SER:O	2:F:92:ALA:HB2	2.19	0.42
1:C:54:LEU:HD23	1:C:54:LEU:HA	1.83	0.42
1:E:146:LYS:HD3	1:E:148[A]:GLN:CG	2.48	0.42
2:H:207:LYS:HB2	2:H:208:PRO:HD3	2.02	0.42
2:D:62:GLU:HB2	5:D:317:HOH:O	2.20	0.42
1:E:126:LEU:O	1:E:184:LYS:HD2	2.20	0.41
2:J:61:ASN:O	2:J:62:GLU:C	2.63	0.41
2:D:27:TYR:CE2	2:D:98:ARG:HD2	2.55	0.41
2:D:39:GLN:HB2	2:D:45:LEU:HD23	2.02	0.41
1:L:147:VAL:HG13	1:L:195[A]:CYS:SG	2.60	0.41
2:F:97[A]:THR:CG2	2:F:106:PHE:HB3	2.41	0.41
2:F:97[B]:THR:HG22	2:F:109:TRP:CE3	2.55	0.41
1:I:141:TYR:CD2	1:I:142:PRO:HA	2.56	0.41
2:F:97[A]:THR:HG22	2:F:98:ARG:N	2.36	0.41
2:F:139:GLU:HG3	2:F:140:SER:N	2.36	0.41
2:D:184:LEU:C	2:D:184:LEU:HD12	2.45	0.41
2:H:19:ARG:NH1	5:H:356:HOH:O	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:VAL:HG22	1:C:176:LEU:HD12	2.03	0.41
1:C:211:ASN:O	1:C:214:GLU:HB2	2.20	0.41
1:I:107:LYS:HA	1:I:141:TYR:OH	2.20	0.41
2:J:30:THR:O	2:J:54:ASN:HB2	2.21	0.41
1:L:75:ILE:HG21	1:L:78:LEU:HD23	2.03	0.41
1:L:31:ASN:O	1:L:50:ASN:HA	2.21	0.40
2:F:122:THR:HG23	5:F:345:HOH:O	2.21	0.40
1:C:22:THR:HG23	5:C:355:HOH:O	2.20	0.40
2:J:97[A]:THR:HG22	2:J:109:TRP:CD2	2.55	0.40
1:E:176:LEU:C	1:E:176:LEU:HD23	2.46	0.40
2:D:12:VAL:CG2	2:D:86:LEU:HD13	2.52	0.40
1:I:32:TYR:CD1	2:J:104:THR:HG21	2.56	0.40
2:J:57:ARG:NH2	2:J:57:ARG:HG3	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:510:HOH:O	5:J:483:HOH:O[2_646]	2.06	0.14
5:L:505:HOH:O	5:H:459:HOH:O[2_846]	2.13	0.07

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	C	217/215 (101%)	211 (97%)	6 (3%)	0	100	100
1	E	218/215 (101%)	214 (98%)	4 (2%)	0	100	100
1	I	216/215 (100%)	211 (98%)	5 (2%)	0	100	100
1	L	219/215 (102%)	214 (98%)	5 (2%)	0	100	100
2	D	217/223 (97%)	207 (95%)	8 (4%)	2 (1%)	14	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	221/223 (99%)	214 (97%)	7 (3%)	0	100	100
2	H	214/223 (96%)	208 (97%)	6 (3%)	0	100	100
2	J	214/223 (96%)	209 (98%)	5 (2%)	0	100	100
All	All	1736/1752 (99%)	1688 (97%)	46 (3%)	2 (0%)	48	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	221	HIS
2	D	220	HIS

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	C	192/188 (102%)	185 (96%)	7 (4%)	31	23
1	E	193/188 (103%)	186 (96%)	7 (4%)	31	23
1	I	191/188 (102%)	184 (96%)	7 (4%)	30	22
1	L	194/188 (103%)	189 (97%)	5 (3%)	40	35
2	D	192/194 (99%)	191 (100%)	1 (0%)	81	84
2	F	196/194 (101%)	193 (98%)	3 (2%)	57	56
2	H	189/194 (97%)	186 (98%)	3 (2%)	55	54
2	J	189/194 (97%)	183 (97%)	6 (3%)	34	27
All	All	1536/1528 (100%)	1497 (98%)	39 (2%)	42	37

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	31	ASN
1	L	105	GLU
1	L	106	LEU
1	L	124[A]	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	124[C]	GLU
2	H	57	ARG
2	H	144	LEU
2	H	184	LEU
1	E	19	VAL
1	E	31	ASN
1	E	33	LEU
1	E	94	THR
1	E	103	LYS
1	E	105	GLU
1	E	169	SER
2	F	111	GLN
2	F	144	LEU
2	F	184	LEU
1	C	1	ASP
1	C	31	ASN
1	C	40	GLN
1	C	103	LYS
1	C	105	GLU
1	C	155	LEU
1	C	157	SER
2	D	57	ARG
1	I	39	LYS
1	I	45	GLN
1	I	47	LEU
1	I	70	GLN
1	I	76	ASN
1	I	105	GLU
1	I	157	SER
2	J	57	ARG
2	J	111	GLN
2	J	139	GLU
2	J	156	VAL
2	J	184	LEU
2	J	195	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	31	ASN
1	L	70	GLN
1	L	76	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	153	ASN
1	L	190	HIS
1	L	199	HIS
2	H	39	GLN
2	H	170	HIS
2	H	218	HIS
2	H	219	HIS
1	E	31	ASN
1	E	79	GLN
1	E	190	HIS
2	F	3	GLN
2	F	59	ASN
2	F	82	GLN
2	F	111	GLN
2	F	206	HIS
2	F	219	HIS
2	F	221	HIS
2	F	223	HIS
1	C	31	ASN
1	C	40	GLN
1	C	50	ASN
1	C	76	ASN
1	C	89	GLN
1	C	156	GLN
1	C	190	HIS
1	C	199	HIS
2	D	39	GLN
2	D	54	ASN
2	D	59	ASN
2	D	170	HIS
2	D	219	HIS
2	D	220	HIS
1	I	3	GLN
1	I	30	HIS
1	I	37	GLN
1	I	38	GLN
1	I	40	GLN
1	I	89	GLN
1	I	148	GLN
1	I	153	ASN
2	J	5	GLN
2	J	52	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	111	GLN
2	J	218	HIS
2	J	219	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
2	PCA	H	1	2	7,8,9	1.93	1 (14%)	9,10,12	2.06	5 (55%)
2	PCA	F	1	2	7,8,9	1.95	1 (14%)	9,10,12	2.36	5 (55%)
2	PCA	J	1	2	7,8,9	1.83	1 (14%)	9,10,12	2.17	5 (55%)
2	PCA	D	1	2	7,8,9	1.89	1 (14%)	9,10,12	2.51	5 (55%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1
2	PCA	F	1	2	-	0/0/11/13	0/1/1/1
2	PCA	J	1	2	-	0/0/11/13	0/1/1/1
2	PCA	D	1	2	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	PCA	CD-N	5.04	1.47	1.34
2	H	1	PCA	CD-N	4.96	1.46	1.34
2	D	1	PCA	CD-N	4.81	1.46	1.34
2	J	1	PCA	CD-N	4.72	1.46	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	PCA	CB-CA-C	-4.43	106.58	112.66
2	F	1	PCA	CB-CA-C	-3.63	107.68	112.66
2	J	1	PCA	CB-CA-C	-3.29	108.14	112.66
2	F	1	PCA	OE-CD-CG	-3.10	121.19	126.72
2	D	1	PCA	CA-N-CD	-3.05	103.14	113.58
2	D	1	PCA	OE-CD-CG	-2.99	121.39	126.72
2	F	1	PCA	CA-N-CD	-2.96	103.44	113.58
2	F	1	PCA	CB-CA-N	2.89	111.20	103.24
2	J	1	PCA	OE-CD-CG	-2.82	121.68	126.72
2	H	1	PCA	CA-N-CD	-2.67	104.43	113.58
2	D	1	PCA	CB-CA-N	2.65	110.53	103.24
2	F	1	PCA	CG-CD-N	2.61	114.78	108.39
2	H	1	PCA	OE-CD-CG	-2.58	122.11	126.72
2	J	1	PCA	CA-N-CD	-2.57	104.76	113.58
2	D	1	PCA	CG-CD-N	2.49	114.49	108.39
2	H	1	PCA	CG-CD-N	2.46	114.41	108.39
2	H	1	PCA	CB-CA-N	2.42	109.89	103.24
2	J	1	PCA	CG-CD-N	2.38	114.20	108.39
2	H	1	PCA	CB-CA-C	-2.31	109.49	112.66
2	J	1	PCA	CB-CA-N	2.16	109.17	103.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	C	216	-	5,5,5	0.41	0	5,5,5	0.43	0
3	GOL	F	224	-	5,5,5	0.41	0	5,5,5	0.36	0
3	GOL	C	217	-	5,5,5	0.39	0	5,5,5	0.53	0
3	GOL	C	221	-	5,5,5	0.45	0	5,5,5	0.52	0
3	GOL	C	218	-	5,5,5	0.41	0	5,5,5	0.32	0
3	GOL	J	225	-	5,5,5	0.37	0	5,5,5	0.47	0
3	GOL	I	217	-	5,5,5	0.43	0	5,5,5	0.20	0
3	GOL	D	224	-	5,5,5	0.35	0	5,5,5	0.51	0
3	GOL	L	218	-	5,5,5	0.38	0	5,5,5	0.33	0
3	GOL	L	217	-	5,5,5	0.32	0	5,5,5	0.52	0
3	GOL	L	216	-	5,5,5	0.36	0	5,5,5	0.38	0
3	GOL	C	220	-	5,5,5	0.44	0	5,5,5	0.32	0
3	GOL	I	216	-	5,5,5	0.48	0	5,5,5	0.40	0
3	GOL	J	226	-	5,5,5	0.42	0	5,5,5	0.48	0
4	SO4	L	219	-	4,4,4	0.28	0	6,6,6	0.14	0
3	GOL	C	219	-	5,5,5	0.37	0	5,5,5	0.39	0
3	GOL	E	216	-	5,5,5	0.48	0	5,5,5	0.15	0
3	GOL	J	224	-	5,5,5	0.39	0	5,5,5	0.37	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	GOL	C	216	-	-	0/4/4/4	-
3	GOL	F	224	-	-	2/4/4/4	-
3	GOL	C	217	-	-	1/4/4/4	-
3	GOL	C	221	-	-	4/4/4/4	-
3	GOL	C	218	-	-	2/4/4/4	-
3	GOL	J	225	-	-	1/4/4/4	-
3	GOL	I	217	-	-	4/4/4/4	-
3	GOL	D	224	-	-	0/4/4/4	-
3	GOL	L	218	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	L	217	-	-	1/4/4/4	-
3	GOL	L	216	-	-	1/4/4/4	-
3	GOL	C	220	-	-	2/4/4/4	-
3	GOL	I	216	-	-	2/4/4/4	-
3	GOL	J	226	-	-	2/4/4/4	-
3	GOL	C	219	-	-	4/4/4/4	-
3	GOL	E	216	-	-	4/4/4/4	-
3	GOL	J	224	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	216	GOL	O1-C1-C2-C3
3	F	224	GOL	O1-C1-C2-C3
3	C	218	GOL	O1-C1-C2-C3
3	C	219	GOL	C1-C2-C3-O3
3	C	220	GOL	O1-C1-C2-C3
3	C	221	GOL	C1-C2-C3-O3
3	I	217	GOL	C1-C2-C3-O3
3	J	224	GOL	O1-C1-C2-O2
3	J	224	GOL	O1-C1-C2-C3
3	J	226	GOL	O1-C1-C2-C3
3	C	221	GOL	O2-C2-C3-O3
3	I	216	GOL	O1-C1-C2-O2
3	E	216	GOL	C1-C2-C3-O3
3	C	219	GOL	O1-C1-C2-C3
3	C	221	GOL	O1-C1-C2-C3
3	I	216	GOL	O1-C1-C2-C3
3	I	217	GOL	O1-C1-C2-C3
3	E	216	GOL	O1-C1-C2-O2
3	F	224	GOL	O1-C1-C2-O2
3	C	218	GOL	O1-C1-C2-O2
3	C	219	GOL	O1-C1-C2-O2
3	C	219	GOL	O2-C2-C3-O3
3	C	220	GOL	O1-C1-C2-O2
3	I	217	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	216	GOL	O2-C2-C3-O3
3	C	221	GOL	O1-C1-C2-O2
3	J	226	GOL	O1-C1-C2-O2
3	I	217	GOL	O1-C1-C2-O2
3	L	216	GOL	O1-C1-C2-O2
3	C	217	GOL	O2-C2-C3-O3
3	L	217	GOL	O1-C1-C2-C3
3	J	225	GOL	O1-C1-C2-O2

There are no ring outliers.

13 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	217	GOL	1	0
3	C	218	GOL	3	0
3	J	225	GOL	1	0
3	I	217	GOL	1	0
3	D	224	GOL	1	0
3	L	217	GOL	2	0
3	L	216	GOL	4	0
3	I	216	GOL	2	0
3	J	226	GOL	3	0
4	L	219	SO4	3	0
3	C	219	GOL	2	0
3	E	216	GOL	2	0
3	J	224	GOL	3	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	C	215/215 (100%)	0.09	4 (1%)	66	70	14, 26, 41, 63	4 (1%)
1	E	215/215 (100%)	0.06	1 (0%)	87	89	12, 25, 41, 56	5 (2%)
1	I	215/215 (100%)	0.24	3 (1%)	73	76	14, 29, 46, 64	3 (1%)
1	L	215/215 (100%)	-0.02	4 (1%)	66	70	12, 23, 40, 56	6 (2%)
2	D	218/223 (97%)	0.26	12 (5%)	30	32	13, 28, 53, 86	2 (0%)
2	F	220/223 (98%)	0.46	9 (4%)	41	44	14, 31, 54, 91	4 (1%)
2	H	215/223 (96%)	0.19	5 (2%)	61	65	11, 26, 46, 84	2 (0%)
2	J	216/223 (96%)	0.50	12 (5%)	30	32	12, 31, 58, 82	1 (0%)
All	All	1729/1752 (98%)	0.22	50 (2%)	53	57	11, 27, 48, 91	27 (1%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	41	PRO	4.2
2	J	220	HIS	4.1
2	D	222	HIS	3.9
2	D	220	HIS	3.5
2	J	33	TRP	3.5
2	J	66	THR	3.4
2	D	42	GLY	3.4
2	J	41	PRO	3.1
2	D	43	GLN	2.9
2	F	137	THR	2.8
2	H	178	SER	2.8
1	L	215	CYS	2.8
2	J	42	GLY	2.8
2	F	15	GLY	2.8
2	F	111	GLN	2.7
1	C	1	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	66	THR	2.6
2	D	44	GLY	2.6
2	H	66	THR	2.6
2	H	139	GLU	2.6
2	J	134	SER	2.6
2	D	210	ASN	2.6
2	F	41	PRO	2.5
1	C	171	ASP	2.5
1	L	157	SER	2.5
2	D	212	LYS	2.4
1	C	76	ASN	2.4
2	J	219	HIS	2.4
2	D	66	THR	2.3
2	J	28	ILE	2.3
2	J	57	ARG	2.3
2	J	139	GLU	2.3
1	L	155	LEU	2.3
2	J	54	ASN	2.3
1	E	57	GLY	2.3
2	F	28	ILE	2.3
2	H	138	SER	2.3
2	H	43	GLN	2.3
2	J	58	ILE	2.2
2	F	13	GLN	2.2
2	F	138	SER	2.2
2	D	221	HIS	2.2
1	C	128	SER	2.1
1	L	124[A]	GLU	2.1
2	D	62	GLU	2.1
1	I	128	SER	2.0
2	F	88	SER	2.0
1	I	27	GLY	2.0
1	I	41	GLY	2.0
2	D	57	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PCA	F	1	8/9	0.86	0.12	32,42,48,49	0
2	PCA	H	1	8/9	0.92	0.09	27,36,45,51	0
2	PCA	J	1	8/9	0.93	0.10	34,35,37,38	0
2	PCA	D	1	8/9	0.94	0.10	21,32,46,50	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	C	219	6/6	0.65	0.24	51,61,67,71	0
3	GOL	C	221	6/6	0.73	0.17	30,44,56,56	0
3	GOL	L	216	6/6	0.74	0.14	34,42,45,49	0
3	GOL	D	224	6/6	0.78	0.17	40,51,61,72	0
3	GOL	E	216	6/6	0.81	0.15	39,45,50,50	0
3	GOL	L	218	6/6	0.82	0.15	37,43,50,55	0
3	GOL	J	226	6/6	0.84	0.16	42,51,53,57	0
3	GOL	J	224	6/6	0.85	0.13	34,48,49,56	0
3	GOL	C	220	6/6	0.85	0.15	47,49,52,55	0
3	GOL	L	217	6/6	0.86	0.13	35,48,49,58	0
3	GOL	I	217	6/6	0.88	0.10	36,42,49,53	0
3	GOL	I	216	6/6	0.89	0.14	30,40,45,47	0
3	GOL	C	217	6/6	0.89	0.10	33,41,42,48	0
3	GOL	J	225	6/6	0.90	0.11	27,43,45,45	0
3	GOL	C	218	6/6	0.92	0.10	24,38,42,54	0
3	GOL	C	216	6/6	0.92	0.09	31,35,41,42	0
3	GOL	F	224	6/6	0.93	0.09	30,35,40,44	0
4	SO4	L	219	5/5	0.97	0.19	11,32,37,37	5

6.5 Other polymers [i](#)

There are no such residues in this entry.