



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 01:35 AM UTC

PDB ID : 5TZZ / pdb_00005tzt
Title : Crystal structure of human CD47 ECD bound to Fab of C47B161
Authors : Cardoso, R.M.F.
Deposited on : 2016-11-22
Resolution : 2.89 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

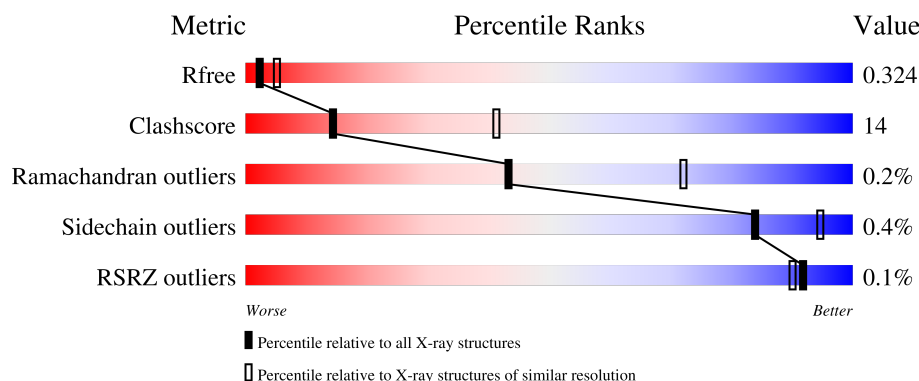
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	B	219	73% 26%
1	L	219	73% 26%
2	A	226	69% 26% .
2	H	226	67% 28% .
3	C	129	% 57% 28% . 14%

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Mol	Chain	Length	Quality of chain
3	D	129	68% 20% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8158 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 Light Chain of Fab C47B161.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	218	Total	C	N	O	S	0	1	0
			1608	1014	265	324	5			
1	L	219	Total	C	N	O	S	0	0	0
			1635	1032	273	324	6			

- Molecule 2 is a protein called Heavy Chain of Fab C47B161.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	217	Total	C	N	O	S	0	0	0
			1577	993	265	311	8			
2	H	217	Total	C	N	O	S	0	0	0
			1566	990	261	308	7			

- Molecule 3 is a protein called Leukocyte surface antigen CD47.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	111	Total	C	N	O	S	0	0	0
			783	496	127	157	3			
3	D	114	Total	C	N	O	S	0	0	0
			799	502	132	162	3			

There are 14 discrepancies between the modelled and reference sequences:

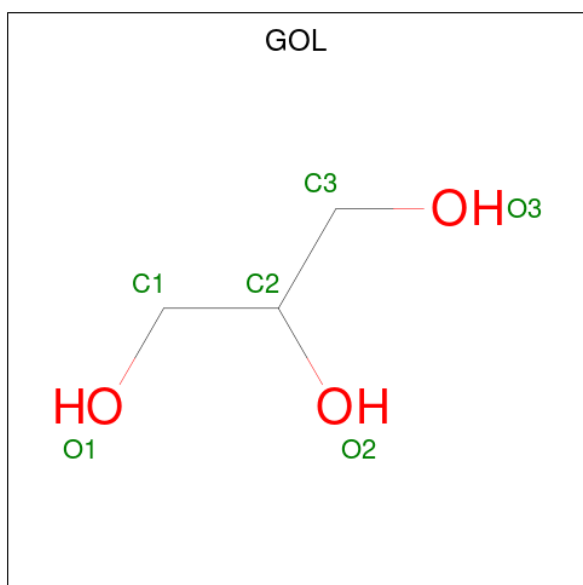
Chain	Residue	Modelled	Actual	Comment	Reference
C	15	GLY	CYS	engineered mutation	UNP Q08722
C	124	HIS	-	expression tag	UNP Q08722
C	125	HIS	-	expression tag	UNP Q08722
C	126	HIS	-	expression tag	UNP Q08722
C	127	HIS	-	expression tag	UNP Q08722
C	128	HIS	-	expression tag	UNP Q08722
C	129	HIS	-	expression tag	UNP Q08722
D	15	GLY	CYS	engineered mutation	UNP Q08722

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Chain	Residue	Modelled	Actual	Comment	Reference
D	124	HIS	-	expression tag	UNP Q08722
D	125	HIS	-	expression tag	UNP Q08722
D	126	HIS	-	expression tag	UNP Q08722
D	127	HIS	-	expression tag	UNP Q08722
D	128	HIS	-	expression tag	UNP Q08722
D	129	HIS	-	expression tag	UNP Q08722

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	L	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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

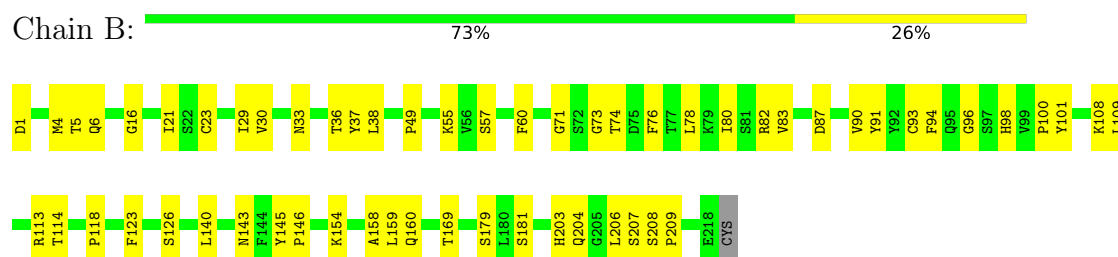
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	27	Total	O	0	0
			27	27		
6	A	24	Total	O	0	0
			24	24		
6	L	27	Total	O	0	0
			27	27		
6	H	26	Total	O	0	0
			26	26		
6	C	9	Total	O	0	0
			9	9		
6	D	5	Total	O	0	0
			5	5		

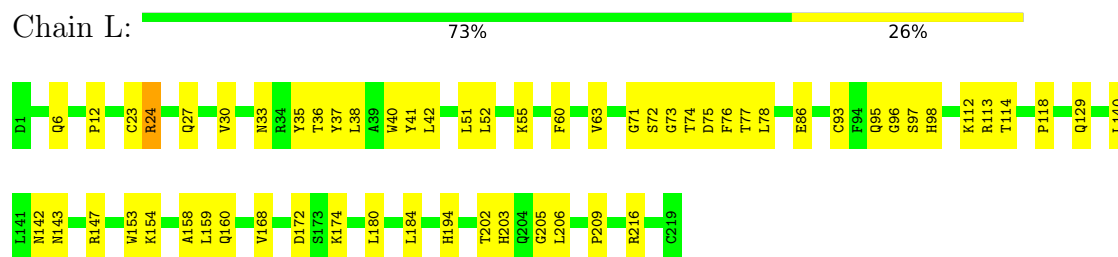
3 Residue-property plots

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.

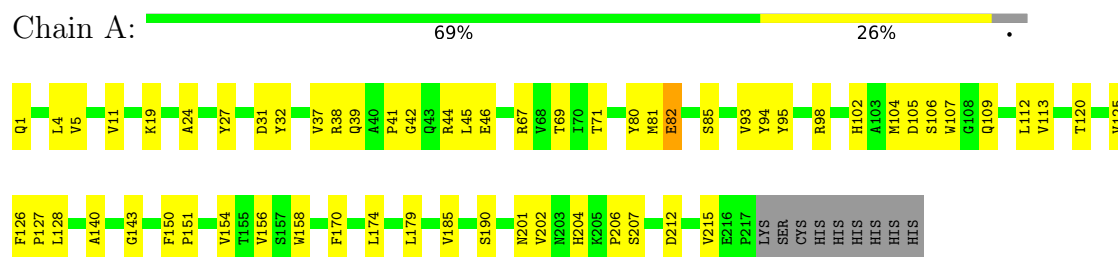
• Molecule 1: Light Chain of Fab C47B161



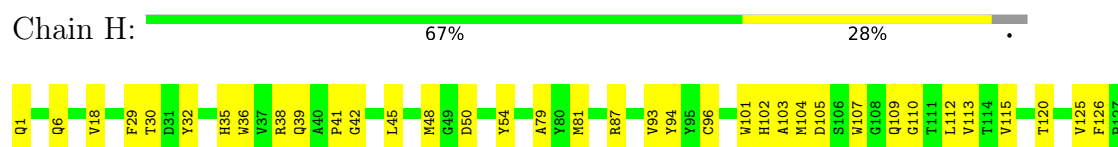
• Molecule 1: Light Chain of Fab C47B161



• Molecule 2: Heavy Chain of Fab C47B161

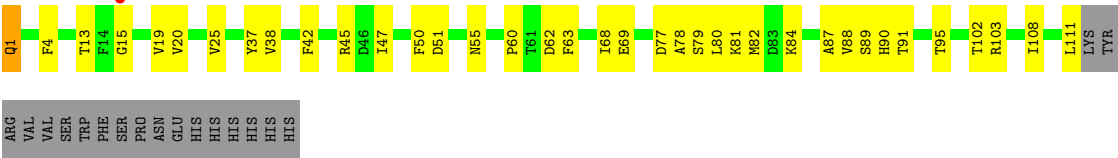


• Molecule 2: Heavy Chain of Fab C47B161





● Molecule 3: Leukocyte surface antigen CD47



● Molecule 3: Leukocyte surface antigen CD47



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.57Å 60.97Å 124.13Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	41.38 – 2.89 41.38 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.0 (41.38-2.89) 97.9 (41.38-2.89)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.257 , 0.328 0.257 , 0.324	Depositor DCC
R_{free} test set	1278 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 83.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.318 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8158	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 7.59% 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: GOL, PCA, NAG

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	B	0.23	0/1651	0.52	1/2258 (0.0%)
1	L	0.24	0/1675	0.54	0/2286
2	A	0.24	0/1611	0.58	4/2209 (0.2%)
2	H	0.30	0/1600	0.59	4/2195 (0.2%)
3	C	0.20	0/789	0.55	0/1082
3	D	0.18	0/804	0.47	0/1101
All	All	0.24	0/8130	0.55	9/11131 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	82	GLU	CA-CB-CG	7.03	128.17	114.10
2	A	81	MET	CA-C-N	5.68	130.56	122.72
2	A	81	MET	C-N-CA	5.68	130.56	122.72
2	H	152	GLU	C-N-CD	-5.62	108.23	120.60
2	H	152	GLU	CA-C-N	5.47	140.12	127.00
2	H	152	GLU	C-N-CA	5.47	140.12	127.00
1	B	74	THR	OG1-CB-CG2	5.43	120.17	109.30
2	H	152	GLU	CB-CA-C	5.37	117.91	109.37
2	A	82	GLU	CB-CA-C	-5.15	101.25	109.75

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	B	1608	0	1454	42	0
1	L	1635	0	1514	51	0
2	A	1577	0	1459	47	0
2	H	1566	0	1443	47	0
3	C	783	0	658	30	0
3	D	799	0	660	21	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	H	12	0	16	0	0
4	L	6	0	8	0	0
5	C	14	0	13	0	0
5	D	28	0	26	0	0
6	A	24	0	0	0	0
6	B	27	0	0	1	0
6	C	9	0	0	1	0
6	D	5	0	0	0	0
6	H	26	0	0	0	0
6	L	27	0	0	3	0
All	All	8158	0	7267	215	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 14.

All (215) 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:A:38:ARG:NH2	2:A:46:GLU:OE2	2.07	0.87
2:A:39:GLN:HB3	2:A:45:LEU:HD23	1.60	0.83
2:H:112:LEU:HD12	2:H:153:PRO:HD3	1.64	0.80
1:L:33:ASN:OD1	1:L:35:TYR:N	2.14	0.80
1:L:24:ARG:NH1	1:L:74:THR:OG1	2.15	0.79
3:C:13:THR:HG23	3:C:15:GLY:H	1.53	0.73
2:H:201:ASN:ND2	2:H:212:ASP:OD2	2.22	0.73
1:L:95:GLN:HE21	1:L:97:SER:H	1.35	0.72
1:L:24:ARG:HH12	1:L:74:THR:HG1	1.37	0.71
3:C:20:VAL:HG22	3:C:81:LYS:HG2	1.73	0.71
2:A:39:GLN:HB3	2:A:45:LEU:CD2	2.20	0.70
1:B:113:ARG:HG2	1:B:114:THR:N	2.07	0.70
3:D:91:THR:HA	3:D:111:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:127:PRO:HB3	2:A:215:VAL:HG23	1.74	0.69
2:A:201:ASN:ND2	2:A:212:ASP:OD2	2.25	0.68
1:L:95:GLN:NE2	1:L:98:HIS:H	1.92	0.68
2:A:67:ARG:NH2	2:A:85:SER:O	2.26	0.67
3:C:47:ILE:HD11	3:C:63:PHE:CZ	2.30	0.66
2:A:94:TYR:HE2	2:A:113:VAL:HG22	1.61	0.65
1:L:12:PRO:HB2	1:L:112:LYS:HD2	1.78	0.65
3:D:83:ASP:OD1	3:D:84:LYS:N	2.30	0.65
2:H:39:GLN:HB3	2:H:93:VAL:HB	1.77	0.65
1:L:72:SER:O	1:L:74:THR:N	2.29	0.65
3:C:68:ILE:HD13	3:C:80:LEU:HA	1.78	0.64
2:H:38:ARG:HE	2:H:94:TYR:HE1	1.44	0.64
3:D:38:VAL:HG12	3:D:50:PHE:HB3	1.80	0.64
3:C:19:VAL:HG23	3:C:82:MET:HB3	1.79	0.63
2:A:31:ASP:HB3	3:D:103:ARG:HH12	1.63	0.62
1:B:83:VAL:HG21	1:B:109:LEU:HD21	1.82	0.62
1:L:33:ASN:HD21	1:L:37:TYR:HE2	1.46	0.62
3:C:47:ILE:HD11	3:C:63:PHE:CE1	2.33	0.62
1:L:158:ALA:O	1:L:160:GLN:NE2	2.33	0.62
1:L:60:PHE:CZ	2:H:105:ASP:HB2	2.34	0.62
2:A:5:VAL:HA	2:A:109:GLN:NE2	2.14	0.62
2:A:11:VAL:HG23	2:A:206:PRO:HB3	1.82	0.61
1:B:203:HIS:CD2	1:B:204:GLN:N	2.69	0.61
1:B:71:GLY:HA3	1:B:76:PHE:HA	1.83	0.60
2:A:104:MET:SD	2:A:104:MET:N	2.74	0.60
1:B:38:LEU:HD11	1:B:93:CYS:HB2	1.82	0.60
2:H:120:THR:HG23	2:H:151:PRO:HD3	1.83	0.60
1:L:194:HIS:O	1:L:216:ARG:NE	2.32	0.60
1:L:41:TYR:HE2	2:H:104:MET:HE2	1.67	0.59
3:D:41:LYS:HG2	3:D:46:ASP:HA	1.85	0.59
3:D:84:LYS:HA	3:D:87:ALA:HB3	1.83	0.59
1:B:4:MET:O	2:A:44:ARG:NH1	2.34	0.59
1:L:168:VAL:HB	1:L:180:LEU:HD12	1.84	0.59
1:B:16:GLY:O	1:B:82:ARG:HD3	2.02	0.59
3:C:42:PHE:CE1	3:C:90:HIS:HB3	2.38	0.58
1:L:41:TYR:CE2	2:H:107:TRP:HZ2	2.21	0.58
1:B:169:THR:HG23	2:A:170:PHE:CD1	2.38	0.58
1:B:208:SER:HB2	1:B:209:PRO:HD2	1.85	0.58
2:A:125:VAL:HG21	2:A:202:VAL:HG21	1.85	0.58
1:B:123:PHE:CD1	2:A:128:LEU:HB3	2.38	0.57
3:C:91:THR:HA	3:C:111:LEU:HD23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:PHE:CZ	2:A:105:ASP:HB2	2.40	0.57
2:A:31:ASP:O	3:D:103:ARG:NH1	2.37	0.57
2:A:32:TYR:CD2	3:D:103:ARG:HD3	2.39	0.56
2:H:125:VAL:HG13	2:H:213:LYS:HG3	1.88	0.56
1:B:6:GLN:HG2	1:B:23:CYS:HB2	1.88	0.56
1:B:118:PRO:HG2	1:B:206:LEU:HD21	1.87	0.56
3:D:32:ASN:OD1	3:D:33:THR:N	2.38	0.56
2:A:109:GLN:NE2	2:A:109:GLN:H	2.04	0.56
1:B:29:ILE:HA	1:B:98:HIS:HE1	1.71	0.56
2:H:104:MET:SD	2:H:104:MET:N	2.79	0.55
1:B:203:HIS:HD2	1:B:204:GLN:H	1.53	0.55
3:D:45:ARG:HG2	3:D:46:ASP:H	1.70	0.55
3:D:100:GLU:HG3	3:D:100:GLU:O	2.07	0.55
1:L:30:VAL:HG22	1:L:36:THR:HG22	1.88	0.55
3:C:89:SER:HB2	3:C:90:HIS:CE1	2.42	0.54
3:C:37:TYR:HD1	3:C:51:ASP:HA	1.72	0.54
2:A:4:LEU:O	2:A:109:GLN:NE2	2.40	0.54
1:L:33:ASN:ND2	1:L:37:TYR:OH	2.40	0.54
2:A:19:LYS:HE3	2:A:80:TYR:HB3	1.90	0.54
3:D:50:PHE:HE2	3:D:55:ASN:HA	1.72	0.54
1:B:140:LEU:HD22	2:A:185:VAL:HG11	1.89	0.54
2:H:18:VAL:HG11	2:H:113:VAL:HG21	1.90	0.53
2:A:27:TYR:CZ	2:A:98:ARG:HD2	2.43	0.53
2:H:39:GLN:HA	2:H:45:LEU:HD22	1.91	0.53
1:L:203:HIS:CE1	1:L:205:GLY:H	2.26	0.53
3:C:45:ARG:HH12	3:C:62:ASP:CG	2.17	0.53
1:B:113:ARG:HG2	1:B:114:THR:H	1.72	0.52
1:B:5:THR:O	1:B:23:CYS:HA	2.09	0.52
3:D:95:THR:HB	3:D:108:ILE:HG22	1.90	0.52
2:A:38:ARG:HD3	2:A:94:TYR:CE1	2.44	0.52
1:L:37:TYR:CD1	1:L:55:LYS:HD3	2.44	0.52
1:L:118:PRO:HG2	1:L:206:LEU:HD21	1.92	0.52
3:C:50:PHE:HE2	3:C:55:ASN:HA	1.75	0.52
2:A:11:VAL:HG22	2:A:151:PRO:HG2	1.91	0.52
2:H:101:TRP:CE2	3:C:1:PCA:H2	2.45	0.51
2:A:5:VAL:HA	2:A:109:GLN:HE22	1.75	0.51
1:B:203:HIS:CD2	1:B:204:GLN:H	2.28	0.51
2:H:29:PHE:HZ	2:H:79:ALA:HB2	1.76	0.51
2:H:170:PHE:O	2:H:182:LEU:HD11	2.11	0.51
1:L:142:ASN:OD1	1:L:143:ASN:N	2.44	0.51
2:H:158:TRP:CH2	2:H:200:CYS:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:24:ARG:NH2	1:L:75:ASP:HB2	2.26	0.50
2:H:152:GLU:HG2	2:H:153:PRO:HA	1.94	0.50
3:C:81:LYS:HD2	6:C:301:HOH:O	2.11	0.50
1:B:143:ASN:H	1:B:179:SER:HB3	1.77	0.50
1:L:6:GLN:HG2	1:L:23:CYS:HB2	1.93	0.50
3:C:20:VAL:HA	3:C:80:LEU:O	2.12	0.50
2:A:71:THR:OG1	2:A:80:TYR:HB2	2.12	0.50
2:A:24:ALA:HB1	2:A:27:TYR:CE1	2.48	0.49
2:A:98:ARG:NH1	2:A:105:ASP:OD2	2.45	0.49
2:H:172:ALA:HA	2:H:182:LEU:HD13	1.92	0.49
3:C:38:VAL:HG21	3:C:78:ALA:HB1	1.95	0.49
1:L:129:GLN:HB2	2:H:126:PHE:CD2	2.48	0.49
2:H:143:GLY:HA2	2:H:158:TRP:CH2	2.48	0.49
3:D:50:PHE:CE2	3:D:55:ASN:HA	2.48	0.49
2:H:36:TRP:CH2	2:H:96:CYS:HB2	2.48	0.49
1:B:80:ILE:HD12	1:B:80:ILE:O	2.12	0.49
1:L:159:LEU:HD12	1:L:160:GLN:H	1.78	0.49
1:L:86:GLU:OE1	1:L:86:GLU:N	2.46	0.48
3:C:37:TYR:CD1	3:C:51:ASP:HA	2.48	0.48
2:H:103:ALA:HB3	3:C:102:THR:HG23	1.94	0.48
3:C:95:THR:HG22	3:C:108:ILE:HG23	1.95	0.48
1:L:41:TYR:HE1	1:L:51:LEU:HD13	1.78	0.48
2:H:216:GLU:HG3	2:H:217:PRO:HD2	1.96	0.48
3:C:77:ASP:OD1	3:C:79:SER:OG	2.25	0.48
1:L:40:TRP:CZ3	1:L:93:CYS:HB3	2.48	0.48
2:A:154:VAL:HG22	2:A:204:HIS:HB2	1.95	0.47
3:C:84:LYS:O	3:C:88:VAL:HG12	2.14	0.47
1:B:55:LYS:O	1:B:57:SER:N	2.42	0.47
1:B:83:VAL:HG23	1:B:87:ASP:HB2	1.97	0.47
2:H:174:LEU:HD12	2:H:179:LEU:O	2.15	0.47
1:B:159:LEU:HD12	1:B:160:GLN:H	1.79	0.47
2:A:37:VAL:O	2:A:95:TYR:N	2.28	0.47
1:L:40:TRP:CH2	1:L:93:CYS:HB3	2.50	0.47
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.49	0.47
3:D:89:SER:HG	3:D:90:HIS:CG	2.33	0.47
1:B:90:VAL:HA	1:B:108:LYS:HA	1.96	0.47
2:A:41:PRO:HA	2:A:42:GLY:HA2	1.54	0.47
1:L:24:ARG:HH21	1:L:75:ASP:HB2	1.78	0.47
3:C:68:ILE:CD1	3:C:80:LEU:HA	2.43	0.47
2:H:140:ALA:HB2	2:H:190:SER:HB3	1.97	0.46
3:D:95:THR:CB	3:D:108:ILE:HG22	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:ASP:OD1	1:B:100:PRO:HG2	2.16	0.46
1:L:172:ASP:OD1	1:L:174:LYS:HG2	2.16	0.46
2:A:69:THR:CG2	2:A:82:GLU:HB3	2.45	0.46
1:B:30:VAL:HG22	1:B:36:THR:CG2	2.46	0.46
2:A:94:TYR:HE2	2:A:113:VAL:CG2	2.28	0.46
1:L:86:GLU:H	1:L:86:GLU:CD	2.23	0.46
1:B:33:ASN:ND2	1:B:37:TYR:OH	2.49	0.46
2:A:98:ARG:NH1	2:A:106:SER:OG	2.47	0.46
2:H:30:THR:HG23	2:H:54:TYR:HA	1.98	0.46
1:B:21:ILE:O	1:B:78:LEU:N	2.38	0.46
2:A:38:ARG:HD3	2:A:94:TYR:HE1	1.80	0.45
3:C:84:LYS:HA	3:C:87:ALA:HB3	1.97	0.45
1:B:30:VAL:HG22	1:B:36:THR:HG22	1.99	0.45
1:L:209:PRO:HD3	6:L:412:HOH:O	2.16	0.45
2:H:205:LYS:N	2:H:206:PRO:HD2	2.32	0.45
1:L:42:LEU:HB2	1:L:52:LEU:HD11	1.98	0.45
3:C:47:ILE:O	3:C:60:PRO:HD2	2.16	0.45
2:H:87:ARG:C	2:H:115:VAL:HG11	2.42	0.45
1:B:83:VAL:CG2	1:B:109:LEU:HD21	2.47	0.45
2:A:143:GLY:HA2	2:A:158:TRP:CH2	2.52	0.45
2:A:174:LEU:HD12	2:A:179:LEU:O	2.17	0.45
2:H:152:GLU:OE2	2:H:180:TYR:CE1	2.70	0.44
1:L:71:GLY:HA3	1:L:76:PHE:HA	1.99	0.44
3:C:63:PHE:CZ	3:C:90:HIS:CG	3.05	0.44
3:D:47:ILE:O	3:D:60:PRO:HD2	2.18	0.44
2:H:151:PRO:O	2:H:204:HIS:NE2	2.45	0.44
1:L:27:GLN:N	1:L:27:GLN:OE1	2.50	0.44
2:H:6:GLN:H	2:H:109:GLN:NE2	2.16	0.44
1:L:113:ARG:HG2	1:L:114:THR:N	2.33	0.43
1:B:126:SER:OG	2:A:126:PHE:HB3	2.18	0.43
1:B:145:TYR:CD2	1:B:146:PRO:HA	2.53	0.43
1:L:129:GLN:NE2	2:H:147:LYS:HE2	2.33	0.43
1:L:38:LEU:HD11	1:L:93:CYS:HB2	2.00	0.43
2:A:120:THR:HG22	2:A:207:SER:HB3	2.01	0.43
2:H:35:HIS:HD2	2:H:50:ASP:CB	2.30	0.43
1:B:49:PRO:HG2	2:A:107:TRP:CE3	2.53	0.43
1:L:60:PHE:HZ	2:H:105:ASP:HB2	1.80	0.43
2:H:41:PRO:HA	2:H:42:GLY:HA2	1.59	0.43
2:A:93:VAL:HG22	2:A:112:LEU:HB2	2.00	0.43
1:L:95:GLN:HE21	1:L:98:HIS:H	1.65	0.43
1:B:96:GLY:HA2	1:B:101:TYR:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:164:THR:O	2:H:167:VAL:HG22	2.19	0.43
1:B:101:TYR:OH	2:A:102:HIS:HD2	2.02	0.42
3:C:4:PHE:CE2	3:C:25:VAL:HG22	2.55	0.42
2:A:140:ALA:HB2	2:A:190:SER:HB3	2.02	0.42
1:L:147:ARG:NH2	6:L:401:HOH:O	2.51	0.42
1:B:140:LEU:HA	1:B:181:SER:HA	2.00	0.42
3:C:68:ILE:HG22	3:C:69:GLU:H	1.85	0.42
2:A:150:PHE:CD2	2:A:151:PRO:HA	2.55	0.42
1:L:41:TYR:CE2	2:H:104:MET:HE2	2.52	0.42
2:H:30:THR:CG2	2:H:54:TYR:HD1	2.33	0.42
1:B:113:ARG:NH1	6:B:401:HOH:O	2.52	0.42
2:H:38:ARG:HB2	2:H:48:MET:SD	2.60	0.42
2:H:174:LEU:HD12	2:H:179:LEU:C	2.45	0.42
1:B:38:LEU:HD12	1:B:94:PHE:O	2.20	0.41
2:H:32:TYR:CZ	3:C:103:ARG:NH1	2.89	0.41
3:C:89:SER:HB2	3:C:90:HIS:ND1	2.35	0.41
1:L:33:ASN:OD1	1:L:33:ASN:C	2.63	0.41
1:L:153:TRP:CG	1:L:184:LEU:HD13	2.55	0.41
1:L:40:TRP:CG	1:L:78:LEU:HD12	2.54	0.41
1:B:154:LYS:HA	1:B:158:ALA:O	2.21	0.41
3:D:14:PHE:O	3:D:14:PHE:CD1	2.73	0.41
2:A:156:VAL:HA	2:A:201:ASN:O	2.20	0.41
1:L:140:LEU:CD2	2:H:185:VAL:HG11	2.51	0.41
2:H:175:GLN:HG3	2:H:179:LEU:O	2.19	0.41
3:D:68:ILE:HG22	3:D:69:GLU:N	2.35	0.41
1:B:91:TYR:HE2	1:B:109:LEU:HB2	1.85	0.41
1:L:38:LEU:HD22	1:L:76:PHE:CD2	2.56	0.41
3:D:41:LYS:HB2	3:D:95:THR:CG2	2.50	0.41
2:H:128:LEU:HD11	2:H:145:LEU:HB2	2.02	0.41
1:B:29:ILE:HA	1:B:98:HIS:CE1	2.53	0.40
2:H:109:GLN:HG2	2:H:110:GLY:N	2.37	0.40
1:L:52:LEU:HA	1:L:63:VAL:HG11	2.02	0.40
3:D:86:ASP:HB3	3:D:90:HIS:CE1	2.56	0.40
1:L:202:THR:HG23	6:L:412:HOH:O	2.22	0.40
3:C:68:ILE:HG22	3:C:69:GLU:N	2.36	0.40
2:A:94:TYR:CE2	2:A:113:VAL:HG22	2.49	0.40
1:L:96:GLY:O	2:H:102:HIS:HB3	2.22	0.40
1:L:154:LYS:HA	1:L:158:ALA:O	2.22	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	B	217/219 (99%)	204 (94%)	12 (6%)	1 (0%)	24	54
1	L	217/219 (99%)	203 (94%)	13 (6%)	1 (0%)	24	54
2	A	215/226 (95%)	208 (97%)	7 (3%)	0	100	100
2	H	215/226 (95%)	209 (97%)	6 (3%)	0	100	100
3	C	109/129 (84%)	102 (94%)	7 (6%)	0	100	100
3	D	110/129 (85%)	104 (94%)	6 (6%)	0	100	100
All	All	1083/1148 (94%)	1030 (95%)	51 (5%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	73	GLY
1	B	73	GLY

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	B	166/194 (86%)	165 (99%)	1 (1%)	78	93
1	L	173/194 (89%)	171 (99%)	2 (1%)	63	86
2	A	162/189 (86%)	162 (100%)	0	100	100
2	H	158/189 (84%)	158 (100%)	0	100	100
3	C	67/117 (57%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	68/117 (58%)	68 (100%)	0	100	100
All	All	794/1000 (79%)	791 (100%)	3 (0%)	84	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	207	SER
1	L	24	ARG
1	L	77	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	143	ASN
1	B	203	HIS
2	A	102	HIS
2	A	159	ASN
2	A	203	ASN
2	A	204	HIS
1	L	6	GLN
1	L	95	GLN
1	L	98	HIS
1	L	129	GLN
3	C	16	ASN
3	C	72	GLN

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	A	1	2	7,8,9	1.92	1 (14%)	9,10,12	2.41	5 (55%)
3	PCA	C	1	3	7,8,9	1.91	1 (14%)	9,10,12	2.25	5 (55%)
2	PCA	H	1	2	7,8,9	1.93	1 (14%)	9,10,12	2.40	5 (55%)
3	PCA	D	1	3	7,8,9	1.94	1 (14%)	9,10,12	2.13	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	A	1	2	-	0/0/11/13	0/1/1/1
3	PCA	C	1	3	-	0/0/11/13	0/1/1/1
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1
3	PCA	D	1	3	-	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)
3	D	1	PCA	CD-N	5.01	1.47	1.34
2	H	1	PCA	CD-N	4.98	1.46	1.34
2	A	1	PCA	CD-N	4.96	1.46	1.34
3	C	1	PCA	CD-N	4.93	1.46	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	PCA	CB-CA-C	-3.99	107.19	112.66
2	H	1	PCA	CB-CA-C	-3.92	107.27	112.66
3	D	1	PCA	OE-CD-CG	-3.07	121.24	126.72
2	H	1	PCA	OE-CD-CG	-3.00	121.37	126.72
2	A	1	PCA	OE-CD-CG	-2.99	121.38	126.72
2	H	1	PCA	CA-N-CD	-2.96	103.46	113.58
2	A	1	PCA	CA-N-CD	-2.95	103.47	113.58
3	C	1	PCA	OE-CD-CG	-2.95	121.46	126.72
3	C	1	PCA	CA-N-CD	-2.92	103.58	113.58
3	C	1	PCA	CB-CA-N	2.90	111.23	103.24
3	D	1	PCA	CB-CA-N	2.85	111.08	103.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	PCA	CA-N-CD	-2.83	103.90	113.58
3	C	1	PCA	CG-CD-N	2.78	115.18	108.39
2	A	1	PCA	CB-CA-N	2.67	110.60	103.24
2	H	1	PCA	CB-CA-N	2.67	110.59	103.24
3	C	1	PCA	CB-CA-C	-2.58	109.12	112.66
3	D	1	PCA	CG-CD-N	2.55	114.62	108.39
2	H	1	PCA	CG-CD-N	2.54	114.61	108.39
2	A	1	PCA	CG-CD-N	2.54	114.60	108.39
3	D	1	PCA	CB-CA-C	-2.31	109.48	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	PCA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
5	NAG	D	201	3	14,14,15	0.28	0	17,19,21	0.32	0
5	NAG	D	202	3	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	C	201	3	14,14,15	0.26	0	17,19,21	0.42	0
4	GOL	H	302	-	5,5,5	0.37	0	5,5,5	0.39	0
4	GOL	A	301	-	5,5,5	0.37	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	301	-	5,5,5	0.38	0	5,5,5	0.22	0
4	GOL	L	301	-	5,5,5	0.39	0	5,5,5	0.25	0
4	GOL	H	301	-	5,5,5	0.38	0	5,5,5	0.28	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
5	NAG	D	201	3	-	2/6/23/26	0/1/1/1
5	NAG	D	202	3	-	0/6/23/26	0/1/1/1
5	NAG	C	201	3	-	1/6/23/26	0/1/1/1
4	GOL	H	302	-	-	2/4/4/4	-
4	GOL	A	301	-	-	4/4/4/4	-
4	GOL	B	301	-	-	2/4/4/4	-
4	GOL	L	301	-	-	4/4/4/4	-
4	GOL	H	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	GOL	O1-C1-C2-C3
4	A	301	GOL	C1-C2-C3-O3
4	L	301	GOL	O1-C1-C2-C3
4	H	301	GOL	O1-C1-C2-C3
4	H	302	GOL	O1-C1-C2-C3
5	D	201	NAG	O5-C5-C6-O6
4	B	301	GOL	O1-C1-C2-O2
4	A	301	GOL	O1-C1-C2-C3
4	L	301	GOL	C1-C2-C3-O3
4	A	301	GOL	O1-C1-C2-O2
4	A	301	GOL	O2-C2-C3-O3
4	H	301	GOL	O1-C1-C2-O2
4	H	302	GOL	O1-C1-C2-O2
4	L	301	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	L	301	GOL	O2-C2-C3-O3
5	C	201	NAG	C1-C2-N2-C7
5	D	201	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9	
1	B	218/219 (99%)	-0.61	0	100	100	29, 60, 82, 108	1 (0%)
1	L	219/219 (100%)	-0.54	0	100	100	30, 61, 87, 107	0
2	A	216/226 (95%)	-0.55	0	100	100	35, 59, 83, 104	0
2	H	216/226 (95%)	-0.53	0	100	100	35, 60, 83, 109	0
3	C	110/129 (85%)	-0.22	1 (0%)	81	75	52, 83, 122, 138	0
3	D	113/129 (87%)	-0.30	0	100	100	53, 86, 119, 149	0
All	All	1092/1148 (95%)	-0.50	1 (0%)	92	90	29, 64, 103, 149	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	15	GLY	2.9

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	PCA	H	1	8/9	0.96	0.09	62,74,78,87	0
2	PCA	A	1	8/9	0.97	0.07	40,59,70,73	0
3	PCA	C	1	8/9	0.98	0.08	39,50,66,68	0
3	PCA	D	1	8/9	0.98	0.06	21,47,54,55	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
4	GOL	A	301	6/6	0.91	0.10	56,62,65,66	0
4	GOL	H	302	6/6	0.93	0.10	67,80,83,83	0
4	GOL	H	301	6/6	0.94	0.09	39,50,54,56	0
5	NAG	D	202	14/15	0.94	0.09	92,108,120,126	0
5	NAG	D	201	14/15	0.95	0.10	90,121,135,150	0
4	GOL	L	301	6/6	0.96	0.12	177,182,190,199	0
5	NAG	C	201	14/15	0.96	0.08	96,101,106,111	0
4	GOL	B	301	6/6	0.97	0.07	80,86,86,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.