



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:44 PM UTC

PDB ID : 6E62 / pdb_00006e62
Title : Crystal structure of malaria transmission-blocking antigen Pfs48/45 6C in complex with antibody 85RF45.1
Authors : Kundu, P.; Semesi, A.; Julien, J.P.
Deposited on : 2018-07-23
Resolution : 2.70 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

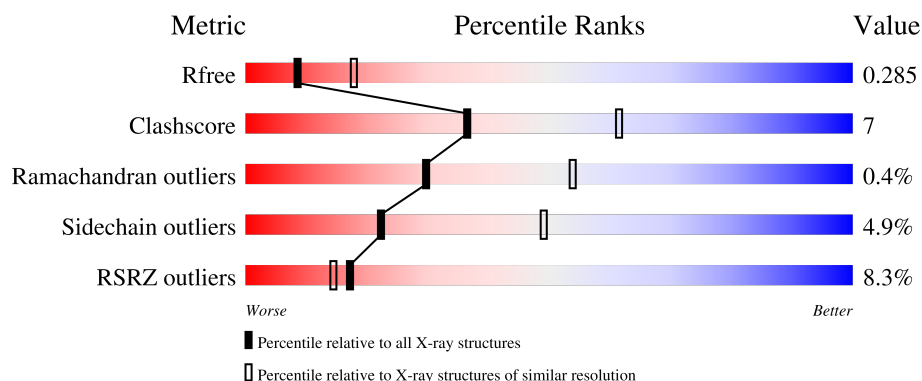
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	139	6% 78% 19% ..
1	P	139	2% 70% 26% ..
2	B	222	8% 86% 11% ..
2	H	222	13% 83% 13% ..
3	C	216	10% 77% 19% ..

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Mol	Chain	Length	Quality of chain
3	L	216	7% 82% 16%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8799 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 Pf48/45.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	137	Total	C	N	O	S	0	0	0
			1059	667	167	218	7			
1	A	137	Total	C	N	O	S	0	0	0
			1059	667	167	218	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	429	GLY	-	expression tag	UNP A8QVT1
A	429	GLY	-	expression tag	UNP A8QVT1

- Molecule 2 is a protein called 85RF45.1 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1650	1045	275	322	8			
2	B	217	Total	C	N	O	S	0	0	0
			1650	1045	275	322	8			

- Molecule 3 is a protein called 85RF45.1 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1625	1013	277	329	6			
3	C	213	Total	C	N	O	S	0	0	0
			1625	1013	277	329	6			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	P	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

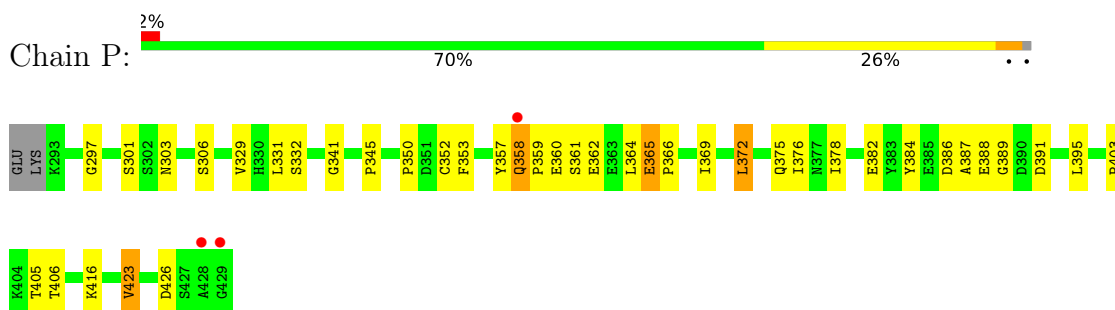
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	20	Total 20	O 20	0	0
6	H	9	Total 9	O 9	0	0
6	L	9	Total 9	O 9	0	0
6	A	26	Total 26	O 26	0	0
6	B	17	Total 17	O 17	0	0
6	C	10	Total 10	O 10	0	0

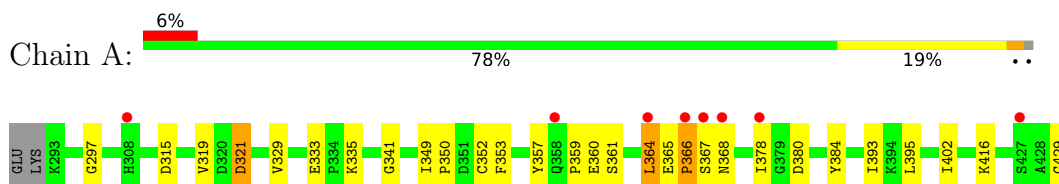
3 Residue-property plots

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.

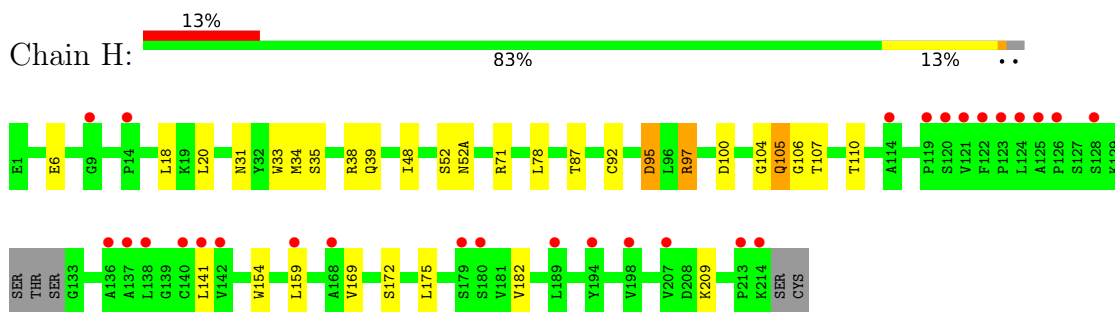
- Molecule 1: Pf48/45



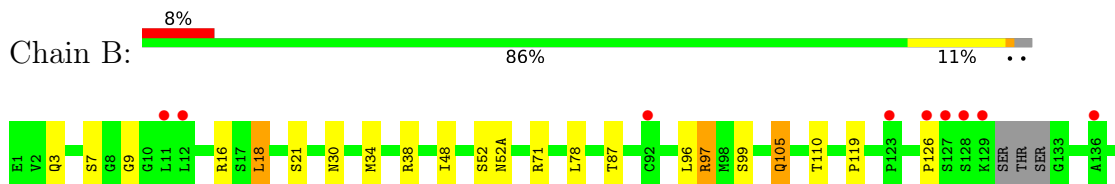
- Molecule 1: Pf48/45

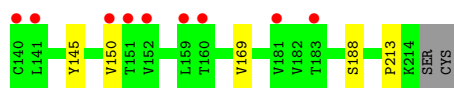


- Molecule 2: 85RF45.1 Fab heavy chain

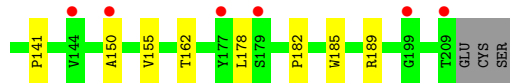
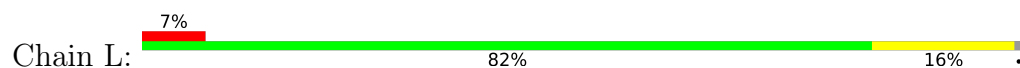


- Molecule 2: 85RF45.1 Fab heavy chain

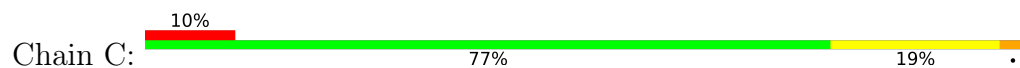




- Molecule 3: 85RF45.1 Fab light chain



- Molecule 3: 85RF45.1 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.51Å 74.45Å 321.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.70 48.70 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.70-2.70) 100.0 (48.70-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.246 , 0.276 0.253 , 0.285	Depositor DCC
R_{free} test set	1858 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	64.2	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 87.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8799	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.36% 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: NAG, GOL

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	0.22	0/1081	0.41	0/1466
1	P	0.18	0/1081	0.39	0/1466
2	B	0.11	0/1690	0.31	0/2299
2	H	0.11	0/1690	0.31	0/2299
3	C	0.13	0/1664	0.33	0/2268
3	L	0.12	0/1664	0.34	0/2268
All	All	0.14	0/8870	0.34	0/12066

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	1059	0	1008	23	0
1	P	1059	0	1008	20	0
2	B	1650	0	1616	17	0
2	H	1650	0	1616	22	0
3	C	1625	0	1567	28	0
3	L	1625	0	1567	24	0
4	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	14	0	13	1	0
5	B	6	0	8	2	0
5	H	6	0	8	2	0
6	A	26	0	0	4	0
6	B	17	0	0	0	0
6	C	10	0	0	1	0
6	H	9	0	0	1	0
6	L	9	0	0	3	0
6	P	20	0	0	2	0
All	All	8799	0	8424	123	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 7.

All (123) 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:L:96:TYR:OH	6:L:301:HOH:O	1.92	0.86
2:B:97:ARG:NH2	3:C:96:TYR:OH	2.14	0.80
1:P:301:SER:O	6:P:601:HOH:O	2.00	0.79
3:C:83:GLU:HG3	3:C:105:THR:HA	1.64	0.78
3:L:54:ARG:NH2	3:L:62:PHE:O	2.18	0.77
1:A:429:GLY:O	6:A:601:HOH:O	2.04	0.75
1:P:303:ASN:OD1	6:P:602:HOH:O	2.06	0.72
2:H:100:ASP:O	6:H:401:HOH:O	2.09	0.69
1:P:384:TYR:HB2	1:P:395:LEU:HB2	1.75	0.68
1:A:384:TYR:HB2	1:A:395:LEU:HB2	1.75	0.67
2:H:31:ASN:O	5:H:301:GOL:O2	2.14	0.65
2:H:97:ARG:NH1	2:H:100:ASP:OD1	2.30	0.64
1:A:378:ILE:HG22	1:A:380:ASP:H	1.62	0.63
3:L:1:GLN:N	6:L:303:HOH:O	2.34	0.61
3:L:25:ARG:NH2	3:L:27(B):ASN:O	2.34	0.61
3:L:26:SER:O	6:L:302:HOH:O	2.16	0.60
1:A:367:SER:O	6:A:602:HOH:O	2.17	0.58
2:H:87:THR:HG23	2:H:110:THR:HA	1.84	0.58
2:B:52:SER:O	2:B:71:ARG:NH1	2.36	0.58
3:C:20:LYS:NZ	6:C:302:HOH:O	2.37	0.57
2:H:159:LEU:HD21	2:H:182:VAL:HG21	1.87	0.57
2:H:52(A):ASN:N	2:H:52(A):ASN:OD1	2.38	0.56
3:L:39:HIS:CG	3:L:42:ARG:HH21	2.24	0.56
3:L:128:ASN:HA	3:L:182:PRO:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:ARG:NH1	3:C:77:ASN:O	2.39	0.56
3:C:150:ALA:HB1	3:C:188:HIS:CD2	2.40	0.56
2:H:154:TRP:HB3	2:H:159:LEU:HD23	1.88	0.56
1:A:315:ASP:OD1	6:A:603:HOH:O	2.18	0.56
1:A:335:LYS:NZ	6:A:605:HOH:O	2.36	0.55
2:B:97:ARG:O	2:B:97:ARG:HD3	2.06	0.55
3:L:132:LEU:HD12	3:L:178:LEU:HD23	1.89	0.55
1:A:366:PRO:HD2	5:B:301:GOL:H32	1.88	0.55
2:B:38:ARG:HB3	2:B:48:ILE:HD11	1.88	0.55
1:P:416:LYS:HE2	3:L:32:TYR:CD1	2.42	0.55
2:H:141:LEU:HD21	3:L:133:VAL:HG21	1.88	0.54
2:B:87:THR:HG23	2:B:110:THR:HA	1.89	0.54
3:L:150:ALA:H	3:L:155:VAL:HG23	1.73	0.54
3:C:14:ASN:ND2	3:C:17:SER:OG	2.40	0.54
3:L:110:LYS:HD3	3:L:141:PRO:HD3	1.90	0.54
3:C:15:LEU:HD22	3:C:78:VAL:O	2.08	0.54
3:L:80:THR:HB	3:C:156:LYS:HE3	1.91	0.53
3:C:20:LYS:HB3	3:C:72:LEU:HD23	1.91	0.53
3:L:150:ALA:H	3:L:155:VAL:CG2	2.22	0.52
2:H:52:SER:O	2:H:71:ARG:NH1	2.42	0.52
1:P:341:GLY:HA2	1:P:353:PHE:CE2	2.45	0.52
3:C:132:LEU:HD12	3:C:178:LEU:HD23	1.92	0.52
1:P:350:PRO:HB3	1:P:369:ILE:HD13	1.92	0.51
1:A:365:GLU:OE1	5:B:301:GOL:O3	2.19	0.51
2:B:34:MET:HB3	2:B:78:LEU:HD22	1.92	0.51
1:P:358:GLN:HG3	1:P:375:GLN:NE2	2.25	0.51
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.91	0.51
2:H:38:ARG:HD3	2:H:48:ILE:HD11	1.93	0.50
2:H:6:GLU:OE1	2:H:106:GLY:N	2.38	0.50
3:C:77:ASN:C	3:C:77:ASN:HD22	2.20	0.50
2:B:7:SER:HB3	2:B:21:SER:HB2	1.93	0.50
2:B:30:ASN:O	2:B:52(A):ASN:HB3	2.12	0.49
1:A:341:GLY:HA3	1:A:395:LEU:HD23	1.94	0.49
2:B:126:PRO:HD2	2:B:213:PRO:HA	1.95	0.49
3:C:4:LEU:HD11	3:C:90:SER:HB2	1.94	0.49
1:A:341:GLY:HA2	1:A:353:PHE:CE2	2.47	0.49
1:P:332:SER:HA	1:P:426:ASP:HB2	1.94	0.49
1:A:364:LEU:HG	3:C:50:ARG:NH2	2.27	0.49
3:L:49:TYR:HD2	3:L:50:ARG:HG2	1.77	0.49
2:B:38:ARG:HD3	2:B:48:ILE:HD11	1.94	0.48
2:H:33:TRP:CZ2	2:H:97:ARG:HD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:MET:HE3	3:C:58:VAL:HG13	1.96	0.48
2:H:38:ARG:HB3	2:H:48:ILE:HD11	1.95	0.48
2:B:9:GLY:HA2	2:B:18:LEU:HD11	1.95	0.48
3:C:66(A):ASP:OD1	3:C:67:SER:OG	2.26	0.48
3:L:54:ARG:HG3	3:L:58:VAL:HB	1.96	0.47
1:A:297:GLY:HA2	1:A:329:VAL:HG21	1.94	0.47
3:C:127:ALA:O	3:C:129:LYS:HG2	2.14	0.47
3:C:82:ASP:N	3:C:82:ASP:OD1	2.45	0.47
1:P:297:GLY:HA2	1:P:329:VAL:HG21	1.97	0.47
1:P:365:GLU:OE2	5:H:301:GOL:O3	2.30	0.47
1:P:372:LEU:HD22	1:P:376:ILE:HG13	1.97	0.47
2:H:33:TRP:HB2	2:H:95:ASP:HB2	1.97	0.47
1:P:388:GLU:HB3	1:P:391:ASP:HB2	1.95	0.47
3:C:122:SER:OG	3:C:126:GLN:NE2	2.38	0.47
2:H:34:MET:HB3	2:H:78:LEU:HD22	1.98	0.46
2:H:105:GLN:H	2:H:105:GLN:HG3	1.53	0.46
2:B:169:VAL:HB	3:C:162:THR:HG22	1.97	0.46
3:C:55:PRO:HD2	3:C:58:VAL:HG21	1.99	0.45
2:B:105:GLN:HE21	2:B:105:GLN:HB2	1.61	0.45
3:L:132:LEU:HD21	3:L:185:TRP:CZ3	2.52	0.44
3:C:15:LEU:HD13	3:C:16:GLY:N	2.33	0.44
1:A:321:ASP:N	1:A:321:ASP:OD1	2.48	0.44
2:H:39:GLN:OE1	3:L:38:HIS:NE2	2.51	0.44
3:L:120:PRO:HD2	3:L:185:TRP:CZ2	2.53	0.44
1:A:365:GLU:OE2	2:B:99:SER:OG	2.25	0.44
2:B:105:GLN:H	2:B:105:GLN:HG3	1.55	0.44
1:P:329:VAL:O	1:P:423:VAL:HA	2.17	0.44
3:C:149:LYS:HD3	3:C:194:GLN:OE1	2.17	0.44
2:H:20:LEU:HD13	2:H:107:THR:HG21	1.99	0.43
2:H:169:VAL:HB	3:L:162:THR:HG22	2.00	0.43
3:C:39:HIS:HE1	3:C:81:GLU:O	2.01	0.43
1:A:360:GLU:HG2	1:A:368:ASN:OD1	2.18	0.43
3:L:132:LEU:HB2	3:L:178:LEU:HB3	2.01	0.43
1:A:365:GLU:HG3	2:B:96:LEU:HD23	2.01	0.43
2:H:209:LYS:HA	2:H:209:LYS:HD3	1.74	0.42
1:A:357:TYR:CZ	1:A:359:PRO:HB3	2.54	0.42
1:P:386:ASP:OD1	1:P:387:ALA:N	2.52	0.42
1:A:349:ILE:HA	1:A:350:PRO:HA	1.89	0.42
3:L:39:HIS:CE1	3:L:84:ALA:HB2	2.54	0.42
3:L:95:MET:HE3	3:L:95:MET:HB2	1.97	0.42
1:A:352:CYS:HA	1:A:353:PHE:HA	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:352:CYS:HA	1:P:353:PHE:HA	1.70	0.42
3:C:82:ASP:O	3:C:84:ALA:N	2.47	0.42
1:P:297:GLY:HA3	1:P:341:GLY:O	2.19	0.42
1:A:378:ILE:HG22	1:A:380:ASP:N	2.30	0.42
2:H:35:SER:OG	2:H:95:ASP:OD2	2.27	0.41
3:L:7:PRO:HD3	3:L:22:LEU:HG	2.01	0.41
1:P:389:GLY:HA3	4:P:501:NAG:H4	2.03	0.41
1:P:357:TYR:CZ	1:P:359:PRO:HB3	2.56	0.41
2:H:92:CYS:O	2:H:104:GLY:N	2.54	0.41
1:A:297:GLY:HA3	1:A:341:GLY:O	2.21	0.41
3:C:61:ARG:HB3	3:C:76:ASP:O	2.21	0.41
3:C:149:LYS:HB2	3:C:192:SER:OG	2.21	0.41
1:A:378:ILE:HD11	1:A:402:ILE:HG22	2.02	0.40
3:C:118:PHE:HB2	3:C:133:VAL:HB	2.03	0.40
1:A:416:LYS:HE2	3:C:32:TYR:CD1	2.57	0.40
1:P:301:SER:HA	1:P:345:PRO:HG3	2.04	0.40
1:P:372:LEU:HD23	1:P:372:LEU:HA	1.91	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	135/139 (97%)	122 (90%)	12 (9%)	1 (1%)	18	41
1	P	135/139 (97%)	123 (91%)	10 (7%)	2 (2%)	8	22
2	B	213/222 (96%)	208 (98%)	5 (2%)	0	100	100
2	H	213/222 (96%)	209 (98%)	4 (2%)	0	100	100
3	C	211/216 (98%)	194 (92%)	16 (8%)	1 (0%)	24	48
3	L	211/216 (98%)	198 (94%)	12 (6%)	1 (0%)	24	48
All	All	1118/1154 (97%)	1054 (94%)	59 (5%)	5 (0%)	30	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	366	PRO
3	L	50	ARG
1	A	366	PRO
3	C	93	THR
1	P	403	PRO

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	125/127 (98%)	119 (95%)	6 (5%)	23	50
1	P	125/127 (98%)	111 (89%)	14 (11%)	6	15
2	B	186/191 (97%)	179 (96%)	7 (4%)	29	58
2	H	186/191 (97%)	180 (97%)	6 (3%)	34	64
3	C	185/188 (98%)	174 (94%)	11 (6%)	18	42
3	L	185/188 (98%)	180 (97%)	5 (3%)	39	69
All	All	992/1012 (98%)	943 (95%)	49 (5%)	22	49

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	306	SER
1	P	331	LEU
1	P	358	GLN
1	P	360	GLU
1	P	361	SER
1	P	362	GLU
1	P	364	LEU
1	P	365	GLU
1	P	372	LEU
1	P	378	ILE
1	P	382	GLU
1	P	405	THR

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Mol	Chain	Res	Type
1	P	406	THR
1	P	423	VAL
2	H	18	LEU
2	H	95	ASP
2	H	97	ARG
2	H	105	GLN
2	H	172	SER
2	H	175	LEU
3	L	14	ASN
3	L	34	SER
3	L	47	MET
3	L	60	ASP
3	L	189	ARG
1	A	319	VAL
1	A	321	ASP
1	A	333	GLU
1	A	361	SER
1	A	364	LEU
1	A	393	ILE
2	B	3	GLN
2	B	16	ARG
2	B	18	LEU
2	B	97	ARG
2	B	105	GLN
2	B	150	VAL
2	B	188	SER
3	C	1	GLN
3	C	12	SER
3	C	14	ASN
3	C	50	ARG
3	C	60	ASP
3	C	74	THR
3	C	77	ASN
3	C	82	ASP
3	C	90	SER
3	C	93	THR
3	C	95	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	337	ASN

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Mol	Chain	Res	Type
1	P	358	GLN
1	P	368	ASN
1	P	377	ASN
2	H	30	ASN
2	H	31	ASN
2	H	39	GLN
2	H	81	GLN
3	L	39	HIS
3	L	53	GLN
3	L	77	ASN
1	A	296	HIS
1	A	324	HIS
1	A	328	ASN
1	A	337	ASN
1	A	358	GLN
2	B	3	GLN
3	C	14	ASN
3	C	39	HIS
3	C	77	ASN
3	C	126	GLN
3	C	188	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](#)

4 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	GOL	H	301	-	5,5,5	1.10	0	5,5,5	0.78	0
5	GOL	B	301	-	5,5,5	0.96	0	5,5,5	1.00	0
4	NAG	P	501	1	14,14,15	0.34	0	17,19,21	0.61	0
4	NAG	A	501	1	14,14,15	0.30	0	17,19,21	0.51	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	GOL	H	301	-	-	2/4/4/4	-
5	GOL	B	301	-	-	2/4/4/4	-
4	NAG	P	501	1	-	4/6/23/26	0/1/1/1
4	NAG	A	501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	301	GOL	O1-C1-C2-O2
5	H	301	GOL	O1-C1-C2-C3
5	B	301	GOL	O1-C1-C2-C3
4	P	501	NAG	O5-C5-C6-O6
4	P	501	NAG	C4-C5-C6-O6
5	B	301	GOL	O1-C1-C2-O2
4	A	501	NAG	C4-C5-C6-O6
4	P	501	NAG	C1-C2-N2-C7
4	A	501	NAG	O5-C5-C6-O6
4	P	501	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	301	GOL	2	0
5	B	301	GOL	2	0
4	P	501	NAG	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	137/139 (98%)	0.08	8 (5%)	29 25	34, 51, 114, 146	0
1	P	137/139 (98%)	0.19	3 (2%)	62 59	38, 57, 107, 129	0
2	B	217/222 (97%)	0.79	18 (8%)	17 14	35, 115, 170, 199	0
2	H	217/222 (97%)	1.00	28 (12%)	7 6	39, 128, 202, 216	0
3	C	213/216 (98%)	1.05	22 (10%)	12 10	45, 127, 190, 206	0
3	L	213/216 (98%)	0.95	15 (7%)	22 19	42, 127, 209, 243	0
All	All	1134/1154 (98%)	0.75	94 (8%)	17 14	34, 97, 195, 243	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	131	THR	6.6
3	L	133	VAL	5.9
2	B	152	VAL	5.7
2	B	159	LEU	4.1
2	B	136	ALA	4.0
1	A	367	SER	3.9
2	H	121	VAL	3.8
2	B	183	THR	3.8
2	B	181	VAL	3.7
2	H	141	LEU	3.7
3	C	112	ALA	3.6
3	C	117	LEU	3.5
2	H	136	ALA	3.5
3	L	118	PHE	3.5
2	H	198	VAL	3.4
1	A	366	PRO	3.4
3	C	11	VAL	3.3
2	H	207	VAL	3.3
2	H	124	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	H	119	PRO	3.2
3	C	12	SER	3.2
3	C	174	ALA	3.1
2	H	122	PHE	3.1
2	H	120	SER	3.1
2	B	129	LYS	3.0
2	B	140	CYS	3.0
2	B	150	VAL	3.0
2	H	123	PRO	2.9
2	H	213	PRO	2.9
3	L	122	SER	2.9
3	C	22	LEU	2.9
2	H	126	PRO	2.9
2	H	125	ALA	2.9
2	H	137	ALA	2.9
3	C	15	LEU	2.9
1	A	368	ASN	2.8
2	B	160	THR	2.8
3	C	13	THR	2.8
2	H	180	SER	2.8
2	B	151	THR	2.8
3	L	209	THR	2.8
3	C	177	TYR	2.8
2	B	126	PRO	2.8
3	L	179	SER	2.8
2	H	142	VAL	2.7
3	C	19	VAL	2.7
3	L	177	TYR	2.6
3	L	67	SER	2.6
2	B	141	LEU	2.6
2	H	9	GLY	2.6
2	H	128	SER	2.5
3	C	202	VAL	2.5
2	B	92	CYS	2.5
3	C	28	ILE	2.5
2	H	138	LEU	2.5
2	H	189	LEU	2.5
2	H	14	PRO	2.5
1	P	428	ALA	2.5
3	C	136	ILE	2.4
3	C	134	CYS	2.4
3	C	21	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	140	CYS	2.3
2	B	127	SER	2.3
2	H	114	ALA	2.3
3	L	15	LEU	2.3
3	C	196	THR	2.3
1	A	308	HIS	2.2
2	H	214	LYS	2.2
2	B	123	PRO	2.2
3	C	139	PHE	2.2
3	L	150	ALA	2.2
1	A	358	GLN	2.2
2	B	128	SER	2.2
2	B	11	LEU	2.2
2	H	168	ALA	2.2
3	L	127	ALA	2.2
1	P	429	GLY	2.2
3	C	209	THR	2.1
2	H	194	TYR	2.1
2	H	179	SER	2.1
3	L	144	VAL	2.1
3	L	199	GLY	2.1
1	A	427	SER	2.1
3	L	130	ALA	2.1
3	C	119	PRO	2.1
1	P	358	GLN	2.1
1	A	364	LEU	2.1
2	H	159	LEU	2.1
2	B	12	LEU	2.1
3	C	72	LEU	2.1
3	C	178	LEU	2.1
3	L	132	LEU	2.0
1	A	378	ILE	2.0
3	C	115	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

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	NAG	P	501	14/15	0.79	0.12	85,100,114,119	0
5	GOL	B	301	6/6	0.80	0.19	70,75,76,78	0
5	GOL	H	301	6/6	0.88	0.18	63,75,84,90	0
4	NAG	A	501	14/15	0.90	0.08	62,68,74,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.