



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:40 PM UTC

PDB ID : 4GAY / pdb_00004gay
Title : Structure of the broadly neutralizing antibody AP33
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Foung, S.K.H.; Taylor, G.L.; Patel, A.H.
Deposited on : 2012-07-26
Resolution : 2.65 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

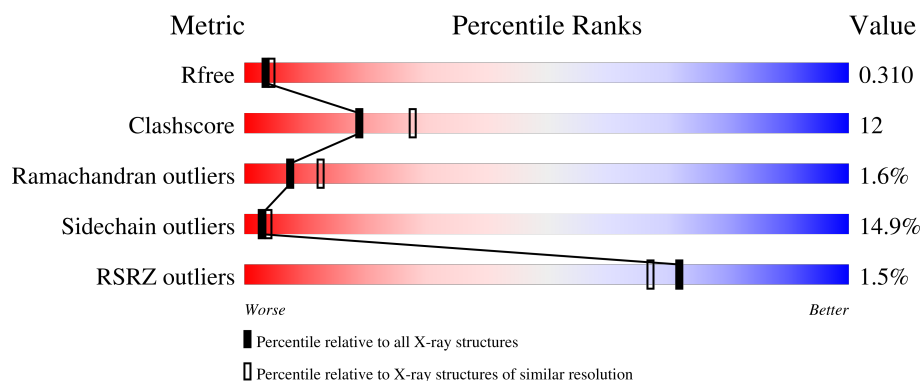
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	218	4% 66% 27% 5%
1	H	218	% 63% 28% 6%
2	B	218	65% 28% 6%
2	L	218	% 62% 29% 7%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6545 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.

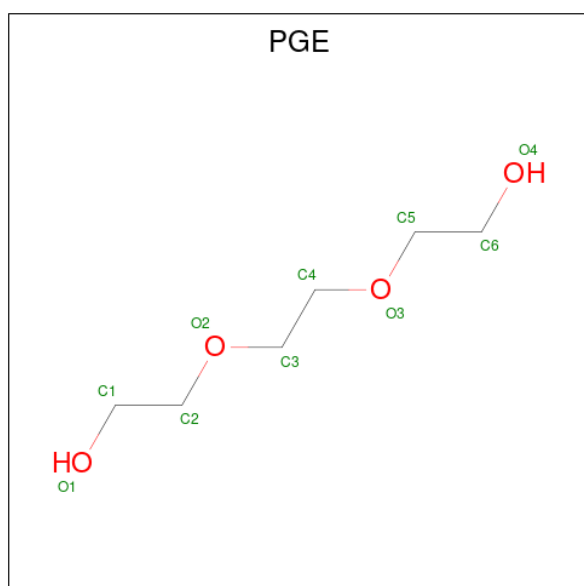
- Molecule 1 is a protein called NEUTRALIZING ANTIBODY AP33 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	212	Total	C	N	O	S	0	0	0
			1623	1030	260	326	7			
1	A	207	Total	C	N	O	S	0	0	0
			1590	1013	251	319	7			

- Molecule 2 is a protein called NEUTRALIZING ANTIBODY AP33 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1639	1025	277	332	5			
2	B	216	Total	C	N	O	S	0	0	0
			1667	1040	285	337	5			

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

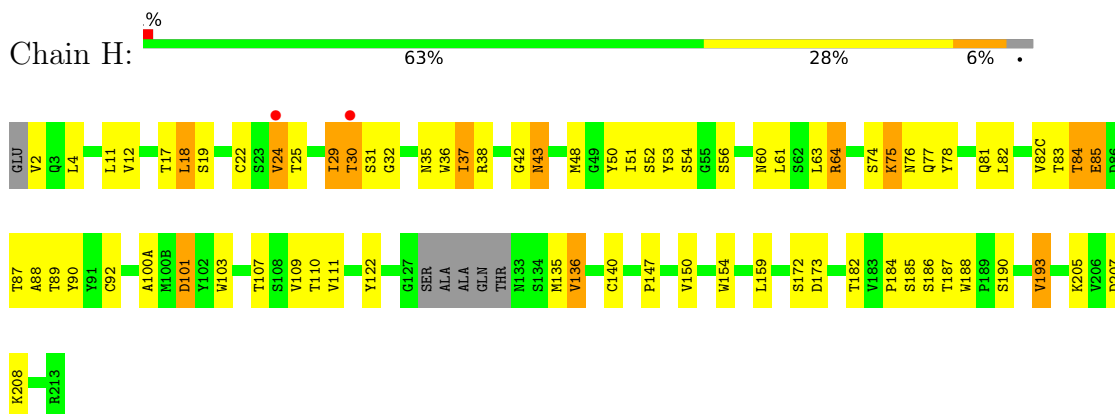
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	4	Total	O	0	0
			4	4		
4	L	2	Total	O	0	0
			2	2		

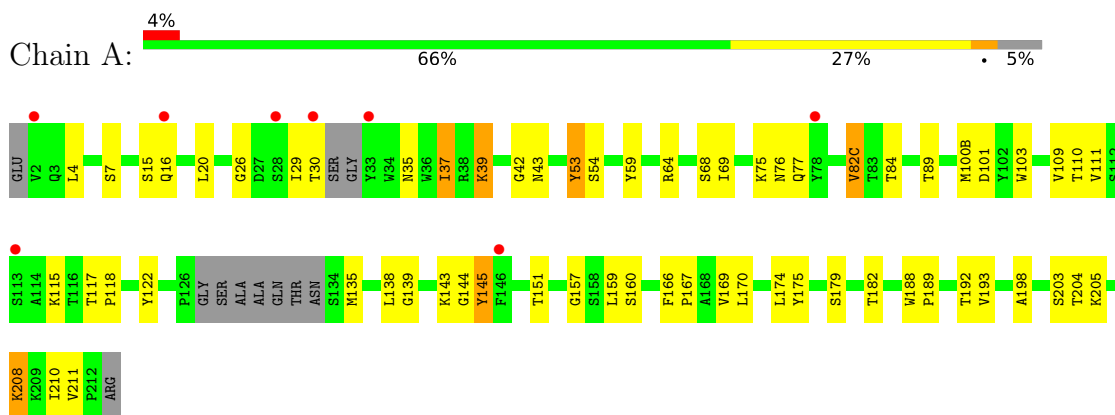
3 Residue-property plots

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.

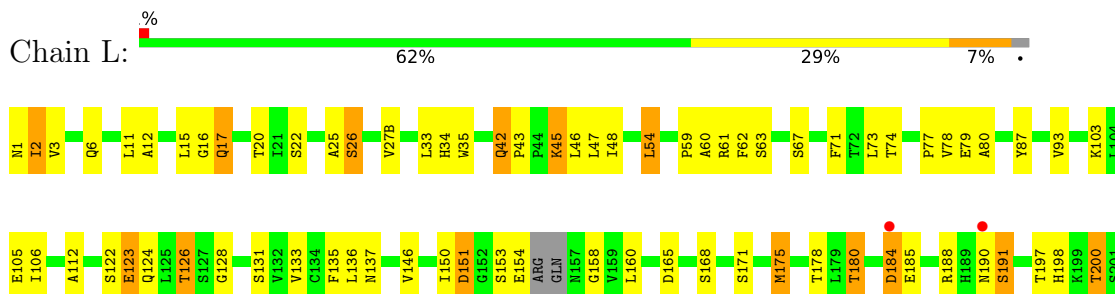
• Molecule 1: NEUTRALIZING ANTIBODY AP33 HEAVY CHAIN

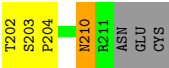


• Molecule 1: NEUTRALIZING ANTIBODY AP33 HEAVY CHAIN

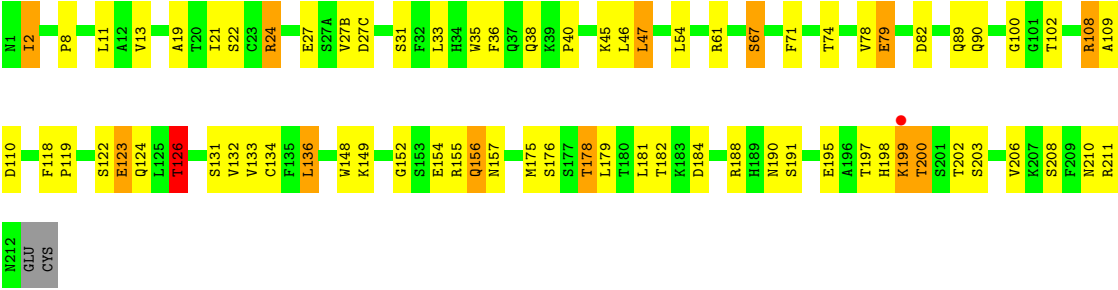


• Molecule 2: NEUTRALIZING ANTIBODY AP33 LIGHT CHAIN





● Molecule 2: NEUTRALIZING ANTIBODY AP33 LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	90.87Å 90.87Å 459.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.87 – 2.65 24.87 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.6 (24.87-2.65) 95.6 (24.87-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.49 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.243 , 0.320 0.238 , 0.310	Depositor DCC
R_{free} test set	1500 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 23.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6545	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE

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	0.72	0/1631	0.93	1/2237 (0.0%)
1	H	0.84	0/1665	1.07	3/2283 (0.1%)
2	B	0.80	0/1706	1.01	3/2323 (0.1%)
2	L	0.83	0/1677	1.09	7/2283 (0.3%)
All	All	0.80	0/6679	1.03	14/9126 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	203	SER	CA-C-N	7.10	127.13	119.89
2	B	203	SER	C-N-CA	7.10	127.13	119.89
2	L	25	ALA	CA-C-N	6.10	128.46	120.28
2	L	25	ALA	C-N-CA	6.10	128.46	120.28
1	A	115	LYS	N-CA-C	5.58	118.72	110.46
2	L	42	GLN	CA-C-N	-5.42	114.80	120.38
2	L	42	GLN	C-N-CA	-5.42	114.80	120.38
2	L	80	ALA	N-CA-C	5.35	117.86	111.71
1	H	88	ALA	CA-C-N	-5.26	115.77	122.77
1	H	88	ALA	C-N-CA	-5.26	115.77	122.77
2	L	128	GLY	N-CA-C	5.21	121.77	115.31
1	H	51	ILE	N-CA-C	-5.19	100.84	108.11
2	L	137	ASN	N-CA-C	5.07	118.01	109.95
2	B	100	GLY	N-CA-C	5.05	120.45	113.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1590	0	1556	32	0
1	H	1623	0	1587	48	0
2	B	1667	0	1597	39	0
2	L	1639	0	1569	44	0
3	A	10	0	14	0	0
3	B	10	0	14	0	0
4	H	4	0	0	0	0
4	L	2	0	0	0	0
All	All	6545	0	6337	152	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 12.

All (152) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:188:TRP:CD1	1:H:193:VAL:HG13	2.18	0.79
2:B:195:GLU:HG2	2:B:206:VAL:HG22	1.67	0.77
1:H:38:ARG:HG3	1:H:48:MET:SD	2.26	0.76
2:B:27(B):VAL:HG11	2:B:90:GLN:HB2	1.68	0.75
2:B:67:SER:O	2:B:71:PHE:CZ	2.41	0.73
2:L:3:VAL:H	2:L:26:SER:HB2	1.55	0.71
1:H:32:GLY:H	1:H:53:TYR:HD2	1.37	0.70
2:B:2:ILE:N	2:B:2:ILE:HD13	2.06	0.70
1:H:30:THR:HA	1:H:53:TYR:HB2	1.73	0.69
1:A:75:LYS:HE2	1:A:75:LYS:HA	1.75	0.69
2:L:33:LEU:HD22	2:L:71:PHE:CG	2.28	0.68
1:H:184:PRO:HB2	1:H:187:THR:HG23	1.77	0.67
1:H:30:THR:C	1:H:53:TYR:HB2	2.20	0.66
2:L:16:GLY:O	2:L:77:PRO:HB3	1.95	0.65
1:A:53:TYR:HD2	1:A:53:TYR:H	1.43	0.65
1:A:138:LEU:HD13	1:A:193:VAL:HG21	1.80	0.63
1:H:100(A):ALA:HB2	2:L:34:HIS:ND1	2.14	0.63
2:B:110:ASP:OD2	2:B:199:LYS:HE2	1.99	0.63
1:H:42:GLY:O	1:H:43:ASN:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:27(B):VAL:O	2:L:27(B):VAL:HG12	1.99	0.62
1:H:30:THR:CA	1:H:53:TYR:HB2	2.29	0.61
2:L:198:HIS:ND1	2:L:200:THR:HB	2.15	0.61
1:H:188:TRP:CD1	1:H:193:VAL:CG1	2.84	0.60
2:L:150:ILE:O	2:L:153:SER:N	2.33	0.60
1:H:4:LEU:HD23	1:H:22:CYS:SG	2.42	0.60
1:A:7:SER:O	1:A:20:LEU:HD23	2.01	0.59
1:H:36:TRP:C	1:H:37:ILE:HD13	2.28	0.59
2:B:122:SER:O	2:B:126:THR:HG22	2.03	0.58
1:A:37:ILE:HG13	1:A:103:TRP:CH2	2.39	0.57
2:B:136:LEU:HD12	2:B:136:LEU:N	2.18	0.57
2:B:61:ARG:CZ	2:B:79:GLU:HG3	2.34	0.56
1:H:101:ASP:HB3	2:L:46:LEU:HD23	1.87	0.56
1:H:188:TRP:HD1	1:H:193:VAL:HG13	1.69	0.55
2:B:13:VAL:HG21	2:B:19:ALA:HB2	1.88	0.55
1:A:39:LYS:HD3	1:A:43:ASN:HA	1.88	0.55
1:H:24:VAL:HG21	1:H:29:ILE:CG2	2.37	0.54
2:B:133:VAL:HG22	2:B:178:THR:HB	1.89	0.54
1:H:75:LYS:HB2	1:H:77:GLN:HG2	1.89	0.53
2:L:17:GLN:HA	2:L:17:GLN:OE1	2.07	0.53
2:L:190:ASN:HB3	2:L:210:ASN:OD1	2.08	0.53
2:L:146:VAL:HG23	2:L:175:MET:HE1	1.91	0.53
2:L:184:ASP:O	2:L:188:ARG:HG3	2.09	0.52
1:H:52:SER:OG	1:H:56:SER:HB3	2.09	0.52
1:H:52:SER:HG	1:H:56:SER:HB3	1.74	0.52
1:A:82(C):VAL:HG12	1:A:82(C):VAL:O	2.09	0.52
2:B:148:TRP:O	2:B:154:GLU:HA	2.10	0.52
2:L:1:ASN:H2	2:L:2:ILE:HA	1.74	0.51
1:H:184:PRO:C	1:H:186:SER:H	2.18	0.51
1:A:4:LEU:HD12	1:A:4:LEU:N	2.25	0.51
1:H:11:LEU:HB2	1:H:147:PRO:HG3	1.93	0.51
2:L:27(B):VAL:O	2:L:27(B):VAL:CG1	2.57	0.51
1:H:136:VAL:HB	1:H:185:SER:HB3	1.93	0.51
1:H:17:THR:CG2	1:H:81:GLN:HG3	2.41	0.51
2:L:123:GLU:O	2:L:126:THR:HG22	2.11	0.51
2:L:131:SER:OG	2:L:180:THR:HG23	2.11	0.51
2:L:54:LEU:HD11	2:L:62:PHE:O	2.11	0.50
2:L:6:GLN:OE1	2:L:87:TYR:HA	2.11	0.50
1:A:42:GLY:O	1:A:43:ASN:HB2	2.11	0.50
1:H:22:CYS:O	1:H:77:GLN:HB2	2.12	0.50
1:H:61:LEU:HA	1:H:64:ARG:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:HG13	1:A:103:TRP:CZ3	2.47	0.50
2:L:12:ALA:HA	2:L:105:GLU:O	2.12	0.50
2:L:133:VAL:HG22	2:L:178:THR:HG22	1.94	0.49
2:L:203:SER:HB3	2:L:204:PRO:HD2	1.94	0.49
1:A:39:LYS:HZ1	2:B:38:GLN:CD	2.21	0.48
2:B:2:ILE:HD13	2:B:2:ILE:H	1.72	0.48
2:L:112:ALA:HB2	2:L:200:THR:HG21	1.95	0.48
1:H:82(C):VAL:HG13	1:H:111:VAL:HG11	1.96	0.48
1:H:122:TYR:CZ	2:L:124:GLN:HG3	2.49	0.47
2:L:78:VAL:HG11	2:L:106:ILE:HD12	1.95	0.47
2:L:158:GLY:O	2:L:180:THR:N	2.44	0.47
1:H:38:ARG:HD3	1:H:90:TYR:CZ	2.49	0.47
2:L:191:SER:OG	2:B:152:GLY:HA3	2.15	0.47
2:B:155:ARG:NH1	2:B:157:ASN:HB2	2.30	0.46
2:L:78:VAL:HG11	2:L:106:ILE:CD1	2.45	0.46
1:H:37:ILE:HG13	1:H:103:TRP:CH2	2.50	0.46
1:H:78:TYR:OH	1:H:92:CYS:HB2	2.15	0.46
2:B:190:ASN:O	2:B:210:ASN:HA	2.16	0.46
1:A:4:LEU:HD12	1:A:4:LEU:H	1.81	0.46
2:B:8:PRO:O	2:B:102:THR:HG23	2.16	0.46
2:B:35:TRP:O	2:B:47:LEU:HB2	2.15	0.46
2:L:150:ILE:O	2:L:151:ASP:C	2.59	0.46
1:A:157:GLY:C	1:A:159:LEU:H	2.24	0.46
1:A:144:GLY:HA2	1:A:174:LEU:HD13	1.99	0.45
2:B:108:ARG:HD3	2:B:109:ALA:O	2.15	0.45
2:L:136:LEU:HD12	2:L:136:LEU:N	2.32	0.45
2:B:2:ILE:H	2:B:2:ILE:CD1	2.29	0.45
2:B:61:ARG:NH1	2:B:82:ASP:OD1	2.50	0.45
2:L:1:ASN:H2	2:L:2:ILE:CA	2.29	0.45
1:A:145:TYR:C	1:A:145:TYR:CD1	2.95	0.45
1:H:87:THR:HG23	1:H:110:THR:HA	1.98	0.45
2:B:184:ASP:O	2:B:188:ARG:HG3	2.17	0.45
1:A:151:THR:HB	1:A:198:ALA:HB3	1.99	0.45
2:L:2:ILE:HD11	2:L:93:VAL:HG21	1.97	0.45
1:A:101:ASP:HB3	2:B:46:LEU:HD22	1.99	0.45
1:A:166:PHE:O	1:A:167:PRO:C	2.60	0.45
1:H:135:MET:HE3	1:H:182:THR:HG22	2.00	0.44
2:B:2:ILE:HG23	2:B:27:GLU:HG2	1.99	0.44
1:H:50:TYR:C	1:H:50:TYR:CD1	2.95	0.44
1:A:118:PRO:O	1:A:144:GLY:O	2.35	0.44
2:L:133:VAL:HG13	2:L:178:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:6:GLN:HA	2:L:22:SER:O	2.17	0.44
1:A:59:TYR:CE2	1:A:69:ILE:HG13	2.53	0.44
1:H:36:TRP:O	1:H:48:MET:HB2	2.17	0.44
1:H:82(C):VAL:HG13	1:H:111:VAL:CG1	2.48	0.43
1:H:208:LYS:HE2	2:L:123:GLU:OE2	2.18	0.43
2:L:112:ALA:CB	2:L:200:THR:HG21	2.48	0.43
2:B:36:PHE:CD1	2:B:46:LEU:HA	2.54	0.43
1:A:170:LEU:HB2	1:A:175:TYR:CE1	2.54	0.43
1:A:53:TYR:N	1:A:53:TYR:CD2	2.84	0.43
2:B:198:HIS:O	2:B:200:THR:N	2.52	0.43
1:H:188:TRP:HD1	1:H:193:VAL:CG1	2.28	0.43
2:L:17:GLN:OE1	2:L:17:GLN:CA	2.67	0.43
1:A:82(C):VAL:HG13	1:A:111:VAL:HG21	2.01	0.43
2:B:175:MET:HG2	2:B:176:SER:N	2.33	0.43
1:H:12:VAL:O	1:H:111:VAL:HA	2.19	0.42
2:L:1:ASN:N	2:L:2:ILE:CA	2.82	0.42
2:L:42:GLN:HB3	2:L:43:PRO:HD2	2.01	0.42
2:L:35:TRP:CE2	2:L:73:LEU:HB2	2.55	0.42
2:L:60:ALA:C	2:L:62:PHE:H	2.26	0.42
2:L:135:PHE:C	2:L:136:LEU:HD12	2.44	0.42
1:A:193:VAL:HG23	1:A:210:ILE:HB	2.00	0.42
2:B:21:ILE:HG12	2:B:102:THR:HG21	2.00	0.42
2:B:27(C):ASP:OD1	2:B:31:SER:OG	2.34	0.42
2:B:122:SER:O	2:B:123:GLU:C	2.62	0.42
1:H:207:ASP:O	1:H:208:LYS:HD2	2.20	0.42
1:H:154:TRP:HB3	1:H:159:LEU:HD23	2.02	0.42
1:A:208:LYS:HA	1:A:208:LYS:HE3	2.02	0.42
1:A:135:MET:HE3	1:A:182:THR:HG22	2.02	0.42
2:B:156:GLN:O	2:B:157:ASN:C	2.63	0.42
1:A:122:TYR:CZ	2:B:124:GLN:HG3	2.55	0.41
2:L:45:LYS:HD3	2:L:46:LEU:O	2.20	0.41
1:A:100(B):MET:CE	2:B:89:GLN:HG3	2.49	0.41
2:B:134:CYS:HB2	2:B:148:TRP:CH2	2.56	0.41
2:B:24:ARG:HG2	2:B:24:ARG:NH1	2.35	0.41
1:A:139:GLY:HA2	1:A:179:SER:O	2.21	0.41
2:B:198:HIS:C	2:B:200:THR:N	2.79	0.41
1:H:60:ASN:OD1	1:H:60:ASN:C	2.63	0.41
1:H:101:ASP:HB3	2:L:46:LEU:CD2	2.50	0.41
1:A:20:LEU:HD11	1:A:109:VAL:HG21	2.02	0.41
1:H:85:GLU:H	1:H:85:GLU:HG2	1.60	0.41
2:B:27(B):VAL:HG12	2:B:27(B):VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:18:LEU:HD22	1:H:109:VAL:HG11	2.01	0.40
1:H:100(A):ALA:HB2	2:L:34:HIS:CE1	2.56	0.40
1:H:63:LEU:O	1:H:64:ARG:C	2.64	0.40
1:A:59:TYR:HE2	1:A:69:ILE:HG13	1.86	0.40
1:A:188:TRP:CD1	1:A:189:PRO:HA	2.57	0.40
2:B:131:SER:HA	2:B:179:LEU:O	2.21	0.40
1:H:82:LEU:C	1:H:82:LEU:HD23	2.46	0.40
2:B:118:PHE:HA	2:B:119:PRO:HD3	1.90	0.40
1:H:35:ASN:OD1	1:H:50:TYR:HB3	2.22	0.40
1:H:60:ASN:HB3	1:H:63:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

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	A	201/218 (92%)	177 (88%)	18 (9%)	6 (3%)	3	5
1	H	208/218 (95%)	192 (92%)	13 (6%)	3 (1%)	9	14
2	B	214/218 (98%)	202 (94%)	10 (5%)	2 (1%)	14	24
2	L	209/218 (96%)	193 (92%)	14 (7%)	2 (1%)	12	20
All	All	832/872 (95%)	764 (92%)	55 (7%)	13 (2%)	7	12

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	59	PRO
2	L	151	ASP
1	A	26	GLY
1	A	29	ILE
1	A	76	ASN

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Mol	Chain	Res	Type
2	B	126	THR
2	B	199	LYS
1	H	43	ASN
1	H	84	THR
1	A	68	SER
1	A	77	GLN
1	A	82(C)	VAL
1	H	29	ILE

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	188/195 (96%)	165 (88%)	23 (12%)	5	7
1	H	191/195 (98%)	164 (86%)	27 (14%)	3	5
2	B	189/191 (99%)	160 (85%)	29 (15%)	3	4
2	L	186/191 (97%)	153 (82%)	33 (18%)	2	2
All	All	754/772 (98%)	642 (85%)	112 (15%)	3	4

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	2	VAL
1	H	18	LEU
1	H	19	SER
1	H	24	VAL
1	H	25	THR
1	H	30	THR
1	H	31	SER
1	H	37	ILE
1	H	54	SER
1	H	64	ARG
1	H	74	SER
1	H	75	LYS
1	H	76	ASN

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Mol	Chain	Res	Type
1	H	83	THR
1	H	84	THR
1	H	85	GLU
1	H	89	THR
1	H	101	ASP
1	H	107	THR
1	H	136	VAL
1	H	140	CYS
1	H	150	VAL
1	H	172	SER
1	H	173	ASP
1	H	190	SER
1	H	193	VAL
1	H	205	LYS
2	L	2	ILE
2	L	11	LEU
2	L	15	LEU
2	L	17	GLN
2	L	20	THR
2	L	26	SER
2	L	45	LYS
2	L	47	LEU
2	L	48	ILE
2	L	54	LEU
2	L	61	ARG
2	L	63	SER
2	L	67	SER
2	L	74	THR
2	L	79	GLU
2	L	103	LYS
2	L	122	SER
2	L	123	GLU
2	L	126	THR
2	L	154	GLU
2	L	160	LEU
2	L	165	ASP
2	L	168	SER
2	L	171	SER
2	L	175	MET
2	L	180	THR
2	L	184	ASP
2	L	185	GLU

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Mol	Chain	Res	Type
2	L	191	SER
2	L	197	THR
2	L	200	THR
2	L	202	THR
2	L	210	ASN
1	A	15	SER
1	A	16	GLN
1	A	30	THR
1	A	35	ASN
1	A	37	ILE
1	A	39	LYS
1	A	53	TYR
1	A	54	SER
1	A	64	ARG
1	A	84	THR
1	A	89	THR
1	A	110	THR
1	A	117	THR
1	A	143	LYS
1	A	145	TYR
1	A	160	SER
1	A	169	VAL
1	A	192	THR
1	A	203	SER
1	A	204	THR
1	A	205	LYS
1	A	208	LYS
1	A	211	VAL
2	B	2	ILE
2	B	11	LEU
2	B	22	SER
2	B	24	ARG
2	B	33	LEU
2	B	40	PRO
2	B	45	LYS
2	B	47	LEU
2	B	54	LEU
2	B	67	SER
2	B	74	THR
2	B	78	VAL
2	B	79	GLU
2	B	108	ARG

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Mol	Chain	Res	Type
2	B	123	GLU
2	B	126	THR
2	B	132	VAL
2	B	136	LEU
2	B	149	LYS
2	B	156	GLN
2	B	178	THR
2	B	181	LEU
2	B	182	THR
2	B	191	SER
2	B	197	THR
2	B	200	THR
2	B	202	THR
2	B	208	SER
2	B	211	ARG

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

Mol	Chain	Res	Type
1	H	16	GLN
1	H	76	ASN
2	L	42	GLN
1	A	76	ASN
1	A	105	GLN
1	A	171	GLN
2	B	1	ASN
2	B	53	ASN
2	B	161	ASN
2	B	190	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

2 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	PGE	A	301	-	9,9,9	0.51	0	8,8,8	0.51	0
3	PGE	B	301	-	9,9,9	0.54	0	8,8,8	0.30	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	PGE	A	301	-	-	5/7/7/7	-
3	PGE	B	301	-	-	5/7/7/7	-

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
3	B	301	PGE	O2-C3-C4-O3
3	A	301	PGE	O3-C5-C6-O4
3	B	301	PGE	O3-C5-C6-O4
3	A	301	PGE	O1-C1-C2-O2
3	A	301	PGE	C1-C2-O2-C3
3	A	301	PGE	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	B	301	PGE	C1-C2-O2-C3
3	A	301	PGE	C3-C4-O3-C5
3	B	301	PGE	C4-C3-O2-C2
3	B	301	PGE	C6-C5-O3-C4

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 ⓘ

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(Å²)	Q<0.9
1	A	207/218 (94%)	0.46	8 (3%)	43	35	32, 53, 67, 74	1 (0%)
1	H	212/218 (97%)	0.00	2 (0%)	81	78	18, 34, 55, 64	1 (0%)
2	B	216/218 (99%)	-0.13	1 (0%)	87	85	24, 35, 49, 54	4 (1%)
2	L	213/218 (97%)	-0.02	2 (0%)	81	78	17, 37, 52, 60	4 (1%)
All	All	848/872 (97%)	0.07	13 (1%)	72	67	17, 40, 61, 74	10 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	190	ASN	2.8
1	A	33	TYR	2.7
2	L	184	ASP	2.6
1	A	30	THR	2.5
1	H	30	THR	2.3
1	A	2	VAL	2.3
1	A	146	PHE	2.3
2	B	199	LYS	2.2
1	A	16	GLN	2.2
1	A	28	SER	2.2
1	A	78	TYR	2.1
1	H	24	VAL	2.1
1	A	113	SER	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 [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	PGE	A	301	10/10	0.84	0.15	41,42,45,47	0
3	PGE	B	301	10/10	0.91	0.10	31,32,32,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.