Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 09:16 AM EDT

PDB ID	:	4GAY
Title	:	Structure of the broadly neutralizing antibody AP33
Authors	:	Potter, J.A.; Owsianka, A.; Jeffery, N.; Matthews, D.; Keck, Z.; Lau, P.; 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 (i) 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 (i)) were used in the production of this report:

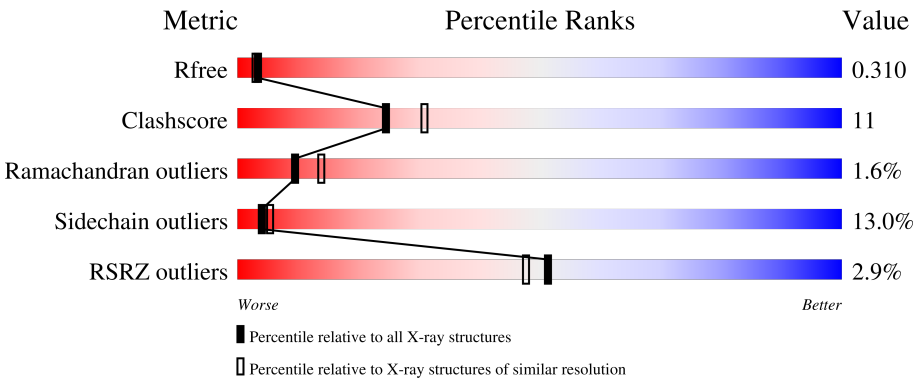
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	5% 68% 25% • 5%
1	H	218	4% 65% 28% • •
2	B	218	% 68% 25% 5% ••
2	L	218	% 66% 25% 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.

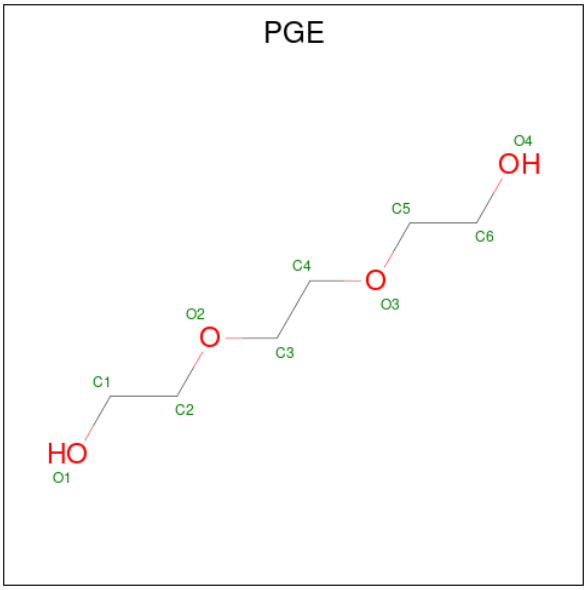
- Molecule 1 is a protein called NEUTRALIZING ANTIBODY AP33 HEAVY CHAIN.

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

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

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

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 4 is water.

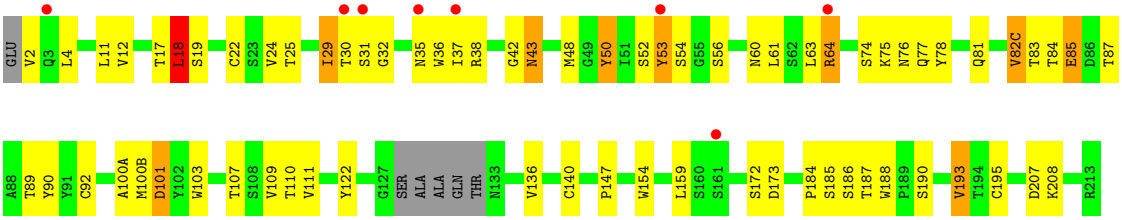
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	H	4	4	4	0	0
			Total	O		
4	L	2	2	2	0	0

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.

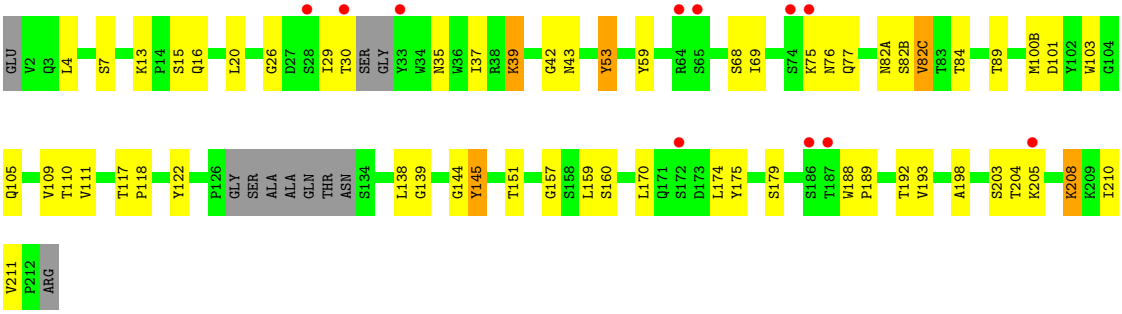
• Molecule 1: NEUTRALIZING ANTIBODY AP33 HEAVY CHAIN

Chain H:



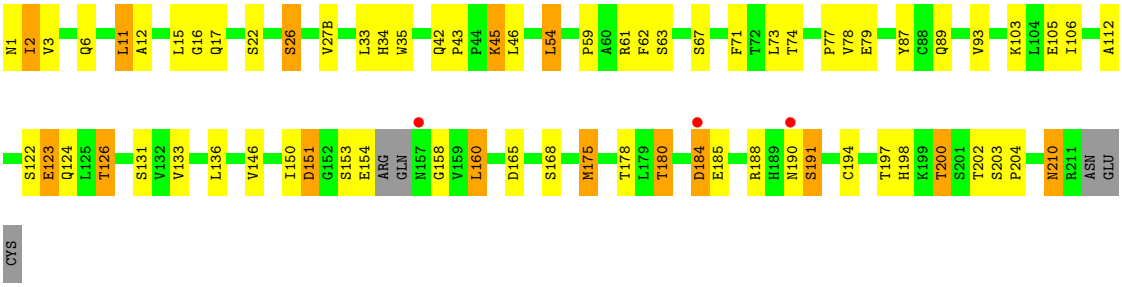
• Molecule 1: NEUTRALIZING ANTIBODY AP33 HEAVY CHAIN

Chain A:



• Molecule 2: NEUTRALIZING ANTIBODY AP33 LIGHT CHAIN

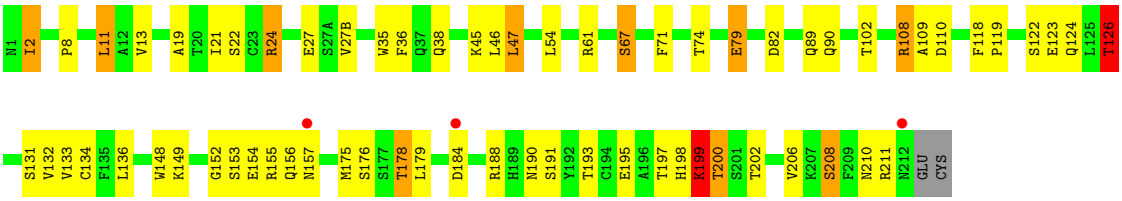
Chain L:



• Molecule 2: NEUTRALIZING ANTIBODY AP33 LIGHT CHAIN

Chain B:

%
68%
25%
5%


N1 I2 P8 L11 A12 V13 A19 T20 I21 S22 C23 R24 E27 S27A V27B W35 F36 Q37 Q38 K45 L46 L47 L54 R61 S67 F71 T74 E79 D82 Q89 Q90 T102 R108 A109 D110 F118 P119 S122 E123 Q124 L125 T126
S131 V132 V133 C134 F135 L136 W148 K149 G152 S153 E154 R155 Q156 N157 M175 S176 S177 T178 L179 D184 R188 H189 N190 S191 Y192 T193 C194 E195 A196 T197 H198 K199 T200 S201 T202 V206 K207 S208 F209 N210 R211 N212 GLU CYS

4 Data and refinement statistics (i)

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 – 2.64	Depositor EDS
% Data completeness (in resolution range)	95.6 (24.87-2.65) 95.6 (24.87-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	1436 reflections (5.17%)	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)	0.32 , 32.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.61	0/1631	0.71	0/2237
1	H	0.68	0/1665	0.78	1/2283 (0.0%)
2	B	0.66	0/1706	0.76	1/2323 (0.0%)
2	L	0.69	0/1677	0.81	4/2283 (0.2%)
All	All	0.66	0/6679	0.77	6/9126 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	18	LEU	CA-CB-CG	7.96	133.60	115.30
2	B	11	LEU	CA-CB-CG	6.76	130.84	115.30
2	L	2	ILE	CG1-CB-CG2	-5.48	99.34	111.40
2	L	160	LEU	CA-CB-CG	5.43	127.79	115.30
2	L	11	LEU	CB-CG-CD1	5.25	119.92	111.00
2	L	11	LEU	CA-CB-CG	5.14	127.12	115.30

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	1590	0	1556	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1623	0	1587	43	0
2	B	1667	0	1597	37	0
2	L	1639	0	1569	42	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	140	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 11.

All (140) 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
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
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:30:THR:C	1:H:53:TYR:HB2	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:39:LYS:HZ1	2:B:38:GLN:CD	2.11	0.55
1:H:36:TRP:C	1:H:37:ILE:HD13	2.28	0.54
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
2:L:146:VAL:HG23	2:L:175:MET:HE1	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:B:193:THR:OG1	2:B:208:SER:OG	2.26	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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:184:PRO:C	1:H:186:SER:H	2.18	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
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
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
2:B:2:ILE:HG23	2:B:27:GLU:HG2	1.99	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
2:L:1:ASN:H2	2:L:2:ILE:HA	1.83	0.44
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
2:B:175:MET:HG2	2:B:176:SER:N	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
2:B:193:THR:HG1	2:B:208:SER:HG	1.63	0.41
1:A:139:GLY:HA2	1:A:179:SER:O	2.21	0.41
1:A:157:GLY:C	1:A:159:LEU:H	2.24	0.41
1:H:100(B):MET:HE1	2:L:89:GLN:HG3	2.02	0.41
1:H:101:ASP:HB3	2:L:46:LEU:CD2	2.50	0.41
2:L:150:ILE:O	2:L:151:ASP:C	2.59	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
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: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:A:145:TYR:CD1	1:A:145:TYR:C	2.95	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%)	4 5
1	H	208/218 (95%)	192 (92%)	13 (6%)	3 (1%)	11 16
2	B	214/218 (98%)	202 (94%)	10 (5%)	2 (1%)	17 26
2	L	209/218 (96%)	193 (92%)	14 (7%)	2 (1%)	15 23
All	All	832/872 (95%)	764 (92%)	55 (7%)	13 (2%)	9 14

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
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 (i)

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%)	166 (88%)	22 (12%)	5 7
1	H	191/195 (98%)	168 (88%)	23 (12%)	5 7
2	B	189/191 (99%)	164 (87%)	25 (13%)	4 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	186/191 (97%)	158 (85%)	28 (15%)	3 3
All	All	754/772 (98%)	656 (87%)	98 (13%)	4 5

All (98) 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	25	THR
1	H	31	SER
1	H	50	TYR
1	H	53	TYR
1	H	54	SER
1	H	64	ARG
1	H	74	SER
1	H	76	ASN
1	H	82(C)	VAL
1	H	83	THR
1	H	85	GLU
1	H	89	THR
1	H	101	ASP
1	H	107	THR
1	H	140	CYS
1	H	172	SER
1	H	173	ASP
1	H	190	SER
1	H	193	VAL
1	H	195	CYS
2	L	11	LEU
2	L	15	LEU
2	L	26	SER
2	L	45	LYS
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

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Mol	Chain	Res	Type
2	L	126	THR
2	L	154	GLU
2	L	160	LEU
2	L	165	ASP
2	L	168	SER
2	L	175	MET
2	L	180	THR
2	L	184	ASP
2	L	185	GLU
2	L	191	SER
2	L	194	CYS
2	L	197	THR
2	L	200	THR
2	L	202	THR
2	L	210	ASN
1	A	13	LYS
1	A	15	SER
1	A	16	GLN
1	A	30	THR
1	A	35	ASN
1	A	39	LYS
1	A	53	TYR
1	A	82(A)	ASN
1	A	82(B)	SER
1	A	84	THR
1	A	89	THR
1	A	105	GLN
1	A	110	THR
1	A	117	THR
1	A	145	TYR
1	A	160	SER
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	45	LYS

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Mol	Chain	Res	Type
2	B	47	LEU
2	B	54	LEU
2	B	67	SER
2	B	74	THR
2	B	79	GLU
2	B	108	ARG
2	B	123	GLU
2	B	126	THR
2	B	132	VAL
2	B	149	LYS
2	B	153	SER
2	B	156	GLN
2	B	178	THR
2	B	191	SER
2	B	197	THR
2	B	199	LYS
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 (7) such sidechains are listed below:

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

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 monosaccharides 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	B	301	-	9,9,9	0.54	0	8,8,8	0.30	0
3	PGE	A	301	-	9,9,9	0.51	0	8,8,8	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
3	PGE	B	301	-	-	5/7/7/7	-
3	PGE	A	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 (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	A	207/218 (94%)	0.35	11 (5%)	26	23	32, 53, 67, 74	1 (0%)
1	H	212/218 (97%)	0.08	8 (3%)	40	36	18, 35, 55, 64	1 (0%)
2	B	216/218 (99%)	-0.16	3 (1%)	75	73	24, 36, 49, 56	4 (1%)
2	L	213/218 (97%)	-0.15	3 (1%)	75	73	17, 38, 52, 60	4 (1%)
All	All	848/872 (97%)	0.03	25 (2%)	51	48	17, 40, 61, 74	10 (1%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	LYS	4.0
1	A	74	SER	3.3
1	H	31	SER	3.3
1	A	187	THR	3.3
2	L	184	ASP	3.0
1	A	64	ARG	2.9
1	H	30	THR	2.9
2	B	184	ASP	2.8
1	A	75	LYS	2.8
1	A	172	SER	2.6
1	A	28	SER	2.6
1	A	30	THR	2.5
1	H	53	TYR	2.5
1	H	3	GLN	2.5
2	L	157	ASN	2.5
1	H	37	ILE	2.4
1	H	35	ASN	2.4
2	B	157	ASN	2.4
2	B	212	ASN	2.4
1	A	65	SER	2.4
1	H	161	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	33	TYR	2.3
1	H	64	ARG	2.2
2	L	190	ASN	2.1
1	A	186	SER	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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
3	PGE	A	301	10/10	0.90	0.25	41,42,45,47	0
3	PGE	B	301	10/10	0.94	0.17	31,32,32,33	0

6.5 Other polymers (i)

There are no such residues in this entry.