



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:23 am BST

PDB ID : 4OAW
Title : Fab structure of anti-HIV gp120 V2 mAb 2158
Authors : Spurrier, B.R.; Kong, X.P.
Deposited on : 2014-01-06
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

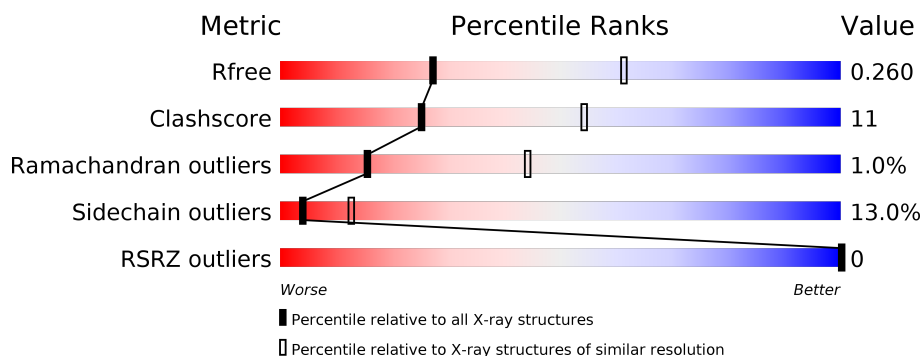
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	214	 67% 27% 6%
1	C	214	 75% 21% 5%
2	B	236	 67% 26% 7%
2	D	236	 67% 30% 3%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6992 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 fragment of anti-HIV1 gp120 V2 mAb 2158.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1636	1021	272	337	6			
1	C	214	Total	C	N	O	S	0	0	0
			1636	1021	272	337	6			

- Molecule 2 is a protein called Heavy chain of Fab fragment of anti-HIV1 gp120 V2 mAb 2158.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	0
			1757	1104	291	354	8			
2	D	236	Total	C	N	O	S	0	0	0
			1757	1104	291	354	8			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	40	Total O 40 40	0	0
5	B	49	Total O 49 49	0	0

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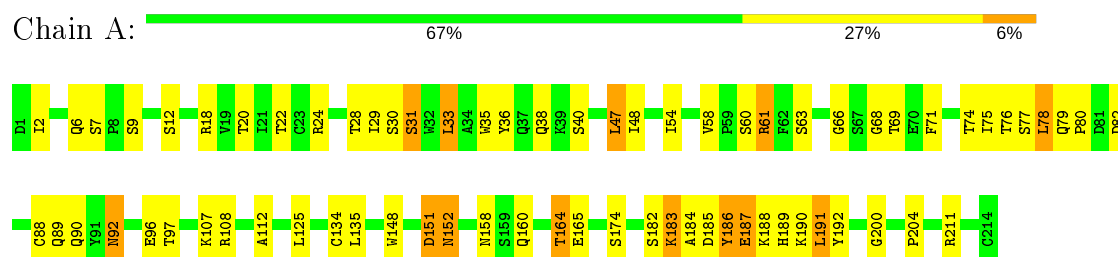
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	32	Total	O	0	0
			32	32		
5	D	43	Total	O	0	0
			43	43		

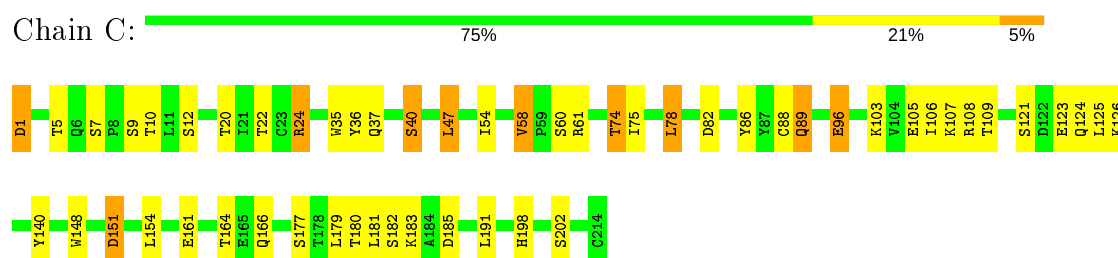
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

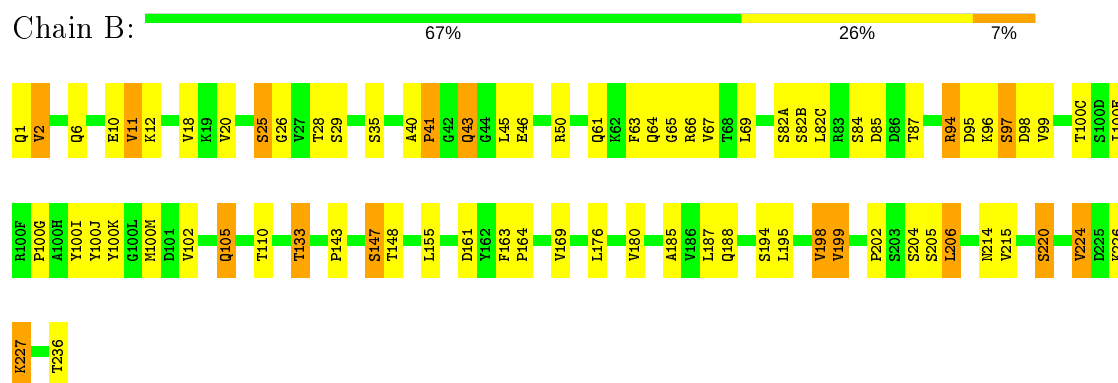
- Molecule 1: Light chain of Fab fragment of anti-HIV1 gp120 V2 mAb 2158



- Molecule 1: Light chain of Fab fragment of anti-HIV1 gp120 V2 mAb 2158

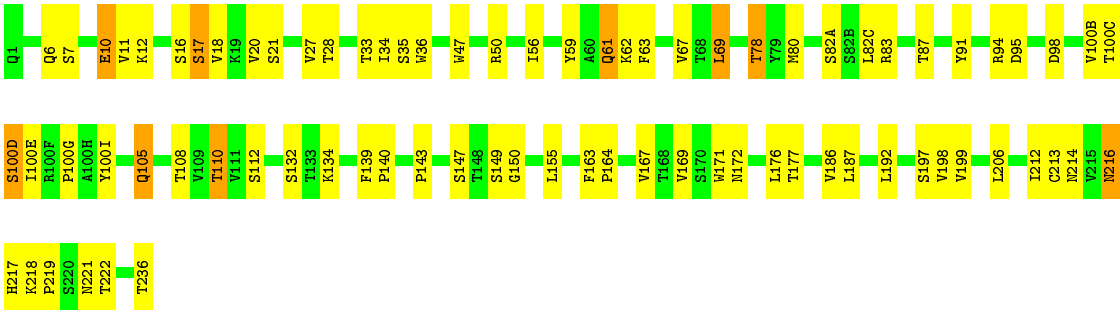


- Molecule 2: Heavy chain of Fab fragment of anti-HIV1 gp120 V2 mAb 2158



- Molecule 2: Heavy chain of Fab fragment of anti-HIV1 gp120 V2 mAb 2158





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	73.71Å 73.71Å 215.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.83 – 2.80 54.95 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.6 (54.83-2.80) 97.2 (54.95-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.182 , 0.254 0.191 , 0.260	Depositor DCC
R_{free} test set	1624 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.047 for -h,-k,l 0.457 for h,-h-k,-l 0.047 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6992	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: GOL, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/1670	0.66	0/2270
1	C	0.49	0/1670	0.65	0/2270
2	B	0.51	0/1795	0.66	0/2448
2	D	0.50	0/1795	0.64	0/2448
All	All	0.50	0/6930	0.65	0/9436

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	TYR	Peptide
2	B	220	SER	Peptide

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	1636	0	1583	43	0
1	C	1636	0	1583	27	0
2	B	1757	0	1743	40	0
2	D	1757	0	1743	42	0
3	A	5	0	0	1	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
4	B	6	0	8	2	0
4	D	6	0	8	2	0
5	A	40	0	0	2	0
5	B	49	0	0	0	0
5	C	32	0	0	2	0
5	D	43	0	0	0	0
All	All	6992	0	6668	145	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 (145) 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:B:87:THR:HG23	2:B:110:THR:HA	1.52	0.90
1:A:186:TYR:O	1:A:192:TYR:OH	1.93	0.87
2:D:87:THR:HG23	2:D:110:THR:HA	1.65	0.78
1:C:151:ASP:HB3	1:C:191:LEU:HB3	1.74	0.70
2:D:56:ILE:HD13	2:D:100(B):VAL:HG13	1.73	0.69
1:A:182:SER:OG	1:A:185:ASP:OD1	2.11	0.69
2:B:143:PRO:HB2	2:B:206:LEU:HD21	1.76	0.68
2:B:180:VAL:HG22	2:B:199:VAL:HG13	1.76	0.68
2:D:6:GLN:N	2:D:105:GLN:OE1	2.25	0.67
1:C:108:ARG:NH1	1:C:109:THR:O	2.28	0.66
1:A:189:HIS:O	1:A:211:ARG:NH1	2.27	0.66
2:B:227:LYS:HD2	2:B:227:LYS:H	1.59	0.66
1:A:61:ARG:NH2	3:A:301:SO4:O3	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:HG3	1:A:75:ILE:HG23	1.78	0.65
2:B:6:GLN:N	2:B:105:GLN:OE1	2.28	0.65
2:B:202:PRO:O	2:B:205:SER:OG	2.15	0.64
2:D:11:VAL:HG13	2:D:110:THR:HB	1.79	0.64
2:B:11:VAL:HG13	2:B:110:THR:HB	1.79	0.64
1:C:106:ILE:O	1:C:166:GLN:NE2	2.33	0.60
2:D:7:SER:HB3	2:D:21:SER:H	1.65	0.60
2:D:10:GLU:HG2	2:D:12:LYS:HE2	1.84	0.60
2:B:18:VAL:HG12	2:B:82(C):LEU:HD11	1.84	0.59
1:A:186:TYR:HB3	1:A:187:GLU:HB2	1.85	0.59
1:A:29:ILE:HG21	1:A:90:GLN:HG3	1.85	0.59
1:A:182:SER:C	1:A:184:ALA:H	2.06	0.59
2:B:96:LYS:HB3	2:B:100(K):TYR:HB2	1.85	0.58
1:A:96:GLU:OE2	2:B:50:ARG:NH2	2.36	0.58
2:B:43:GLN:HE22	2:B:46:GLU:CD	2.06	0.58
2:D:16:SER:OG	2:D:17:SER:N	2.36	0.57
2:D:12:LYS:HG3	2:D:18:VAL:HB	1.86	0.57
2:D:63:PHE:O	2:D:67:VAL:HG12	2.04	0.57
2:B:147:SER:OG	2:B:147:SER:O	2.22	0.56
1:C:40:SER:O	5:C:430:HOH:O	2.17	0.56
2:D:34:ILE:HG13	2:D:78:THR:HG21	1.87	0.56
1:C:54:ILE:HG23	1:C:58:VAL:HG22	1.89	0.55
2:D:35:SER:HB2	2:D:95:ASP:OD2	2.06	0.55
2:D:169:VAL:HG21	2:D:197:SER:HB2	1.89	0.55
1:C:125:LEU:O	1:C:183:LYS:HD2	2.06	0.55
1:A:30:SER:OG	1:A:31:SER:N	2.40	0.54
2:B:227:LYS:CD	2:B:227:LYS:H	2.20	0.54
2:D:94:ARG:NH2	4:D:302:GOL:H11	2.22	0.54
2:D:167:VAL:HG23	2:D:217:HIS:HB2	1.90	0.54
1:A:185:ASP:HA	1:A:188:LYS:HE3	1.89	0.54
1:A:35:TRP:CZ3	1:A:88:CYS:HB3	2.43	0.54
1:C:35:TRP:CZ3	1:C:88:CYS:HB3	2.43	0.54
2:D:35:SER:OG	2:D:47:TRP:NE1	2.39	0.53
2:B:161:ASP:OD1	2:B:188:GLN:NE2	2.38	0.53
2:D:47:TRP:HZ2	2:D:50:ARG:HB2	1.74	0.53
2:D:98:ASP:HB2	2:D:100(I):TYR:HB3	1.91	0.53
2:D:143:PRO:HA	2:D:147:SER:OG	2.09	0.52
2:B:66:ARG:HD2	2:B:82(B):SER:HB2	1.90	0.52
1:A:48:ILE:HG12	1:A:54:ILE:HD13	1.90	0.52
1:C:96:GLU:OE1	2:D:50:ARG:NH2	2.37	0.52
1:C:36:TYR:OH	1:C:89:GLN:NE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100(C):THR:OG1	2:D:100(D):SER:N	2.42	0.51
1:A:47:LEU:HA	1:A:58:VAL:HG21	1.92	0.51
2:D:82(A):SER:O	2:D:82(C):LEU:N	2.44	0.51
2:D:112:SER:HB3	2:D:163:PHE:CZ	2.46	0.51
2:B:98:ASP:HB2	2:B:100(I):TYR:HB3	1.93	0.51
1:A:151:ASP:HB3	1:A:191:LEU:HB3	1.92	0.50
2:B:11:VAL:HG21	2:B:164:PRO:HG3	1.93	0.50
1:C:121:SER:HB3	2:D:140:PRO:HD2	1.92	0.50
2:B:100(E):ILE:O	2:B:100(G):PRO:HD3	2.11	0.50
1:C:124:GLN:HG3	2:D:139:PHE:CE2	2.47	0.50
2:D:163:PHE:CE2	2:D:164:PRO:HB3	2.47	0.50
2:B:82(A):SER:O	2:B:82(C):LEU:N	2.44	0.50
1:C:1:ASP:OD2	2:D:61:GLN:NE2	2.45	0.50
2:D:216:ASN:HD22	2:D:217:HIS:N	2.10	0.49
2:D:169:VAL:HA	2:D:214:ASN:O	2.12	0.49
2:B:40:ALA:HB3	2:B:43:GLN:HE21	1.77	0.49
1:A:135:LEU:HD22	2:B:198:VAL:HG21	1.94	0.49
2:B:63:PHE:O	2:B:65:GLY:N	2.46	0.49
1:C:182:SER:OG	1:C:185:ASP:OD2	2.30	0.48
1:A:164:THR:HG22	1:A:174:SER:H	1.78	0.48
2:D:169:VAL:HG21	2:D:197:SER:CB	2.44	0.48
2:B:176:LEU:HD21	2:B:199:VAL:HG11	1.96	0.48
1:A:164:THR:HG23	1:A:165:GLU:O	2.14	0.48
1:A:190:LYS:NZ	5:A:429:HOH:O	2.44	0.47
1:A:28:THR:HA	1:A:68:GLY:O	2.14	0.47
2:B:97:SER:HB3	2:B:99:VAL:O	2.14	0.47
2:B:94:ARG:O	2:B:100(M):MET:HA	2.14	0.47
2:D:33:THR:HG21	2:D:50:ARG:HD3	1.97	0.47
1:A:24:ARG:HA	1:A:69:THR:O	2.15	0.47
2:B:45:LEU:HA	2:B:45:LEU:HD23	1.76	0.47
1:C:20:THR:HG22	1:C:74:THR:OG1	2.15	0.46
1:A:20:THR:HG22	1:A:74:THR:HG23	1.98	0.46
1:A:33:LEU:HD11	1:A:88:CYS:HB2	1.96	0.46
2:B:94:ARG:HD3	4:B:303:GOL:H31	1.98	0.46
1:C:61:ARG:NH1	1:C:82:ASP:OD1	2.48	0.46
1:C:140:TYR:O	1:C:198:HIS:HE1	1.99	0.46
2:D:27:VAL:HB	4:D:302:GOL:O1	2.16	0.45
2:B:28:THR:H	4:B:303:GOL:HO1	1.59	0.45
1:C:47:LEU:HA	1:C:58:VAL:HG11	1.97	0.45
2:B:169:VAL:HA	2:B:214:ASN:O	2.17	0.45
1:C:37:GLN:HB2	1:C:86:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:TRP:CE2	1:C:179:LEU:HB2	2.52	0.45
1:A:61:ARG:HD3	1:A:77:SER:O	2.18	0.44
1:A:76:THR:OG1	1:A:77:SER:N	2.51	0.44
2:B:25:SER:HA	2:B:26:GLY:HA2	1.59	0.44
1:A:182:SER:C	1:A:184:ALA:N	2.71	0.43
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.67	0.43
2:B:215:VAL:HB	2:B:224:VAL:HG13	1.99	0.43
1:C:126:LYS:NZ	5:C:405:HOH:O	2.51	0.43
1:C:123:GLU:HA	1:C:126:LYS:HG3	2.00	0.43
1:A:152:ASN:O	1:A:152:ASN:ND2	2.37	0.43
1:A:90:GLN:HE21	1:A:92:ASN:HB3	1.83	0.43
2:D:112:SER:HB3	2:D:163:PHE:HZ	1.83	0.43
1:C:24:ARG:HB2	1:C:24:ARG:HH11	1.84	0.43
1:A:38:GLN:HA	5:A:409:HOH:O	2.18	0.43
2:B:12:LYS:HG3	2:B:18:VAL:HB	2.01	0.43
1:A:61:ARG:NH1	1:A:82:ASP:OD2	2.37	0.43
2:B:50:ARG:NH1	2:B:95:ASP:OD1	2.50	0.43
2:D:36:TRP:CE2	2:D:80:MET:HB2	2.54	0.42
2:D:11:VAL:HG21	2:D:164:PRO:HG3	2.00	0.42
1:A:75:ILE:HG21	1:A:78:LEU:HD23	2.00	0.42
2:B:185:ALA:HA	2:B:195:LEU:HB3	2.00	0.42
1:A:36:TYR:OH	1:A:89:GLN:NE2	2.53	0.42
2:B:133:THR:HG1	2:B:220:SER:HG	1.56	0.42
1:A:12:SER:HB3	1:A:107:LYS:HE2	2.01	0.42
2:B:2:VAL:HG13	2:B:102:VAL:HG21	2.01	0.42
2:D:171:TRP:HB3	2:D:176:LEU:HD23	2.01	0.42
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.87	0.41
1:A:160:GLN:HE22	2:B:188:GLN:HA	1.84	0.41
1:A:79:GLN:HG3	1:A:80:PRO:HD2	2.01	0.41
2:D:11:VAL:HG11	2:D:163:PHE:HE2	1.84	0.41
1:C:78:LEU:HA	1:C:78:LEU:HD23	1.82	0.41
1:A:2:ILE:O	1:A:97:THR:HG21	2.20	0.41
1:C:103:LYS:HG2	1:C:105:GLU:HG2	2.02	0.41
2:D:59:TYR:HE1	2:D:69:LEU:HD22	1.85	0.41
1:A:112:ALA:HB2	1:A:200:GLY:O	2.20	0.41
1:A:66:GLY:HA3	1:A:71:PHE:HA	2.03	0.41
2:B:163:PHE:CE2	2:B:164:PRO:HB3	2.56	0.41
1:C:61:ARG:HG2	1:C:75:ILE:HG23	2.03	0.41
1:A:134:CYS:HB2	1:A:148:TRP:CH2	2.56	0.41
2:D:192:LEU:HD23	2:D:192:LEU:HA	1.91	0.41
2:B:100(E):ILE:HD12	2:B:100(J):TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:ALA:HA	2:B:41:PRO:HD3	1.88	0.40
1:C:151:ASP:N	1:C:151:ASP:OD1	2.54	0.40
1:C:161:GLU:HG2	1:C:177:SER:HB2	2.02	0.40
1:A:183:LYS:O	1:A:187:GLU:HG2	2.22	0.40
1:A:61:ARG:HE	1:A:61:ARG:HB3	1.76	0.40
2:D:172:ASN:OD1	2:D:212:ILE:HD12	2.21	0.40
2:D:36:TRP:CD2	2:D:80:MET:HB2	2.56	0.40
2:D:100(E):ILE:O	2:D:100(G):PRO:HD3	2.21	0.40
2:D:6:GLN:OE1	2:D:91:TYR:HA	2.21	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	212/214 (99%)	188 (89%)	20 (9%)	4 (2%)	8	26
1	C	212/214 (99%)	193 (91%)	19 (9%)	0	100	100
2	B	234/236 (99%)	213 (91%)	18 (8%)	3 (1%)	12	36
2	D	234/236 (99%)	214 (92%)	18 (8%)	2 (1%)	17	46
All	All	892/900 (99%)	808 (91%)	75 (8%)	9 (1%)	15	44

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
2	B	25	SER
2	B	64	GLN
1	A	183	LYS
1	A	40	SER
2	D	219	PRO

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Mol	Chain	Res	Type
1	A	204	PRO
2	D	150	GLY
2	B	41	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	188/189 (100%)	169 (90%)	19 (10%)	7	22
1	C	188/189 (100%)	165 (88%)	23 (12%)	5	15
2	B	203/203 (100%)	172 (85%)	31 (15%)	2	8
2	D	203/203 (100%)	174 (86%)	29 (14%)	3	10
All	All	782/784 (100%)	680 (87%)	102 (13%)	4	13

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	7	SER
1	A	9	SER
1	A	18	ARG
1	A	22	THR
1	A	31	SER
1	A	33	LEU
1	A	47	LEU
1	A	60	SER
1	A	61	ARG
1	A	63	SER
1	A	78	LEU
1	A	108	ARG
1	A	151	ASP
1	A	152	ASN
1	A	158	ASN
1	A	164	THR
1	A	187	GLU

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Mol	Chain	Res	Type
1	A	191	LEU
2	B	1	GLN
2	B	2	VAL
2	B	10	GLU
2	B	11	VAL
2	B	20	VAL
2	B	29	SER
2	B	35	SER
2	B	43	GLN
2	B	61	GLN
2	B	67	VAL
2	B	69	LEU
2	B	84	SER
2	B	85	ASP
2	B	94	ARG
2	B	97	SER
2	B	100(C)	THR
2	B	105	GLN
2	B	133	THR
2	B	147	SER
2	B	148	THR
2	B	155	LEU
2	B	187	LEU
2	B	194	SER
2	B	198	VAL
2	B	199	VAL
2	B	204	SER
2	B	206	LEU
2	B	224	VAL
2	B	226	LYS
2	B	227	LYS
2	B	236	THR
1	C	1	ASP
1	C	5	THR
1	C	7	SER
1	C	9	SER
1	C	10	THR
1	C	12	SER
1	C	22	THR
1	C	24	ARG
1	C	40	SER
1	C	47	LEU

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Mol	Chain	Res	Type
1	C	58	VAL
1	C	60	SER
1	C	74	THR
1	C	78	LEU
1	C	89	GLN
1	C	96	GLU
1	C	107	LYS
1	C	151	ASP
1	C	154	LEU
1	C	164	THR
1	C	180	THR
1	C	181	LEU
1	C	202	SER
2	D	10	GLU
2	D	17	SER
2	D	20	VAL
2	D	28	THR
2	D	61	GLN
2	D	62	LYS
2	D	69	LEU
2	D	78	THR
2	D	83	ARG
2	D	100(D)	SER
2	D	105	GLN
2	D	108	THR
2	D	110	THR
2	D	132	SER
2	D	134	LYS
2	D	149	SER
2	D	155	LEU
2	D	177	THR
2	D	186	VAL
2	D	187	LEU
2	D	198	VAL
2	D	199	VAL
2	D	206	LEU
2	D	213	CYS
2	D	216	ASN
2	D	218	LYS
2	D	221	ASN
2	D	222	THR
2	D	236	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	90	GLN
2	B	43	GLN
1	C	89	GLN
2	D	216	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	SO4	C	301	-	4,4,4	0.19	0	6,6,6	0.17	0
3	SO4	B	302	-	4,4,4	0.17	0	6,6,6	0.21	0
3	SO4	D	301	-	4,4,4	0.20	0	6,6,6	0.15	0
3	SO4	C	302	-	4,4,4	0.21	0	6,6,6	0.20	0
4	GOL	D	302	-	5,5,5	0.43	0	5,5,5	0.73	0
3	SO4	A	301	-	4,4,4	0.15	0	6,6,6	0.10	0
4	GOL	B	303	-	5,5,5	0.32	0	5,5,5	0.67	0
3	SO4	B	301	-	4,4,4	0.28	0	6,6,6	0.18	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
4	GOL	D	302	-	-	0/4/4/4	-
4	GOL	B	303	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	303	GOL	O1-C1-C2-C3
4	B	303	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	302	GOL	2	0
3	A	301	SO4	1	0
4	B	303	GOL	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	214/214 (100%)	-0.16	0 100 100	29, 47, 65, 73	0
1	C	214/214 (100%)	-0.18	0 100 100	30, 45, 64, 71	0
2	B	236/236 (100%)	-0.16	0 100 100	27, 42, 58, 72	0
2	D	236/236 (100%)	-0.18	0 100 100	31, 43, 58, 75	0
All	All	900/900 (100%)	-0.17	0 100 100	27, 45, 63, 75	0

There are no RSRZ outliers to report.

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 carbohydrates 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	SO4	D	301	5/5	0.94	0.14	65,65,81,86	0
3	SO4	B	302	5/5	0.96	0.13	69,75,89,89	0
4	GOL	B	303	6/6	0.96	0.23	43,45,50,50	0
3	SO4	B	301	5/5	0.96	0.14	62,70,88,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	C	302	5/5	0.97	0.17	53,62,70,83	0
4	GOL	D	302	6/6	0.97	0.24	43,45,48,48	0
3	SO4	C	301	5/5	0.98	0.12	62,64,78,78	0
3	SO4	A	301	5/5	0.98	0.11	71,72,75,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.