



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:10 pm BST

PDB ID : 4RQQ
Title : Crystal structure of human Fab PGDM1400, a broadly reactive and potent HIV-1 neutralizing antibody
Authors : Julien, J.-P.; Wilson, I.A.
Deposited on : 2014-11-04
Resolution : 3.10 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

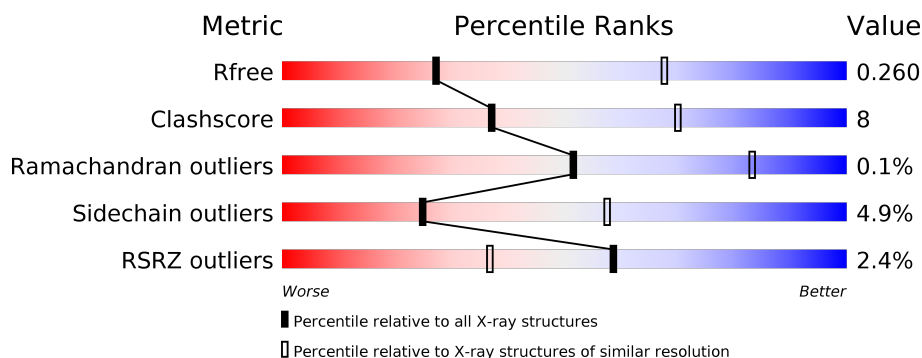
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	219	<div> <div>81%</div> <div>16%</div> <div>..</div> </div>
1	C	219	<div>6%</div> <div>75%</div> <div>21%</div> <div>.</div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10427 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 Human anti-HIV-1 antibody PGDM1400 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1659	1034	287	333	5			
1	A	215	Total	C	N	O	S	0	0	0
			1659	1034	287	333	5			
1	C	213	Total	C	N	O	S	0	0	0
			1644	1026	282	331	5			

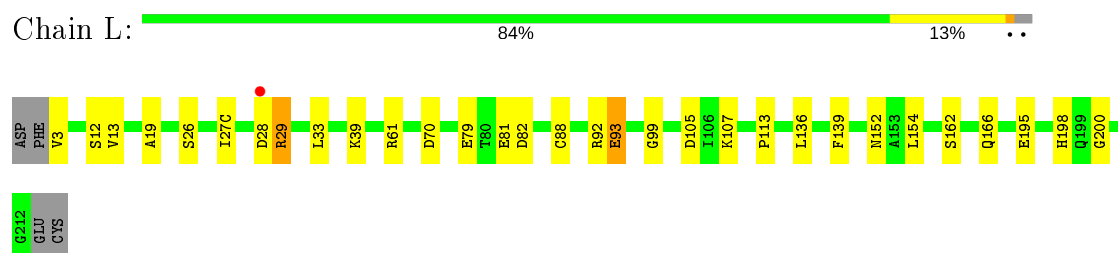
- Molecule 2 is a protein called Human anti-HIV-1 antibody PGDM1400 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	241	Total	C	N	O	S	0	0	0
			1831	1156	310	359	6			
2	B	240	Total	C	N	O	S	0	0	0
			1825	1153	309	357	6			
2	D	238	Total	C	N	O	S	0	0	0
			1809	1142	306	355	6			

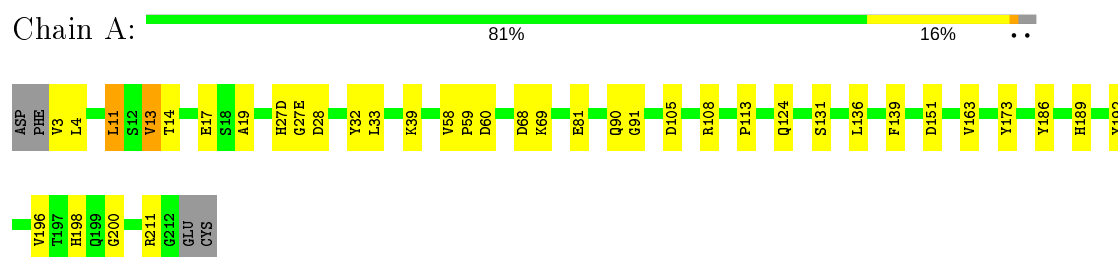
3 Residue-property plots [i](#)

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.

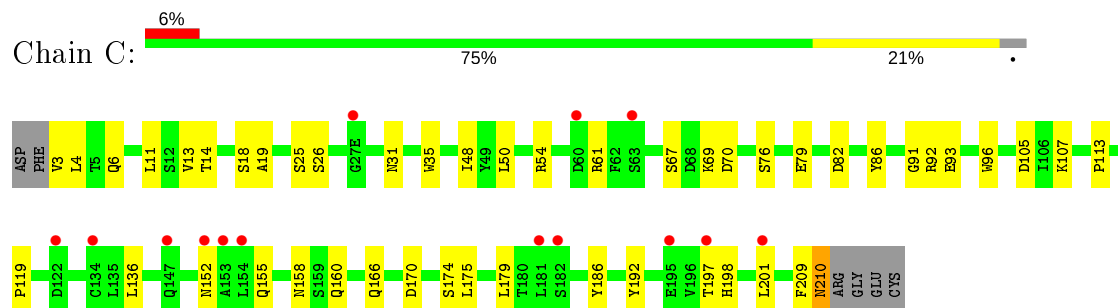
- Molecule 1: Human anti-HIV-1 antibody PGDM1400 light chain



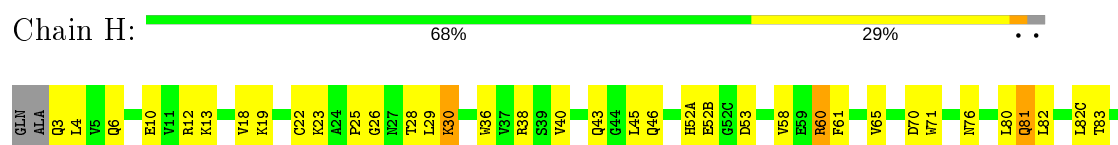
- Molecule 1: Human anti-HIV-1 antibody PGDM1400 light chain

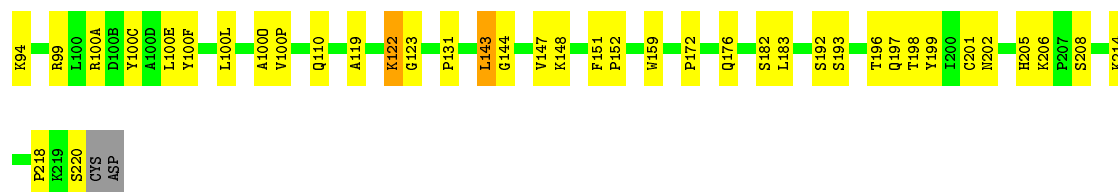


- Molecule 1: Human anti-HIV-1 antibody PGDM1400 light chain

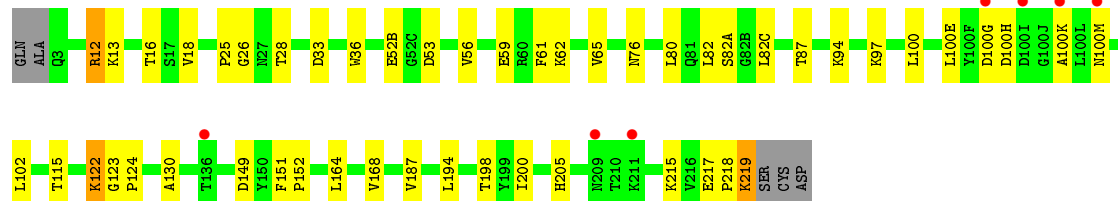
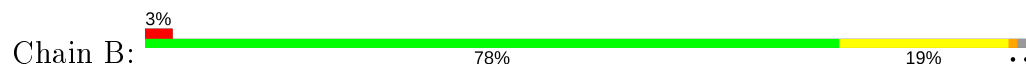


- Molecule 2: Human anti-HIV-1 antibody PGDM1400 heavy chain

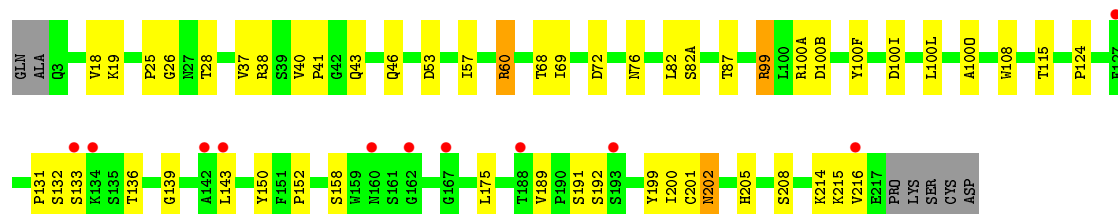
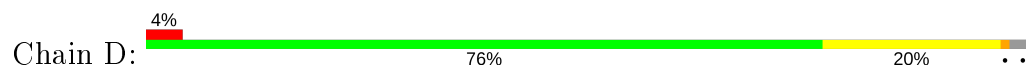




- Molecule 2: Human anti-HIV-1 antibody PGDM1400 heavy chain



- Molecule 2: Human anti-HIV-1 antibody PGDM1400 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.70 Å 149.17 Å 109.93 Å 90.00° 100.90° 90.00°	Depositor
Resolution (Å)	38.81 – 3.10 38.81 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.7 (38.81-3.10) 96.7 (38.81-3.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.12 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.221 , 0.253 0.233 , 0.260	Depositor DCC
R_{free} test set	1544 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	57.7	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	10427	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: TYS

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	0.23	0/1696	0.40	0/2300
1	C	0.23	0/1681	0.42	0/2281
1	L	0.22	0/1696	0.42	0/2300
2	B	0.24	0/1853	0.43	0/2525
2	D	0.22	0/1836	0.42	0/2502
2	H	0.23	0/1859	0.43	0/2533
All	All	0.23	0/10621	0.42	0/14441

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	1659	0	1610	24	0
1	C	1644	0	1594	28	0
1	L	1659	0	1610	15	0
2	B	1825	0	1792	30	0
2	D	1809	0	1772	27	0
2	H	1831	0	1797	43	0
All	All	10427	0	10175	161	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 8.

All (161) 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:C:3:VAL:N	1:C:26:SER:HG	1.66	0.93
1:L:3:VAL:N	1:L:26:SER:HG	1.78	0.82
2:D:26:GLY:O	2:D:76:ASN:ND2	2.21	0.74
1:C:113:PRO:HD3	1:C:198:HIS:HD2	1.52	0.73
2:H:29:LEU:O	2:H:94:LYS:NZ	2.23	0.71
2:H:25:PRO:O	2:H:28:THR:OG1	2.08	0.71
2:B:26:GLY:O	2:B:76:ASN:ND2	2.21	0.70
2:D:100(A):ARG:NH1	2:D:100(F):TYS:O1	2.26	0.69
1:C:186:TYR:O	1:C:192:TYR:OH	2.11	0.68
2:H:100(A):ARG:HD2	2:H:100(O):ALA:HB1	1.74	0.68
1:A:27(D):HIS:HB3	1:A:32:TYR:HE2	1.61	0.66
2:D:133:SER:HA	2:D:136:THR:HG22	1.80	0.64
1:C:136:LEU:HB2	1:C:175:LEU:HB3	1.80	0.64
1:A:186:TYR:O	1:A:192:TYR:OH	2.16	0.64
2:H:70:ASP:OD1	2:H:71:TRP:N	2.30	0.64
1:A:136:LEU:HD21	1:A:196:VAL:HG21	1.79	0.63
2:H:40:VAL:HB	2:H:43:GLN:HB3	1.80	0.63
2:B:25:PRO:O	2:B:28:THR:OG1	2.16	0.63
2:D:18:VAL:HG12	2:D:82:LEU:HB2	1.79	0.63
1:A:39:LYS:NZ	1:A:81:GLU:O	2.32	0.62
2:B:215:LYS:NZ	2:B:217:GLU:OE2	2.31	0.62
1:C:113:PRO:HD3	1:C:198:HIS:CD2	2.34	0.62
2:B:122:LYS:NZ	2:B:123:GLY:O	2.31	0.61
1:A:3:VAL:HG12	1:A:4:LEU:H	1.65	0.61
1:C:160:GLN:NE2	2:D:175:LEU:O	2.32	0.61
1:A:14:THR:HB	1:A:17:GLU:HG3	1.83	0.60
2:H:131:PRO:HG3	2:H:143:LEU:HD23	1.82	0.60
1:C:61:ARG:NH1	1:C:82:ASP:OD2	2.36	0.59
1:L:27(C):ILE:O	1:L:92:ARG:NH1	2.35	0.59
2:D:53:ASP:OD1	2:D:99:ARG:NH2	2.30	0.59
2:D:158:SER:OG	2:D:202:ASN:OD1	2.18	0.58
2:H:122:LYS:NZ	2:H:123:GLY:O	2.37	0.58
1:A:91:GLY:HA3	2:B:102:LEU:HB3	1.86	0.58
1:C:92:ARG:HG3	1:C:93:GLU:HG3	1.87	0.57
2:D:60:ARG:HH21	2:D:60:ARG:HB2	1.70	0.57
2:H:131:PRO:HG3	2:H:143:LEU:HB3	1.86	0.57
2:B:100(G):ASP:HB2	2:B:100(K):ALA:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:6:GLN:HG2	2:H:22:CYS:HB2	1.87	0.57
2:H:61:PHE:HB3	2:H:65:VAL:HG21	1.86	0.56
2:H:176:GLN:OE1	2:H:182:SER:OG	2.23	0.56
2:B:124:PRO:HD3	2:B:205:HIS:CD2	2.40	0.55
2:D:40:VAL:HB	2:D:43:GLN:HB3	1.88	0.55
2:B:87:THR:HG23	2:B:115:THR:HA	1.88	0.55
2:H:30:LYS:HE2	2:H:30:LYS:H	1.72	0.55
2:B:124:PRO:HD3	2:B:205:HIS:HD2	1.72	0.55
1:C:136:LEU:HD13	1:C:175:LEU:HD22	1.89	0.55
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.87	0.55
2:B:52(B):GLU:OE1	2:B:97:LYS:NZ	2.25	0.54
2:H:13:LYS:NZ	2:H:119:ALA:O	2.30	0.54
2:B:12:ARG:HG3	2:B:16:THR:OG1	2.08	0.54
2:H:205:HIS:HD2	2:H:208:SER:H	1.57	0.53
2:B:18:VAL:HG12	2:B:82(C):LEU:HD11	1.91	0.53
2:H:26:GLY:O	2:H:76:ASN:ND2	2.38	0.53
1:L:198:HIS:CD2	1:L:200:GLY:H	2.27	0.53
1:C:210:ASN:N	1:C:210:ASN:OD1	2.43	0.52
2:D:57:ILE:HD11	2:D:69:ILE:HG12	1.90	0.52
1:A:151:ASP:OD2	1:A:189:HIS:ND1	2.38	0.52
1:L:13:VAL:HG21	1:L:19:ALA:HB2	1.92	0.52
1:A:113:PRO:HD3	1:A:198:HIS:CD2	2.45	0.52
1:A:3:VAL:HG12	1:A:4:LEU:N	2.25	0.51
1:A:105:ASP:OD1	1:A:173:TYR:OH	2.24	0.51
1:L:61:ARG:NH1	1:L:82:ASP:OD2	2.38	0.51
2:D:139:GLY:O	2:D:191:SER:N	2.30	0.51
2:D:25:PRO:O	2:D:28:THR:OG1	2.18	0.51
1:A:189:HIS:O	1:A:211:ARG:NH1	2.44	0.51
1:L:39:LYS:NZ	1:L:81:GLU:O	2.34	0.50
2:H:143:LEU:HD21	2:H:199:TYR:CD2	2.47	0.50
2:B:164:LEU:HD21	2:B:187:VAL:HG11	1.93	0.50
2:H:18:VAL:HG12	2:H:82(C):LEU:HD11	1.94	0.50
2:B:61:PHE:HB3	2:B:65:VAL:HG21	1.95	0.49
2:D:53:ASP:CG	2:D:99:ARG:HH22	2.14	0.49
2:D:87:THR:HG23	2:D:115:THR:HA	1.95	0.49
1:L:113:PRO:HD3	1:L:198:HIS:CD2	2.47	0.49
2:H:197:GLN:OE1	2:H:198:THR:N	2.45	0.49
1:A:60:ASP:OD1	1:A:60:ASP:N	2.46	0.48
2:H:100(L):LEU:HD11	2:H:100(O):ALA:HB2	1.94	0.48
2:D:131:PRO:HD3	2:D:216:VAL:HG12	1.95	0.48
1:C:13:VAL:HG21	1:C:19:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:HIS:CD2	1:A:200:GLY:H	2.32	0.48
2:B:12:ARG:HA	2:B:12:ARG:HD3	1.66	0.48
2:H:38:ARG:HB3	2:H:46:GLN:HB3	1.96	0.47
2:H:100(C):TYR:HB3	2:H:100(P):VAL:HG12	1.95	0.47
2:D:100(L):LEU:HD11	2:D:100(O):ALA:HB2	1.97	0.47
2:H:143:LEU:HD21	2:H:199:TYR:HD2	1.80	0.47
1:L:88:CYS:O	1:L:99:GLY:N	2.48	0.47
2:B:130:ALA:HB2	2:B:219:LYS:HD3	1.97	0.47
2:H:19:LYS:HG2	2:H:81:GLN:HG3	1.97	0.47
1:A:27(D):HIS:HE1	2:B:100:LEU:HD21	1.80	0.46
1:A:68:ASP:HB3	1:A:69:LYS:H	1.54	0.46
2:B:33:ASP:O	2:B:94:LYS:HA	2.15	0.46
1:C:105:ASP:OD1	1:C:166:GLN:NE2	2.48	0.46
1:C:31:ASN:OD1	1:C:67:SER:HA	2.16	0.46
1:A:124:GLN:HE22	1:A:131:SER:HB2	1.79	0.46
2:H:53:ASP:OD2	2:H:99:ARG:NH2	2.42	0.46
1:C:119:PRO:HB3	1:C:209:PHE:CE2	2.51	0.46
2:H:58:VAL:HG12	2:H:60:ARG:HG3	1.97	0.46
2:H:23:LYS:HD2	2:H:23:LYS:HA	1.53	0.45
2:B:59:GLU:HA	2:B:62:LYS:HE3	1.99	0.45
2:H:151:PHE:HA	2:H:152:PRO:HA	1.70	0.45
2:H:131:PRO:HD2	2:H:218:PRO:HA	1.98	0.45
2:H:52(B):GLU:OE1	2:H:99:ARG:NH1	2.48	0.45
2:H:205:HIS:CD2	2:H:208:SER:H	2.34	0.45
2:D:72:ASP:O	2:D:76:ASN:N	2.49	0.45
2:B:168:VAL:HG22	2:B:187:VAL:HG22	1.98	0.45
2:D:201:CYS:N	2:D:214:LYS:O	2.46	0.45
1:C:18:SER:HA	1:C:76:SER:HA	1.99	0.45
2:D:38:ARG:HH21	2:D:46:GLN:HE22	1.65	0.45
2:H:3:GLN:O	2:H:4:LEU:HD23	2.17	0.45
2:D:124:PRO:HB3	2:D:150:TYR:HB3	1.99	0.44
2:H:193:SER:HA	2:H:196:THR:HB	1.99	0.44
1:C:4:LEU:HD23	1:C:25:SER:HB3	2.00	0.44
2:H:100(E):LEU:HD21	2:B:28:THR:HG21	1.99	0.44
1:A:13:VAL:HG21	1:A:19:ALA:HB2	2.00	0.44
1:L:12:SER:HB3	1:L:107:LYS:HB2	2.00	0.44
1:A:113:PRO:HB3	1:A:139:PHE:HB3	2.00	0.44
2:B:123:GLY:HA2	2:B:205:HIS:HD2	1.82	0.44
1:L:29:ARG:HA	1:L:29:ARG:HD2	1.68	0.44
1:C:35:TRP:HD1	1:C:48:ILE:HB	1.83	0.43
1:C:113:PRO:HD2	1:C:201:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:162:SER:HB2	2:H:172:PRO:HG2	2.01	0.43
1:A:27(D):HIS:CE1	2:B:100:LEU:HD21	2.53	0.43
2:H:52(A):HIS:NE2	2:H:52(B):GLU:OE2	2.51	0.43
2:B:194:LEU:HD22	2:B:218:PRO:HG3	2.01	0.43
1:C:92:ARG:NH1	1:C:92:ARG:O	2.43	0.43
2:B:122:LYS:NZ	2:B:149:ASP:O	2.49	0.43
2:B:82:LEU:HB3	2:B:82(C):LEU:HD21	2.00	0.43
1:C:69:LYS:NZ	1:C:70:ASP:OD1	2.33	0.43
2:D:200:ILE:HG13	2:D:215:LYS:HB3	2.01	0.43
1:C:25:SER:O	1:C:69:LYS:HD3	2.18	0.43
2:B:13:LYS:O	2:B:16:THR:OG1	2.31	0.43
2:B:151:PHE:HA	2:B:152:PRO:HA	1.81	0.43
2:D:132:SER:OG	2:D:133:SER:N	2.52	0.43
2:H:144:GLY:HA2	2:H:159:TRP:CZ2	2.54	0.43
1:C:155:GLN:HB3	1:C:158:ASN:HD21	1.83	0.42
2:D:131:PRO:HB3	2:D:143:LEU:HB3	2.00	0.42
2:H:10:GLU:HG2	2:H:18:VAL:HG23	2.01	0.42
2:H:36:TRP:CE2	2:H:80:LEU:HB2	2.54	0.42
2:H:65:VAL:HG22	2:H:82:LEU:HD13	2.00	0.42
2:B:36:TRP:CE2	2:B:80:LEU:HB2	2.55	0.42
1:L:105:ASP:OD1	1:L:166:GLN:NE2	2.52	0.42
1:A:113:PRO:HB2	1:A:136:LEU:HD22	2.02	0.42
1:A:4:LEU:HD11	1:A:90:GLN:HB3	2.01	0.42
2:H:100(A):ARG:NH1	2:H:100(F):TYS:O1	2.53	0.41
2:H:201:CYS:SG	2:H:214:LYS:HB3	2.60	0.41
1:C:82:ASP:HB3	1:C:86:TYR:OH	2.19	0.41
2:H:45:LEU:HA	2:H:45:LEU:HD23	1.93	0.41
1:C:31:ASN:O	1:C:50:LEU:HA	2.19	0.41
2:D:152:PRO:O	2:D:205:HIS:HE1	2.03	0.41
1:C:14:THR:N	1:C:107:LYS:HB3	2.36	0.41
1:A:11:LEU:HD22	1:A:13:VAL:HG22	2.02	0.41
2:D:189:VAL:HG21	2:D:199:TYR:CE2	2.54	0.41
1:A:58:VAL:HA	1:A:59:PRO:HD3	1.94	0.41
2:H:13:LYS:HD3	2:H:13:LYS:HA	1.88	0.41
1:C:6:GLN:NE2	1:C:86:TYR:O	2.39	0.41
2:D:37:VAL:HG21	2:D:108:TRP:CH2	2.56	0.40
2:D:205:HIS:HD2	2:D:208:SER:OG	2.04	0.40
1:L:93:GLU:HG3	1:L:93:GLU:H	1.63	0.40
1:C:198:HIS:HB3	1:C:201:LEU:CD1	2.51	0.40
1:C:91:GLY:HA2	1:C:96:TRP:CD1	2.57	0.40
2:B:200:ILE:HG12	2:B:215:LYS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:28:ASP:OD1	1:L:28:ASP:N	2.54	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	213/219 (97%)	207 (97%)	5 (2%)	1 (0%)	29	64
1	C	211/219 (96%)	200 (95%)	11 (5%)	0	100	100
1	L	213/219 (97%)	203 (95%)	10 (5%)	0	100	100
2	B	237/245 (97%)	224 (94%)	13 (6%)	0	100	100
2	D	235/245 (96%)	226 (96%)	8 (3%)	1 (0%)	34	69
2	H	238/245 (97%)	225 (94%)	13 (6%)	0	100	100
All	All	1347/1392 (97%)	1285 (95%)	60 (4%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27(E)	GLY
2	D	41	PRO

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	190/194 (98%)	184 (97%)	6 (3%)	39	69
1	C	189/194 (97%)	180 (95%)	9 (5%)	25	58
1	L	190/194 (98%)	181 (95%)	9 (5%)	26	59
2	B	203/207 (98%)	193 (95%)	10 (5%)	25	57
2	D	201/207 (97%)	192 (96%)	9 (4%)	27	60
2	H	204/207 (99%)	189 (93%)	15 (7%)	13	42
All	All	1177/1203 (98%)	1119 (95%)	58 (5%)	25	57

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	29	ARG
1	L	33	LEU
1	L	70	ASP
1	L	79	GLU
1	L	93	GLU
1	L	136	LEU
1	L	152	ASN
1	L	154	LEU
1	L	195	GLU
2	H	12	ARG
2	H	30	LYS
2	H	60	ARG
2	H	81	GLN
2	H	83	THR
2	H	110	GLN
2	H	122	LYS
2	H	143	LEU
2	H	147	VAL
2	H	148	LYS
2	H	183	LEU
2	H	192	SER
2	H	202	ASN
2	H	206	LYS
2	H	220	SER
1	A	11	LEU
1	A	13	VAL
1	A	28	ASP
1	A	33	LEU
1	A	108	ARG
1	A	163	VAL

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Mol	Chain	Res	Type
2	B	12	ARG
2	B	53	ASP
2	B	56	VAL
2	B	82(A)	SER
2	B	100(E)	LEU
2	B	100(H)	ASP
2	B	100(M)	ASN
2	B	122	LYS
2	B	198	THR
2	B	219	LYS
1	C	11	LEU
1	C	54	ARG
1	C	79	GLU
1	C	152	ASN
1	C	170	ASP
1	C	174	SER
1	C	179	LEU
1	C	197	THR
1	C	210	ASN
2	D	19	LYS
2	D	60	ARG
2	D	68	THR
2	D	82(A)	SER
2	D	99	ARG
2	D	100(B)	ASP
2	D	100(I)	ASP
2	D	192	SER
2	D	202	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	30	ASN
1	L	198	HIS
1	L	199	GLN
2	H	110	GLN
2	H	205	HIS
1	A	27(D)	HIS
1	A	45	GLN
1	A	124	GLN
1	A	155	GLN
1	A	198	HIS

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Mol	Chain	Res	Type
2	B	43	GLN
2	B	205	HIS
1	C	137	ASN
2	D	46	GLN
2	D	169	HIS
2	D	205	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	TYS	D	100(F)	2	15,16,17	1.26	3 (20%)	18,22,24	0.91	1 (5%)
2	TYS	H	100(F)	2	15,16,17	1.30	3 (20%)	18,22,24	1.07	1 (5%)
2	TYS	B	100(F)	2	15,16,17	1.32	3 (20%)	18,22,24	0.97	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TYS	D	100(F)	2	-	4/10/11/13	0/1/1/1
2	TYS	H	100(F)	2	-	0/10/11/13	0/1/1/1
2	TYS	B	100(F)	2	-	3/10/11/13	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	100(F)	TYS	OH-CZ	-3.10	1.37	1.42
2	H	100(F)	TYS	OH-CZ	-2.99	1.37	1.42
2	D	100(F)	TYS	OH-CZ	-2.93	1.37	1.42
2	H	100(F)	TYS	OH-S	-2.83	1.54	1.58
2	B	100(F)	TYS	OH-S	-2.79	1.54	1.58
2	D	100(F)	TYS	OH-S	-2.54	1.54	1.58
2	B	100(F)	TYS	O3-S	2.21	1.64	1.50
2	D	100(F)	TYS	O3-S	2.20	1.63	1.50
2	H	100(F)	TYS	O3-S	2.20	1.63	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	100(F)	TYS	CG-CB-CA	-3.34	107.33	114.10
2	B	100(F)	TYS	CB-CA-C	-2.59	106.61	111.47
2	D	100(F)	TYS	CG-CB-CA	-2.36	109.33	114.10

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	100(F)	TYS	CZ-OH-S-O3
2	D	100(F)	TYS	N-CA-CB-CG
2	D	100(F)	TYS	CE1-CZ-OH-S
2	D	100(F)	TYS	CE2-CZ-OH-S
2	D	100(F)	TYS	C-CA-CB-CG
2	B	100(F)	TYS	CZ-OH-S-O1
2	B	100(F)	TYS	CZ-OH-S-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	100(F)	TYS	1	0
2	H	100(F)	TYS	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	215/219 (98%)	-0.18	0 100 100	32, 45, 66, 78	0
1	C	213/219 (97%)	0.55	14 (6%) 18 7	56, 91, 113, 123	0
1	L	215/219 (98%)	-0.17	1 (0%) 91 81	31, 45, 70, 116	0
2	B	239/245 (97%)	0.01	7 (2%) 51 28	35, 52, 82, 114	0
2	D	237/245 (96%)	0.28	11 (4%) 32 16	48, 73, 116, 154	0
2	H	240/245 (97%)	-0.11	0 100 100	26, 49, 74, 111	0
All	All	1359/1392 (97%)	0.06	33 (2%) 59 37	26, 55, 107, 154	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	182	SER	6.8
1	C	181	LEU	5.5
1	C	201	LEU	3.6
2	D	133	SER	3.5
1	C	154	LEU	3.2
1	C	122	ASP	2.9
2	B	136	THR	2.8
2	D	216	VAL	2.8
1	C	27(E)	GLY	2.7
1	C	152	ASN	2.7
2	D	134	LYS	2.6
1	C	134	CYS	2.6
2	D	188	THR	2.6
2	B	100(G)	ASP	2.6
1	C	197	THR	2.6
2	B	100(I)	ASP	2.4
1	C	195	GLU	2.4
2	B	211	LYS	2.4
1	L	28	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	63	SER	2.3
2	D	162	GLY	2.3
2	D	127	PHE	2.2
1	C	153	ALA	2.2
2	B	209	ASN	2.2
2	D	167	GLY	2.2
1	C	147	GLN	2.2
2	B	100(M)	ASN	2.1
2	D	142	ALA	2.1
2	D	143	LEU	2.1
2	D	160	ASN	2.1
2	B	100(K)	ALA	2.1
2	D	193	SER	2.1
1	C	60	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TYS	B	100(F)	16/17	0.86	0.40	65,70,101,105	0
2	TYS	D	100(F)	16/17	0.94	0.27	64,69,72,81	0
2	TYS	H	100(F)	16/17	0.96	0.22	48,57,67,68	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.