



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:34 am BST

PDB ID : 4JO3
Title : Crystal structure of rabbit mAb R20 Fab in complex with V3 C-terminus of HIV-1 Consensus B gp120
Authors : Pan, R.M.; Kong, X.P.
Deposited on : 2013-03-16
Resolution : 2.60 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

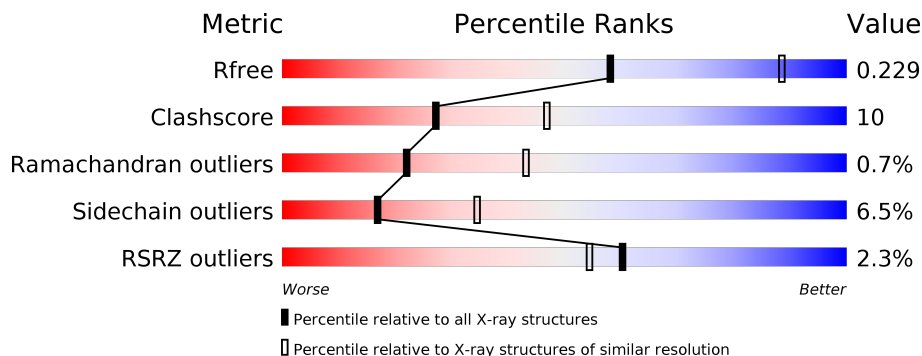
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	L	214	79% (green), 19% (yellow), 2% (orange), 2% (red)
1	M	214	79% (green), 20% (yellow), 1% (orange), 1% (red)
2	H	227	4% (red), 79% (green), 18% (yellow), 1% (orange)
2	I	227	4% (red), 74% (green), 22% (yellow), 1% (orange)
3	P	15	7% (red), 40% (green), 20% (yellow), 40% (grey)
3	Q	15	47% (green), 13% (yellow), 40% (grey)

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7039 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 monoclonal anti-HIV-1 gp120 V3 antibody R20 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	214	1583	984	256	335	8	0	0	0
1	M	214	1583	984	256	335	8	0	0	0

- Molecule 2 is a protein called monoclonal anti-HIV-1 gp120 V3 antibody R20 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	227	1677	1063	273	331	10	0	0	0
2	I	227	1677	1063	273	331	10	0	0	0

- Molecule 3 is a protein called gp120.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	P	9	70	43	13	14	0	0	0
3	Q	9	70	43	13	14	0	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total O S 5 4 1	0	0
4	M	1	Total O S 5 4 1	0	0

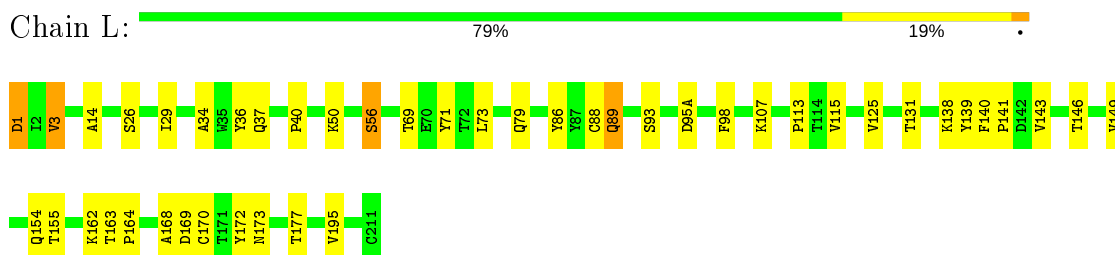
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	92	Total O 92 92	0	0
5	H	78	Total O 78 78	0	0
5	M	86	Total O 86 86	0	0
5	I	111	Total O 111 111	0	0
5	Q	2	Total O 2 2	0	0

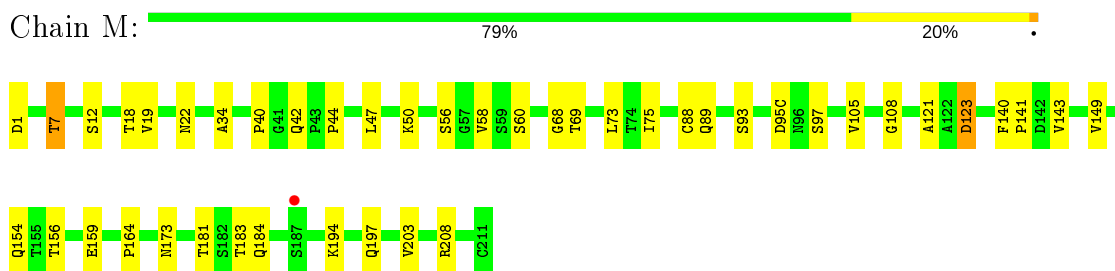
3 Residue-property plots [i](#)

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.

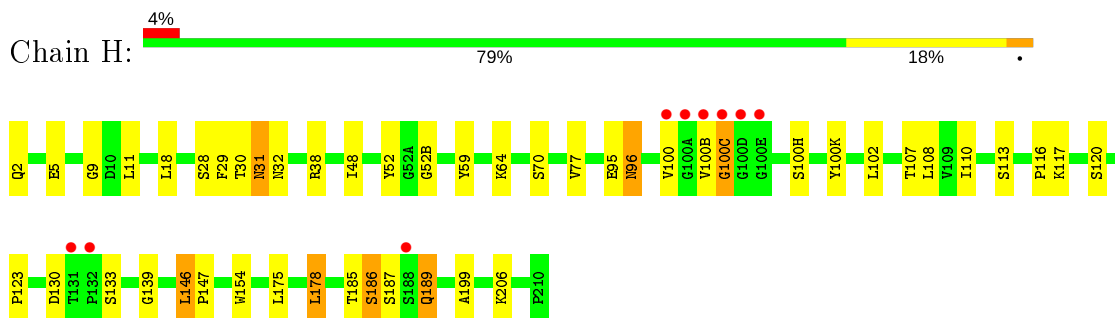
- Molecule 1: monoclonal anti-HIV-1 gp120 V3 antibody R20 light chain



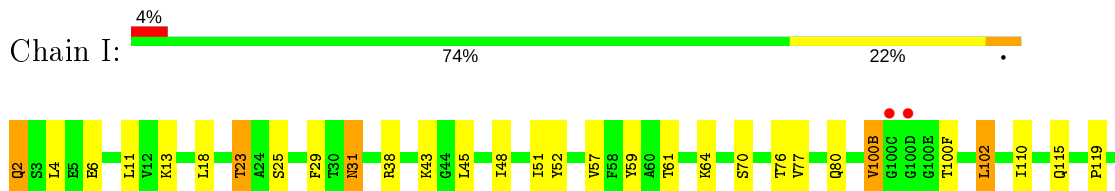
- Molecule 1: monoclonal anti-HIV-1 gp120 V3 antibody R20 light chain

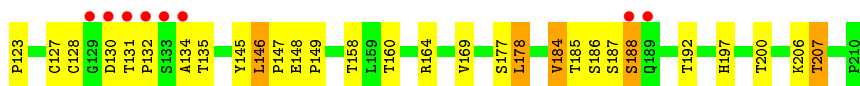


- Molecule 2: monoclonal anti-HIV-1 gp120 V3 antibody R20 heavy chain

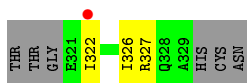


- Molecule 2: monoclonal anti-HIV-1 gp120 V3 antibody R20 heavy chain





- Molecule 3: gp120



- Molecule 3: gp120



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.22Å 118.98Å 134.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.05 – 2.60 38.05 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.6 (38.05-2.60) 96.4 (38.05-2.58)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.58Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.184 , 0.234 0.179 , 0.229	Depositor DCC
R_{free} test set	1770 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtrriage
Anisotropy	0.449	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7039	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2430e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	L	0.43	0/1613	0.59	0/2209
1	M	0.44	0/1613	0.60	0/2209
2	H	0.44	0/1720	0.59	0/2357
2	I	0.47	0/1720	0.62	0/2357
3	P	0.29	0/69	0.55	0/91
3	Q	0.46	0/69	0.60	0/91
All	All	0.44	0/6804	0.60	0/9314

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	L	1583	0	1523	28	0
1	M	1583	0	1523	26	0
2	H	1677	0	1628	40	0
2	I	1677	0	1628	53	0
3	P	70	0	71	4	0
3	Q	70	0	71	2	0
4	M	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	78	0	0	3	1
5	I	111	0	0	5	1
5	L	92	0	0	5	0
5	M	86	0	0	1	0
5	Q	2	0	0	0	0
All	All	7039	0	6444	132	1

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 10.

All (132) 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:H:186:SER:HB2	2:H:189:GLN:HG3	1.41	0.99
2:I:2:GLN:N	2:I:2:GLN:NE2	2.19	0.89
2:I:51:ILE:HG13	2:I:57:VAL:HG12	1.55	0.88
2:I:146:LEU:HD22	2:I:147:PRO:HA	1.57	0.86
2:H:146:LEU:HD22	2:H:147:PRO:HA	1.61	0.82
2:H:5:GLU:O	5:H:376:HOH:O	1.98	0.79
2:H:100(B):VAL:HG12	2:H:100(C):GLY:H	1.49	0.76
2:I:197:HIS:HD2	2:I:200:THR:OG1	1.69	0.76
2:I:23:THR:HB	2:I:76:THR:HG22	1.70	0.73
1:M:108:GLY:O	5:M:436:HOH:O	2.07	0.73
2:I:2:GLN:HA	2:I:25:SER:O	1.89	0.72
2:H:2:GLN:N	2:H:2:GLN:OE1	2.23	0.71
1:M:19:VAL:HG12	1:M:75:ILE:HB	1.73	0.70
2:H:206:LYS:NZ	5:H:301:HOH:O	2.26	0.69
1:M:208:ARG:HG2	1:M:208:ARG:HH21	1.58	0.68
1:L:50:LYS:NZ	5:L:350:HOH:O	2.21	0.68
2:I:80:GLN:HG3	5:I:406:HOH:O	1.93	0.68
1:M:93:SER:CB	3:Q:327:ARG:HD2	2.23	0.68
2:H:189:GLN:HE22	2:I:160:THR:H	1.39	0.68
2:I:2:GLN:N	2:I:2:GLN:CD	2.44	0.67
1:L:125:VAL:HG23	5:L:335:HOH:O	1.93	0.67
2:H:38:ARG:HB3	2:H:48:ILE:HD11	1.77	0.67
2:I:29:PHE:CE1	2:I:77:VAL:HG23	2.31	0.66
2:I:38:ARG:HB3	2:I:48:ILE:HD11	1.78	0.65
1:L:56:SER:HB3	1:M:50:LYS:HD3	1.77	0.65
2:I:4:LEU:HG	2:I:102:LEU:HD13	1.79	0.64
2:I:100(F):THR:HG23	5:I:410:HOH:O	1.97	0.64
2:I:178:LEU:C	2:I:178:LEU:HD12	2.18	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:31:ASN:H	2:H:31:ASN:HD22	1.45	0.63
2:I:61:THR:HG21	5:I:405:HOH:O	1.99	0.63
2:H:100:VAL:HG21	3:P:326:ILE:HD13	1.80	0.62
1:L:93:SER:CB	3:P:327:ARG:HD2	2.28	0.62
2:I:2:GLN:NE2	5:I:389:HOH:O	2.34	0.61
2:H:189:GLN:NE2	2:I:160:THR:H	1.99	0.61
2:I:2:GLN:HE21	2:I:2:GLN:CA	2.15	0.60
1:M:40:PRO:HG2	1:M:164:PRO:HG3	1.86	0.58
2:H:186:SER:HB3	2:I:158:THR:C	2.23	0.58
2:H:100(B):VAL:HG12	2:H:100(C):GLY:N	2.19	0.58
1:L:162:LYS:HE3	1:L:172:TYR:CE2	2.39	0.58
1:L:56:SER:O	1:M:50:LYS:HE2	2.05	0.56
1:M:123:ASP:N	1:M:123:ASP:OD2	2.33	0.56
1:M:159:GLU:HB3	2:I:169:VAL:HG11	1.87	0.56
2:H:123:PRO:HD3	2:H:206:LYS:HD3	1.88	0.56
1:M:121:ALA:HB2	2:I:123:PRO:HD2	1.88	0.55
2:I:197:HIS:CD2	2:I:200:THR:OG1	2.57	0.55
2:H:186:SER:HB2	2:H:189:GLN:CG	2.28	0.55
2:I:119:PRO:HB3	2:I:145:TYR:HB3	1.89	0.55
1:L:93:SER:HB2	3:P:327:ARG:HD2	1.89	0.55
2:I:2:GLN:HE21	2:I:2:GLN:N	2.05	0.54
1:M:12:SER:HA	1:M:105:VAL:O	2.08	0.54
1:L:131:THR:O	5:L:303:HOH:O	2.18	0.54
2:H:178:LEU:HD12	2:H:178:LEU:C	2.28	0.54
2:H:146:LEU:CD2	2:H:147:PRO:HA	2.36	0.53
1:L:177:THR:HG23	5:L:308:HOH:O	2.09	0.52
2:H:29:PHE:CE1	2:H:77:VAL:HG23	2.45	0.52
1:M:44:PRO:HG3	2:I:45:LEU:HD11	1.91	0.51
2:H:108:LEU:HG	2:H:110:ILE:HD11	1.91	0.51
1:M:181:THR:OG1	1:M:184:GLN:HG3	2.09	0.51
2:H:186:SER:HB3	2:I:158:THR:O	2.11	0.51
1:L:79:GLN:HB3	2:I:2:GLN:OE1	2.11	0.51
2:H:96:ASN:O	2:H:100(K):TYR:HA	2.11	0.50
2:I:11:LEU:HD22	2:I:146:LEU:HD13	1.93	0.50
2:H:52:TYR:CE2	2:H:52(B):GLY:HA3	2.46	0.50
1:L:79:GLN:OE1	2:I:2:GLN:HG2	2.11	0.50
2:I:31:ASN:HB2	2:I:52:TYR:OH	2.12	0.50
2:H:146:LEU:HD22	2:H:147:PRO:CA	2.39	0.49
2:I:135:THR:HA	2:I:185:THR:O	2.12	0.49
1:M:208:ARG:NH2	1:M:208:ARG:HG2	2.26	0.49
2:I:2:GLN:CA	2:I:2:GLN:NE2	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:139:GLY:HA2	2:H:154:TRP:CH2	2.47	0.49
2:I:51:ILE:HD12	2:I:70:SER:HA	1.94	0.49
2:H:28:SER:O	2:H:30:THR:HG23	2.13	0.49
2:I:192:THR:OG1	2:I:207:THR:HB	2.12	0.48
1:M:121:ALA:CB	2:I:123:PRO:HD2	2.43	0.48
2:I:127:CYS:O	2:I:130:ASP:HB2	2.13	0.48
2:I:148:GLU:HB3	2:I:149:PRO:HA	1.95	0.47
1:L:149:VAL:HG23	1:L:154:GLN:HG2	1.96	0.47
1:M:7:THR:HG22	1:M:22:ASN:HD22	1.80	0.47
2:H:100(H):SER:HB3	3:P:322:ILE:HD13	1.96	0.47
1:L:3:VAL:HG13	1:L:26:SER:HB3	1.96	0.47
1:M:173:ASN:OD1	2:I:164:ARG:HD3	2.14	0.47
2:H:11:LEU:HD23	2:H:116:PRO:HG3	1.96	0.47
1:L:37:GLN:HB2	1:L:86:TYR:CE1	2.48	0.47
2:H:38:ARG:CB	2:H:48:ILE:HD11	2.45	0.46
2:I:110:ILE:HG12	2:I:147:PRO:HB2	1.97	0.46
2:H:30:THR:C	2:H:32:ASN:H	2.19	0.46
2:I:115:GLN:HB2	5:I:348:HOH:O	2.14	0.46
2:I:187:SER:O	2:I:188:SER:C	2.53	0.46
2:I:186:SER:OG	2:I:187:SER:N	2.44	0.46
2:H:189:GLN:NE2	2:I:160:THR:OG1	2.48	0.45
1:L:169:ASP:O	1:L:170:CYS:HB2	2.16	0.45
1:L:168:ALA:HA	2:I:2:GLN:HE22	1.82	0.44
1:M:95(C):ASP:C	1:M:95(C):ASP:OD1	2.56	0.44
2:H:9:GLY:HA3	2:H:107:THR:OG1	2.17	0.44
2:H:123:PRO:HD3	2:H:206:LYS:CD	2.46	0.44
1:L:1:ASP:HB3	1:L:95(A):ASP:O	2.17	0.44
1:L:140:PHE:CG	1:L:141:PRO:HA	2.53	0.44
1:L:40:PRO:HG2	1:L:164:PRO:HB3	2.00	0.44
1:M:140:PHE:CG	1:M:141:PRO:HA	2.53	0.44
1:M:181:THR:HG23	1:M:184:GLN:OE1	2.17	0.44
2:H:108:LEU:HG	2:H:110:ILE:CD1	2.47	0.43
1:L:34:ALA:O	1:L:88:CYS:HA	2.18	0.43
2:I:178:LEU:C	2:I:178:LEU:CD1	2.87	0.43
2:I:135:THR:HG23	2:I:184:VAL:O	2.18	0.43
1:M:47:LEU:HA	1:M:58:VAL:HG21	2.00	0.43
1:L:14:ALA:HA	1:L:107:LYS:HB2	1.99	0.43
1:L:29:ILE:HD11	1:L:71:TYR:CE2	2.53	0.43
1:M:34:ALA:O	1:M:88:CYS:HA	2.19	0.43
1:L:113:PRO:HA	1:L:139:TYR:HB3	2.00	0.43
2:H:147:PRO:HD2	2:H:199:ALA:CB	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:139:TYR:CE1	1:L:143:VAL:HG13	2.54	0.42
1:M:149:VAL:HG23	1:M:154:GLN:CG	2.49	0.42
2:H:95:GLU:OE2	2:H:100(K):TYR:HB3	2.19	0.42
1:L:36:TYR:HE2	1:L:89:GLN:HE21	1.67	0.42
2:H:2:GLN:NE2	5:H:344:HOH:O	2.53	0.42
2:I:110:ILE:N	2:I:110:ILE:HD12	2.34	0.42
1:M:194:LYS:HG3	1:M:203:VAL:HG22	2.02	0.42
2:I:185:THR:OG1	2:I:186:SER:N	2.54	0.41
2:I:59:TYR:HB2	2:I:64:LYS:HB2	2.02	0.41
1:L:163:THR:CG2	1:L:173:ASN:HB2	2.51	0.41
1:L:115:VAL:HG21	1:L:195:VAL:HB	2.03	0.41
2:H:117:LYS:HD3	2:H:175:LEU:HD13	2.01	0.41
2:H:100(B):VAL:CG1	2:H:100(C):GLY:H	2.28	0.41
2:H:29:PHE:CZ	2:H:77:VAL:HG23	2.55	0.41
2:I:100(B):VAL:HG21	3:Q:329:ALA:HB1	2.03	0.41
2:I:13:LYS:HE3	2:I:115:GLN:HE22	1.86	0.41
1:M:143:VAL:HG12	1:M:197:GLN:HB2	2.03	0.41
1:L:98:PHE:O	5:L:365:HOH:O	2.22	0.40
2:H:59:TYR:HB2	2:H:64:LYS:HB2	2.03	0.40
1:M:89:GLN:HA	1:M:97:SER:O	2.21	0.40
2:I:6:GLU:OE2	2:I:6:GLU:N	2.42	0.40
2:I:185:THR:OG1	2:I:188:SER:HB3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:349:HOH:O	5:I:374:HOH:O[3_655]	2.18	0.02

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	L	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	29	52
1	M	212/214 (99%)	199 (94%)	12 (6%)	1 (0%)	29	52
2	H	225/227 (99%)	215 (96%)	9 (4%)	1 (0%)	34	57
2	I	225/227 (99%)	212 (94%)	10 (4%)	3 (1%)	12	24
3	P	7/15 (47%)	4 (57%)	3 (43%)	0	100	100
3	Q	7/15 (47%)	6 (86%)	1 (14%)	0	100	100
All	All	888/912 (97%)	841 (95%)	41 (5%)	6 (1%)	22	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	134	ALA
1	L	138	LYS
2	I	132	PRO
2	I	188	SER
2	H	100(C)	GLY
1	M	68	GLY

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	L	181/181 (100%)	173 (96%)	8 (4%)	28	53
1	M	181/181 (100%)	170 (94%)	11 (6%)	18	38
2	H	187/187 (100%)	172 (92%)	15 (8%)	12	24
2	I	187/187 (100%)	172 (92%)	15 (8%)	12	24
3	P	7/12 (58%)	7 (100%)	0	100	100
3	Q	7/12 (58%)	7 (100%)	0	100	100
All	All	750/760 (99%)	701 (94%)	49 (6%)	17	34

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

Mol	Chain	Res	Type
1	L	1	ASP
1	L	3	VAL
1	L	56	SER
1	L	69	THR
1	L	73	LEU
1	L	89	GLN
1	L	146	THR
1	L	155	THR
2	H	18	LEU
2	H	31	ASN
2	H	70	SER
2	H	96	ASN
2	H	102	LEU
2	H	113	SER
2	H	120	SER
2	H	130	ASP
2	H	133	SER
2	H	146	LEU
2	H	178	LEU
2	H	185	THR
2	H	186	SER
2	H	187	SER
2	H	189	GLN
1	M	1	ASP
1	M	7	THR
1	M	18	THR
1	M	42	GLN
1	M	56	SER
1	M	60	SER
1	M	69	THR
1	M	73	LEU
1	M	123	ASP
1	M	156	THR
1	M	183	THR
2	I	2	GLN
2	I	18	LEU
2	I	23	THR
2	I	31	ASN
2	I	43	LYS
2	I	100(B)	VAL
2	I	102	LEU
2	I	128	CYS
2	I	131	THR

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Mol	Chain	Res	Type
2	I	146	LEU
2	I	177	SER
2	I	178	LEU
2	I	184	VAL
2	I	206	LYS
2	I	207	THR

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

Mol	Chain	Res	Type
1	L	89	GLN
1	L	137	ASN
1	L	207	ASN
2	H	31	ASN
2	H	189	GLN
1	M	154	GLN
2	I	31	ASN
2	I	32	ASN
2	I	115	GLN
2	I	197	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z > 2$
4	SO4	M	302	-	4,4,4	0.22	0	6,6,6	0.21	0
4	SO4	M	301	-	4,4,4	0.13	0	6,6,6	0.24	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	L	214/214 (100%)	-0.48	0 100 100	22, 32, 44, 64	0
1	M	214/214 (100%)	-0.40	1 (0%) 91 89	23, 35, 50, 65	0
2	H	227/227 (100%)	-0.29	9 (3%) 38 31	21, 32, 71, 95	0
2	I	227/227 (100%)	-0.37	10 (4%) 34 27	22, 30, 75, 105	0
3	P	9/15 (60%)	0.30	1 (11%) 5 3	44, 48, 59, 62	0
3	Q	9/15 (60%)	-0.46	0 100 100	34, 37, 44, 51	0
All	All	900/912 (98%)	-0.38	21 (2%) 60 54	21, 32, 59, 105	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	100(C)	GLY	5.1
2	I	132	PRO	5.0
2	H	100(B)	VAL	3.8
2	H	100(D)	GLY	3.8
2	I	129	GLY	3.7
2	H	188	SER	3.7
2	I	131	THR	3.6
2	H	100(E)	GLY	3.6
2	H	132	PRO	3.1
2	I	188	SER	2.9
2	I	100(C)	GLY	2.9
2	H	131	THR	2.9
2	I	133	SER	2.8
2	I	100(D)	GLY	2.4
3	P	322	ILE	2.4
1	M	187	SER	2.4
2	H	100	VAL	2.3
2	H	100(A)	GLY	2.3
2	I	189	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	I	134	ALA	2.2
2	I	130	ASP	2.0

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
4	SO4	M	302	5/5	0.86	0.38	60,63,91,98	0
4	SO4	M	301	5/5	0.96	0.10	59,62,72,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.