



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 03:51 pm BST

PDB ID : 4JO4  
Title : Crystal structure of rabbit mAb R20 Fab  
Authors : Pan, R.M.; Kong, X.P.  
Deposited on : 2013-03-16  
Resolution : 2.27 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](mailto: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.

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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

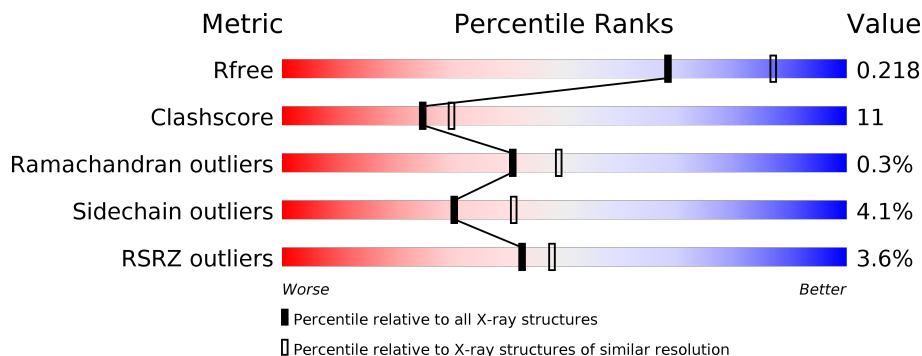
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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  $\geq 3$ , 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	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">%      79%      19%      •</p>
1	M	214	<div style="display: flex; align-items: center;"> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">87%      11%      •</p>
2	H	227	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">7%      76%      20%      •</p>
2	I	227	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">6%      84%      15%      •</p>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7344 atoms, of which 48 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.

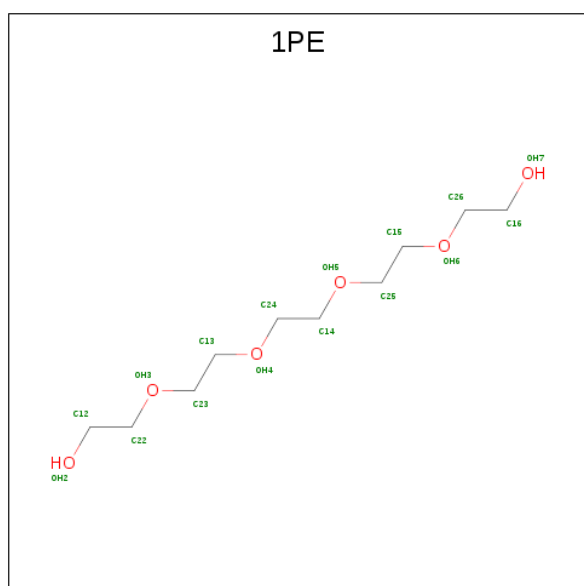
- Molecule 1 is a protein called monoclonal anti-HIV-1 gp120 V3 antibody R20 light chain.

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

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

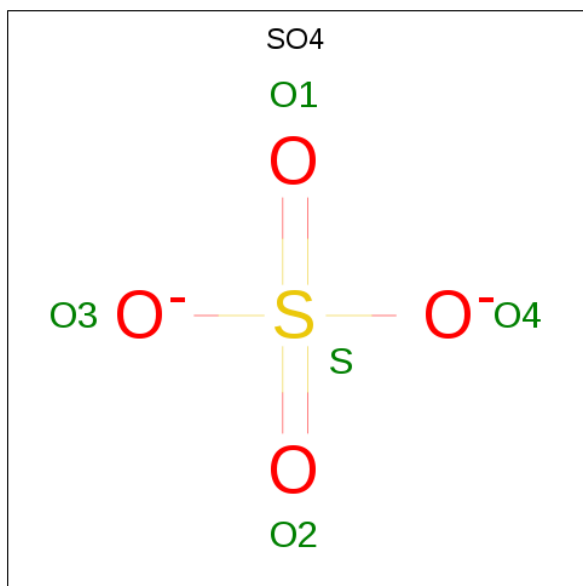
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	227	Total 1677	C 1063	N 273	O 331	S 10	0	0	0
2	I	227	Total 1677	C 1063	N 273	O 331	S 10	0	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	H	O	0	0
			38	10	22	6		
3	I	1	Total	C	H	O	0	0
			23	6	13	4		
3	I	1	Total	C	H	O	0	0
			23	6	13	4		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

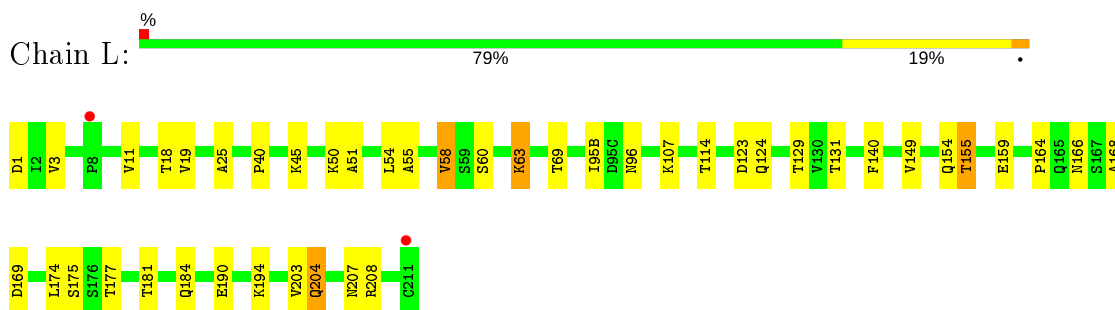
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	165	Total	O	0	0
			165	165		
5	H	206	Total	O	0	0
			206	206		
5	M	180	Total	O	0	0
			180	180		
5	I	179	Total	O	0	0
			179	179		

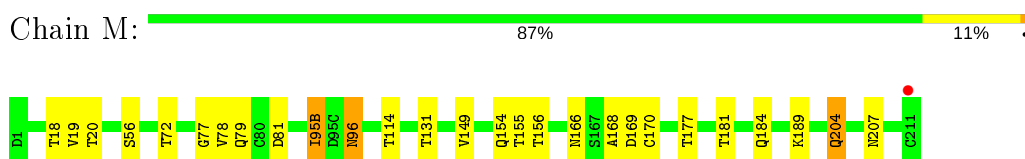
### 3 Residue-property plots [i](#)

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.

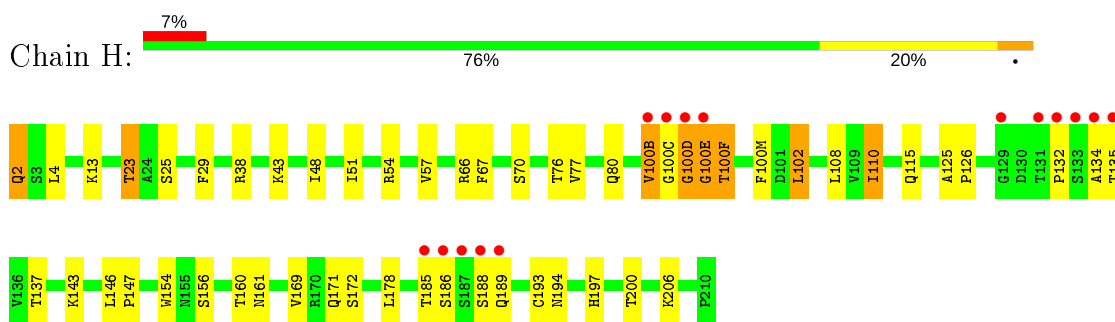
- Molecule 1: monoclonal anti-HIV-1 gp120 V3 antibody R20 light chain



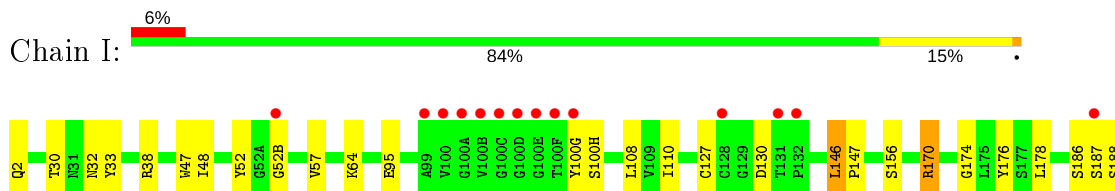
- Molecule 1: monoclonal anti-HIV-1 gp120 V3 antibody R20 light chain



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.65Å 119.69Å 135.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.27 – 2.27 38.27 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.27-2.27) 99.5 (38.27-2.02)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.03Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.184 , 0.226 0.177 , 0.218	Depositor DCC
$R_{free}$ test set	3791 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtrriage
Anisotropy	0.087	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7344	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 1PE

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	0.38	0/1613	0.56	0/2209
1	M	0.39	0/1613	0.55	0/2209
2	H	0.39	0/1720	0.57	0/2357
2	I	0.38	0/1720	0.55	0/2357
All	All	0.39	0/6666	0.56	0/9132

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	39	0
1	M	1583	0	1523	25	0
2	H	1677	0	1628	54	0
2	I	1677	0	1628	35	0
3	H	16	22	22	2	0
3	I	20	26	26	4	0
4	H	5	0	0	1	0
4	I	5	0	0	0	0
5	H	206	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	179	0	0	5	0
5	L	165	0	0	3	1
5	M	180	0	0	1	1
All	All	7296	48	6350	140	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 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)
2:H:2:GLN:N	2:H:2:GLN:OE1	1.84	1.09
2:H:100(C):GLY:HA3	2:H:100(D):GLY:C	1.73	1.05
1:L:159:GLU:HG2	2:H:169:VAL:HG11	1.47	0.96
1:L:159:GLU:CG	2:H:169:VAL:HG11	1.96	0.95
1:L:159:GLU:HG3	5:L:459:HOH:O	1.66	0.94
2:H:100(C):GLY:HA3	2:H:100(E):GLY:N	1.82	0.94
2:H:2:GLN:NE2	1:M:81:ASP:H	1.71	0.87
2:H:156:SER:H	2:H:194:ASN:HD21	1.24	0.85
1:L:154:GLN:NE2	5:L:448:HOH:O	2.09	0.85
2:I:156:SER:H	2:I:194:ASN:HD21	1.26	0.84
1:L:166:ASN:HD22	1:L:169:ASP:H	1.30	0.80
2:I:110:ILE:HD12	2:I:147:PRO:HB2	1.63	0.79
1:M:166:ASN:HD22	1:M:169:ASP:H	1.31	0.77
2:H:100(M):PHE:O	5:H:498:HOH:O	2.03	0.77
2:H:2:GLN:HE22	1:M:81:ASP:H	1.33	0.76
2:H:13:LYS:HE3	2:H:115:GLN:HE22	1.52	0.74
2:H:108:LEU:HD21	2:H:110:ILE:HD11	1.68	0.73
1:L:159:GLU:HG3	2:H:169:VAL:HG11	1.71	0.71
2:I:190:PRO:O	5:I:530:HOH:O	2.08	0.71
3:I:302:1PE:C13	5:I:535:HOH:O	2.39	0.70
2:I:110:ILE:HD12	2:I:147:PRO:CB	2.21	0.69
2:H:100(C):GLY:CA	2:H:100(D):GLY:C	2.57	0.69
1:L:166:ASN:ND2	1:L:168:ALA:H	1.94	0.66
2:H:197:HIS:HD2	2:H:200:THR:OG1	1.79	0.66
2:I:147:PRO:O	2:I:197:HIS:HE1	1.78	0.66
2:H:2:GLN:HE22	1:M:81:ASP:N	1.94	0.65
1:M:181:THR:H	1:M:184:GLN:HE21	1.42	0.65
2:H:156:SER:H	2:H:194:ASN:ND2	1.94	0.65
1:L:124:GLN:HE22	1:L:131:THR:H	1.43	0.65
2:I:170:ARG:HG3	2:I:176:TYR:CZ	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:161:ASN:ND2	2:I:189:GLN:HB2	2.11	0.65
1:L:181:THR:H	1:L:184:GLN:NE2	1.96	0.64
1:M:204:GLN:HA	1:M:204:GLN:HE21	1.64	0.63
1:L:159:GLU:HG2	2:H:169:VAL:CG1	2.26	0.63
2:H:134:ALA:O	2:H:186:SER:HA	1.99	0.62
1:L:131:THR:HG23	1:L:177:THR:CG2	2.29	0.62
1:L:181:THR:H	1:L:184:GLN:HE21	1.48	0.62
2:H:178:LEU:HD12	2:H:178:LEU:C	2.20	0.62
1:M:166:ASN:ND2	1:M:168:ALA:H	1.98	0.61
2:H:13:LYS:CE	2:H:115:GLN:HE22	2.14	0.61
1:L:124:GLN:NE2	1:L:131:THR:H	1.98	0.61
2:H:110:ILE:HG13	5:H:567:HOH:O	1.99	0.61
2:H:147:PRO:O	2:H:197:HIS:HE1	1.83	0.61
1:L:40:PRO:HG2	1:L:164:PRO:HG3	1.84	0.59
2:H:29:PHE:CE1	2:H:77:VAL:HG13	2.39	0.58
2:I:110:ILE:HG13	5:I:509:HOH:O	2.04	0.58
4:H:302:SO4:O1	5:H:595:HOH:O	2.16	0.57
2:H:13:LYS:HE3	2:H:115:GLN:NE2	2.19	0.57
2:H:23:THR:HB	2:H:76:THR:HG22	1.86	0.57
2:I:178:LEU:C	2:I:178:LEU:HD12	2.24	0.57
2:I:100(G):TYR:HB2	3:I:301:1PE:H141	1.87	0.57
1:L:194:LYS:HG3	1:L:203:VAL:HG22	1.87	0.57
2:I:197:HIS:HD2	2:I:200:THR:OG1	1.88	0.57
2:H:2:GLN:HA	2:H:25:SER:O	2.05	0.57
2:H:185:THR:HG23	2:H:186:SER:N	2.20	0.56
2:I:156:SER:H	2:I:194:ASN:ND2	1.98	0.56
2:I:2:GLN:OE1	2:I:2:GLN:N	2.39	0.55
1:L:50:LYS:HE3	1:M:56:SER:OG	2.07	0.55
2:H:2:GLN:CD	2:H:2:GLN:N	2.51	0.55
1:L:166:ASN:ND2	1:L:169:ASP:H	2.02	0.55
2:I:127:CYS:O	2:I:130:ASP:HB2	2.06	0.54
1:M:189:LYS:HG2	1:M:207:ASN:OD1	2.07	0.54
2:I:170:ARG:HG3	2:I:176:TYR:CE1	2.43	0.53
2:H:161:ASN:HD22	2:I:189:GLN:HB2	1.73	0.53
1:M:131:THR:CG2	1:M:177:THR:CG2	2.86	0.53
2:H:4:LEU:HG	2:H:102:LEU:HD13	1.91	0.53
2:H:188:SER:C	2:H:189:GLN:HG3	2.28	0.53
1:L:63:LYS:HD3	5:L:383:HOH:O	2.08	0.53
2:H:125:ALA:HB1	2:H:126:PRO:HD2	1.91	0.53
1:M:96:ASN:ND2	2:I:47:TRP:H	2.07	0.53
2:I:110:ILE:CD1	2:I:147:PRO:HB2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:204:GLN:HE21	1:L:204:GLN:HA	1.74	0.52
2:H:160:THR:OG1	2:I:189:GLN:NE2	2.42	0.52
1:M:95(B):ILE:HG12	5:M:339:HOH:O	2.09	0.52
1:M:166:ASN:HB3	1:M:169:ASP:OD2	2.11	0.51
1:L:40:PRO:HG2	1:L:164:PRO:CG	2.41	0.51
1:M:77:GLY:O	1:M:79:GLN:HG3	2.11	0.51
2:H:51:ILE:HG13	2:H:57:VAL:HG12	1.92	0.50
2:I:2:GLN:HB2	5:I:552:HOH:O	2.12	0.50
2:I:38:ARG:HB3	2:I:48:ILE:HD11	1.95	0.49
1:M:181:THR:H	1:M:184:GLN:NE2	2.09	0.49
1:L:129:THR:CG2	2:H:143:LYS:HZ3	2.25	0.48
1:M:19:VAL:HG23	1:M:78:VAL:HG21	1.95	0.48
2:H:186:SER:C	2:H:188:SER:H	2.16	0.48
2:I:146:LEU:HD22	2:I:147:PRO:HA	1.95	0.48
2:H:54:ARG:NH1	3:H:301:1PE:H221	2.29	0.48
1:M:131:THR:HG23	1:M:177:THR:CG2	2.44	0.48
1:L:129:THR:HG22	2:H:143:LYS:HZ3	1.80	0.47
1:M:20:THR:HG23	1:M:72:THR:CG2	2.43	0.47
1:L:124:GLN:HE22	1:L:131:THR:N	2.12	0.47
2:H:54:ARG:HH12	3:H:301:1PE:H221	1.79	0.47
2:I:186:SER:OG	2:I:189:GLN:HG2	2.14	0.47
1:L:174:LEU:HD13	1:L:175:SER:N	2.30	0.47
2:I:170:ARG:HH11	2:I:174:GLY:HA2	1.79	0.47
1:L:166:ASN:HD21	1:L:168:ALA:HB3	1.80	0.47
2:I:100(H):SER:H	3:I:301:1PE:H131	1.80	0.46
1:L:55:ALA:O	1:L:58:VAL:HG13	2.16	0.46
2:H:188:SER:O	2:H:189:GLN:HG3	2.16	0.46
1:L:25:ALA:O	1:L:69:THR:HB	2.15	0.46
2:I:108:LEU:HD21	2:I:110:ILE:HD11	1.99	0.45
2:I:33:TYR:HB2	2:I:95:GLU:O	2.16	0.45
1:L:123:ASP:N	1:L:123:ASP:OD1	2.43	0.45
2:H:38:ARG:HB3	2:H:48:ILE:HD11	1.99	0.45
2:H:2:GLN:CG	1:M:79:GLN:HB3	2.46	0.45
1:M:155:THR:HG23	1:M:156:THR:HG23	1.98	0.45
1:L:54:LEU:HD21	1:L:60:SER:HA	1.98	0.45
2:H:80:GLN:HG3	5:H:495:HOH:O	2.16	0.45
1:M:149:VAL:HG23	1:M:154:GLN:HG2	1.98	0.44
1:L:208:ARG:HG2	1:L:208:ARG:HH21	1.82	0.44
1:L:155:THR:HG23	1:L:155:THR:O	2.16	0.44
2:I:146:LEU:CD2	2:I:147:PRO:HA	2.47	0.44
2:I:52:TYR:CE2	2:I:52(B):GLY:HA3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:190:GLU:HG3	1:L:207:ASN:OD1	2.17	0.44
1:L:50:LYS:O	1:L:51:ALA:HB3	2.17	0.43
1:L:174:LEU:HD13	1:L:174:LEU:C	2.38	0.43
1:M:169:ASP:O	1:M:170:CYS:HB2	2.17	0.43
2:H:2:GLN:HG3	1:M:79:GLN:HB3	1.99	0.43
2:I:186:SER:C	2:I:188:SER:H	2.20	0.43
2:H:100(B):VAL:HA	2:H:100(F):THR:HG22	2.00	0.43
2:H:66:ARG:O	2:H:67:PHE:HD2	2.02	0.43
1:L:107:LYS:HA	1:L:140:PHE:CZ	2.54	0.43
2:I:187:SER:O	2:I:210:PRO:HG2	2.19	0.43
1:L:11:VAL:HG13	1:L:19:VAL:HG21	2.00	0.43
2:H:206:LYS:HB2	2:H:206:LYS:HE2	1.66	0.43
1:L:1:ASP:HB3	1:L:95(B):ILE:HA	2.01	0.43
1:M:166:ASN:HD22	1:M:168:ALA:H	1.65	0.42
2:H:154:TRP:CH2	2:H:193:CYS:HB3	2.54	0.42
2:I:30:THR:C	2:I:32:ASN:H	2.22	0.42
3:I:302:1PE:H132	5:I:535:HOH:O	2.13	0.42
2:H:143:LYS:NZ	5:H:533:HOH:O	2.37	0.41
2:H:185:THR:CG2	2:H:186:SER:N	2.83	0.41
2:I:170:ARG:HD2	2:I:174:GLY:HA2	2.02	0.41
2:H:2:GLN:OE1	2:H:2:GLN:CA	2.64	0.41
2:H:80:GLN:NE2	5:H:474:HOH:O	2.45	0.41
1:L:149:VAL:HG23	1:L:154:GLN:CG	2.51	0.41
1:L:149:VAL:HG23	1:L:154:GLN:HG2	2.02	0.41
2:H:146:LEU:HD12	2:H:147:PRO:HA	2.03	0.41
1:M:204:GLN:HA	1:M:204:GLN:NE2	2.33	0.40
2:I:197:HIS:CD2	2:I:200:THR:OG1	2.70	0.40
2:I:193:CYS:SG	2:I:206:LYS:HB3	2.61	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:L:465:HOH:O	5:M:454:HOH:O 4_455	2.15	0.05

## 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%)	204 (96%)	8 (4%)	0	100	100
1	M	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
2	H	225/227 (99%)	215 (96%)	7 (3%)	3 (1%)	12	11
2	I	225/227 (99%)	214 (95%)	11 (5%)	0	100	100
All	All	874/882 (99%)	838 (96%)	33 (4%)	3 (0%)	41	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	100(D)	GLY
2	H	132	PRO
2	H	100(E)	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%)	172 (95%)	9 (5%)	24	32
1	M	181/181 (100%)	176 (97%)	5 (3%)	43	57
2	H	187/187 (100%)	175 (94%)	12 (6%)	17	21
2	I	187/187 (100%)	183 (98%)	4 (2%)	53	68
All	All	736/736 (100%)	706 (96%)	30 (4%)	30	41

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	VAL
1	L	18	THR
1	L	45	LYS
1	L	58	VAL
1	L	63	LYS
1	L	96	ASN
1	L	114	THR
1	L	155	THR
1	L	204	GLN
2	H	2	GLN
2	H	23	THR
2	H	43	LYS
2	H	70	SER
2	H	100(B)	VAL
2	H	100(F)	THR
2	H	102	LEU
2	H	110	ILE
2	H	135	THR
2	H	137	THR
2	H	171	GLN
2	H	172	SER
1	M	18	THR
1	M	95(B)	ILE
1	M	96	ASN
1	M	114	THR
1	M	204	GLN
2	I	57	VAL
2	I	64	LYS
2	I	146	LEU
2	I	170	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	37	GLN
1	L	38	GLN
1	L	42	GLN
1	L	96	ASN
1	L	124	GLN
1	L	137	ASN
1	L	154	GLN
1	L	166	ASN
1	L	184	GLN

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Mol	Chain	Res	Type
1	L	204	GLN
2	H	2	GLN
2	H	32	ASN
2	H	39	GLN
2	H	115	GLN
2	H	161	ASN
2	H	194	ASN
2	H	197	HIS
1	M	24	GLN
1	M	38	GLN
1	M	42	GLN
1	M	96	ASN
1	M	137	ASN
1	M	166	ASN
1	M	184	GLN
1	M	204	GLN
2	I	39	GLN
2	I	96	ASN
2	I	115	GLN
2	I	171	GLN
2	I	189	GLN
2	I	194	ASN
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](#)

5 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	1PE	I	301	-	9,9,15	0.61	0	8,8,14	1.54	0
3	1PE	H	301	-	15,15,15	0.73	0	14,14,14	1.39	1 (7%)
3	1PE	I	302	-	9,9,15	0.53	0	8,8,14	1.67	1 (12%)
4	SO4	H	302	-	4,4,4	0.16	0	6,6,6	0.41	0
4	SO4	I	303	-	4,4,4	0.16	0	6,6,6	0.20	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	1PE	I	301	-	-	3/7/7/13	-
3	1PE	H	301	-	-	8/13/13/13	-
3	1PE	I	302	-	-	6/7/7/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	302	1PE	OH3-C22-C12	2.22	119.84	110.07
3	H	301	1PE	C25-OH5-C14	2.07	122.27	113.29

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	302	1PE	OH5-C14-C24-OH4
3	I	301	1PE	OH4-C13-C23-OH3
3	H	301	1PE	OH5-C14-C24-OH4
3	I	302	1PE	C23-C13-OH4-C24
3	I	302	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
3	H	301	1PE	OH2-C12-C22-OH3
3	I	301	1PE	C14-C24-OH4-C13
3	H	301	1PE	C14-C24-OH4-C13
3	H	301	1PE	C16-C26-OH6-C15
3	H	301	1PE	C13-C23-OH3-C22
3	I	302	1PE	C13-C23-OH3-C22
3	I	302	1PE	C12-C22-OH3-C23
3	H	301	1PE	C12-C22-OH3-C23
3	I	301	1PE	C13-C23-OH3-C22
3	I	302	1PE	C14-C24-OH4-C13
3	H	301	1PE	C15-C25-OH5-C14
3	H	301	1PE	OH4-C13-C23-OH3

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	301	1PE	2	0
3	H	301	1PE	2	0
3	I	302	1PE	2	0
4	H	302	SO4	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	L	214/214 (100%)	-0.28	2 (0%) 84 87	18, 30, 40, 53	0
1	M	214/214 (100%)	-0.31	1 (0%) 91 93	17, 27, 43, 57	0
2	H	227/227 (100%)	-0.13	15 (6%) 18 22	16, 23, 72, 91	0
2	I	227/227 (100%)	0.01	14 (6%) 20 25	16, 27, 66, 103	0
All	All	882/882 (100%)	-0.17	32 (3%) 42 48	16, 26, 52, 103	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	100(D)	GLY	10.2
2	I	100(B)	VAL	10.0
2	I	100(D)	GLY	8.5
2	H	100(C)	GLY	8.5
2	H	134	ALA	7.4
2	H	100(B)	VAL	5.5
2	I	100(C)	GLY	4.9
2	H	129	GLY	4.9
2	I	100(E)	GLY	4.8
2	I	100(F)	THR	4.7
2	H	188	SER	4.5
2	H	187	SER	4.3
2	H	132	PRO	4.2
2	H	131	THR	4.1
2	I	100(A)	GLY	3.9
2	H	186	SER	3.9
2	H	100(E)	GLY	3.6
2	I	100	VAL	3.5
2	I	187	SER	3.3
2	I	132	PRO	3.2
2	H	189	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
2	I	131	THR	3.1
2	H	185	THR	3.1
2	H	133	SER	3.0
2	I	100(G)	TYR	2.9
2	I	128	CYS	2.6
2	I	99	ALA	2.3
1	L	211	CYS	2.2
1	M	211	CYS	2.2
1	L	8	PRO	2.1
2	I	52(B)	GLY	2.1
2	H	135	THR	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	1PE	I	302	10/16	0.85	0.19	31,40,45,46	0
3	1PE	I	301	10/16	0.88	0.20	47,56,64,68	0
3	1PE	H	301	16/16	0.91	0.17	34,47,65,66	0
4	SO4	I	303	5/5	0.96	0.17	38,41,52,59	0
4	SO4	H	302	5/5	0.99	0.12	29,31,37,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.