



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 12:17 AM EDT

PDB ID : 3MLW  
Title : Crystal structure of anti-HIV-1 V3 Fab 1006-15D in complex with an MN V3 peptide  
Authors : Kong, X.-P.  
Deposited on : 2010-04-18  
Resolution : 2.70 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

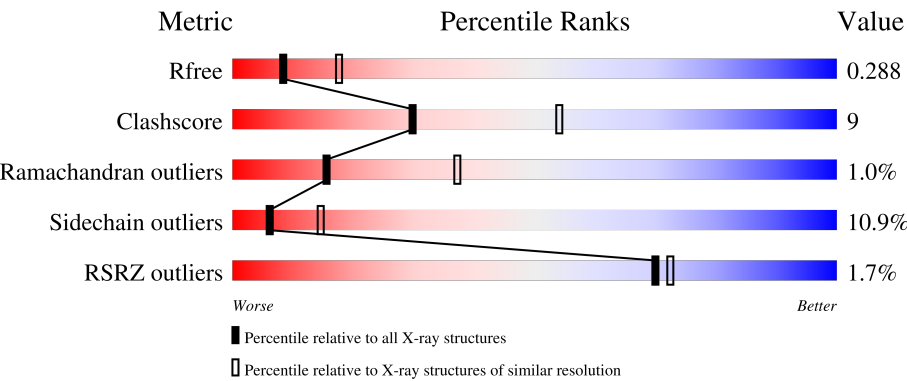
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	215	<div><div></div><div>78%19%.</div></div>
1	M	215	<div><div>5%</div><div>75%19%6%</div></div>
2	H	228	<div><div>%</div><div>75%23%.</div></div>
2	I	228	<div><div>%</div><div>82%16%.</div></div>
3	P	23	<div><div></div><div>43%30%26%</div></div>

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Mol	Chain	Length	Quality of chain
3	Q	23	<div><div></div><div>57%</div><div>9%</div><div>•</div><div>•</div><div>26%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7170 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 monoclonal anti-HIV-1 gp120 V3 antibody 1006-15D Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1621	1010	275	332	4			
1	M	215	Total	C	N	O	S	0	0	0
			1621	1010	275	332	4			

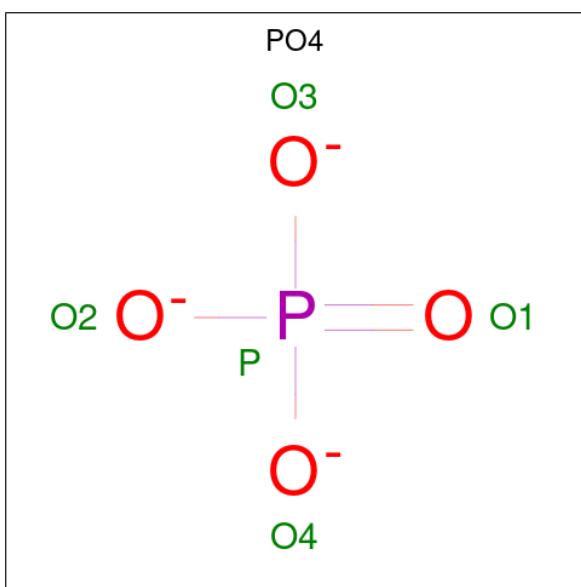
- Molecule 2 is a protein called Human monoclonal anti-HIV-1 gp120 V3 antibody 1006-15D Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	228	Total	C	N	O	S	0	0	0
			1726	1088	289	340	9			
2	I	228	Total	C	N	O	S	0	0	0
			1726	1088	289	340	9			

- Molecule 3 is a protein called HIV-1 gp120 third variable region (V3) crown.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	17	Total	C	N	O	0	0	0
			143	92	31	20			
3	Q	17	Total	C	N	O	0	0	0
			142	90	31	21			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		
4	M	1	Total	O	P	0	0
			5	4	1		
4	I	1	Total	O	P	0	0
			5	4	1		
4	I	1	Total	O	P	0	0
			5	4	1		

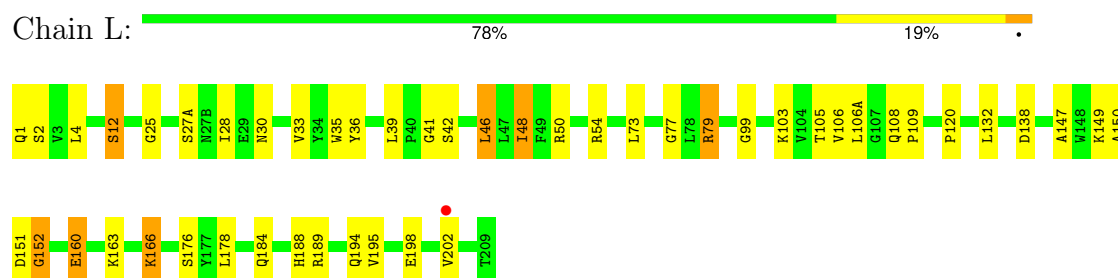
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	36	Total	O	0	0
			36	36		
5	H	53	Total	O	0	0
			53	53		
5	P	2	Total	O	0	0
			2	2		
5	M	24	Total	O	0	0
			24	24		
5	I	41	Total	O	0	0
			41	41		
5	Q	5	Total	O	0	0
			5	5		

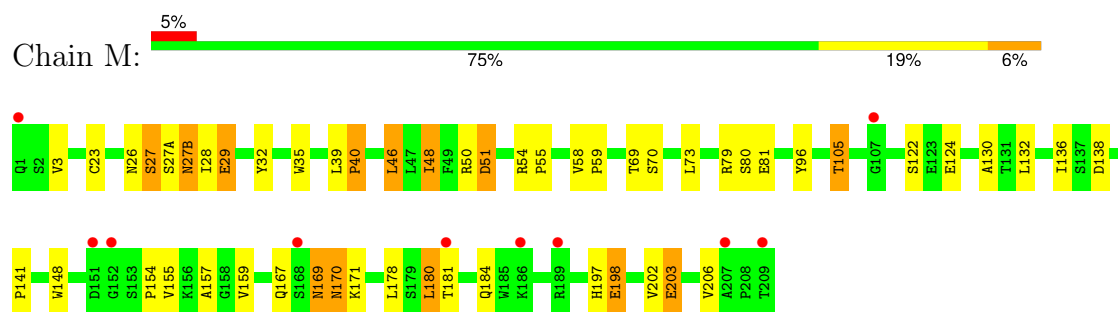
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

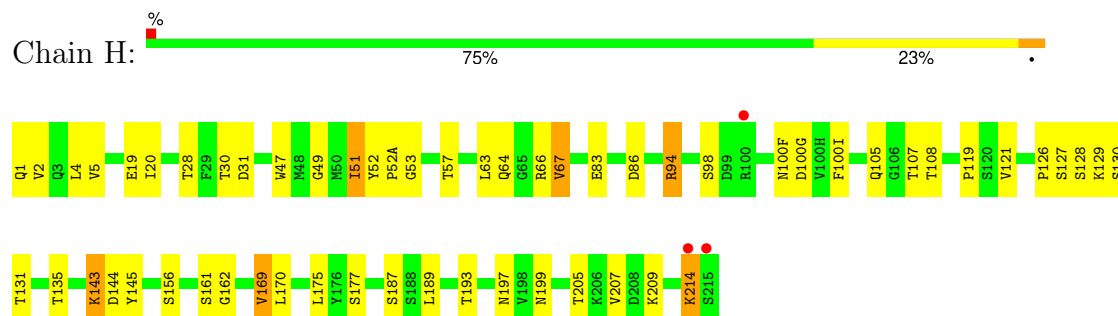
- Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody 1006-15D Fab light chain



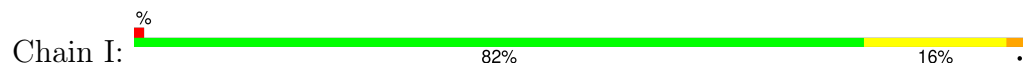
- Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody 1006-15D Fab light chain

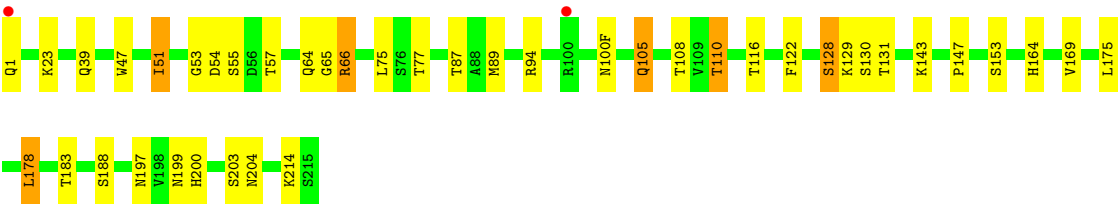


- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 1006-15D Fab heavy chain



- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 1006-15D Fab heavy chain

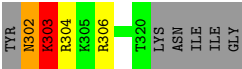




- Molecule 3: HIV-1 gp120 third variable region (V3) crown



- Molecule 3: HIV-1 gp120 third variable region (V3) crown



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.92Å 82.31Å 149.83Å 90.00° 110.35° 90.00°	Depositor
Resolution (Å)	42.27 – 2.70 42.27 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.3 (42.27-2.70) 93.3 (42.27-2.70)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0091	Depositor
R, $R_{free}$	0.214 , 0.291 0.212 , 0.288	Depositor DCC
$R_{free}$ test set	1473 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.1	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7170	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.47	0/1662	0.65	1/2269 (0.0%)
1	M	0.45	0/1662	0.59	0/2269
2	H	0.48	0/1771	0.64	0/2411
2	I	0.49	0/1771	0.62	0/2411
3	P	0.47	0/146	0.70	0/192
3	Q	0.47	0/145	0.68	0/192
All	All	0.47	0/7157	0.63	1/9744 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	46	LEU	CA-CB-CG	6.24	129.66	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	L	1621	0	1559	32	0
1	M	1621	0	1559	31	0
2	H	1726	0	1676	33	0
2	I	1726	0	1676	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	143	0	156	12	0
3	Q	142	0	149	5	0
4	H	10	0	0	1	0
4	I	10	0	0	0	0
4	L	5	0	0	1	0
4	M	5	0	0	0	0
5	H	53	0	0	2	0
5	I	41	0	0	4	0
5	L	36	0	0	0	0
5	M	24	0	0	0	0
5	P	2	0	0	0	0
5	Q	5	0	0	0	0
All	All	7170	0	6775	129	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 9.

All (129) 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:L:166:LYS:H	1:L:166:LYS:HD2	1.30	0.95
2:H:51:ILE:HG12	2:H:57:THR:HG22	1.50	0.93
2:I:105:GLN:HE21	2:I:105:GLN:H	1.08	0.93
2:I:105:GLN:H	2:I:105:GLN:NE2	1.77	0.82
3:Q:303:LYS:HG2	3:Q:304:ARG:H	1.43	0.81
1:M:27(B):ASN:HD22	1:M:28:ILE:H	1.26	0.81
2:H:100(F):ASN:HA	5:H:268:HOH:O	1.80	0.80
2:I:51:ILE:HG23	2:I:57:THR:HG22	1.65	0.77
1:L:50:ARG:NH1	2:H:100(G):ASP:OD1	2.18	0.76
2:H:156:SER:H	2:H:197:ASN:HD21	1.31	0.75
1:L:166:LYS:HD2	1:L:166:LYS:N	2.06	0.69
1:L:30:ASN:HB2	3:P:315:ARG:HH21	1.57	0.69
3:Q:303:LYS:CG	3:Q:304:ARG:H	2.06	0.68
2:I:105:GLN:HE21	2:I:105:GLN:N	1.88	0.68
1:L:108:GLN:HB2	1:L:109:PRO:HD2	1.76	0.68
2:H:127:SER:H	2:H:130:SER:HB3	1.59	0.66
1:L:30:ASN:HB2	3:P:315:ARG:NH2	2.10	0.66
2:H:2:VAL:HG11	2:H:94:ARG:NH2	2.12	0.64
3:P:303:LYS:HD2	3:P:304:ARG:HG2	1.80	0.64
2:H:20:ILE:HG21	2:H:107:THR:HG21	1.81	0.62
1:L:132:LEU:HD12	1:L:178:LEU:HD23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:48:ILE:HD11	1:M:73:LEU:HD13	1.83	0.61
2:H:30:THR:OG1	2:H:53:GLY:HA2	2.01	0.60
3:P:303:LYS:N	3:P:321:LYS:HG3	2.16	0.60
1:L:108:GLN:HB2	1:L:109:PRO:CD	2.32	0.59
3:Q:302:ASN:HD22	3:Q:302:ASN:N	2.01	0.59
2:I:51:ILE:CG2	2:I:57:THR:HG22	2.32	0.58
3:Q:303:LYS:HG2	3:Q:304:ARG:N	2.14	0.58
1:L:4:LEU:HB2	1:L:99:GLY:HA2	1.86	0.57
1:L:12:SER:HB2	1:L:198:GLU:OE1	2.04	0.57
2:I:23:LYS:HG3	2:I:77:THR:OG1	2.05	0.57
2:H:143:LYS:HE3	2:H:144:ASP:OD1	2.04	0.57
1:L:25:GLY:N	1:L:28:ILE:HD11	2.20	0.56
3:P:320:THR:O	3:P:320:THR:HG23	2.06	0.56
1:M:132:LEU:HD12	1:M:178:LEU:HD23	1.89	0.55
1:L:41:GLY:H	4:L:210:PO4:P	2.29	0.54
1:L:28:ILE:HG22	1:L:33:VAL:HG22	1.89	0.54
1:L:48:ILE:HD11	1:L:73:LEU:HD13	1.88	0.54
1:M:202:VAL:HG22	1:M:203:GLU:H	1.72	0.54
1:M:35:TRP:HB2	1:M:48:ILE:CG1	2.38	0.54
2:I:200:HIS:HD2	2:I:203:SER:HB3	1.73	0.53
1:L:79:ARG:O	1:L:106:VAL:HG21	2.09	0.53
1:M:27:SER:HA	1:M:29:GLU:HB2	1.90	0.53
1:M:202:VAL:HG22	1:M:203:GLU:N	2.23	0.53
1:L:151:ASP:OD2	1:L:189:ARG:HB2	2.09	0.52
2:I:64:GLN:HB3	2:I:66:ARG:HG2	1.91	0.52
2:I:188:SER:HB3	5:I:220:HOH:O	2.09	0.52
2:H:30:THR:HG1	2:H:53:GLY:HA2	1.74	0.52
1:M:169:ASN:O	1:M:171:LYS:N	2.43	0.52
1:M:169:ASN:H	1:M:169:ASN:HD22	1.56	0.52
1:L:28:ILE:HG22	1:L:33:VAL:CG2	2.40	0.52
1:L:30:ASN:CB	3:P:315:ARG:HH21	2.21	0.51
3:P:304:ARG:C	3:P:306:ARG:H	2.14	0.51
1:L:35:TRP:HB2	1:L:48:ILE:HG12	1.92	0.51
1:L:77:GLY:O	1:L:79:ARG:HG2	2.11	0.51
1:M:96:TYR:HB3	2:I:47:TRP:CG	2.47	0.50
2:I:200:HIS:HD2	2:I:203:SER:CB	2.24	0.50
1:M:26:ASN:HB3	1:M:27(A):SER:H	1.77	0.50
1:M:181:THR:H	1:M:184:GLN:HG3	1.78	0.49
2:H:30:THR:HA	2:H:52(A):PRO:HB2	1.94	0.49
2:I:147:PRO:O	2:I:200:HIS:HE1	1.96	0.49
2:I:51:ILE:HG23	2:I:57:THR:CG2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:155:VAL:HG22	1:M:157:ALA:H	1.78	0.48
2:H:209:LYS:HE3	5:H:254:HOH:O	2.12	0.48
1:M:105:THR:HG21	1:M:141:PRO:HB3	1.95	0.48
2:I:87:THR:HG23	2:I:110:THR:HA	1.94	0.48
2:H:52:TYR:CZ	3:P:305:LYS:HB2	2.48	0.48
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.95	0.47
1:M:181:THR:OG1	1:M:184:GLN:HG2	2.14	0.47
2:I:64:GLN:C	2:I:66:ARG:H	2.17	0.47
2:H:4:LEU:HD11	2:H:94:ARG:HB3	1.96	0.47
4:H:216:PO4:O3	3:P:304:ARG:NH1	2.47	0.47
1:M:138:ASP:HA	1:M:171:LYS:HB3	1.96	0.47
2:I:39:GLN:HA	5:I:258:HOH:O	2.13	0.47
2:I:100(F):ASN:ND2	5:I:225:HOH:O	2.47	0.47
2:I:51:ILE:CG2	2:I:57:THR:CG2	2.93	0.47
1:L:184:GLN:O	1:L:188:HIS:HD2	1.97	0.47
1:M:28:ILE:HD11	1:M:70:SER:HA	1.97	0.47
3:P:320:THR:HA	3:P:321:LYS:HA	1.67	0.46
2:I:128:SER:HA	2:I:131:THR:HG22	1.97	0.46
1:L:25:GLY:H	1:L:28:ILE:HD11	1.79	0.46
1:M:124:GLU:HG3	2:I:122:PHE:CE2	2.50	0.46
2:H:156:SER:N	2:H:197:ASN:HD21	2.07	0.46
1:L:166:LYS:N	1:L:166:LYS:CD	2.75	0.46
2:I:64:GLN:O	2:I:66:ARG:N	2.49	0.45
3:Q:303:LYS:CG	3:Q:304:ARG:N	2.78	0.45
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.48	0.45
1:L:120:PRO:HD3	1:L:132:LEU:HD23	1.98	0.45
1:M:39:LEU:O	1:M:40:PRO:C	2.55	0.45
1:M:46:LEU:HD13	1:M:55:PRO:HG3	1.99	0.44
1:L:147:ALA:O	1:L:194:GLN:HB3	2.17	0.44
1:L:35:TRP:HB2	1:L:48:ILE:CG1	2.47	0.44
1:M:148:TRP:CD1	1:M:159:VAL:HG12	2.52	0.44
2:H:63:LEU:HD22	2:H:67:VAL:HG13	1.99	0.44
2:I:178:LEU:C	2:I:178:LEU:HD12	2.38	0.44
1:M:197:HIS:O	1:M:198:GLU:C	2.56	0.44
2:I:55:SER:HB2	5:I:228:HOH:O	2.17	0.44
2:H:2:VAL:HG11	2:H:94:ARG:HH21	1.83	0.44
1:M:35:TRP:HB2	1:M:48:ILE:HG13	1.99	0.43
1:L:36:TYR:OH	2:H:100(I):PHE:HB2	2.18	0.43
3:P:320:THR:O	3:P:320:THR:CG2	2.66	0.43
1:L:166:LYS:H	1:L:166:LYS:CD	2.14	0.43
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:58:VAL:HA	1:M:59:PRO:HD3	1.87	0.42
1:M:35:TRP:CD1	1:M:48:ILE:HG13	2.55	0.42
1:L:150:ALA:O	1:L:152:GLY:N	2.48	0.42
2:H:121:VAL:HG13	2:H:207:VAL:HG11	2.02	0.42
2:H:143:LYS:HB2	2:H:177:SER:OG	2.20	0.42
1:L:160:GLU:HB2	2:H:169:VAL:HG22	2.01	0.42
2:H:28:THR:HB	2:H:31:ASP:OD1	2.20	0.42
2:I:153:SER:OG	2:I:197:ASN:HB2	2.19	0.42
1:M:130:ALA:HB3	1:M:180:LEU:O	2.20	0.42
2:H:63:LEU:HD22	2:H:67:VAL:CG1	2.50	0.41
1:M:23:CYS:HB2	1:M:35:TRP:CH2	2.54	0.41
2:I:200:HIS:CD2	2:I:203:SER:CB	3.03	0.41
2:H:127:SER:N	2:H:130:SER:HB3	2.32	0.41
2:I:54:ASP:N	2:I:54:ASP:OD1	2.52	0.41
1:L:160:GLU:HB2	2:H:169:VAL:CG2	2.50	0.41
1:M:32:TYR:CG	1:M:50:ARG:HG2	2.55	0.41
2:H:66:ARG:NH2	2:H:83:GLU:HG2	2.36	0.41
2:H:126:PRO:O	2:H:214:LYS:HE3	2.20	0.41
2:H:161:SER:HA	2:H:162:GLY:HA2	1.81	0.41
3:P:303:LYS:HD2	3:P:304:ARG:H	1.86	0.41
1:M:54:ARG:HD2	1:M:58:VAL:HG12	2.02	0.41
1:M:154:PRO:O	1:M:155:VAL:HB	2.21	0.41
1:L:120:PRO:HD3	1:L:132:LEU:CD2	2.51	0.40
2:H:64:GLN:NE2	2:H:66:ARG:HD3	2.36	0.40
2:H:127:SER:O	2:H:131:THR:HG22	2.21	0.40
1:M:167:GLN:HE21	2:I:164:HIS:CE1	2.39	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	213/215 (99%)	194 (91%)	17 (8%)	2 (1%)	17	40
1	M	213/215 (99%)	190 (89%)	19 (9%)	4 (2%)	8	20
2	H	226/228 (99%)	215 (95%)	11 (5%)	0	100	100
2	I	226/228 (99%)	213 (94%)	11 (5%)	2 (1%)	17	40
3	P	15/23 (65%)	14 (93%)	1 (7%)	0	100	100
3	Q	15/23 (65%)	14 (93%)	0	1 (7%)	1	1
All	All	908/932 (97%)	840 (92%)	59 (6%)	9 (1%)	15	37

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	40	PRO
1	L	2	SER
1	M	170	ASN
2	I	65	GLY
1	M	198	GLU
3	Q	303	LYS
1	M	51	ASP
1	L	152	GLY
2	I	53	GLY

### 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	L	183/183 (100%)	163 (89%)	20 (11%)	6	14
1	M	183/183 (100%)	164 (90%)	19 (10%)	7	16
2	H	194/194 (100%)	172 (89%)	22 (11%)	6	13
2	I	194/194 (100%)	173 (89%)	21 (11%)	6	15
3	P	14/19 (74%)	14 (100%)	0	100	100
3	Q	14/19 (74%)	11 (79%)	3 (21%)	1	3
All	All	782/792 (99%)	697 (89%)	85 (11%)	6	14

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	GLN
1	L	12	SER
1	L	27(A)	SER
1	L	39	LEU
1	L	42	SER
1	L	46	LEU
1	L	48	ILE
1	L	54	ARG
1	L	79	ARG
1	L	103	LYS
1	L	105	THR
1	L	106(A)	LEU
1	L	138	ASP
1	L	149	LYS
1	L	160	GLU
1	L	163	LYS
1	L	166	LYS
1	L	176	SER
1	L	195	VAL
1	L	202	VAL
2	H	1	GLN
2	H	5	VAL
2	H	19	GLU
2	H	51	ILE
2	H	67	VAL
2	H	94	ARG
2	H	98	SER
2	H	105	GLN
2	H	108	THR
2	H	128	SER
2	H	129	LYS
2	H	135	THR
2	H	143	LYS
2	H	169	VAL
2	H	170	LEU
2	H	175	LEU
2	H	187	SER
2	H	189	LEU
2	H	193	THR
2	H	199	ASN
2	H	205	THR
2	H	214	LYS

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Mol	Chain	Res	Type
1	M	3	VAL
1	M	27	SER
1	M	27(B)	ASN
1	M	29	GLU
1	M	46	LEU
1	M	48	ILE
1	M	51	ASP
1	M	69	THR
1	M	79	ARG
1	M	80	SER
1	M	81	GLU
1	M	105	THR
1	M	122	SER
1	M	136	ILE
1	M	169	ASN
1	M	170	ASN
1	M	180	LEU
1	M	203	GLU
1	M	206	VAL
2	I	1	GLN
2	I	51	ILE
2	I	66	ARG
2	I	75	LEU
2	I	89	MET
2	I	94	ARG
2	I	105	GLN
2	I	108	THR
2	I	110	THR
2	I	116	THR
2	I	128	SER
2	I	129	LYS
2	I	130	SER
2	I	143	LYS
2	I	169	VAL
2	I	175	LEU
2	I	178	LEU
2	I	183	THR
2	I	199	ASN
2	I	204	ASN
2	I	214	LYS
3	Q	302	ASN
3	Q	303	LYS

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Mol	Chain	Res	Type
3	Q	306	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	108	GLN
1	L	126	GLN
1	L	188	HIS
2	H	64	GLN
2	H	171	GLN
2	H	197	ASN
3	P	308	HIS
1	M	26	ASN
1	M	27(B)	ASN
1	M	167	GLN
1	M	169	ASN
1	M	170	ASN
1	M	194	GLN
2	I	1	GLN
2	I	32	HIS
2	I	81	GLN
2	I	96	HIS
2	I	101	HIS
2	I	105	GLN
2	I	200	HIS
3	Q	308	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 monosaccharides in this entry.

## 5.6 Ligand geometry

6 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	PO4	L	210	-	4,4,4	0.91	0	6,6,6	0.55	0
4	PO4	I	217	-	4,4,4	0.87	0	6,6,6	0.53	0
4	PO4	H	217	-	4,4,4	0.88	0	6,6,6	0.59	0
4	PO4	I	216	-	4,4,4	0.85	0	6,6,6	0.76	0
4	PO4	H	216	-	4,4,4	0.94	0	6,6,6	0.54	0
4	PO4	M	210	-	4,4,4	0.93	0	6,6,6	0.47	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	210	PO4	1	0
4	H	216	PO4	1	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

### 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	215/215 (100%)	-0.15	1 (0%) 91 92	30, 44, 54, 61	0
1	M	215/215 (100%)	0.32	10 (4%) 31 30	36, 54, 75, 78	0
2	H	228/228 (100%)	-0.18	3 (1%) 77 78	30, 42, 55, 69	0
2	I	228/228 (100%)	0.03	2 (0%) 84 85	32, 51, 64, 76	0
3	P	17/23 (73%)	-0.12	0 100 100	44, 48, 57, 58	0
3	Q	17/23 (73%)	0.02	0 100 100	46, 48, 55, 57	0
All	All	920/932 (98%)	0.00	16 (1%) 70 72	30, 47, 68, 78	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	152	GLY	4.1
1	M	168	SER	4.0
2	I	100	ARG	3.9
2	I	1	GLN	3.8
2	H	215	SER	3.6
1	M	186	LYS	3.5
1	M	209	THR	3.4
1	M	189	ARG	2.5
1	M	1	GLN	2.4
2	H	214	LYS	2.3
1	M	181	THR	2.2
1	M	107	GLY	2.2
1	M	151	ASP	2.1
1	M	207	ALA	2.1
2	H	100	ARG	2.1
1	L	202	VAL	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
4	PO4	M	210	5/5	0.89	0.23	94,95,95,95	0
4	PO4	L	210	5/5	0.91	0.18	112,112,112,112	0
4	PO4	I	216	5/5	0.91	0.15	75,76,76,76	0
4	PO4	I	217	5/5	0.94	0.11	79,80,80,80	0
4	PO4	H	217	5/5	0.95	0.18	84,85,85,85	0
4	PO4	H	216	5/5	0.95	0.17	93,93,93,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.