



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:39 AM GMT

PDB ID : 3MLV
Title : Crystal structure of anti-HIV-1 V3 Fab 2557 in complex with an NOF V3 peptide
Authors : Kong, X.-P.
Deposited on : 2010-04-18
Resolution : 2.48 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

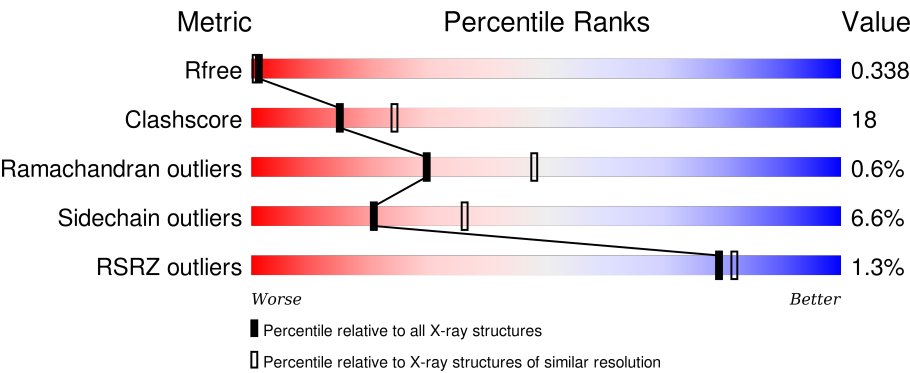
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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.



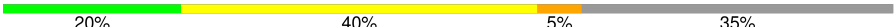
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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. 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 <=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	219	<div><div></div><div>73%24%.</div></div>
1	M	219	<div><div>%</div><div>71%27%.</div></div>
2	H	226	<div><div>3%</div><div>65%28%. .</div></div>
2	N	226	<div><div>%</div><div>61%32%5%. .</div></div>
3	P	20	<div><div>20%40%5%35%</div></div>

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Mol	Chain	Length	Quality of chain
3	Q	20	 A horizontal bar chart showing the quality of chain Q. The bar is divided into four segments: green (20%), yellow (40%), orange (5%), and grey (35%).

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7276 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 2557 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	218	Total	C	N	O	S	0	0	0
			1636	1030	268	333	5			
1	M	219	Total	C	N	O	S	0	0	0
			1642	1033	269	335	5			

- Molecule 2 is a protein called Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	1	0
			1679	1070	270	332	7			
2	N	221	Total	C	N	O	S	0	0	0
			1671	1065	269	331	6			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	0	0	0
			107	67	24	16			
3	Q	13	Total	C	N	O	0	0	0
			107	67	24	16			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	119	Total	O	0	0
			119	119		
4	H	76	Total	O	0	0
			76	76		
4	P	10	Total	O	0	0
			10	10		

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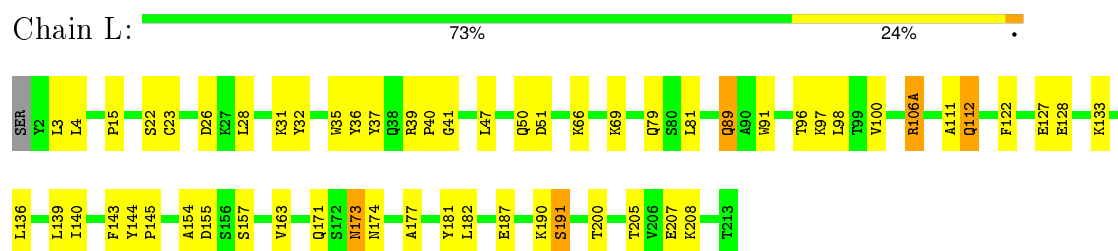
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	108	Total 108	O 108	0	0
4	N	113	Total 113	O 113	0	0
4	Q	8	Total 8	O 8	0	0

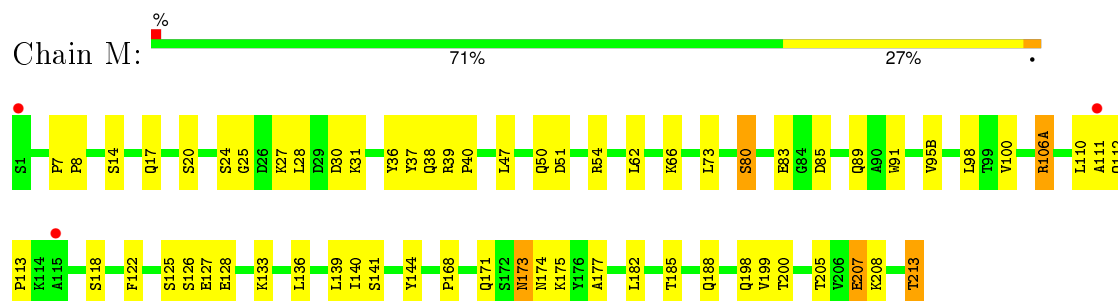
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

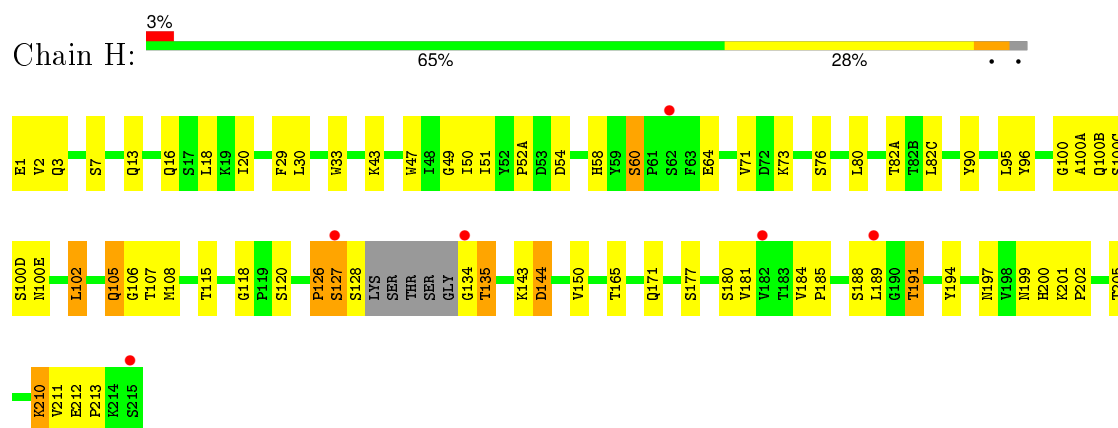
- Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab light chain



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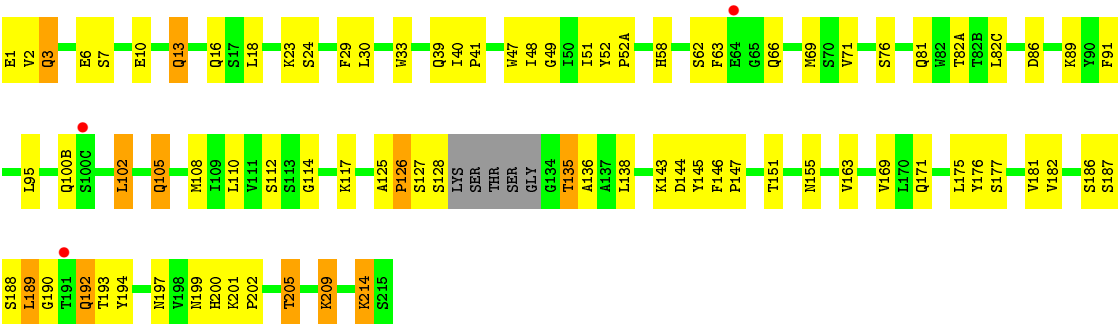


- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab heavy chain

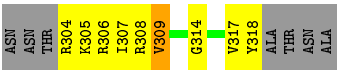
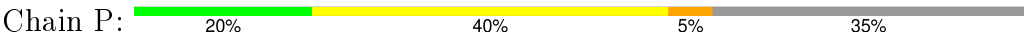


- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab heavy chain

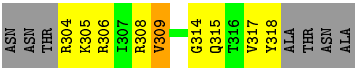
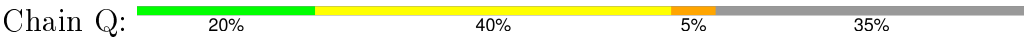




- Molecule 3: HIV-1 gp120 third variable region (V3) crown



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.55Å 42.74Å 116.06Å 87.91° 85.22° 85.97°	Depositor
Resolution (Å)	35.54 – 2.48 40.81 – 2.48	Depositor EDS
% Data completeness (in resolution range)	89.0 (35.54-2.48) 89.3 (40.81-2.48)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.233 , 0.342 0.227 , 0.338	Depositor DCC
R_{free} test set	1319 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.6	EDS
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 25771 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7276	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 83.42 % 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 2.1787e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.44	0/1676	0.60	0/2287
1	M	0.42	0/1682	0.59	0/2295
2	H	0.43	0/1722	0.62	0/2345
2	N	0.43	0/1714	0.60	0/2335
3	P	0.42	0/108	0.68	0/143
3	Q	0.45	0/108	0.68	0/143
All	All	0.43	0/7010	0.60	0/9548

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

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	1636	0	1602	58	0
1	M	1642	0	1610	52	0
2	H	1679	0	1636	64	0
2	N	1671	0	1628	66	0
3	P	107	0	117	11	0
3	Q	107	0	117	15	0
4	H	76	0	0	2	0
4	L	119	0	0	12	0
4	M	108	0	0	6	0
4	N	113	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	10	0	0	1	0
4	Q	8	0	0	1	0
All	All	7276	0	6710	238	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 18.

All (238) 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:139:LEU:HD13	2:H:181:VAL:HG11	1.42	1.01
1:M:139:LEU:HD13	2:N:181:VAL:HG21	1.45	0.96
2:N:24:SER:HB2	4:N:325:HOH:O	1.66	0.94
4:L:321:HOH:O	3:P:308:ARG:HD3	1.70	0.88
2:N:105:GLN:HE21	2:N:105:GLN:H	1.18	0.87
1:L:91:TRP:HB2	3:P:309:VAL:HG22	1.63	0.80
2:H:200:HIS:HB3	2:H:205:THR:HG22	1.64	0.80
2:H:135:THR:H	2:H:185:PRO:HA	1.47	0.80
2:N:105:GLN:NE2	2:N:105:GLN:H	1.80	0.79
1:M:91:TRP:HB2	3:Q:309:VAL:HG22	1.63	0.79
2:H:13:GLN:H	2:H:16:GLN:NE2	1.80	0.79
2:N:200:HIS:HB3	2:N:205:THR:HG22	1.64	0.78
2:H:135:THR:HA	2:H:184:VAL:O	1.84	0.77
1:L:3:LEU:HG	4:L:316:HOH:O	1.83	0.77
2:N:144:ASP:HA	2:N:176:TYR:O	1.86	0.75
1:M:85:ASP:OD1	1:M:106(A):ARG:HD3	1.87	0.75
1:M:111:ALA:HB3	4:M:268:HOH:O	1.87	0.74
1:M:171:GLN:HE21	1:M:173:ASN:HD21	1.36	0.74
1:M:139:LEU:HD13	2:N:181:VAL:CG2	2.18	0.73
1:L:139:LEU:CD1	2:H:181:VAL:HG11	2.18	0.73
2:N:114:GLY:HA3	4:N:284:HOH:O	1.90	0.72
1:L:36:TYR:HE1	1:L:89:GLN:HG2	1.54	0.72
1:L:106(A):ARG:HG2	1:L:106(A):ARG:HH11	1.56	0.71
2:N:18:LEU:HB2	2:N:82(C):LEU:HD11	1.73	0.70
3:P:306:ARG:HG3	4:P:323:HOH:O	1.89	0.70
2:H:194:TYR:H	2:H:210:LYS:HZ3	1.39	0.70
2:N:1:GLU:O	2:N:1:GLU:HG3	1.92	0.70
2:H:105:GLN:HE21	2:H:105:GLN:H	1.38	0.70
1:M:36:TYR:HE1	1:M:89:GLN:HG2	1.56	0.69
1:M:38:GLN:HE22	2:N:39:GLN:HE22	1.41	0.69
1:L:122:PHE:HE2	1:L:139:LEU:HD12	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:198:GLN:HG3	4:M:314:HOH:O	1.93	0.68
1:L:22:SER:HB3	4:L:219:HOH:O	1.92	0.68
1:L:15:PRO:HG3	4:L:354:HOH:O	1.92	0.67
1:M:37:TYR:HB2	1:M:47:LEU:HD11	1.76	0.67
1:L:37:TYR:HB2	1:L:47:LEU:HD11	1.77	0.66
1:L:79:GLN:HE21	1:L:81:LEU:HB2	1.60	0.65
2:H:51:ILE:HD13	2:H:71:VAL:HG13	1.78	0.65
1:M:38:GLN:HE22	2:N:39:GLN:NE2	1.95	0.64
1:M:31:LYS:HE3	3:Q:309:VAL:HG13	1.79	0.64
2:H:100:GLY:C	2:H:100(B):GLN:H	2.00	0.64
2:H:210:LYS:HD3	2:H:211:VAL:N	2.13	0.63
2:N:105:GLN:N	2:N:105:GLN:HE21	1.95	0.63
2:N:201:LYS:HA	4:N:225:HOH:O	1.98	0.63
2:N:66:GLN:NE2	2:N:86:ASP:OD1	2.31	0.63
1:L:91:TRP:HB2	3:P:309:VAL:CG2	2.28	0.63
2:H:105:GLN:NE2	2:H:105:GLN:H	1.95	0.63
2:N:2:VAL:HG12	2:N:102:LEU:HD11	1.79	0.63
2:H:210:LYS:NZ	2:H:211:VAL:O	2.31	0.62
2:H:2:VAL:HG12	2:H:102:LEU:HD11	1.81	0.61
3:Q:306:ARG:HG2	3:Q:318:TYR:O	1.99	0.61
2:N:143:LYS:HD2	2:N:177:SER:OG	2.00	0.61
1:M:122:PHE:HE2	1:M:139:LEU:HD12	1.66	0.61
2:H:108[A]:MET:HG3	4:H:438:HOH:O	2.00	0.61
1:M:125:SER:HB2	1:M:127:GLU:OE1	2.00	0.61
1:M:31:LYS:HE3	3:Q:309:VAL:CG1	2.31	0.61
2:H:194:TYR:H	2:H:210:LYS:NZ	1.98	0.60
2:H:30:LEU:HD22	2:H:73:LYS:HD2	1.84	0.60
2:H:134:GLY:HA2	2:H:135:THR:OG1	2.02	0.59
1:L:154:ALA:O	1:L:155:ASP:HB2	2.02	0.59
2:N:163:VAL:HG22	2:N:182:VAL:HG22	1.84	0.59
1:M:31:LYS:NZ	3:Q:315:GLN:HE22	2.00	0.59
2:H:127:SER:O	2:H:128:SER:HB2	2.02	0.59
1:M:171:GLN:HE21	1:M:173:ASN:ND2	2.01	0.58
1:L:171:GLN:HE21	1:L:173:ASN:ND2	2.02	0.58
3:Q:308:ARG:NH2	3:Q:314:GLY:H	2.01	0.57
1:L:106(A):ARG:NH1	1:L:106(A):ARG:HG2	2.19	0.57
1:L:4:LEU:HD22	1:L:28:LEU:HD11	1.86	0.57
1:L:51:ASP:OD1	1:L:66:LYS:HE2	2.05	0.57
1:L:79:GLN:NE2	1:L:81:LEU:HB2	2.19	0.57
1:M:31:LYS:HZ2	3:Q:315:GLN:HE22	1.50	0.56
2:N:23:LYS:HE2	4:N:234:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:171:GLN:HB2	1:L:173:ASN:ND2	2.19	0.56
1:L:97:LYS:HE2	4:L:330:HOH:O	2.04	0.56
1:M:38:GLN:NE2	2:N:39:GLN:HE22	2.03	0.56
2:N:47:TRP:CZ2	2:N:49:GLY:HA2	2.40	0.56
2:N:3:GLN:HA	2:N:102:LEU:HD21	1.88	0.56
2:H:135:THR:N	2:H:185:PRO:HA	2.20	0.56
2:N:209:LYS:HE3	4:N:247:HOH:O	2.05	0.56
1:L:171:GLN:HE21	1:L:173:ASN:HD21	1.53	0.55
1:M:50:GLN:NE2	2:N:100(B):GLN:O	2.37	0.55
2:N:81:GLN:HG2	4:N:223:HOH:O	2.06	0.55
1:L:36:TYR:CE1	1:L:89:GLN:HG2	2.38	0.55
3:Q:317:VAL:O	3:Q:318:TYR:HB2	2.07	0.55
1:M:185:THR:OG1	1:M:188:GLN:HG3	2.06	0.55
2:N:24:SER:HB3	2:N:76:SER:HB3	1.89	0.55
2:H:30:LEU:HA	2:H:52(A):PRO:HB2	1.87	0.55
3:Q:306:ARG:HA	3:Q:318:TYR:HB2	1.88	0.55
2:H:118:GLY:HA3	2:H:205:THR:HG21	1.89	0.54
2:H:3:GLN:HA	2:H:102:LEU:HD21	1.89	0.54
1:L:32:TYR:HB3	1:L:50:GLN:HA	1.88	0.54
1:L:111:ALA:HB3	4:L:253:HOH:O	2.08	0.54
1:M:98:LEU:HD21	3:Q:317:VAL:HG21	1.89	0.54
2:N:89:LYS:HB2	2:N:108:MET:SD	2.48	0.53
2:H:134:GLY:HA2	2:H:135:THR:O	2.08	0.53
2:N:155:ASN:HA	4:N:268:HOH:O	2.08	0.53
2:H:105:GLN:HE21	2:H:105:GLN:N	2.04	0.53
1:M:36:TYR:CE1	1:M:89:GLN:HG2	2.41	0.53
2:H:127:SER:O	2:H:128:SER:CB	2.56	0.53
1:L:100:VAL:HB	2:H:47:TRP:CG	2.44	0.52
2:H:73:LYS:HG3	4:H:227:HOH:O	2.09	0.52
3:P:317:VAL:O	3:P:318:TYR:HB2	2.09	0.52
2:H:13:GLN:H	2:H:16:GLN:HE21	1.57	0.52
1:L:4:LEU:HD21	1:L:28:LEU:HD21	1.91	0.52
2:N:189:LEU:HD23	2:N:190:GLY:N	2.24	0.52
1:M:91:TRP:CB	3:Q:309:VAL:HG22	2.36	0.52
2:H:150:VAL:HG12	2:H:200:HIS:CD2	2.45	0.52
1:M:112:GLN:HG3	1:M:144:TYR:CD2	2.45	0.51
2:H:200:HIS:HB3	2:H:205:THR:CG2	2.38	0.51
2:N:51:ILE:HB	2:N:69:MET:HE3	1.93	0.51
2:N:13:GLN:H	2:N:16:GLN:NE2	2.08	0.51
2:N:193:THR:HG23	4:N:378:HOH:O	2.09	0.51
2:N:125:ALA:HB3	2:N:214:LYS:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:110:LEU:HD11	4:N:406:HOH:O	2.10	0.50
2:H:126:PRO:HB3	2:H:189:LEU:HD12	1.93	0.50
1:M:140:ILE:HG12	1:M:199:VAL:HG21	1.93	0.50
1:L:190:LYS:HD3	1:L:190:LYS:O	2.12	0.49
2:N:40:ILE:HG23	2:N:41:PRO:HD2	1.94	0.49
2:H:210:LYS:C	2:H:210:LYS:HD3	2.33	0.49
2:N:117:LYS:HE2	4:N:261:HOH:O	2.11	0.49
2:H:13:GLN:N	2:H:16:GLN:NE2	2.56	0.49
1:L:187:GLU:O	1:L:191:SER:HB2	2.12	0.48
3:Q:308:ARG:HH22	3:Q:314:GLY:H	1.61	0.48
2:H:47:TRP:HE1	2:H:50:ILE:HG23	1.76	0.48
2:N:30:LEU:HA	2:N:52(A):PRO:HB2	1.95	0.48
2:H:30:LEU:HD21	2:H:73:LYS:HB3	1.96	0.48
2:H:13:GLN:N	2:H:16:GLN:HE21	2.12	0.48
1:L:39:ARG:NH2	1:L:81:LEU:O	2.42	0.48
1:M:80:SER:O	1:M:83:GLU:HG3	2.13	0.48
2:H:100:GLY:C	2:H:100(B):GLN:N	2.67	0.48
2:H:29:PHE:CD2	2:H:76:SER:HA	2.48	0.48
2:N:89:LYS:HE2	2:N:91:PHE:CZ	2.48	0.48
2:N:29:PHE:CD2	2:N:76:SER:HA	2.49	0.47
2:N:169:VAL:HG22	2:N:177:SER:O	2.14	0.47
2:N:143:LYS:HE3	2:N:171:GLN:OE1	2.14	0.47
1:L:173:ASN:N	1:L:173:ASN:HD22	2.12	0.47
2:N:33:TRP:HB2	2:N:95:LEU:HB3	1.95	0.47
2:N:201:LYS:N	2:N:202:PRO:CD	2.77	0.47
1:L:112:GLN:HG2	4:L:253:HOH:O	2.14	0.47
1:L:136:LEU:HD12	1:L:182:LEU:HD23	1.97	0.47
2:H:18:LEU:HB2	2:H:82(C):LEU:HD11	1.96	0.47
1:M:31:LYS:O	1:M:66:LYS:NZ	2.48	0.47
2:N:58:HIS:HA	4:N:328:HOH:O	2.14	0.47
1:M:110:LEU:HA	1:M:144:TYR:OH	2.16	0.46
2:N:33:TRP:CZ2	3:Q:305:LYS:HE3	2.50	0.46
1:L:128:GLU:HG2	1:L:133:LYS:HB2	1.97	0.46
2:N:145:TYR:N	2:N:145:TYR:CD2	2.76	0.46
2:N:18:LEU:CB	2:N:82(C):LEU:HD11	2.44	0.46
1:L:97:LYS:HD2	1:L:97:LYS:HA	1.71	0.46
1:M:175:LYS:HE3	4:M:282:HOH:O	2.16	0.46
1:M:198:GLN:HA	1:M:207:GLU:HB2	1.97	0.46
1:M:100:VAL:HB	2:N:47:TRP:CD1	2.50	0.46
1:M:208:LYS:HA	1:M:208:LYS:HD3	1.73	0.46
1:M:200:THR:OG1	1:M:205:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:144:TYR:CG	1:L:145:PRO:HA	2.51	0.46
2:H:143:LYS:HA	2:H:177:SER:HB2	1.98	0.46
2:N:151:THR:OG1	2:N:199:ASN:HB3	2.15	0.46
1:L:91:TRP:CB	3:P:309:VAL:CG2	2.94	0.45
1:L:98:LEU:CD1	3:P:307:ILE:HD12	2.46	0.45
2:H:199:ASN:ND2	2:H:201:LYS:HE3	2.32	0.45
2:H:212:GLU:HB2	2:H:213:PRO:HD2	1.98	0.45
2:N:192:GLN:HB3	2:N:194:TYR:CE2	2.51	0.45
1:L:127:GLU:HG3	4:L:254:HOH:O	2.17	0.45
1:L:41:GLY:HA3	4:L:270:HOH:O	2.17	0.45
1:L:106(A):ARG:CG	1:L:106(A):ARG:HH11	2.29	0.45
1:L:200:THR:OG1	1:L:205:THR:HG22	2.17	0.45
1:M:112:GLN:NE2	4:M:300:HOH:O	2.43	0.45
1:L:133:LYS:HD2	4:L:360:HOH:O	2.15	0.45
2:H:201:LYS:N	2:H:202:PRO:CD	2.79	0.45
1:L:26:ASP:O	1:L:69:LYS:HE2	2.17	0.45
2:H:143:LYS:HA	2:H:177:SER:CB	2.46	0.45
2:H:143:LYS:HG3	2:H:144:ASP:CG	2.38	0.45
1:M:54:ARG:HD3	1:M:62:LEU:O	2.17	0.45
2:N:66:GLN:HG3	4:N:254:HOH:O	2.16	0.44
1:L:143:PHE:CE1	1:L:177:ALA:HA	2.52	0.44
2:N:48:ILE:HA	2:N:63:PHE:CD2	2.51	0.44
2:N:125:ALA:CB	2:N:214:LYS:HG2	2.47	0.44
2:H:96:TYR:O	2:H:100(E):ASN:HA	2.18	0.44
2:H:165:THR:HA	2:H:180:SER:HA	2.00	0.44
1:L:97:LYS:HD2	2:H:58:HIS:ND1	2.33	0.44
1:L:31:LYS:HE3	3:P:309:VAL:HG13	2.00	0.44
2:N:138:LEU:HD12	2:N:138:LEU:C	2.38	0.44
1:M:95(B):VAL:HG12	4:M:216:HOH:O	2.17	0.44
1:L:98:LEU:HD21	3:P:317:VAL:HG21	1.99	0.44
1:M:112:GLN:HG3	1:M:144:TYR:CE2	2.53	0.44
1:M:31:LYS:NZ	3:Q:315:GLN:NE2	2.66	0.43
1:L:96:THR:HG23	4:L:256:HOH:O	2.17	0.43
2:N:6:GLU:H	2:N:105:GLN:HE22	1.67	0.43
2:N:127:SER:O	2:N:128:SER:C	2.56	0.43
1:M:136:LEU:HD12	1:M:182:LEU:HD23	1.99	0.43
2:H:90:TYR:O	2:H:106:GLY:HA2	2.17	0.43
1:L:100:VAL:HB	2:H:47:TRP:CD2	2.53	0.43
2:N:66:GLN:HG2	2:N:66:GLN:O	2.18	0.43
2:H:189:LEU:O	2:H:189:LEU:HD23	2.18	0.43
2:H:7:SER:O	2:H:107:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:25:GLY:HA3	1:M:28:LEU:HG	2.01	0.43
1:M:27:LYS:O	1:M:31:LYS:HB2	2.17	0.43
2:H:80:LEU:HA	2:H:80:LEU:HD12	1.83	0.43
1:L:39:ARG:HG3	1:L:40:PRO:HD2	2.00	0.43
2:H:33:TRP:HB2	2:H:95:LEU:HB3	2.02	0.42
1:M:14:SER:HB2	1:M:17:GLN:NE2	2.33	0.42
2:H:188:SER:O	2:H:191:THR:HG23	2.18	0.42
1:M:62:LEU:HD11	1:M:73:LEU:HD11	2.01	0.42
1:L:171:GLN:OE1	1:L:177:ALA:HB2	2.19	0.42
2:N:188:SER:O	2:N:192:GLN:N	2.38	0.42
2:N:144:ASP:HB2	2:N:175:LEU:CB	2.49	0.42
2:N:126:PRO:HB3	2:N:189:LEU:HD12	2.01	0.42
2:N:51:ILE:HD13	2:N:71:VAL:HG13	2.00	0.42
2:H:143:LYS:O	2:H:144:ASP:HB2	2.20	0.42
1:M:39:ARG:O	1:M:40:PRO:C	2.57	0.42
1:L:31:LYS:O	1:L:66:LYS:NZ	2.52	0.42
2:H:144:ASP:OD1	2:H:171:GLN:NE2	2.37	0.42
2:H:100(A):ALA:O	2:H:100(B):GLN:HG2	2.20	0.42
2:H:47:TRP:CE3	2:H:60:SER:HB3	2.55	0.42
1:M:128:GLU:HG2	1:M:133:LYS:HB2	2.01	0.42
1:M:213:THR:C	4:M:339:HOH:O	2.59	0.42
1:M:168:PRO:HA	1:M:177:ALA:O	2.20	0.42
3:Q:304:ARG:N	4:Q:327:HOH:O	2.53	0.42
2:N:186:SER:O	2:N:189:LEU:HD22	2.20	0.41
1:L:140:ILE:O	1:L:177:ALA:HA	2.20	0.41
1:M:112:GLN:HB2	1:M:113:PRO:CD	2.51	0.41
1:M:118:SER:HB2	1:M:141:SER:OG	2.20	0.41
2:N:135:THR:HB	2:N:136:ALA:H	1.70	0.41
1:M:7:PRO:HA	1:M:8:PRO:HD3	1.86	0.41
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.55	0.41
1:L:97:LYS:CE	4:L:310:HOH:O	2.68	0.41
1:L:23:CYS:HB2	1:L:35:TRP:CH2	2.55	0.41
1:L:122:PHE:HE2	1:L:139:LEU:CD1	2.30	0.41
3:P:308:ARG:HH22	3:P:314:GLY:HA2	1.86	0.41
2:N:192:GLN:NE2	2:N:193:THR:H	2.19	0.41
2:H:54:ASP:OD1	3:P:305:LYS:NZ	2.51	0.41
1:L:208:LYS:HD3	1:L:208:LYS:HA	1.87	0.41
2:H:100(C):SER:O	2:H:100(D):SER:HB3	2.21	0.41
1:L:163:VAL:HA	1:L:181:TYR:O	2.21	0.41
2:H:3:GLN:HB2	2:H:3:GLN:HE21	1.64	0.40
1:M:50:GLN:O	1:M:51:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:33:TRP:CH2	2:N:52:TYR:HB2	2.56	0.40
2:N:146:PHE:HA	2:N:147:PRO:HA	1.91	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	L	216/219 (99%)	210 (97%)	6 (3%)	0	100	100
1	M	217/219 (99%)	211 (97%)	6 (3%)	0	100	100
2	H	218/226 (96%)	206 (94%)	9 (4%)	3 (1%)	14	22
2	N	217/226 (96%)	206 (95%)	9 (4%)	2 (1%)	21	36
3	P	11/20 (55%)	10 (91%)	1 (9%)	0	100	100
3	Q	11/20 (55%)	11 (100%)	0	0	100	100
All	All	890/930 (96%)	854 (96%)	31 (4%)	5 (1%)	30	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	126	PRO
2	H	135	THR
2	H	144	ASP
2	H	126	PRO
2	N	214	LYS

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	185/186 (100%)	177 (96%)	8 (4%)	35	59
1	M	186/186 (100%)	176 (95%)	10 (5%)	27	47
2	H	191/194 (98%)	177 (93%)	14 (7%)	17	31
2	N	190/194 (98%)	174 (92%)	16 (8%)	14	24
3	P	11/16 (69%)	9 (82%)	2 (18%)	2	3
3	Q	11/16 (69%)	10 (91%)	1 (9%)	12	20
All	All	774/792 (98%)	723 (93%)	51 (7%)	21	36

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	89	GLN
1	L	106(A)	ARG
1	L	112	GLN
1	L	157	SER
1	L	173	ASN
1	L	174	ASN
1	L	191	SER
1	L	207	GLU
2	H	1	GLU
2	H	20	ILE
2	H	43	LYS
2	H	60	SER
2	H	64	GLU
2	H	82(A)	THR
2	H	102	LEU
2	H	105	GLN
2	H	115	THR
2	H	120	SER
2	H	127	SER
2	H	191	THR
2	H	197	ASN
2	H	210	LYS
3	P	304	ARG
3	P	309	VAL
1	M	20	SER
1	M	24	SER

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Mol	Chain	Res	Type
1	M	30	ASP
1	M	80	SER
1	M	106(A)	ARG
1	M	126	SER
1	M	173	ASN
1	M	174	ASN
1	M	207	GLU
1	M	213	THR
2	N	3	GLN
2	N	7	SER
2	N	10	GLU
2	N	13	GLN
2	N	62	SER
2	N	82(A)	THR
2	N	102	LEU
2	N	105	GLN
2	N	112	SER
2	N	135	THR
2	N	187	SER
2	N	189	LEU
2	N	192	GLN
2	N	197	ASN
2	N	205	THR
2	N	209	LYS
3	Q	309	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	79	GLN
1	L	89	GLN
1	L	112	GLN
1	L	173	ASN
2	H	3	GLN
2	H	16	GLN
2	H	83	GLN
2	H	105	GLN
1	M	17	GLN
1	M	112	GLN
1	M	173	ASN
1	M	174	ASN
1	M	201	HIS

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Mol	Chain	Res	Type
2	N	16	GLN
2	N	39	GLN
2	N	105	GLN
2	N	192	GLN
3	Q	315	GLN

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](#)

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 [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	218/219 (99%)	-0.24	0 100 100	10, 18, 26, 44	0
1	M	219/219 (100%)	-0.24	3 (1%) 78 80	10, 18, 26, 48	0
2	H	221/226 (97%)	-0.07	6 (2%) 58 61	10, 19, 45, 60	0
2	N	221/226 (97%)	-0.07	3 (1%) 78 80	11, 20, 39, 63	0
3	P	13/20 (65%)	-0.29	0 100 100	16, 22, 29, 39	0
3	Q	13/20 (65%)	-0.06	0 100 100	18, 21, 40, 41	0
All	All	905/930 (97%)	-0.15	12 (1%) 79 82	10, 19, 36, 63	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	100(C)	SER	5.1
2	H	189	LEU	4.0
1	M	1	SER	3.7
1	M	111	ALA	2.9
2	H	127	SER	2.7
2	N	64	GLU	2.4
2	H	134	GLY	2.2
2	H	182	VAL	2.2
2	H	215	SER	2.2
2	H	62	SER	2.1
1	M	115	ALA	2.1
2	N	191	THR	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.