



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:38 PM UTC

PDB ID : 3MLV / pdb_00003mlv
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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

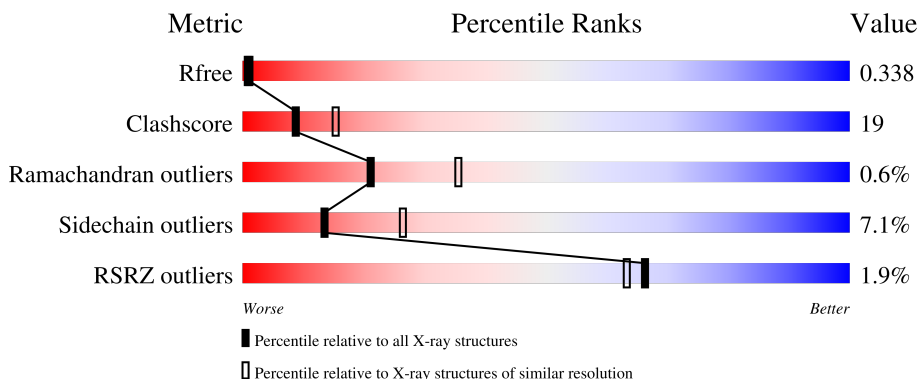
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (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 of 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	219	71% 26% .
1	M	219	0% 70% 27% .
2	H	226	3% 64% 29% 5% .
2	N	226	4% 58% 34% 6% .
3	P	20	15% 40% 10% 35%

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Mol	Chain	Length	Quality of chain
3	Q	20	 20% 35% 10% 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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O			
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
			Total	O		
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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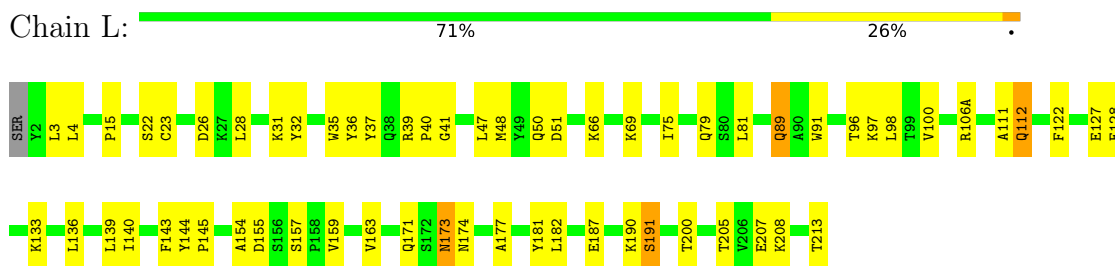
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	108	Total 108	O 108	0	0
4	N	113	Total 113	O 113	0	0
4	Q	8	Total 8	O 8	0	0

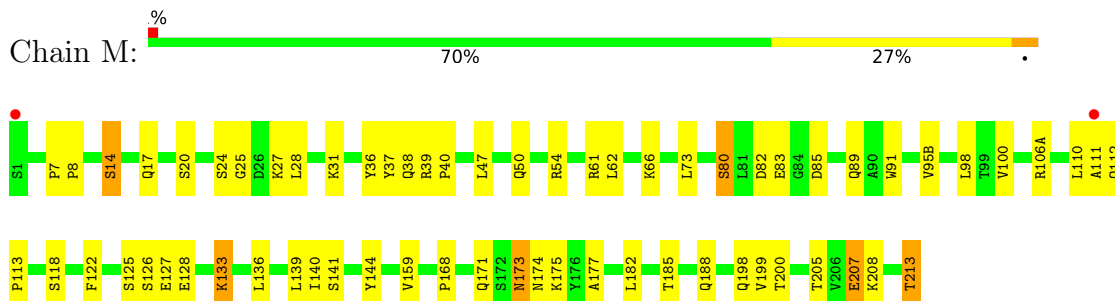
3 Residue-property plots [i](#)

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.

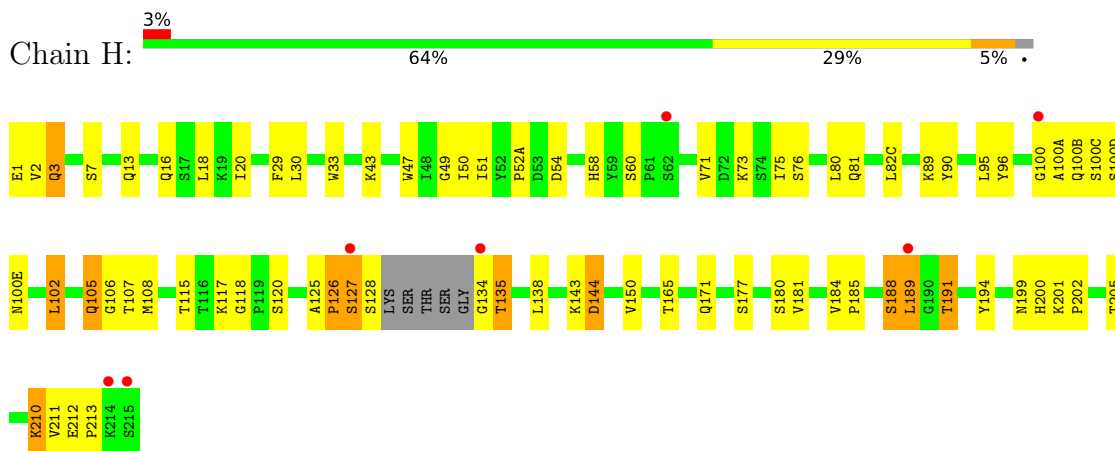
- Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab light chain



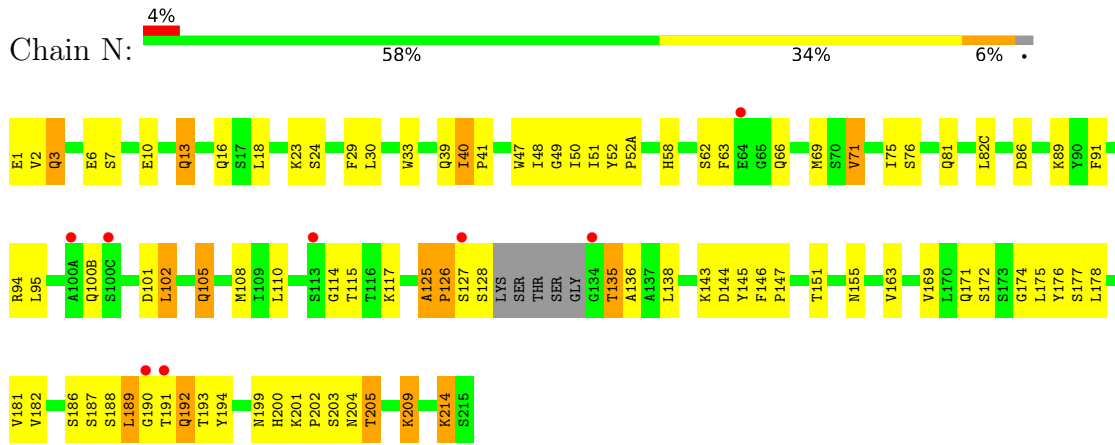
- Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab light chain



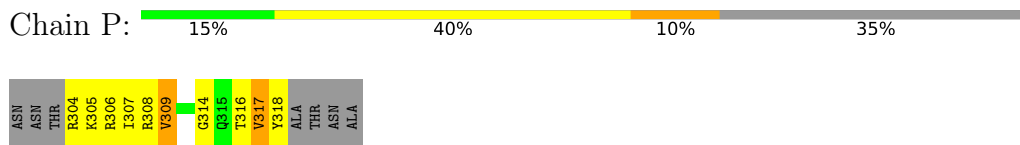
- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab heavy chain



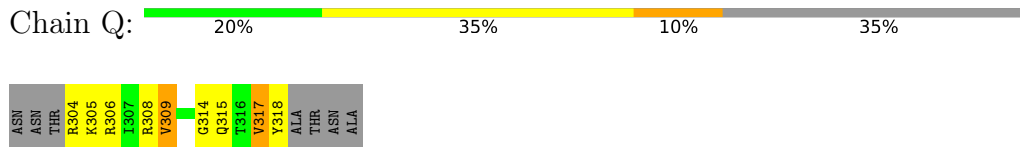
- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab heavy chain



• 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 i

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 35.54 – 2.48	Depositor EDS
% Data completeness (in resolution range)	89.0 (35.54-2.48) 89.4 (35.54-2.48)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.48Å)	Xtrriage
Refinement program	PHENIX 1.6.1_357, REFMAC 5.2.0019	Depositor
R, R_{free}	0.233 , 0.342 0.229 , 0.338	Depositor DCC
R_{free} test set	1322 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtrriage
Anisotropy	0.277	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtrriage
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

Xtrriage'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.*

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](#)

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	0.53	0/1676	0.84	0/2287
1	M	0.52	0/1682	0.86	2/2295 (0.1%)
2	H	0.52	0/1722	0.93	6/2345 (0.3%)
2	N	0.53	0/1714	0.88	2/2335 (0.1%)
3	P	0.44	0/108	1.00	0/143
3	Q	0.63	0/108	1.03	0/143
All	All	0.53	0/7010	0.88	10/9548 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	125	ALA	CA-C-N	6.58	128.06	119.84
2	N	125	ALA	C-N-CA	6.58	128.06	119.84
2	H	117	LYS	N-CA-C	5.91	117.51	108.52
2	H	125	ALA	CA-C-N	5.78	127.07	119.84
2	H	125	ALA	C-N-CA	5.78	127.07	119.84
2	H	3	GLN	N-CA-C	5.72	117.23	108.42
2	H	125	ALA	N-CA-C	5.38	116.47	109.64
2	H	81	GLN	N-CA-C	5.34	118.14	109.06
1	M	14	SER	CA-C-N	5.01	126.11	119.84
1	M	14	SER	C-N-CA	5.01	126.11	119.84

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	1636	0	1602	60	0
1	M	1642	0	1610	53	0
2	H	1679	0	1636	70	0
2	N	1671	0	1628	72	0
3	P	107	0	117	12	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
4	P	10	0	0	1	0
4	Q	8	0	0	1	0
All	All	7276	0	6710	254	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 19.

All (254) 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:H	2:N:105:GLN:NE2	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:50:ILE:O	2:N:69:MET:HE1	1.87	0.75
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:P:306:ARG:HG3	4:P:323:HOH:O	1.89	0.70
2:N:18:LEU:HB2	2:N:82(C):LEU:HD11	1.73	0.70
2:H:194:TYR:H	2:H:210:LYS:HZ3	1.39	0.70
2:N:1:GLU:HG3	2:N:1:GLU:O	1.92	0.70
2:H:105:GLN:H	2:H:105:GLN:HE21	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
2:H:100:GLY:C	2:H:100(B):GLN:H	2.00	0.68
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:210:LYS:HD3	2:H:211:VAL:N	2.13	0.63
2:N:105:GLN:HE21	2:N:105:GLN:N	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:H	2:H:105:GLN:NE2	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
2:H:108[A]:MET:HG3	4:H:438:HOH:O	2.00	0.61
1:M:122:PHE:HE2	1:M:139:LEU:HD12	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	1:L:106(A):ARG:NH1	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
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
1:M:185:THR:OG1	1:M:188:GLN:HG3	2.06	0.55
3:Q:317:VAL:O	3:Q:318:TYR:HB2	2.07	0.55
2:H:30:LEU:HA	2:H:52(A):PRO:HB2	1.87	0.55
2:N:24:SER:HB3	2:N:76:SER:HB3	1.89	0.55
2:H:89:LYS:NZ	2:H:108[B]:MET:HE2	2.22	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
2:H:210:LYS:HD3	2:H:210:LYS:C	2.33	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
2:H:127:SER:O	2:H:128:SER:CB	2.56	0.53
1:M:36:TYR:CE1	1:M:89:GLN:HG2	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:100:GLY:C	2:H:100(B):GLN:N	2.67	0.52
1:M:112:GLN:HG3	1:M:144:TYR:CD2	2.45	0.51
2:H:89:LYS:HD2	2:H:108[B]:MET:HE2	1.92	0.51
2:H:200:HIS:HB3	2:H:205:THR:CG2	2.38	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
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:N:117:LYS:HE2	4:N:261:HOH:O	2.11	0.49
2:H:143:LYS:HG3	2:H:144:ASP:CG	2.38	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
2:N:138:LEU:C	2:N:138:LEU:HD12	2.38	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:N:127:SER:O	2:N:128:SER:C	2.56	0.48
2:H:30:LEU:HD21	2:H:73:LYS:HB3	1.96	0.48
1:L:39:ARG:NH2	1:L:81:LEU:O	2.42	0.48
2:H:13:GLN:N	2:H:16:GLN:HE21	2.12	0.48
1:M:80:SER:O	1:M:83:GLU:HG3	2.13	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:H:89:LYS:HZ3	2:H:108[B]:MET:HE2	1.78	0.47
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
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:143:LYS:HE3	2:N:171:GLN:OE1	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:213:THR:C	4:M:339:HOH:O	2.59	0.46
1:L:128:GLU:HG2	1:L:133:LYS:HB2	1.97	0.46
2:N:33:TRP:CZ2	3:Q:305:LYS:HE3	2.50	0.46
2:N:145:TYR:CD2	2:N:145:TYR:N	2.76	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
2:N:18:LEU:CB	2:N:82(C):LEU:HD11	2.44	0.46
1:M:39:ARG:O	1:M:40:PRO:C	2.57	0.46
1:M:100:VAL:HB	2:N:47:TRP:CD1	2.50	0.46
1:M:198:GLN:HA	1:M:207:GLU:HB2	1.97	0.46
1:M:200:THR:OG1	1:M:205:THR:HG22	2.15	0.46
1:M:208:LYS:HA	1:M:208:LYS:HD3	1.73	0.46
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
1:L:127:GLU:HG3	4:L:254:HOH:O	2.17	0.45
2:N:192:GLN:HB3	2:N:194:TYR:CE2	2.51	0.45
1:L:41:GLY:HA3	4:L:270:HOH:O	2.17	0.45
1:L:106(A):ARG:HH11	1:L:106(A):ARG:CG	2.29	0.45
1:L:200:THR:OG1	1:L:205:THR:HG22	2.17	0.45
1:L:133:LYS:HD2	4:L:360:HOH:O	2.15	0.45
1:M:112:GLN:NE2	4:M:300:HOH:O	2.43	0.45
1:L:26:ASP:O	1:L:69:LYS:HE2	2.17	0.45
2:H:201:LYS:N	2:H:202:PRO:CD	2.79	0.45
2:H:143:LYS:HA	2:H:177:SER:CB	2.46	0.45
2:H:189:LEU:HD23	2:H:189:LEU:C	2.42	0.45
1:M:54:ARG:HD3	1:M:62:LEU:O	2.17	0.45
1:L:143:PHE:CE1	1:L:177:ALA:HA	2.52	0.44
1:L:190:LYS:HD3	1:L:190:LYS:C	2.41	0.44
2:N:66:GLN:HG3	4:N:254:HOH:O	2.16	0.44
2:N:203:SER:O	2:N:204:ASN:C	2.58	0.44
2:N:48:ILE:HA	2:N:63:PHE:CD2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:96:TYR:O	2:H:100(E):ASN:HA	2.18	0.44
2:H:138:LEU:HD12	2:H:138:LEU:C	2.41	0.44
2:H:165:THR:HA	2:H:180:SER:HA	2.00	0.44
2:N:125:ALA:CB	2:N:214:LYS:HG2	2.47	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
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
2:H:54:ASP:OD1	3:P:305:LYS:NZ	2.51	0.44
1:L:96:THR:HG23	4:L:256:HOH:O	2.17	0.43
1:M:31:LYS:NZ	3:Q:315:GLN:NE2	2.66	0.43
1:M:61:ARG:HH22	1:M:82:ASP:CG	2.26	0.43
1:M:136:LEU:HD12	1:M:182:LEU:HD23	1.99	0.43
2:N:6:GLU:H	2:N:105:GLN:HE22	1.67	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:H:7:SER:O	2:H:107:THR:HG23	2.18	0.43
2:H:189:LEU:HD23	2:H:189:LEU:O	2.18	0.43
1:M:25:GLY:HA3	1:M:28:LEU:HG	2.01	0.43
2:N:66:GLN:HG2	2:N:66:GLN:O	2.18	0.43
1:M:27:LYS:O	1:M:31:LYS:HB2	2.17	0.43
2:H:80:LEU:HD12	2:H:80:LEU:HA	1.83	0.43
2:N:33:TRP:CE3	2:N:51:ILE:C	2.97	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
2:H:188:SER:O	2:H:191:THR:HG23	2.18	0.42
1:M:14:SER:HB2	1:M:17:GLN:NE2	2.33	0.42
1:M:133:LYS:HZ2	1:M:133:LYS:HB3	1.85	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:51:ILE:HD13	2:N:71:VAL:HG13	2.00	0.42
2:N:126:PRO:HB3	2:N:189:LEU:HD12	2.01	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:75:ILE:O	2:H:76:SER:C	2.63	0.42
2:N:172:SER:C	2:N:174:GLY:N	2.75	0.42
2:H:47:TRP:CE3	2:H:60:SER:HB3	2.55	0.42
2:H:100(A):ALA:O	2:H:100(B):GLN:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:128:GLU:HG2	1:M:133:LYS:HB2	2.01	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:94:ARG:HH21	2:N:101:ASP:CG	2.28	0.41
2:N:186:SER:O	2:N:189:LEU:HD22	2.20	0.41
2:H:143:LYS:O	2:H:144:ASP:HB2	2.20	0.41
2:N:178:LEU:C	2:N:178:LEU:HD12	2.45	0.41
1:L:140:ILE:O	1:L:177:ALA:HA	2.20	0.41
1:M:7:PRO:HA	1:M:8:PRO:HD3	1.86	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
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.55	0.41
1:L:23:CYS:HB2	1:L:35:TRP:CH2	2.55	0.41
1:L:48:MET:HE2	1:L:48:MET:HB2	1.94	0.41
1:L:97:LYS:CE	4:L:310:HOH:O	2.68	0.41
1:L:122:PHE:HE2	1:L:139:LEU:CD1	2.30	0.41
1:L:163:VAL:HA	1:L:181:TYR:O	2.21	0.41
1:L:208:LYS:HA	1:L:208:LYS:HD3	1.87	0.41
2:H:100(C):SER:O	2:H:100(D):SER:HB3	2.21	0.41
3:P:305:LYS:O	3:P:306:ARG:C	2.63	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:3:GLN:HE21	2:H:3:GLN:HB2	1.64	0.40
2:N:75:ILE:O	2:N:76:SER:C	2.63	0.40
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%)	9	15
2	N	217/226 (96%)	206 (95%)	9 (4%)	2 (1%)	14	25
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%)	21	35

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%)	175 (95%)	10 (5%)	20	38
1	M	186/186 (100%)	176 (95%)	10 (5%)	20	38
2	H	191/194 (98%)	179 (94%)	12 (6%)	16	31
2	N	190/194 (98%)	173 (91%)	17 (9%)	9	18
3	P	11/16 (69%)	7 (64%)	4 (36%)	0	0
3	Q	11/16 (69%)	9 (82%)	2 (18%)	2	3
All	All	774/792 (98%)	719 (93%)	55 (7%)	13	26

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	75	ILE
1	L	89	GLN
1	L	112	GLN
1	L	157	SER
1	L	159	VAL
1	L	173	ASN
1	L	174	ASN
1	L	191	SER
1	L	207	GLU
1	L	213	THR
2	H	1	GLU
2	H	20	ILE
2	H	43	LYS
2	H	102	LEU
2	H	105	GLN
2	H	115	THR
2	H	120	SER
2	H	127	SER
2	H	188	SER
2	H	189	LEU
2	H	191	THR
2	H	210	LYS
3	P	304	ARG
3	P	309	VAL
3	P	316	THR
3	P	317	VAL
1	M	20	SER
1	M	24	SER
1	M	80	SER
1	M	126	SER
1	M	133	LYS
1	M	159	VAL
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	40	ILE
2	N	62	SER
2	N	71	VAL

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Mol	Chain	Res	Type
2	N	102	LEU
2	N	105	GLN
2	N	115	THR
2	N	135	THR
2	N	187	SER
2	N	189	LEU
2	N	191	THR
2	N	192	GLN
2	N	205	THR
2	N	209	LYS
3	Q	309	VAL
3	Q	317	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) 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
1	L	174	ASN
1	L	201	HIS
2	H	3	GLN
2	H	16	GLN
2	H	81	GLN
2	H	105	GLN
2	H	199	ASN
1	M	17	GLN
1	M	38	GLN
1	M	42	GLN
1	M	112	GLN
1	M	173	ASN
1	M	174	ASN
1	M	201	HIS
2	N	3	GLN
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 oligosaccharides 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%)	-0.13	0 100 100	10, 18, 26, 44	0
1	M	219/219 (100%)	-0.11	2 (0%) 81 79	10, 18, 26, 48	0
2	H	221/226 (97%)	0.03	7 (3%) 50 47	9, 19, 45, 60	1 (0%)
2	N	221/226 (97%)	0.07	8 (3%) 46 42	11, 20, 39, 63	0
3	P	13/20 (65%)	0.05	0 100 100	16, 22, 29, 39	0
3	Q	13/20 (65%)	0.31	0 100 100	18, 21, 40, 41	0
All	All	905/930 (97%)	-0.03	17 (1%) 66 63	9, 19, 36, 63	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	100(C)	SER	5.4
2	H	215	SER	3.7
1	M	1	SER	3.6
2	N	64	GLU	3.2
1	M	111	ALA	3.2
2	N	190	GLY	2.9
2	H	214	LYS	2.9
2	H	127	SER	2.8
2	N	191	THR	2.6
2	H	62	SER	2.3
2	H	100	GLY	2.3
2	N	127	SER	2.3
2	H	134	GLY	2.2
2	H	189	LEU	2.2
2	N	134	GLY	2.2
2	N	113	SER	2.2
2	N	100(A)	ALA	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 oligosaccharides 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.