



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:58 AM UTC

PDB ID : 3MLX / pdb\_00003mlx  
Title : Crystal structure of anti-HIV-1 V3 Fab 3074 in complex with an MN V3 peptide  
Authors : Kong, X.-P.  
Deposited on : 2010-04-18  
Resolution : 1.90 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>.

---

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

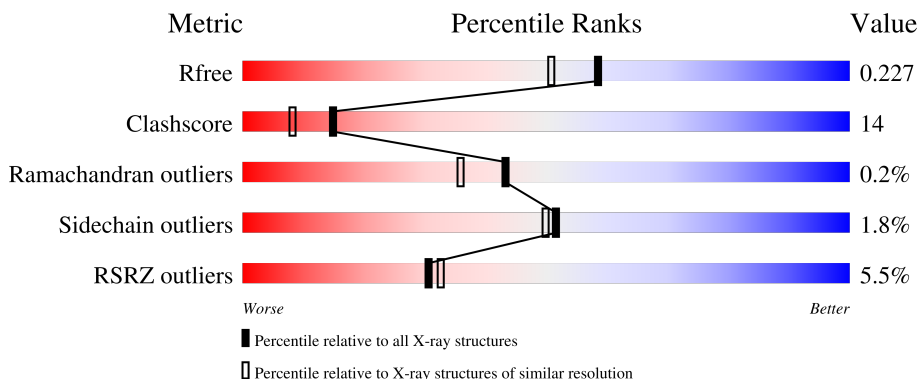
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

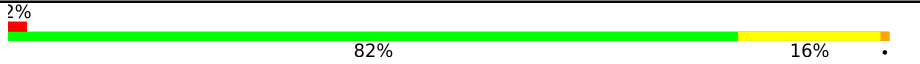
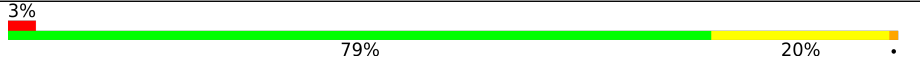


The reported resolution of this entry is 1.90 Å.

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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	211	
1	M	211	
2	H	228	
2	I	228	
3	P	23	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	Q	23	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment (17%), a green segment (35%), a yellow segment (22%), and a grey segment (39%). The percentages are labeled below the segments. A small black dot is visible on the yellow segment.</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7531 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 3074 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	211	1567	978	267	317	5	0	0	0
1	M	211	1567	978	267	317	5	0	0	0

- Molecule 2 is a protein called Human monoclonal anti-HIV-1 gp120 V3 antibody 3074 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	228	1709	1080	281	342	6	0	0	0
2	I	228	1709	1080	281	342	6	0	0	0

- 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	14	114	74	23	17	0	0	0
3	Q	14	114	74	23	17	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	L	175	175	175	0	0
4	H	218	218	218	0	0
4	P	12	12	12	0	0

*Continued on next page...*

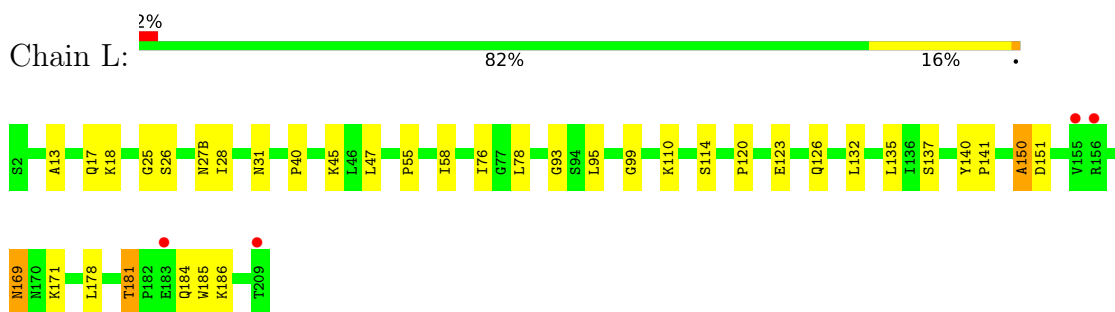
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	M	148	Total 148	O 148	0	0
4	I	193	Total 193	O 193	0	0
4	Q	5	Total 5	O 5	0	0

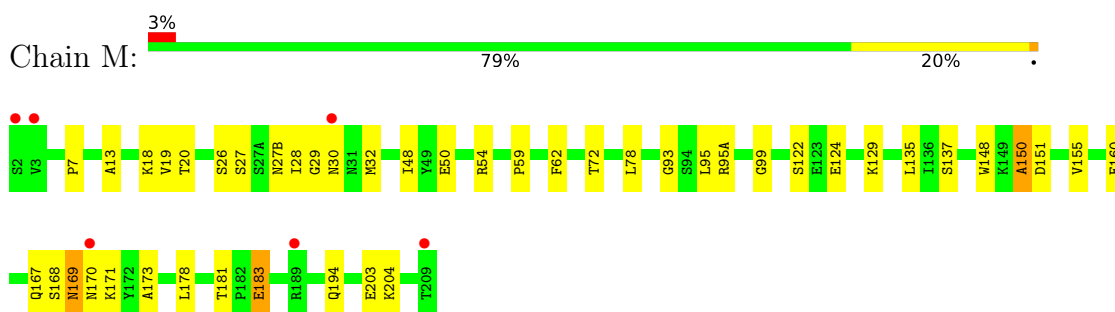
### 3 Residue-property plots [i](#)

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.

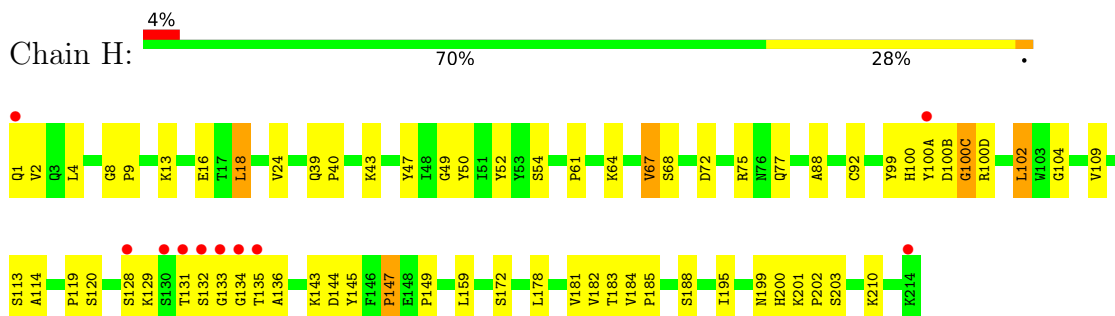
- Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody 3074 Fab light chain



- Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody 3074 Fab light chain

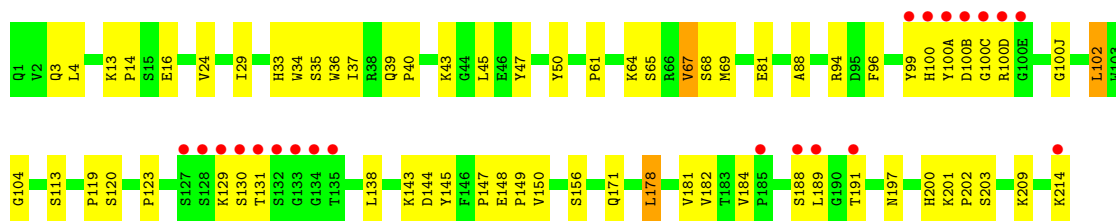


- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 3074 Fab heavy chain

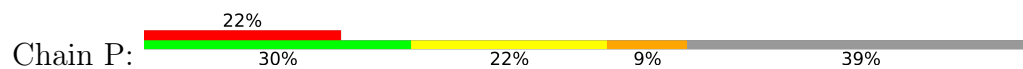


- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 3074 Fab heavy chain

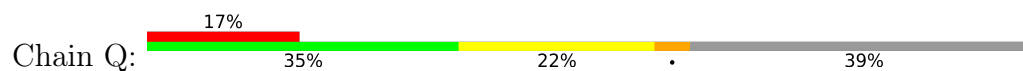




- Molecule 3: HIV-1 gp120 third variable region (V3) crown



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



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.87Å 128.80Å 60.19Å 90.00° 92.66° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.7 (50.00-1.90) 93.7 (50.00-1.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 1.87Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.192 , 0.228 0.192 , 0.227	Depositor DCC
$R_{free}$ test set	7275 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for l,k,-h 0.032 for h,-k,-l 0.021 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7531	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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

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	0.35	0/1605	0.90	5/2192 (0.2%)
1	M	0.34	0/1605	0.91	5/2192 (0.2%)
2	H	0.35	0/1754	0.95	8/2391 (0.3%)
2	I	0.35	0/1754	0.90	7/2391 (0.3%)
3	P	0.40	0/117	0.84	0/156
3	Q	0.33	0/117	0.78	0/156
All	All	0.35	0/6952	0.91	25/9478 (0.3%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	143	LYS	N-CA-C	7.74	122.05	109.59
2	H	143	LYS	N-CA-C	7.61	122.24	109.76
1	M	181	THR	N-CA-C	-6.90	101.11	110.36
2	H	144	ASP	N-CA-C	6.51	119.15	111.02
2	I	67	VAL	N-CA-C	6.24	118.37	108.89
2	H	67	VAL	N-CA-C	5.88	118.31	109.20
2	H	120	SER	N-CA-C	-5.84	100.19	109.76
1	M	150	ALA	N-CA-C	-5.79	97.74	107.99
1	M	99	GLY	N-CA-C	-5.76	103.70	112.51
1	L	181	THR	N-CA-C	-5.68	102.75	110.36
1	L	99	GLY	N-CA-C	-5.57	103.99	112.51
2	I	148	GLU	N-CA-C	-5.57	102.18	110.20
1	L	150	ALA	N-CA-C	-5.56	98.69	108.20
2	H	8	GLY	CA-C-N	5.51	125.03	119.19
2	H	8	GLY	C-N-CA	5.51	125.03	119.19
2	H	92	CYS	N-CA-C	-5.36	101.83	110.14
1	M	137	SER	N-CA-C	5.29	117.02	109.14
2	I	104	GLY	N-CA-C	-5.27	104.13	112.66
2	I	144	ASP	N-CA-C	5.20	117.52	111.02
1	L	114	SER	N-CA-C	-5.17	101.27	109.96
1	L	137	SER	N-CA-C	5.16	116.83	109.14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	120	SER	N-CA-C	-5.14	100.86	109.24
2	H	104	GLY	N-CA-C	-5.11	104.38	112.66
2	I	35	SER	N-CA-C	5.03	116.64	109.14
1	M	7	PRO	N-CA-C	-5.03	105.20	110.58

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	1567	0	1531	33	0
1	M	1567	0	1531	38	0
2	H	1709	0	1654	55	0
2	I	1709	0	1654	57	0
3	P	114	0	117	13	0
3	Q	114	0	117	8	0
4	H	218	0	0	6	0
4	I	193	0	0	2	0
4	L	175	0	0	3	0
4	M	148	0	0	1	0
4	P	12	0	0	0	0
4	Q	5	0	0	0	0
All	All	7531	0	6604	184	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 14.

All (184) 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:M:27(B):ASN:HD22	1:M:28:ILE:H	0.92	0.90
1:M:27(B):ASN:ND2	1:M:28:ILE:H	1.74	0.85
1:L:27(B):ASN:HD22	1:L:28:ILE:H	1.23	0.85
2:I:156:SER:H	2:I:197:ASN:HD21	1.20	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:40:PRO:HG2	2:I:43:LYS:HB2	1.57	0.84
1:M:26:SER:H	1:M:27(B):ASN:HD21	1.23	0.84
1:M:27(B):ASN:HD22	1:M:28:ILE:N	1.77	0.77
2:I:123:PRO:HD3	2:I:209:LYS:HE2	1.65	0.77
2:H:40:PRO:HG2	2:H:43:LYS:HB2	1.65	0.77
1:M:135:LEU:HD13	2:I:181:VAL:HG21	1.66	0.77
2:I:24:VAL:HG21	2:I:29:ILE:HD11	1.67	0.76
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.67	0.75
1:M:135:LEU:CD1	2:I:181:VAL:HG21	2.17	0.75
2:I:100:HIS:HB3	2:I:100(B):ASP:OD1	1.88	0.72
2:I:99:TYR:HB2	3:Q:307:ILE:HG23	1.71	0.72
1:L:132:LEU:HD22	1:L:178:LEU:HD23	1.73	0.71
2:H:18:LEU:HD12	2:H:109:VAL:HG11	1.71	0.71
1:L:27(B):ASN:ND2	1:L:28:ILE:H	1.89	0.69
1:L:123:GLU:O	1:L:126:GLN:HG2	1.91	0.69
1:M:26:SER:H	1:M:27(B):ASN:ND2	1.90	0.67
2:H:2:VAL:HB	2:H:102:LEU:HD21	1.77	0.67
1:L:135:LEU:HD12	2:H:181:VAL:HG21	1.78	0.66
1:M:169:ASN:ND2	1:M:171:LYS:H	1.92	0.66
2:H:75:ARG:HE	2:H:77:GLN:NE2	1.94	0.65
2:I:119:PRO:HB3	2:I:145:TYR:HB3	1.79	0.64
1:L:26:SER:H	1:L:27(B):ASN:HD21	1.46	0.64
1:M:54:ARG:HD3	1:M:62:PHE:O	1.98	0.63
2:H:99:TYR:HB3	3:P:307:ILE:CG2	2.29	0.63
2:H:75:ARG:HE	2:H:77:GLN:HE22	1.46	0.63
2:I:147:PRO:O	2:I:200:HIS:HE1	1.83	0.62
1:M:160:GLU:HG3	2:I:171:GLN:OE1	1.98	0.62
2:I:201:LYS:HD2	4:I:252:HOH:O	1.99	0.62
2:I:188:SER:HA	2:I:191:THR:HG22	1.82	0.62
2:I:100:HIS:HB2	2:I:100(D):ARG:HB2	1.81	0.61
1:M:95(A):ARG:HD3	2:I:61:PRO:HD2	1.82	0.61
2:I:24:VAL:CG2	2:I:29:ILE:HD11	2.31	0.61
1:L:169:ASN:ND2	1:L:171:LYS:H	1.97	0.60
2:I:33:HIS:HE1	2:I:99:TYR:OH	1.83	0.60
1:L:40:PRO:HD2	4:L:260:HOH:O	2.00	0.60
2:I:182:VAL:HG12	2:I:184:VAL:HG13	1.83	0.60
1:L:18:LYS:HB2	1:L:76:ILE:HD13	1.83	0.60
1:L:45:LYS:HE2	1:L:58:ILE:HD11	1.83	0.60
1:M:122:SER:H	2:I:214:LYS:NZ	2.00	0.60
2:I:24:VAL:HG21	2:I:29:ILE:CD1	2.30	0.60
2:H:147:PRO:O	2:H:200:HIS:HE1	1.85	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:200:HIS:HD2	2:H:203:SER:OG	1.86	0.58
1:L:169:ASN:C	1:L:169:ASN:HD22	2.11	0.58
3:P:307:ILE:C	3:P:307:ILE:HD13	2.28	0.58
2:I:200:HIS:CE1	2:I:202:PRO:HG2	2.39	0.58
3:P:307:ILE:HD13	3:P:308:HIS:N	2.19	0.58
1:L:181:THR:H	1:L:184:GLN:HE21	1.51	0.58
2:H:135:THR:CG2	2:H:183:THR:HG22	2.34	0.57
1:M:122:SER:H	2:I:214:LYS:HZ3	1.53	0.57
2:I:99:TYR:HB2	3:Q:307:ILE:CG2	2.34	0.57
2:H:200:HIS:CE1	2:H:202:PRO:HG2	2.40	0.57
1:L:26:SER:H	1:L:27(B):ASN:ND2	2.03	0.56
2:I:200:HIS:HD2	2:I:203:SER:OG	1.87	0.56
2:I:94:ARG:CZ	2:I:102:LEU:HD22	2.36	0.56
2:I:178:LEU:C	2:I:178:LEU:HD12	2.31	0.56
2:H:1:GLN:HB3	4:H:334:HOH:O	2.05	0.55
2:I:99:TYR:CE1	3:Q:309:ILE:HG13	2.42	0.55
1:L:181:THR:H	1:L:184:GLN:NE2	2.06	0.54
1:M:20:THR:HG23	1:M:72:THR:CG2	2.38	0.54
2:I:68:SER:OG	2:I:81:GLU:HB2	2.08	0.54
2:H:67:VAL:HG22	2:H:68:SER:N	2.22	0.54
1:L:13:ALA:HB3	1:L:78:LEU:CD1	2.38	0.54
1:M:20:THR:HG23	1:M:72:THR:HG23	1.92	0.52
2:H:172:SER:HA	4:H:566:HOH:O	2.09	0.52
3:P:307:ILE:HD12	3:P:309:ILE:HD13	1.91	0.52
2:I:14:PRO:HD2	2:I:113:SER:HB3	1.92	0.52
2:H:18:LEU:C	2:H:18:LEU:HD23	2.34	0.52
1:M:183:GLU:H	1:M:183:GLU:CD	2.18	0.52
2:H:131:THR:C	2:H:133:GLY:H	2.18	0.51
2:H:184:VAL:HB	2:H:185:PRO:HD2	1.91	0.51
2:I:13:LYS:NZ	2:I:113:SER:HA	2.26	0.51
2:I:37:ILE:HD13	2:I:47:TYR:HA	1.92	0.51
2:H:188:SER:HA	4:H:725:HOH:O	2.10	0.51
2:H:129:LYS:HE3	4:H:472:HOH:O	2.10	0.50
1:L:169:ASN:ND2	1:L:169:ASN:C	2.68	0.50
2:H:18:LEU:CD1	2:H:109:VAL:HG11	2.38	0.50
2:H:100:HIS:CG	2:H:100(D):ARG:HH11	2.28	0.50
1:M:13:ALA:HB3	1:M:78:LEU:CD1	2.41	0.50
2:I:100:HIS:CE1	3:Q:306:ARG:HG2	2.46	0.50
1:M:169:ASN:C	1:M:169:ASN:HD22	2.18	0.50
1:M:169:ASN:O	1:M:170:ASN:HB2	2.11	0.50
2:H:13:LYS:HB2	2:H:16:GLU:OE1	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:40:PRO:HG2	2:I:43:LYS:CB	2.36	0.49
2:I:64:LYS:O	2:I:65:SER:CB	2.60	0.49
2:H:132:SER:C	2:H:134:GLY:H	2.20	0.49
2:H:199:ASN:HD22	2:H:200:HIS:N	2.10	0.49
1:L:31:ASN:ND2	4:L:244:HOH:O	2.44	0.49
2:I:99:TYR:HE1	3:Q:309:ILE:HG13	1.75	0.49
2:H:72:ASP:OD1	2:H:75:ARG:HD3	2.12	0.49
1:M:19:VAL:HG13	1:M:78:LEU:HD11	1.95	0.49
2:H:61:PRO:O	2:H:64:LYS:HG2	2.12	0.49
2:I:96:PHE:CZ	2:I:100(J):GLY:HA3	2.48	0.48
1:L:140:TYR:HA	1:L:141:PRO:C	2.39	0.48
1:M:194:GLN:HG2	1:M:203:GLU:HG3	1.95	0.48
1:L:135:LEU:CD1	2:H:181:VAL:HG21	2.43	0.48
2:I:100(A):TYR:C	2:I:100(C):GLY:H	2.21	0.48
3:Q:319:THR:O	3:Q:320:THR:C	2.56	0.48
1:L:110:LYS:HG2	1:L:141:PRO:HD3	1.95	0.48
2:H:129:LYS:NZ	2:H:136:ALA:HA	2.28	0.48
2:H:100:HIS:CE1	3:P:306:ARG:HG2	2.49	0.48
2:H:1:GLN:HA	2:H:1:GLN:OE1	2.14	0.47
1:M:26:SER:N	1:M:27(B):ASN:HD21	2.01	0.47
2:I:50:TYR:C	2:I:50:TYR:CD1	2.92	0.47
1:L:150:ALA:O	1:L:151:ASP:HB2	2.15	0.47
1:L:135:LEU:CD1	2:H:181:VAL:CG2	2.93	0.46
2:I:129:LYS:HE2	2:I:189:LEU:HD13	1.96	0.46
2:H:99:TYR:O	3:P:307:ILE:HG22	2.15	0.46
1:L:17:GLN:NE2	1:L:17:GLN:HA	2.31	0.46
2:H:200:HIS:NE2	2:H:202:PRO:HG2	2.30	0.46
2:I:138:LEU:C	2:I:138:LEU:HD12	2.40	0.46
2:H:135:THR:HG22	2:H:183:THR:HG22	1.98	0.46
3:P:307:ILE:HD12	3:P:309:ILE:CD1	2.47	0.45
1:L:13:ALA:HB3	1:L:78:LEU:HD12	1.97	0.45
2:I:156:SER:H	2:I:197:ASN:ND2	2.00	0.45
2:I:201:LYS:N	2:I:202:PRO:HD2	2.32	0.45
2:I:130:SER:O	2:I:131:THR:HB	2.16	0.45
2:H:128:SER:O	2:H:129:LYS:HG3	2.16	0.45
2:H:100:HIS:CG	2:H:100(D):ARG:NH1	2.85	0.45
2:H:47:TYR:CZ	2:H:49:GLY:HA2	2.51	0.45
2:H:100:HIS:HE1	3:P:306:ARG:HG2	1.82	0.45
1:L:47:LEU:O	1:L:55:PRO:HD2	2.16	0.44
1:M:32:MET:HE2	1:M:50:GLU:C	2.42	0.44
1:M:169:ASN:HD22	1:M:171:LYS:H	1.63	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3:GLN:C	2:I:4:LEU:HD12	2.43	0.44
2:H:201:LYS:N	2:H:202:PRO:HD2	2.33	0.44
1:M:18:LYS:HG2	4:M:509:HOH:O	2.16	0.44
1:M:59:PRO:HG2	1:M:62:PHE:HD1	1.82	0.44
2:H:195:ILE:HD13	2:H:210:LYS:HA	2.00	0.44
3:P:315:ARG:HH11	3:P:315:ARG:HG2	1.83	0.44
1:M:93:GLY:C	1:M:95:LEU:H	2.25	0.44
1:M:59:PRO:HG2	1:M:62:PHE:CD1	2.53	0.44
2:H:9:PRO:HG3	4:H:292:HOH:O	2.16	0.44
1:M:124:GLU:HG2	1:M:129:LYS:O	2.16	0.44
2:I:188:SER:HA	2:I:191:THR:CG2	2.48	0.44
2:H:4:LEU:HD22	2:H:24:VAL:HG22	2.00	0.43
3:P:315:ARG:HH12	3:P:317:PHE:HD1	1.66	0.43
2:I:39:GLN:HB2	2:I:45:LEU:HD23	2.00	0.43
2:I:29:ILE:HG23	2:I:34:TRP:NE1	2.34	0.43
2:H:18:LEU:HD23	2:H:18:LEU:O	2.18	0.43
1:M:167:GLN:HB2	1:M:169:ASN:ND2	2.34	0.43
2:H:159:LEU:CD2	2:H:182:VAL:HG21	2.48	0.43
2:I:171:GLN:HG3	4:I:264:HOH:O	2.19	0.43
1:L:93:GLY:C	1:L:95:LEU:H	2.27	0.43
2:I:100:HIS:HE1	3:Q:306:ARG:HG2	1.83	0.43
3:Q:315:ARG:HG2	3:Q:315:ARG:HH11	1.84	0.43
2:H:100(A):TYR:H	3:P:305:LYS:N	2.16	0.43
2:H:52:TYR:HD2	2:H:54:SER:HG	1.66	0.42
1:L:186:LYS:HE2	4:L:685:HOH:O	2.18	0.42
1:M:27:SER:HA	1:M:29:GLY:HA3	2.00	0.42
1:L:25:GLY:HA3	1:L:27(B):ASN:HD21	1.84	0.42
2:I:129:LYS:HE2	2:I:189:LEU:CD1	2.50	0.42
1:L:26:SER:N	1:L:27(B):ASN:HD21	2.14	0.42
2:H:67:VAL:CG2	2:H:68:SER:N	2.83	0.42
2:H:113:SER:O	2:H:114:ALA:HB3	2.19	0.42
1:M:148:TRP:HB2	1:M:155:VAL:HG13	2.01	0.42
2:H:100(B):ASP:OD2	2:H:100(D):ARG:NH1	2.53	0.41
2:H:100(B):ASP:OD1	2:H:100(C):GLY:N	2.44	0.41
2:H:178:LEU:C	2:H:178:LEU:HD12	2.45	0.41
2:I:67:VAL:CG1	2:I:68:SER:N	2.83	0.41
2:H:39:GLN:C	2:H:88:ALA:HB1	2.46	0.41
2:I:13:LYS:O	2:I:16:GLU:HG3	2.20	0.41
1:M:168:SER:C	1:M:170:ASN:H	2.29	0.41
3:P:307:ILE:O	3:P:307:ILE:HG23	2.21	0.41
1:M:169:ASN:ND2	1:M:169:ASN:C	2.79	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:135:THR:HG21	2:H:183:THR:HG22	2.03	0.41
2:I:150:VAL:HG12	2:I:200:HIS:ND1	2.36	0.41
1:L:120:PRO:HD2	1:L:185:TRP:CE2	2.56	0.41
1:L:169:ASN:HD21	1:L:171:LYS:HB2	1.86	0.41
1:M:167:GLN:OE1	1:M:173:ALA:HB2	2.21	0.41
2:I:39:GLN:C	2:I:88:ALA:HB1	2.46	0.41
2:I:33:HIS:CE1	2:I:99:TYR:OH	2.71	0.40
4:H:251:HOH:O	3:P:306:ARG:HG3	2.20	0.40
1:L:17:GLN:CA	1:L:17:GLN:HE21	2.34	0.40
1:L:18:LYS:CB	1:L:76:ILE:HD13	2.51	0.40
2:I:100:HIS:CB	2:I:100(D):ARG:HB2	2.49	0.40
1:M:48:ILE:CD1	1:M:54:ARG:HG2	2.52	0.40
2:I:36:TRP:HD1	2:I:69:MET:HE3	1.85	0.40
2:H:50:TYR:CD1	2:H:50:TYR:C	2.98	0.40
1:M:150:ALA:O	1:M:151:ASP:HB2	2.21	0.40
1:M:204:LYS:HD3	1:M:204:LYS:HA	1.94	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	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
1	M	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
2	H	226/228 (99%)	214 (95%)	11 (5%)	1 (0%)	30	22
2	I	226/228 (99%)	213 (94%)	13 (6%)	0	100	100
3	P	12/23 (52%)	11 (92%)	0	1 (8%)	0	0
3	Q	12/23 (52%)	11 (92%)	1 (8%)	0	100	100
All	All	894/924 (97%)	852 (95%)	40 (4%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	P	306	ARG
2	H	100(C)	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	177/177 (100%)	176 (99%)	1 (1%)	78 81
1	M	177/177 (100%)	173 (98%)	4 (2%)	44 40
2	H	195/195 (100%)	191 (98%)	4 (2%)	47 44
2	I	195/195 (100%)	192 (98%)	3 (2%)	57 56
3	P	11/19 (58%)	10 (91%)	1 (9%)	9 3
3	Q	11/19 (58%)	10 (91%)	1 (9%)	9 3
All	All	766/782 (98%)	752 (98%)	14 (2%)	51 50

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	169	ASN
2	H	18	LEU
2	H	102	LEU
2	H	147	PRO
2	H	149	PRO
3	P	307	ILE
1	M	30	ASN
1	M	169	ASN
1	M	178	LEU
1	M	183	GLU
2	I	102	LEU
2	I	149	PRO
2	I	178	LEU
3	Q	307	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	17	GLN
1	L	27(B)	ASN
1	L	30	ASN
1	L	31	ASN
1	L	79	GLN
1	L	126	GLN
1	L	169	ASN
1	L	184	GLN
2	H	77	GLN
2	H	100(G)	GLN
2	H	105	GLN
2	H	171	GLN
2	H	192	GLN
2	H	199	ASN
2	H	200	HIS
2	H	204	ASN
1	M	27(B)	ASN
1	M	79	GLN
1	M	169	ASN
2	I	3	GLN
2	I	5	GLN
2	I	33	HIS
2	I	77	GLN
2	I	192	GLN
2	I	197	ASN
2	I	200	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 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, 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	211/211 (100%)	0.00	4 (1%) 66 70	16, 22, 33, 53	0
1	M	211/211 (100%)	0.19	6 (2%) 55 59	16, 24, 37, 52	0
2	H	228/228 (100%)	0.19	10 (4%) 39 41	15, 22, 47, 76	0
2	I	228/228 (100%)	0.32	21 (9%) 14 15	15, 23, 61, 80	0
3	P	14/23 (60%)	1.16	5 (35%) 1 0	21, 30, 58, 63	0
3	Q	14/23 (60%)	1.27	4 (28%) 1 1	26, 38, 58, 63	0
All	All	906/924 (98%)	0.21	50 (5%) 30 32	15, 23, 47, 80	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	131	THR	7.2
2	H	131	THR	6.7
1	L	209	THR	5.1
1	M	2	SER	4.7
2	I	130	SER	4.6
2	H	132	SER	4.4
2	I	132	SER	4.4
2	I	100(A)	TYR	4.3
2	I	100	HIS	4.2
1	M	3	VAL	4.1
2	I	128	SER	4.0
2	H	130	SER	3.8
2	I	129	LYS	3.7
2	H	133	GLY	3.7
2	I	100(B)	ASP	3.6
2	I	100(E)	GLY	3.6
2	I	134	GLY	3.5
2	I	135	THR	3.5
2	I	99	TYR	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	P	319	THR	3.2
1	M	209	THR	3.1
3	P	307	ILE	3.0
2	I	127	SER	2.9
3	Q	320	THR	2.9
3	P	320	THR	2.8
3	Q	306	ARG	2.8
2	H	100(A)	TYR	2.8
2	I	100(D)	ARG	2.8
2	I	100(C)	GLY	2.8
2	I	133	GLY	2.7
2	H	135	THR	2.6
1	M	170	ASN	2.6
1	L	183	GLU	2.5
2	H	134	GLY	2.5
1	M	189	ARG	2.4
2	I	188	SER	2.4
2	H	128	SER	2.4
2	I	214	LYS	2.4
2	I	189	LEU	2.3
2	I	185	PRO	2.3
3	Q	307	ILE	2.3
1	L	155	VAL	2.2
1	L	156	ARG	2.2
1	M	30	ASN	2.1
2	H	1	GLN	2.1
2	I	191	THR	2.0
3	Q	319	THR	2.0
3	P	306	ARG	2.0
2	H	214	LYS	2.0
3	P	305	LYS	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 oligosaccharides in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.