



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:55 am BST

PDB ID : 1NAN
Title : MCH CLASS I H-2KB MOLECULE COMPLEXED WITH PBM1 PEPTIDE
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Deposited on : 2002-11-28
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

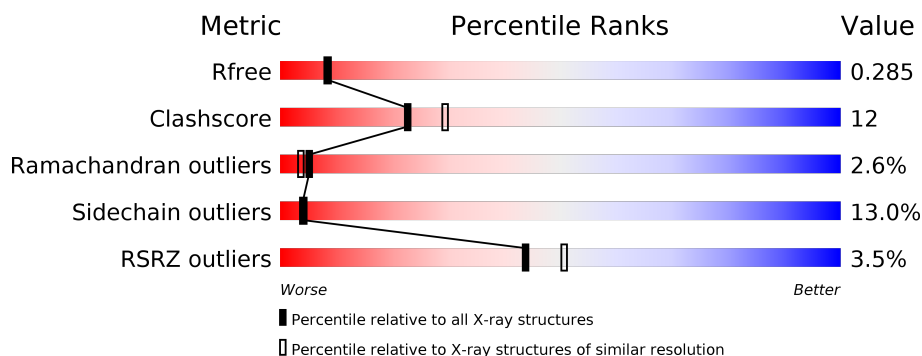
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	H	278	<div> <div>4%</div> <div>68% 24% 7%</div> </div>
1	L	278	<div> <div>6%</div> <div>65% 27% 6%</div> </div>
2	I	99	<div> <div>83% 14%</div> </div>
2	P	99	<div> <div>81% 18%</div> </div>
3	M	8	<div> <div>63% 25% 13%</div> </div>
3	Q	8	<div> <div>88% 13%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6462 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 H-2 class I histocompatibility antigen, K-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	278	Total	C	N	O	S	0	0	0
			2262	1428	397	428	9			
1	L	278	Total	C	N	O	S	0	0	0
			2262	1428	397	428	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	I	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- Molecule 3 is a protein called pBM1 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	8	Total	C	N	O	0	0	0
			70	46	10	14			
3	Q	8	Total	C	N	O	0	0	0
			70	46	10	14			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	46	Total	O	0	0
			46	46		
4	L	51	Total	O	0	0
			51	51		
4	P	28	Total	O	0	0
			28	28		
4	I	24	Total	O	0	0
			24	24		

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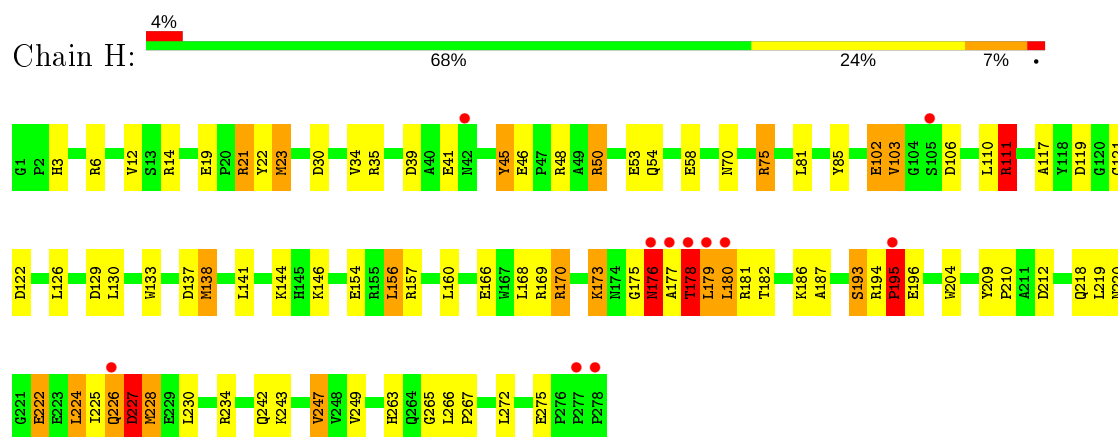
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	6	Total	O	0	0
			6	6		
4	Q	1	Total	O	0	0
			1	1		

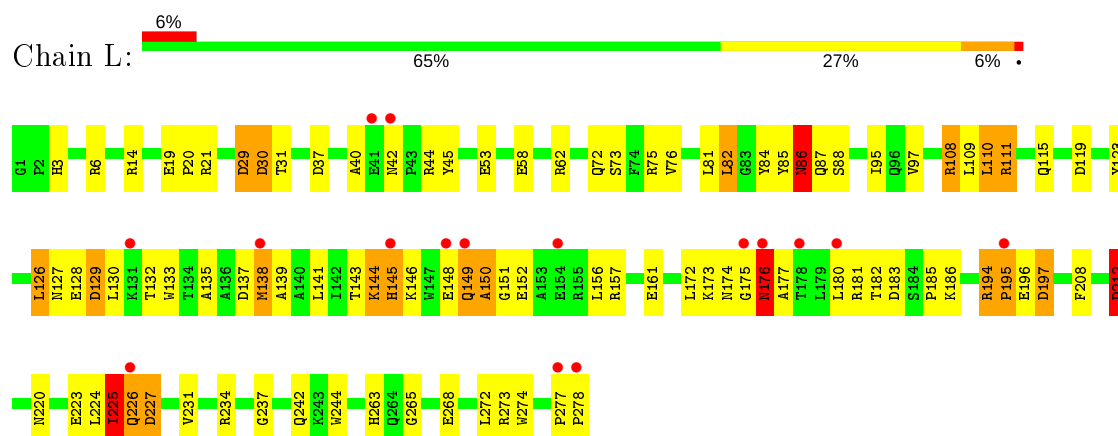
3 Residue-property plots [i](#)

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

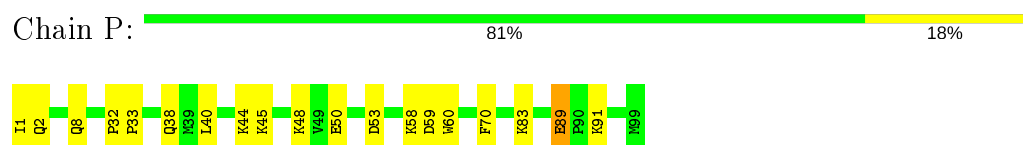
- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain



- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

Chain I:

83%

14%



• Molecule 3: pBM1 peptide

Chain M:

63%

25%

13%



• Molecule 3: pBM1 peptide

Chain Q:

88%

13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.98Å 88.61Å 89.17Å 90.00° 111.60° 90.00°	Depositor
Resolution (Å)	12.00 – 2.30 61.26 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-2.30) 97.9 (61.26-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.279 0.229 , 0.285	Depositor DCC
R_{free} test set	4177 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.823	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6462	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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 38.98 % 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 3.3972e-04. 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, 0.333 respectively for untwinned datasets, and 0.375, 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	H	0.50	0/2326	0.77	5/3161 (0.2%)
1	L	0.52	0/2326	0.78	8/3161 (0.3%)
2	I	0.56	0/847	0.78	3/1148 (0.3%)
2	P	0.55	0/847	0.79	1/1148 (0.1%)
3	M	0.58	0/71	0.82	0/94
3	Q	0.58	0/71	0.83	0/94
All	All	0.52	0/6488	0.78	17/8806 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	137	ASP	CB-CG-OD2	7.23	124.81	118.30
1	L	212	ASP	CB-CG-OD2	6.93	124.53	118.30
1	L	119	ASP	CB-CG-OD2	6.67	124.30	118.30
1	H	129	ASP	CB-CG-OD2	6.10	123.79	118.30
1	H	137	ASP	CB-CG-OD2	5.99	123.69	118.30
1	H	212	ASP	CB-CG-OD2	5.68	123.41	118.30
1	H	122	ASP	CB-CG-OD2	5.44	123.19	118.30
2	I	85	ASP	CB-CG-OD2	5.38	123.14	118.30
1	L	129	ASP	CB-CG-OD2	5.34	123.11	118.30
1	L	37	ASP	CB-CG-OD2	5.33	123.09	118.30
2	I	59	ASP	CB-CG-OD2	5.31	123.08	118.30
1	H	227	ASP	CB-CG-OD2	5.26	123.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	29	ASP	CB-CG-OD2	5.21	122.99	118.30
1	L	183	ASP	CB-CG-OD2	5.16	122.94	118.30
2	I	76	ASP	CB-CG-OD2	5.16	122.94	118.30
1	L	30	ASP	CB-CG-OD2	5.08	122.87	118.30
2	P	53	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	195	PRO	Peptide

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	H	2262	0	2150	55	0
1	L	2262	0	2150	64	0
2	I	821	0	796	13	0
2	P	821	0	796	10	0
3	M	70	0	65	5	0
3	Q	70	0	65	0	0
4	H	46	0	0	4	0
4	I	24	0	0	1	0
4	L	51	0	0	2	0
4	M	6	0	0	1	0
4	P	28	0	0	0	0
4	Q	1	0	0	0	0
All	All	6462	0	6022	142	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 12.

All (142) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1:ILE:H1	2:I:1:ILE:HD12	1.33	0.93
1:H:19:GLU:OE1	1:H:75:ARG:NH2	2.02	0.92
1:H:194:ARG:O	1:H:196:GLU:HA	1.70	0.90
1:H:21:ARG:HH11	1:H:21:ARG:HG3	1.37	0.89
2:I:1:ILE:N	2:I:1:ILE:CD1	2.38	0.86
1:H:50:ARG:HD2	1:H:53:GLU:OE2	1.78	0.84
1:H:226:GLN:O	1:H:227:ASP:HB2	1.79	0.82
1:H:234:ARG:HE	1:H:242:GLN:HE21	1.31	0.77
1:L:194:ARG:CG	1:L:195:PRO:HD2	2.13	0.77
1:L:20:PRO:HG2	1:L:75:ARG:HG2	1.66	0.77
2:I:1:ILE:N	2:I:1:ILE:HD12	1.93	0.77
1:H:21:ARG:NH1	1:H:21:ARG:HG3	1.98	0.75
1:H:156:LEU:HD22	1:H:160:LEU:HD11	1.67	0.75
1:L:196:GLU:O	1:L:197:ASP:CB	2.35	0.74
1:L:263:HIS:CD2	1:L:265:GLY:H	2.07	0.73
1:H:103:VAL:HG13	1:H:168:LEU:HD23	1.70	0.72
1:L:234:ARG:HE	1:L:242:GLN:HE21	1.36	0.72
1:L:194:ARG:CD	1:L:195:PRO:HD2	2.20	0.71
1:L:6:ARG:NH2	1:L:30:ASP:OD1	2.23	0.71
1:L:194:ARG:HD3	1:L:195:PRO:HD2	1.74	0.70
1:L:133:TRP:HB2	1:L:144:LYS:HG3	1.73	0.70
1:L:224:LEU:O	1:L:226:GLN:N	2.26	0.69
1:L:40:ALA:O	4:L:324:HOH:O	2.10	0.68
1:L:194:ARG:HG2	1:L:195:PRO:HD2	1.73	0.68
1:L:223:GLU:OE2	4:L:285:HOH:O	2.10	0.67
1:L:145:HIS:O	1:L:149:GLN:HG3	1.96	0.66
1:H:234:ARG:HH11	2:P:8:GLN:NE2	1.94	0.66
1:H:234:ARG:HE	1:H:242:GLN:NE2	1.94	0.65
1:H:3:HIS:HE1	1:H:178:THR:HB	1.62	0.65
1:L:146:LYS:O	1:L:150:ALA:HB3	1.95	0.65
1:L:126:LEU:HD21	1:L:130:LEU:HD23	1.80	0.64
1:L:234:ARG:HH11	2:I:8:GLN:NE2	1.95	0.64
1:H:34:VAL:HG21	1:H:45:TYR:CE2	2.34	0.63
1:H:175:GLY:O	1:H:179:LEU:HB2	1.99	0.63
1:H:263:HIS:CD2	1:H:265:GLY:H	2.18	0.62
1:L:133:TRP:O	1:L:144:LYS:HE2	1.99	0.62
2:I:1:ILE:H3	2:I:1:ILE:CD1	2.12	0.61
2:I:59:ASP:O	2:I:60:TRP:HB2	2.00	0.61
1:L:127:ASN:C	1:L:129:ASP:H	2.02	0.61
3:M:2:ASN:ND2	3:M:3:PHE:H	1.97	0.61
1:H:110:LEU:O	1:H:111:ARG:HB2	2.00	0.61
1:L:196:GLU:O	1:L:197:ASP:HB2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1:ILE:HD13	2:I:1:ILE:H3	1.66	0.60
1:L:110:LEU:O	1:L:111:ARG:HB3	2.00	0.60
1:L:196:GLU:HA	1:L:196:GLU:OE1	2.00	0.60
1:L:277:PRO:O	1:L:278:PRO:C	2.40	0.60
2:I:34:HIS:HE1	2:I:36:GLU:OE2	1.86	0.59
1:L:126:LEU:HD21	1:L:130:LEU:HA	1.84	0.59
1:L:127:ASN:O	1:L:129:ASP:N	2.35	0.59
1:L:126:LEU:HD21	1:L:130:LEU:CD2	2.34	0.58
3:M:2:ASN:HD22	3:M:3:PHE:H	1.51	0.58
1:H:225:ILE:HA	1:H:228:MET:HE2	1.86	0.57
1:L:234:ARG:HE	1:L:242:GLN:NE2	2.00	0.57
4:H:312:HOH:O	2:P:58:LYS:HE2	2.04	0.57
2:I:34:HIS:CE1	2:I:36:GLU:OE2	2.58	0.56
1:H:193:SER:HA	4:H:313:HOH:O	2.05	0.56
1:L:263:HIS:HD2	1:L:265:GLY:H	1.52	0.56
1:L:212:ASP:OD2	1:L:212:ASP:N	2.36	0.56
1:H:21:ARG:NH1	1:H:23:MET:HE1	2.20	0.56
1:H:3:HIS:CE1	1:H:178:THR:HB	2.41	0.55
1:H:34:VAL:HG21	1:H:45:TYR:HE2	1.71	0.55
1:H:133:TRP:HB2	1:H:144:LYS:HG3	1.89	0.55
1:H:178:THR:O	1:H:178:THR:OG1	2.26	0.54
1:L:133:TRP:HB2	1:L:144:LYS:CG	2.38	0.53
1:H:156:LEU:HD22	1:H:160:LEU:CD1	2.38	0.53
1:L:146:LYS:HA	1:L:149:GLN:HE21	1.74	0.53
1:H:194:ARG:O	1:H:195:PRO:C	2.46	0.52
1:H:106:ASP:OD1	1:H:106:ASP:N	2.43	0.52
1:H:117:ALA:HB2	2:P:60:TRP:CE2	2.45	0.52
1:H:21:ARG:HE	1:H:39:ASP:HB2	1.74	0.51
1:H:102:GLU:HG3	1:H:111:ARG:HB3	1.91	0.51
1:H:19:GLU:HB3	1:H:75:ARG:NH2	2.25	0.51
1:H:138:MET:O	1:H:141:LEU:HB2	2.11	0.50
1:L:174:ASN:HD22	1:L:174:ASN:N	2.09	0.50
1:H:219:LEU:HB3	1:H:224:LEU:HD21	1.92	0.50
1:L:97:VAL:HA	1:L:115:GLN:O	2.11	0.49
1:L:109:LEU:HD22	1:L:161:GLU:HG2	1.94	0.49
1:H:21:ARG:NH1	1:H:21:ARG:CG	2.70	0.49
1:L:123:TYR:OH	1:L:143:THR:OG1	2.29	0.48
1:H:218:GLN:HA	1:H:222:GLU:O	2.14	0.48
2:P:32:PRO:HB2	2:P:33:PRO:HD2	1.95	0.48
1:L:182:THR:CG2	1:L:182:THR:O	2.62	0.48
1:L:3:HIS:ND1	1:L:29:ASP:OD1	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:237:GLY:HA3	4:I:106:HOH:O	2.13	0.48
4:H:312:HOH:O	2:P:58:LYS:CE	2.60	0.48
1:H:187:ALA:HA	1:H:204:TRP:O	2.14	0.47
2:I:59:ASP:O	2:I:60:TRP:CB	2.63	0.47
1:H:121:CYS:SG	2:P:1:ILE:HG13	2.55	0.47
1:H:130:LEU:HB3	1:H:157:ARG:HG3	1.95	0.47
1:L:231:VAL:HG13	1:L:244:TRP:CZ2	2.50	0.47
1:H:247:VAL:HG13	1:H:249:VAL:CG1	2.45	0.47
1:L:196:GLU:O	1:L:197:ASP:HB3	2.11	0.47
1:H:266:LEU:HA	1:H:267:PRO:HD2	1.77	0.47
1:H:6:ARG:NH2	1:H:30:ASP:OD1	2.48	0.46
1:H:81:LEU:HD22	1:H:85:TYR:HE2	1.79	0.46
1:H:263:HIS:HD2	1:H:265:GLY:H	1.63	0.46
1:H:81:LEU:HG	3:M:8:ILE:HD11	1.96	0.46
2:P:59:ASP:O	2:P:60:TRP:HB2	2.16	0.46
1:H:230:LEU:HD22	1:H:243:LYS:HE3	1.97	0.46
1:L:226:GLN:HB3	1:L:226:GLN:HE21	1.58	0.46
1:L:85:TYR:O	1:L:86:ASN:C	2.55	0.46
2:I:55:SER:HB2	2:I:63:TYR:CZ	2.51	0.45
1:L:175:GLY:O	1:L:177:ALA:N	2.49	0.45
1:L:157:ARG:HE	1:L:161:GLU:CD	2.20	0.45
1:L:172:LEU:O	1:L:176:ASN:N	2.50	0.45
1:L:19:GLU:OE1	1:L:75:ARG:NH1	2.44	0.45
1:L:82:LEU:HD22	1:L:87:GLN:HB2	1.98	0.45
2:I:59:ASP:OD1	2:I:59:ASP:C	2.56	0.44
1:H:14:ARG:NH1	1:H:21:ARG:HG2	2.33	0.44
1:L:108:ARG:HH11	1:L:108:ARG:CG	2.31	0.44
1:L:274:TRP:CH2	1:L:277:PRO:HD3	2.52	0.44
1:L:194:ARG:O	1:L:195:PRO:C	2.56	0.44
2:P:89:GLU:CD	2:P:89:GLU:H	2.21	0.44
1:H:176:ASN:O	1:H:178:THR:N	2.50	0.44
3:M:2:ASN:ND2	4:M:23:HOH:O	2.51	0.43
1:H:126:LEU:HD22	1:H:156:LEU:HD13	1.99	0.43
1:H:169:ARG:NH2	4:H:301:HOH:O	2.51	0.43
2:I:40:LEU:HD23	2:I:45:LYS:HA	2.01	0.43
1:L:129:ASP:C	1:L:129:ASP:OD1	2.57	0.43
1:L:224:LEU:O	1:L:225:ILE:C	2.56	0.43
3:M:2:ASN:ND2	3:M:3:PHE:N	2.65	0.43
1:L:225:ILE:C	1:L:227:ASP:H	2.22	0.43
2:P:38:GLN:HG2	2:P:45:LYS:HE3	2.00	0.43
1:L:72:GLN:NE2	1:L:76:VAL:HG23	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:MET:HE3	1:H:23:MET:HB2	1.85	0.42
1:L:149:GLN:O	1:L:151:GLY:N	2.52	0.42
1:H:133:TRP:HH2	1:H:156:LEU:HD12	1.84	0.42
1:L:174:ASN:ND2	1:L:174:ASN:N	2.67	0.42
2:P:40:LEU:HD23	2:P:45:LYS:HA	2.01	0.41
1:H:22:TYR:OH	1:H:70:ASN:HB3	2.21	0.41
1:L:135:ALA:HB3	1:L:141:LEU:HD23	2.02	0.41
1:L:81:LEU:HD22	1:L:85:TYR:HE2	1.85	0.41
1:H:178:THR:O	1:H:180:LEU:N	2.50	0.41
1:L:175:GLY:O	1:L:176:ASN:C	2.59	0.41
1:L:81:LEU:HD12	1:L:95:ILE:HD11	2.03	0.41
1:H:35:ARG:HB3	1:H:48:ARG:HD3	2.02	0.41
1:H:209:TYR:CG	1:H:210:PRO:HA	2.56	0.40
1:L:85:TYR:O	1:L:86:ASN:ND2	2.54	0.40
1:L:135:ALA:CB	1:L:141:LEU:HD23	2.52	0.40
1:L:84:TYR:CD2	1:L:139:ALA:HB1	2.57	0.40
1:H:170:ARG:O	1:H:173:LYS:HB2	2.22	0.40
1:L:185:PRO:CA	1:L:208:PHE:HB3	2.51	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	H	276/278 (99%)	258 (94%)	9 (3%)	9 (3%)	4	2
1	L	276/278 (99%)	249 (90%)	16 (6%)	11 (4%)	3	1
2	I	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
2	P	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
3	M	6/8 (75%)	6 (100%)	0	0	100	100
3	Q	6/8 (75%)	6 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	758/770 (98%)	706 (93%)	32 (4%)	20 (3%)	5 4

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	177	ALA
1	H	178	THR
1	L	138	MET
1	L	176	ASN
1	L	225	ILE
1	H	111	ARG
1	H	179	LEU
1	L	128	GLU
1	L	197	ASP
1	H	176	ASN
1	L	111	ARG
1	L	220	ASN
1	H	119	ASP
1	H	227	ASP
1	L	86	ASN
1	H	173	LYS
1	L	150	ALA
1	L	195	PRO
1	L	148	GLU
1	H	195	PRO

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	H	236/236 (100%)	201 (85%)	35 (15%)	3 3
1	L	236/236 (100%)	200 (85%)	36 (15%)	2 2
2	I	94/94 (100%)	87 (93%)	7 (7%)	13 17
2	P	94/94 (100%)	86 (92%)	8 (8%)	10 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	8/8 (100%)	7 (88%)	1 (12%)	4	5
3	Q	8/8 (100%)	7 (88%)	1 (12%)	4	5
All	All	676/676 (100%)	588 (87%)	88 (13%)	4	4

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	VAL
1	H	21	ARG
1	H	23	MET
1	H	41	GLU
1	H	45	TYR
1	H	46	GLU
1	H	50	ARG
1	H	54	GLN
1	H	58	GLU
1	H	75	ARG
1	H	102	GLU
1	H	103	VAL
1	H	111	ARG
1	H	138	MET
1	H	146	LYS
1	H	154	GLU
1	H	156	LEU
1	H	166	GLU
1	H	170	ARG
1	H	176	ASN
1	H	178	THR
1	H	180	LEU
1	H	181	ARG
1	H	182	THR
1	H	186	LYS
1	H	193	SER
1	H	220	ASN
1	H	222	GLU
1	H	224	LEU
1	H	226	GLN
1	H	227	ASP
1	H	228	MET
1	H	247	VAL
1	H	272	LEU

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Mol	Chain	Res	Type
1	H	275	GLU
1	L	14	ARG
1	L	21	ARG
1	L	31	THR
1	L	42	ASN
1	L	44	ARG
1	L	45	TYR
1	L	53	GLU
1	L	58	GLU
1	L	62	ARG
1	L	73	SER
1	L	82	LEU
1	L	86	ASN
1	L	88	SER
1	L	108	ARG
1	L	110	LEU
1	L	126	LEU
1	L	132	THR
1	L	138	MET
1	L	144	LYS
1	L	145	HIS
1	L	149	GLN
1	L	152	GLU
1	L	156	LEU
1	L	173	LYS
1	L	176	ASN
1	L	180	LEU
1	L	181	ARG
1	L	186	LYS
1	L	194	ARG
1	L	212	ASP
1	L	225	ILE
1	L	226	GLN
1	L	227	ASP
1	L	268	GLU
1	L	272	LEU
1	L	273	ARG
2	P	2	GLN
2	P	44	LYS
2	P	48	LYS
2	P	50	GLU
2	P	70	PHE

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Mol	Chain	Res	Type
2	P	83	LYS
2	P	89	GLU
2	P	91	LYS
2	I	1	ILE
2	I	44	LYS
2	I	50	GLU
2	I	70	PHE
2	I	85	ASP
2	I	89	GLU
2	I	91	LYS
3	M	2	ASN
3	Q	4	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	HIS
1	H	127	ASN
1	H	176	ASN
1	H	242	GLN
1	H	263	HIS
1	L	72	GLN
1	L	86	ASN
1	L	114	GLN
1	L	149	GLN
1	L	174	ASN
1	L	226	GLN
1	L	242	GLN
1	L	263	HIS
2	P	8	GLN
2	P	29	GLN
2	P	38	GLN
2	I	8	GLN
2	I	34	HIS
3	M	2	ASN

5.3.3 RNA ⓘ

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

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, 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	H	278/278 (100%)	0.49	11 (3%)	38	45	27, 42, 64, 78	10 (3%)
1	L	278/278 (100%)	0.48	16 (5%)	23	29	25, 42, 64, 77	4 (1%)
2	I	99/99 (100%)	0.08	0	100	100	25, 37, 49, 56	4 (4%)
2	P	99/99 (100%)	0.10	0	100	100	26, 38, 49, 60	2 (2%)
3	M	8/8 (100%)	0.09	0	100	100	33, 36, 44, 44	0
3	Q	8/8 (100%)	0.21	0	100	100	30, 42, 56, 59	0
All	All	770/770 (100%)	0.38	27 (3%)	44	51	25, 40, 63, 78	20 (2%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	178	THR	12.4
1	H	177	ALA	11.1
1	H	278	PRO	6.0
1	H	180	LEU	5.6
1	L	277	PRO	5.5
1	H	179	LEU	5.2
1	H	176	ASN	4.8
1	L	178	THR	4.5
1	H	277	PRO	4.5
1	H	195	PRO	4.1
1	H	226	GLN	3.4
1	L	278	PRO	3.2
1	H	42	ASN	3.2
1	L	154	GLU	3.1
1	L	226	GLN	3.1
1	L	195	PRO	3.1
1	L	131	LYS	3.0
1	L	175	GLY	2.9
1	L	148	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	105	SER	2.7
1	L	41	GLU	2.7
1	L	149	GLN	2.7
1	L	138	MET	2.6
1	L	42	ASN	2.4
1	L	176	ASN	2.3
1	L	145	HIS	2.1
1	L	180	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.