Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2023 – 04:36 am GMT

PDB ID	:	1UWX
Title	:	P1.2 serosubtype antigen derived from N. meningitidis PorA in complex with Fab fragment
Authors	:	Tzitzilonis, C.; Prince, S.M.; Collins, R.F.; Maiden, M.C.J.; Feavers, I.M.; Derrick, J.P.
Deposited on	:	2004-02-12
Resolution	:	2.20 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:

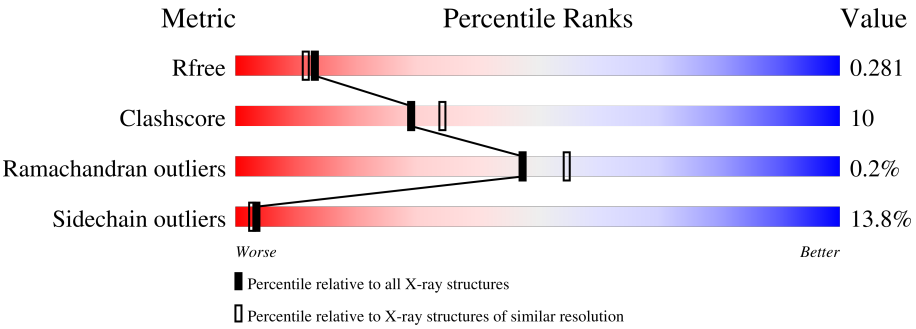
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	63	78% 13% • 8%
1	B	63	79% 11% 5% 5%
2	H	225	74% 18% • •
2	M	225	75% 16% 5% •
3	K	213	77% 17% 5%
3	L	213	74% 20% • •
4	P	13	62% 23% 8% 8%

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Mol	Chain	Length	Quality of chain
4	Q	13	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8120 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 PROTEIN G-PRIME.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	58	Total	C	N	O	0	0	1
			441	277	70	94			
1	B	60	Total	C	N	O	0	0	0
			466	293	73	100			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	LYS	GLU	engineered mutation	UNP Q54181
B	24	LYS	GLU	engineered mutation	UNP Q54181

- Molecule 2 is a protein called ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1686	1083	270	327	6			
2	M	218	Total	C	N	O	S	0	0	0
			1686	1083	270	327	6			

- Molecule 3 is a protein called ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	212	Total	C	N	O	S	0	0	1
			1616	1015	268	327	6			
3	L	212	Total	C	N	O	S	0	0	1
			1616	1015	268	327	6			

- Molecule 4 is a protein called CLASS 1 OUTER MEMBRANE PROTEIN VARIABLE REGION 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	13	Total	C	N	O	0	0	0
			107	68	19	20			
4	Q	13	Total	C	N	O	0	0	0
			107	68	19	20			

- Molecule 5 is water.

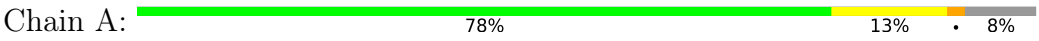
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	41	Total	O	0	0
			41	41		
5	B	29	Total	O	0	0
			29	29		
5	H	103	Total	O	0	0
			103	103		
5	K	45	Total	O	0	0
			45	45		
5	L	94	Total	O	0	0
			94	94		
5	M	73	Total	O	0	0
			73	73		
5	P	7	Total	O	0	0
			7	7		
5	Q	3	Total	O	0	0
			3	3		

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. 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. 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: PROTEIN G-PRIME

Chain A:

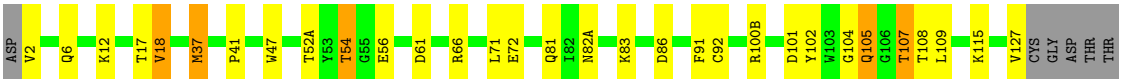


• Molecule 1: PROTEIN G-PRIME

Chain B:

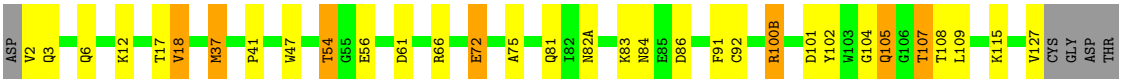
• Molecule 2: ANTIBODY

Chain H:



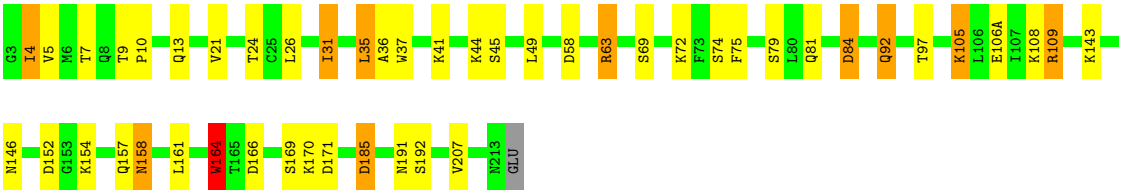
• Molecule 2: ANTIBODY

Chain M:



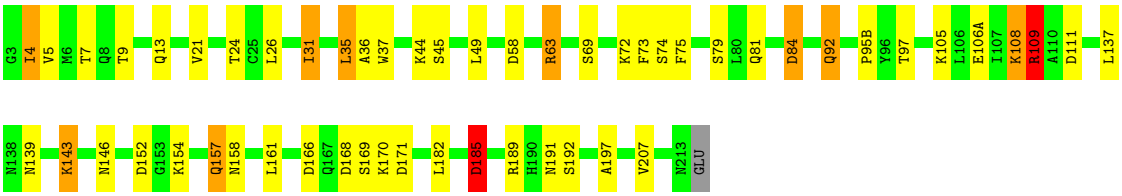
• Molecule 3: ANTIBODY

Chain K:



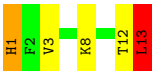
• Molecule 3: ANTIBODY

Chain L:



• Molecule 4: CLASS 1 OUTER MEMBRANE PROTEIN VARIABLE REGION 2

Chain P:



• Molecule 4: CLASS 1 OUTER MEMBRANE PROTEIN VARIABLE REGION 2

Chain Q:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.43Å 110.57Å 138.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.0 (20.00-2.20) 77.7 (20.89-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.223 , 0.265 0.264 , 0.281	Depositor DCC
R_{free} test set	2487 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 35.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8120	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 35.20 % 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 6.0577e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	A	0.99	2/447 (0.4%)	1.03	2/608 (0.3%)
1	B	0.85	2/473 (0.4%)	0.97	3/641 (0.5%)
2	H	0.79	1/1736 (0.1%)	0.91	8/2366 (0.3%)
2	M	0.73	1/1736 (0.1%)	0.92	9/2366 (0.4%)
3	K	0.62	0/1653	0.87	6/2245 (0.3%)
3	L	0.73	0/1653	0.89	10/2245 (0.4%)
4	P	0.70	0/110	1.07	1/148 (0.7%)
4	Q	0.62	0/110	0.75	0/148
All	All	0.74	6/7918 (0.1%)	0.91	39/10767 (0.4%)

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
2	M	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	GLU	CD-OE2	-6.12	1.19	1.25
1	B	32	GLU	CD-OE2	-6.05	1.19	1.25
1	A	32	GLU	CD-OE1	-5.74	1.19	1.25
1	B	32	GLU	CD-OE1	-5.47	1.19	1.25
2	H	211	GLU	CD-OE2	-5.10	1.20	1.25
2	M	211	GLU	CD-OE2	-5.04	1.20	1.25

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	213	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	32	GLU	OE1-CD-OE2	-8.41	113.21	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	164	TRP	CA-CB-CG	8.21	129.30	113.70
2	H	213	ARG	NE-CZ-NH2	8.16	124.38	120.30
3	L	166	ASP	CB-CG-OD2	7.95	125.45	118.30
2	M	177	LEU	CA-CB-CG	7.94	133.57	115.30
4	P	13	LEU	CA-CB-CG	7.70	133.01	115.30
2	H	177	LEU	CA-CB-CG	7.68	132.96	115.30
2	M	213	ARG	NE-CZ-NH2	-7.48	116.56	120.30
2	M	101	ASP	CB-CG-OD2	7.40	124.96	118.30
3	K	166	ASP	CB-CG-OD2	7.32	124.88	118.30
2	H	213	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	B	32	GLU	OE1-CD-OE2	-6.62	115.36	123.30
3	L	171	ASP	CB-CG-OD2	6.53	124.18	118.30
2	H	173	ASP	CB-CG-OD2	6.49	124.14	118.30
3	K	171	ASP	CB-CG-OD2	6.42	124.08	118.30
3	K	185	ASP	CB-CG-OD2	6.32	123.99	118.30
3	K	152	ASP	CB-CG-OD2	6.31	123.98	118.30
2	M	211	GLU	OE1-CD-OE2	-6.21	115.85	123.30
1	A	52	ASP	CB-CG-OD2	6.20	123.88	118.30
3	L	111	ASP	CB-CG-OD1	6.13	123.82	118.30
3	L	185	ASP	CB-CG-OD2	6.13	123.82	118.30
2	M	61	ASP	CB-CG-OD2	6.11	123.80	118.30
2	H	18	VAL	CB-CA-C	-6.05	99.91	111.40
2	H	61	ASP	CB-CG-OD2	5.84	123.55	118.30
3	K	84	ASP	CB-CG-OD2	5.83	123.54	118.30
2	H	101	ASP	CB-CG-OD2	5.81	123.53	118.30
3	L	182	LEU	CA-CB-CG	5.68	128.36	115.30
2	M	213	ARG	N-CA-C	5.67	126.31	111.00
3	L	109	ARG	NE-CZ-NH2	-5.63	117.48	120.30
3	L	84	ASP	CB-CG-OD2	5.62	123.35	118.30
2	M	18	VAL	CB-CA-C	-5.52	100.91	111.40
1	B	41	ASP	CB-CG-OD2	5.49	123.24	118.30
3	L	152	ASP	CB-CG-OD2	5.48	123.23	118.30
3	L	168	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	45	ASP	CB-CG-OD2	5.20	122.98	118.30
3	L	58	ASP	CB-CG-OD2	5.19	122.97	118.30
2	M	173	ASP	CB-CG-OD2	5.15	122.94	118.30
2	H	211	GLU	OE1-CD-OE2	-5.03	117.26	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	213	ARG	Peptide

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	A	441	0	428	8	0
1	B	466	0	454	8	0
2	H	1686	0	1623	41	0
2	M	1686	0	1623	44	0
3	K	1616	0	1566	20	0
3	L	1616	0	1566	25	0
4	P	107	0	108	5	0
4	Q	107	0	108	0	0
5	A	41	0	0	6	0
5	B	29	0	0	6	0
5	H	103	0	0	7	0
5	K	45	0	0	9	1
5	L	94	0	0	9	1
5	M	73	0	0	8	0
5	P	7	0	0	1	0
5	Q	3	0	0	0	0
All	All	8120	0	7476	146	1

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 10.

All (146) 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:B:12:ILE:HG21	5:B:2017:HOH:O	1.07	1.25
1:A:13:ASN:HB3	5:A:2006:HOH:O	1.47	1.13
2:M:171:GLN:HG2	2:M:172:SER:N	1.67	1.05
2:H:171:GLN:HG2	2:H:172:SER:N	1.69	1.01
2:H:171:GLN:HG2	2:H:172:SER:H	1.23	1.00
2:M:171:GLN:HG2	2:M:172:SER:H	1.24	0.98
2:M:108:THR:HG22	5:M:2005:HOH:O	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:105:LYS:HE3	5:L:2072:HOH:O	1.67	0.92
2:H:108:THR:HG22	5:H:2010:HOH:O	1.69	0.91
3:K:158:ASN:HB3	5:K:2030:HOH:O	1.70	0.91
2:H:105:GLN:HE21	2:H:105:GLN:H	1.12	0.90
2:M:6:GLN:H	2:M:105:GLN:HE22	1.14	0.90
2:H:6:GLN:H	2:H:105:GLN:HE22	1.18	0.87
2:M:105:GLN:HE21	2:M:105:GLN:H	1.20	0.87
3:L:146:ASN:HB2	5:L:2056:HOH:O	1.75	0.85
1:A:58:THR:HG22	5:A:2036:HOH:O	1.78	0.84
3:K:105:LYS:HE3	5:K:2034:HOH:O	1.80	0.82
3:L:105:LYS:CE	5:L:2072:HOH:O	2.24	0.82
3:K:63:ARG:NH1	3:K:84:ASP:OD2	2.16	0.78
2:H:151:THR:HG22	5:H:2090:HOH:O	1.83	0.77
2:H:213:ARG:HB3	5:H:2099:HOH:O	1.85	0.76
4:P:13:LEU:O	5:P:2007:HOH:O	2.02	0.76
2:H:54:THR:HG21	5:H:2024:HOH:O	1.86	0.75
1:B:13:ASN:HB2	1:B:60:THR:HB	1.69	0.74
2:H:6:GLN:HE22	2:H:91:PHE:HA	1.57	0.70
2:M:156:SER:H	2:M:196:ASN:HD21	1.39	0.70
1:A:60:THR:CG2	5:A:2036:HOH:O	2.39	0.69
2:H:156:SER:H	2:H:196:ASN:HD21	1.41	0.68
1:B:41:ASP:HB3	5:M:2037:HOH:O	1.93	0.68
2:M:100(B):ARG:NE	5:M:2028:HOH:O	2.25	0.68
3:K:58:ASP:HB3	5:K:2006:HOH:O	1.93	0.68
1:A:20:GLU:OE2	5:A:2012:HOH:O	2.10	0.67
2:M:127:VAL:HG12	5:M:2072:HOH:O	1.94	0.67
3:K:161:LEU:HD11	2:M:169:VAL:HG22	1.77	0.67
2:M:2:VAL:HG11	2:M:102:TYR:CD2	2.30	0.66
2:H:127:VAL:HB	2:H:213:ARG:HG3	1.78	0.65
1:A:60:THR:HG23	5:A:2036:HOH:O	1.96	0.65
3:L:63:ARG:NH1	3:L:84:ASP:OD2	2.27	0.65
2:M:84:ASN:HB3	5:M:2017:HOH:O	1.97	0.64
1:A:13:ASN:HB2	1:A:60:THR:HB	1.78	0.64
2:M:2:VAL:CG1	2:M:102:TYR:CD2	2.81	0.64
2:M:2:VAL:HG11	2:M:102:TYR:CE2	2.33	0.64
2:M:54:THR:HG22	2:M:56:GLU:H	1.64	0.63
3:K:158:ASN:CB	5:K:2030:HOH:O	2.36	0.63
2:M:6:GLN:HE22	2:M:91:PHE:HA	1.63	0.62
2:H:81:GLN:HE21	2:H:82(A):ASN:HD21	1.47	0.62
3:L:108:LYS:HE3	5:L:2034:HOH:O	2.00	0.62
2:H:54:THR:HG22	2:H:56:GLU:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:109:ARG:HH11	3:K:109:ARG:HG3	1.65	0.62
3:K:105:LYS:CE	5:K:2034:HOH:O	2.42	0.61
2:H:37:MET:HE3	2:H:47:TRP:HA	1.84	0.60
2:M:37:MET:HE3	2:M:47:TRP:HA	1.82	0.60
4:P:3:VAL:HG22	4:P:12:THR:HB	1.84	0.58
2:M:213:ARG:HD2	5:M:2070:HOH:O	2.02	0.58
2:M:81:GLN:HE21	2:M:82(A):ASN:HD21	1.51	0.57
2:M:2:VAL:CG1	2:M:102:TYR:CE2	2.87	0.57
2:H:12:LYS:HE2	2:H:17:THR:O	2.05	0.56
2:H:205:LYS:HG2	5:H:2091:HOH:O	2.04	0.56
2:H:205:LYS:HB2	2:H:205:LYS:HZ3	1.71	0.56
2:H:213:ARG:HD3	5:H:2100:HOH:O	2.05	0.56
3:L:109:ARG:HG3	3:L:109:ARG:NH1	2.18	0.56
2:M:6:GLN:HE21	2:M:104:GLY:HA3	1.71	0.56
2:H:105:GLN:HE21	2:H:105:GLN:N	1.93	0.56
2:H:159:LEU:HD13	2:H:181:VAL:HG21	1.88	0.56
3:L:109:ARG:HG3	3:L:109:ARG:HH11	1.71	0.56
3:K:109:ARG:HG3	3:K:109:ARG:NH1	2.17	0.55
2:M:12:LYS:HE2	2:M:17:THR:O	2.07	0.54
2:H:205:LYS:HB2	2:H:205:LYS:NZ	2.23	0.54
4:P:1:HIS:ND1	4:P:1:HIS:N	2.51	0.53
5:K:2031:HOH:O	2:M:171:GLN:HB2	2.09	0.53
2:H:171:GLN:CG	2:H:172:SER:N	2.55	0.52
2:M:145:TYR:CE2	2:M:150:VAL:HG13	2.45	0.52
2:H:213:ARG:NH2	5:H:2100:HOH:O	2.38	0.52
3:L:4:ILE:HG22	5:L:2027:HOH:O	2.10	0.51
1:B:9:LYS:HE2	5:B:2002:HOH:O	2.11	0.51
3:K:4:ILE:C	3:K:4:ILE:HD13	2.32	0.50
2:H:66:ARG:NH1	2:H:86:ASP:OD1	2.45	0.49
2:H:6:GLN:OE1	2:H:107:THR:CG2	2.60	0.49
3:L:35:LEU:HD22	3:L:73:PHE:CD2	2.47	0.49
2:M:37:MET:CE	2:M:47:TRP:HA	2.42	0.49
2:H:171:GLN:CG	2:H:172:SER:H	2.11	0.49
2:M:37:MET:HE1	2:M:47:TRP:HD1	1.77	0.49
1:B:64:GLU:HG2	5:B:2029:HOH:O	2.12	0.49
1:A:60:THR:HG22	5:A:2036:HOH:O	2.07	0.49
2:H:37:MET:CE	2:H:47:TRP:HA	2.41	0.49
3:L:4:ILE:HD13	3:L:4:ILE:C	2.33	0.49
2:M:54:THR:HG22	2:M:56:GLU:HB2	1.93	0.49
1:B:24:LYS:HD2	5:B:2010:HOH:O	2.12	0.49
3:L:37:TRP:CE2	3:L:75:PHE:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:35:LEU:HG	3:K:36:ALA:N	2.29	0.48
3:K:161:LEU:CD1	2:M:169:VAL:HG22	2.44	0.48
2:M:205:LYS:HZ3	2:M:205:LYS:HB2	1.78	0.47
3:L:191:ASN:HB2	5:L:2082:HOH:O	2.13	0.47
2:M:2:VAL:HG12	2:M:102:TYR:CD2	2.48	0.47
3:K:31:ILE:HG12	3:K:92:GLN:HG3	1.96	0.47
4:P:3:VAL:CG2	4:P:12:THR:HB	2.45	0.47
2:H:6:GLN:OE1	2:H:107:THR:HG23	2.15	0.47
3:L:157:GLN:HE21	3:L:157:GLN:HB2	1.49	0.47
2:M:100(B):ARG:NH2	5:M:2024:HOH:O	2.48	0.47
3:K:161:LEU:HD12	5:K:2031:HOH:O	2.14	0.47
2:M:6:GLN:OE1	2:M:107:THR:CG2	2.63	0.47
2:M:105:GLN:H	2:M:105:GLN:NE2	2.00	0.47
3:K:31:ILE:HG12	3:K:92:GLN:CG	2.46	0.46
2:M:156:SER:H	2:M:196:ASN:ND2	2.10	0.46
2:H:169:VAL:HG22	3:L:161:LEU:HD11	1.97	0.46
3:L:31:ILE:HG12	3:L:92:GLN:CG	2.46	0.46
3:L:95(B):PRO:HD2	5:L:2027:HOH:O	2.15	0.46
4:P:3:VAL:O	4:P:3:VAL:HG23	2.14	0.45
2:H:152:LEU:HA	2:H:196:ASN:O	2.17	0.45
3:K:191:ASN:HB2	5:K:2041:HOH:O	2.16	0.45
2:H:102:TYR:CD1	2:H:102:TYR:N	2.82	0.45
1:B:9:LYS:HD3	5:B:2006:HOH:O	2.17	0.45
2:H:164:HIS:HE1	3:L:139:ASN:HD21	1.65	0.45
3:L:137:LEU:CD2	3:L:197:ALA:HB2	2.47	0.45
3:L:105:LYS:HE2	5:L:2072:HOH:O	2.02	0.45
2:H:54:THR:HG22	2:H:56:GLU:HB2	1.97	0.45
3:L:108:LYS:CE	5:L:2034:HOH:O	2.61	0.45
2:M:37:MET:HE1	2:M:47:TRP:CD1	2.52	0.45
2:M:105:GLN:HE21	2:M:105:GLN:N	2.00	0.44
2:M:171:GLN:CG	2:M:172:SER:H	2.12	0.44
2:H:145:TYR:CE2	2:H:150:VAL:HG13	2.53	0.44
2:M:54:THR:CG2	2:M:56:GLU:HB2	2.48	0.43
2:M:6:GLN:NE2	2:M:92:CYS:H	2.15	0.43
2:H:6:GLN:HE21	2:H:104:GLY:HA3	1.84	0.43
2:H:156:SER:H	2:H:196:ASN:ND2	2.14	0.43
1:A:49:THR:OG1	1:A:58:THR:HB	2.19	0.42
1:B:24:LYS:NZ	5:B:2011:HOH:O	2.52	0.42
3:L:143:LYS:HB2	3:L:143:LYS:HE2	1.91	0.42
2:M:205:LYS:HB2	2:M:205:LYS:NZ	2.34	0.42
2:M:66:ARG:NH1	2:M:86:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:3:GLN:HG2	5:M:2002:HOH:O	2.19	0.42
3:L:31:ILE:HG12	3:L:92:GLN:HG3	2.01	0.42
3:K:164:TRP:N	3:K:164:TRP:CE3	2.88	0.42
2:M:6:GLN:OE1	2:M:107:THR:HG22	2.20	0.42
2:H:164:HIS:HE1	3:L:139:ASN:ND2	2.18	0.41
2:H:188:TRP:CG	2:H:189:PRO:HA	2.55	0.41
3:K:37:TRP:CE2	3:K:75:PHE:HB2	2.55	0.41
3:K:146:ASN:HB2	5:K:2024:HOH:O	2.19	0.41
2:H:52(A):THR:HA	2:H:71:LEU:HD11	2.03	0.41
3:L:35:LEU:HG	3:L:36:ALA:N	2.35	0.41
2:H:2:VAL:HG12	2:H:102:TYR:CD2	2.55	0.41
2:M:188:TRP:CG	2:M:189:PRO:HA	2.56	0.41
2:H:6:GLN:NE2	2:H:92:CYS:H	2.19	0.40
3:K:63:ARG:HH12	3:K:84:ASP:CG	2.17	0.40
3:L:185:ASP:O	3:L:189:ARG:HG3	2.21	0.40
2:M:72:GLU:HG2	2:M:75:ALA:HB3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:2045:HOH:O	5:L:2019:HOH:O[2_655]	2.17	0.03

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	A	56/63 (89%)	55 (98%)	1 (2%)	0	100	100
1	B	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
2	H	214/225 (95%)	209 (98%)	4 (2%)	1 (0%)	29	31
2	M	214/225 (95%)	207 (97%)	6 (3%)	1 (0%)	29	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	210/213 (99%)	205 (98%)	5 (2%)	0	100	100
3	L	210/213 (99%)	203 (97%)	7 (3%)	0	100	100
4	P	11/13 (85%)	11 (100%)	0	0	100	100
4	Q	11/13 (85%)	11 (100%)	0	0	100	100
All	All	984/1028 (96%)	958 (97%)	24 (2%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	41	PRO
2	M	41	PRO

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	A	47/52 (90%)	44 (94%)	3 (6%)	17	20
1	B	50/52 (96%)	47 (94%)	3 (6%)	19	22
2	H	186/191 (97%)	168 (90%)	18 (10%)	8	7
2	M	186/191 (97%)	166 (89%)	20 (11%)	6	6
3	K	183/185 (99%)	146 (80%)	37 (20%)	1	1
3	L	183/185 (99%)	150 (82%)	33 (18%)	1	1
4	P	13/13 (100%)	10 (77%)	3 (23%)	1	0
4	Q	13/13 (100%)	11 (85%)	2 (15%)	2	2
All	All	861/882 (98%)	742 (86%)	119 (14%)	3	3

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	12	ILE

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Mol	Chain	Res	Type
1	A	60	THR
1	B	6	THR
1	B	12	ILE
1	B	60	THR
2	H	18	VAL
2	H	37	MET
2	H	54	THR
2	H	72	GLU
2	H	83	LYS
2	H	100(B)	ARG
2	H	105	GLN
2	H	107	THR
2	H	109	LEU
2	H	115	LYS
2	H	141	LEU
2	H	151	THR
2	H	171	GLN
2	H	172	SER
2	H	177	LEU
2	H	190	SER
2	H	205	LYS
2	H	213	ARG
3	K	4	ILE
3	K	5	VAL
3	K	7	THR
3	K	9	THR
3	K	10	PRO
3	K	13	GLN
3	K	21	VAL
3	K	24	THR
3	K	26	LEU
3	K	31	ILE
3	K	35	LEU
3	K	41	LYS
3	K	44	LYS
3	K	45	SER
3	K	49	LEU
3	K	63	ARG
3	K	69	SER
3	K	72	LYS
3	K	74	SER
3	K	79	SER

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Mol	Chain	Res	Type
3	K	81	GLN
3	K	92	GLN
3	K	97	THR
3	K	105	LYS
3	K	106(A)	GLU
3	K	108	LYS
3	K	109	ARG
3	K	143	LYS
3	K	154	LYS
3	K	157	GLN
3	K	158	ASN
3	K	164	TRP
3	K	169	SER
3	K	170	LYS
3	K	185	ASP
3	K	192	SER
3	K	207	VAL
3	L	4	ILE
3	L	5	VAL
3	L	7	THR
3	L	9	THR
3	L	13	GLN
3	L	21	VAL
3	L	24	THR
3	L	26	LEU
3	L	31	ILE
3	L	35	LEU
3	L	44	LYS
3	L	45	SER
3	L	49	LEU
3	L	63	ARG
3	L	69	SER
3	L	72	LYS
3	L	74	SER
3	L	79	SER
3	L	81	GLN
3	L	92	GLN
3	L	97	THR
3	L	106(A)	GLU
3	L	108	LYS
3	L	109	ARG
3	L	143	LYS

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Mol	Chain	Res	Type
3	L	154	LYS
3	L	157	GLN
3	L	158	ASN
3	L	169	SER
3	L	170	LYS
3	L	185	ASP
3	L	192	SER
3	L	207	VAL
2	M	18	VAL
2	M	37	MET
2	M	54	THR
2	M	72	GLU
2	M	83	LYS
2	M	100(B)	ARG
2	M	105	GLN
2	M	107	THR
2	M	109	LEU
2	M	115	LYS
2	M	134	SER
2	M	141	LEU
2	M	151	THR
2	M	171	GLN
2	M	172	SER
2	M	177	LEU
2	M	186	SER
2	M	196	ASN
2	M	205	LYS
2	M	213	ARG
4	P	1	HIS
4	P	8	LYS
4	P	13	LEU
4	Q	10	GLN
4	Q	13	LEU

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

Mol	Chain	Res	Type
2	H	6	GLN
2	H	82(A)	ASN
2	H	105	GLN
2	H	164	HIS
2	H	196	ASN

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Mol	Chain	Res	Type
3	K	13	GLN
3	K	139	ASN
3	K	157	GLN
3	K	211	ASN
3	L	13	GLN
3	L	139	ASN
3	L	157	GLN
3	L	211	ASN
2	M	6	GLN
2	M	82(A)	ASN
2	M	105	GLN
2	M	164	HIS
2	M	196	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.