



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2025 – 01:40 PM JST

PDB ID : 8ZUA
Title : The complex structure of MPXV M1R and neutralizing antibody A138
Authors : Ge, J.W.
Deposited on : 2024-06-08
Resolution : 3.49 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)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

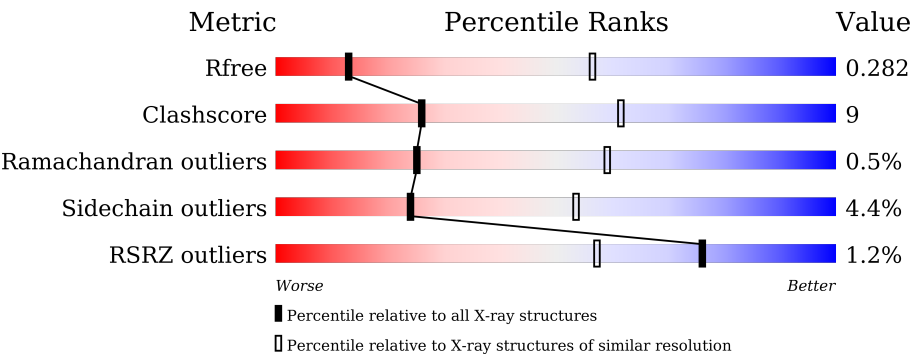
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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}	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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	A	218	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>74%26%</div></div>
1	B	218	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>78%18%.•</div></div>
1	E	218	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>83%15%.•</div></div>
1	J	218	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>79%18%.•</div></div>
2	C	187	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>68%19%.•11%</div></div>
2	F	187	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>61%26%.•11%</div></div>

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Mol	Chain	Length	Quality of chain
2	H	187	<div><div><div>%</div><div><div></div><div>65%</div><div>24%</div><div>• 11%</div></div></div></div>
2	K	187	<div><div><div></div><div>66%</div><div>21%</div><div>• 11%</div></div></div>
3	D	213	<div><div><div>%</div><div><div></div><div>77%</div><div>17%</div><div>7%</div></div></div></div>
3	G	213	<div><div><div>2%</div><div><div></div><div>75%</div><div>17%</div><div>• 7%</div></div></div></div>
3	I	213	<div><div><div>2%</div><div><div></div><div>73%</div><div>19%</div><div>• 7%</div></div></div></div>
3	L	213	<div><div><div>4%</div><div><div></div><div>66%</div><div>25%</div><div>• 7%</div></div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17537 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 A138 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1634	1030	275	323	6			
1	B	218	Total	C	N	O	S	0	0	0
			1618	1022	268	322	6			
1	E	218	Total	C	N	O	S	0	0	0
			1634	1030	275	323	6			
1	J	217	Total	C	N	O	S	0	0	0
			1621	1022	271	322	6			

- Molecule 2 is a protein called Entry-fusion complex associated protein OPG095.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	167	Total	C	N	O	S	0	0	0
			1247	766	210	261	10			
2	C	167	Total	C	N	O	S	0	0	0
			1253	769	213	261	10			
2	H	167	Total	C	N	O	S	0	0	0
			1249	767	213	259	10			
2	K	167	Total	C	N	O	S	0	0	0
			1243	764	210	259	10			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	146	MET	LEU	conflict	UNP M1LBP0
F	182	HIS	-	expression tag	UNP M1LBP0
F	183	HIS	-	expression tag	UNP M1LBP0
F	184	HIS	-	expression tag	UNP M1LBP0
F	185	HIS	-	expression tag	UNP M1LBP0
F	186	HIS	-	expression tag	UNP M1LBP0
F	187	HIS	-	expression tag	UNP M1LBP0
C	146	MET	LEU	conflict	UNP M1LBP0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	182	HIS	-	expression tag	UNP M1LBP0
C	183	HIS	-	expression tag	UNP M1LBP0
C	184	HIS	-	expression tag	UNP M1LBP0
C	185	HIS	-	expression tag	UNP M1LBP0
C	186	HIS	-	expression tag	UNP M1LBP0
C	187	HIS	-	expression tag	UNP M1LBP0
H	146	MET	LEU	conflict	UNP M1LBP0
H	182	HIS	-	expression tag	UNP M1LBP0
H	183	HIS	-	expression tag	UNP M1LBP0
H	184	HIS	-	expression tag	UNP M1LBP0
H	185	HIS	-	expression tag	UNP M1LBP0
H	186	HIS	-	expression tag	UNP M1LBP0
H	187	HIS	-	expression tag	UNP M1LBP0
K	146	MET	LEU	conflict	UNP M1LBP0
K	182	HIS	-	expression tag	UNP M1LBP0
K	183	HIS	-	expression tag	UNP M1LBP0
K	184	HIS	-	expression tag	UNP M1LBP0
K	185	HIS	-	expression tag	UNP M1LBP0
K	186	HIS	-	expression tag	UNP M1LBP0
K	187	HIS	-	expression tag	UNP M1LBP0

- Molecule 3 is a protein called A138 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	198	Total 1508	C 944	N 253	O 307	S 4	0	0	0
3	D	199	Total 1514	C 947	N 254	O 309	S 4	0	0	0
3	I	199	Total 1508	C 944	N 251	O 309	S 4	0	0	0
3	L	199	Total 1508	C 944	N 251	O 309	S 4	0	0	0

- Molecule 1: A138 heavy chain





- Molecule 2: Entry-fusion complex associated protein OPG095



- Molecule 2: Entry-fusion complex associated protein OPG095



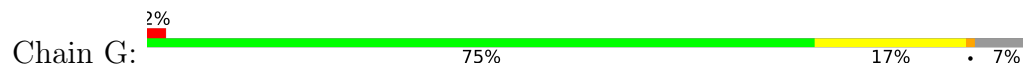
- Molecule 2: Entry-fusion complex associated protein OPG095

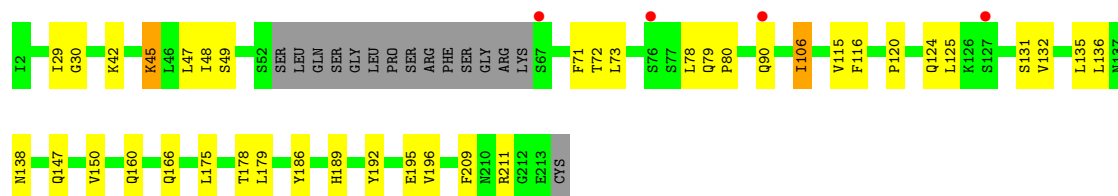


- Molecule 2: Entry-fusion complex associated protein OPG095

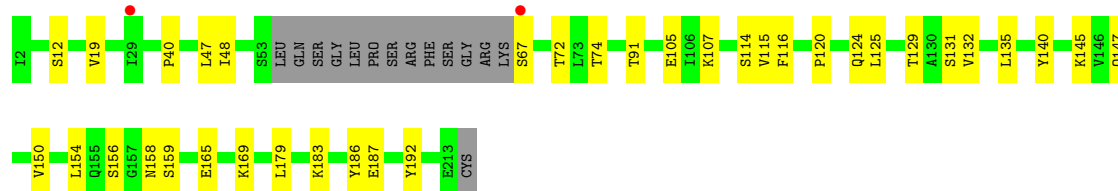
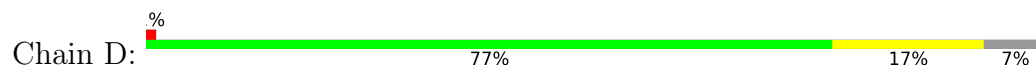


- Molecule 3: A138 light chain

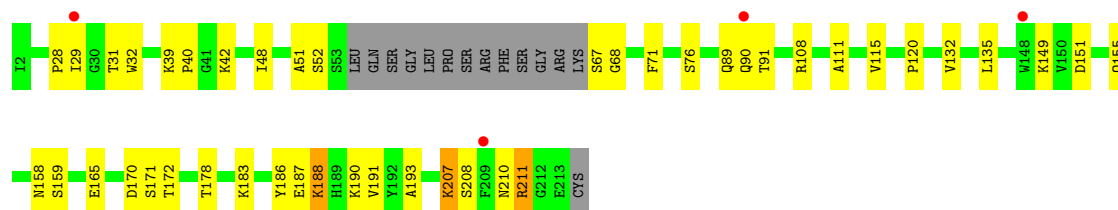




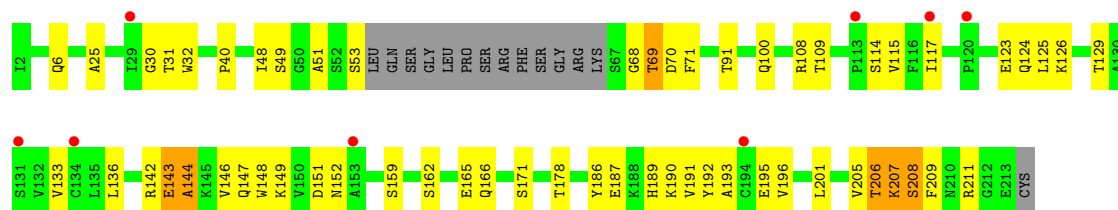
• Molecule 3: A138 light chain



• Molecule 3: A138 light chain



• Molecule 3: A138 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.39Å 136.68Å 123.77Å 90.00° 96.55° 90.00°	Depositor
Resolution (Å)	46.67 – 3.49 46.67 – 3.49	Depositor EDS
% Data completeness (in resolution range)	97.1 (46.67-3.49) 97.3 (46.67-3.49)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.237 , 0.286 0.238 , 0.282	Depositor DCC
R_{free} test set	1603 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	64.3	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	17537	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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	0.39	0/1673	0.69	0/2277
1	B	0.41	0/1657	0.68	0/2258
1	E	0.40	0/1673	0.63	0/2277
1	J	0.39	0/1660	0.68	0/2260
2	C	0.37	0/1266	0.65	0/1718
2	F	0.34	0/1260	0.61	0/1711
2	H	0.41	0/1262	0.71	0/1713
2	K	0.39	0/1256	0.65	0/1706
3	D	0.37	0/1545	0.64	0/2101
3	G	0.38	0/1539	0.65	0/2093
3	I	0.37	0/1539	0.68	0/2094
3	L	0.41	0/1539	0.70	0/2094
All	All	0.39	0/17869	0.67	0/24302

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	38	ARG	Sidechain

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	A	1634	0	1596	36	0
1	B	1618	0	1568	36	0
1	E	1634	0	1596	22	0
1	J	1621	0	1576	29	1
2	C	1253	0	1233	25	0
2	F	1247	0	1222	31	1
2	H	1249	0	1229	30	0
2	K	1243	0	1218	22	0
3	D	1514	0	1476	26	0
3	G	1508	0	1471	26	0
3	I	1508	0	1465	28	0
3	L	1508	0	1465	37	0
All	All	17537	0	17115	323	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 9.

All (323) 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)
3:I:28:PRO:HB3	3:I:67:SER:HA	1.48	0.93
1:A:34:MET:HB3	1:A:79:LEU:HD22	1.70	0.72
3:I:151:ASP:HA	3:I:191:VAL:HB	1.72	0.71
1:A:151:ASP:OD1	1:A:178:GLN:NE2	2.24	0.71
2:K:58:SER:OG	2:K:64:GLN:NE2	2.25	0.70
2:C:8:GLN:HA	2:C:11:VAL:HG22	1.72	0.70
2:H:13:THR:O	2:H:17:ARG:HG3	1.92	0.70
2:H:17:ARG:NH2	2:H:74:GLU:OE1	2.25	0.69
3:L:187:GLU:HG2	3:L:211:ARG:NH1	2.08	0.69
2:C:133:ILE:HG21	2:C:168:THR:HG21	1.74	0.68
3:D:145:LYS:HE3	3:D:147:GLN:HG3	1.76	0.68
2:H:100:SER:O	2:H:104:VAL:HG13	1.94	0.68
3:L:195:GLU:HB2	3:L:206:THR:HG23	1.74	0.68
2:C:42:TYR:HB2	2:C:132:ILE:HG22	1.76	0.68
1:J:105:TYR:O	3:L:91:THR:HB	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ARG:NH1	1:B:46:GLU:OE1	2.27	0.67
1:E:149:VAL:HB	1:E:185:LEU:HB3	1.76	0.66
3:D:125:LEU:HD21	3:D:186:TYR:HD2	1.60	0.66
2:C:28:ALA:HB2	2:C:58:SER:HB3	1.77	0.66
3:D:120:PRO:HD3	3:D:132:VAL:HG22	1.75	0.66
3:I:31:THR:H	3:I:52:SER:HB3	1.60	0.65
2:F:8:GLN:HA	2:F:11:VAL:HG22	1.77	0.65
1:A:8:GLY:O	1:A:18:LEU:HD12	1.98	0.64
2:K:50:ASN:HB3	2:K:145:ASN:OD1	1.98	0.64
3:I:32:TRP:HB3	3:I:91:THR:HG22	1.80	0.63
1:E:22:CYS:HB3	1:E:79:LEU:HB3	1.80	0.63
1:E:104:ASN:HD22	3:I:51:ALA:HB2	1.63	0.63
1:J:57:THR:HG21	2:K:55:ASN:ND2	2.14	0.63
1:B:100:GLU:HB2	1:B:103:SER:HB3	1.80	0.63
3:D:124:GLN:HG2	3:D:129:THR:O	1.99	0.62
2:K:165:GLN:O	2:K:169:LYS:HG2	2.00	0.62
2:H:122:VAL:HG22	2:H:155:LYS:HG2	1.82	0.62
2:K:14:LEU:HD21	2:K:163:LEU:HD21	1.80	0.62
1:J:40:ALA:HB1	1:J:41:PRO:HD2	1.82	0.61
2:K:28:ALA:HB2	2:K:58:SER:HB3	1.83	0.61
2:F:28:ALA:HB2	2:F:58:SER:HB3	1.83	0.61
3:D:116:PHE:HD2	3:D:135:LEU:HD23	1.66	0.61
3:L:187:GLU:HG2	3:L:211:ARG:HH12	1.63	0.61
1:J:98:ARG:HE	1:J:108:ASP:HB2	1.67	0.60
3:I:193:ALA:HA	3:I:208:SER:HA	1.82	0.60
3:G:189:HIS:O	3:G:211:ARG:HD3	2.02	0.59
2:H:116:CYS:HA	2:H:121:VAL:HG21	1.83	0.59
3:L:125:LEU:HD21	3:L:186:TYR:CD2	2.38	0.59
2:H:90:MET:SD	2:H:170:ALA:HB2	2.43	0.59
3:G:79:GLN:HG3	3:G:80:PRO:HD2	1.85	0.59
3:I:120:PRO:HD3	3:I:132:VAL:HG22	1.83	0.58
2:F:43:ILE:O	2:F:44:ARG:C	2.41	0.58
3:L:193:ALA:HB1	3:L:206:THR:HG22	1.85	0.58
1:B:27:PHE:CE2	1:B:98:ARG:HD3	2.37	0.58
3:I:108:ARG:NH1	3:I:111:ALA:HB2	2.19	0.58
3:G:73:LEU:HD11	3:I:48:ILE:HD11	1.86	0.57
1:A:129:PHE:CD2	3:G:124:GLN:HG3	2.39	0.57
2:H:122:VAL:HG13	2:H:155:LYS:HE3	1.87	0.57
1:A:61:ALA:O	1:A:65:LYS:HB2	2.05	0.57
1:B:51:ILE:HD11	1:B:70:ILE:HG12	1.87	0.57
3:I:149:LYS:HB2	3:I:193:ALA:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:SER:OG	1:A:21:SER:OG	2.23	0.57
2:F:13:THR:O	2:F:17:ARG:HG2	2.05	0.56
1:A:207:HIS:HD2	1:A:209:PRO:HD2	1.70	0.56
1:J:83:MET:HE1	1:J:116:VAL:HG21	1.86	0.56
1:A:207:HIS:CD2	1:A:209:PRO:HD2	2.39	0.56
1:B:51:ILE:HG23	1:B:58:ILE:HG12	1.87	0.56
2:H:14:LEU:HD21	2:H:163:LEU:HD11	1.88	0.56
2:K:8:GLN:HA	2:K:11:VAL:HG22	1.87	0.56
1:A:143:ALA:HB3	1:A:191:VAL:HG23	1.88	0.56
3:G:45:LYS:HE2	3:I:76:SER:HB2	1.88	0.56
1:B:51:ILE:CG2	1:B:58:ILE:HG12	2.37	0.55
3:L:124:GLN:HG2	3:L:129:THR:O	2.07	0.55
2:K:48:GLY:O	2:K:143:PRO:HB2	2.06	0.55
3:L:69:THR:OG1	3:L:70:ASP:N	2.39	0.55
2:H:28:ALA:HB2	2:H:58:SER:OG	2.06	0.55
2:F:35:ASP:HB2	2:F:152:GLY:O	2.07	0.55
1:B:52:SER:O	1:B:72:ARG:NH1	2.40	0.55
3:L:147:GLN:HB2	3:L:195:GLU:O	2.07	0.55
1:A:69:THR:OG1	1:A:82:GLN:HB3	2.08	0.54
1:A:91:THR:HG23	1:A:117:THR:HA	1.89	0.54
2:F:116:CYS:O	2:F:155:LYS:HB2	2.08	0.54
2:C:6:SER:N	2:C:9:THR:HG1	2.05	0.54
1:J:40:ALA:O	1:J:42:GLY:N	2.41	0.54
3:L:148:TRP:HD1	3:L:159:SER:HG	1.53	0.54
2:C:13:THR:O	2:C:17:ARG:HG2	2.09	0.54
1:E:135:SER:O	1:E:136:LYS:C	2.46	0.54
1:J:98:ARG:O	1:J:107:PHE:HA	2.08	0.53
2:F:14:LEU:HD21	2:F:163:LEU:HD21	1.90	0.53
2:C:65:LEU:HD11	2:C:112:VAL:HG12	1.89	0.53
2:K:100:SER:O	2:K:104:VAL:HG23	2.08	0.53
1:A:101:ALA:HA	1:A:105:TYR:CE1	2.43	0.53
1:B:137:SER:HA	3:D:116:PHE:HD1	1.74	0.53
2:C:131:VAL:HG11	2:C:148:PHE:CE2	2.43	0.53
1:J:103:SER:OG	1:J:108:ASP:OD1	2.21	0.53
1:B:138:THR:OG1	3:D:115:VAL:O	2.24	0.53
3:D:125:LEU:HD21	3:D:186:TYR:CD2	2.43	0.53
2:H:14:LEU:HD13	2:H:75:THR:OG1	2.09	0.53
2:K:22:LEU:HD11	2:K:151:THR:HG22	1.91	0.53
1:A:133:PRO:HD3	1:A:218:VAL:HG12	1.90	0.53
3:L:6:GLN:H	3:L:100:GLN:HG2	1.74	0.53
2:C:30:ALA:HA	2:C:55:ASN:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:183:LYS:HG2	3:I:187:GLU:HG3	1.89	0.52
1:J:143:ALA:HB3	1:J:191:VAL:O	2.09	0.52
1:B:6:GLU:OE2	1:B:111:GLY:HA3	2.10	0.52
2:F:51:ILE:HG12	2:F:146:MET:HB2	1.91	0.52
3:I:29:ILE:HB	3:I:90:GLN:HE21	1.75	0.51
1:J:40:ALA:HB3	1:J:43:LYS:HB2	1.93	0.51
1:A:104:ASN:O	1:A:105:TYR:C	2.48	0.51
1:B:34:MET:HB3	1:B:79:LEU:HD22	1.91	0.51
1:B:51:ILE:HG12	1:B:70:ILE:HD13	1.92	0.51
1:B:105:TYR:O	3:D:91:THR:HB	2.10	0.51
1:B:51:ILE:CD1	1:B:70:ILE:HG12	2.41	0.51
3:L:192:TYR:HB2	3:L:209:PHE:CE1	2.46	0.51
2:F:45:GLN:HG2	2:F:134:ASP:O	2.11	0.51
2:F:46:ASN:OD1	2:F:47:HIS:N	2.44	0.51
1:J:17:SER:HA	1:J:83:MET:O	2.10	0.51
1:B:133:PRO:HD3	1:B:218:VAL:HG12	1.93	0.50
2:F:47:HIS:O	2:F:138:GLY:N	2.45	0.50
1:E:52:SER:O	1:E:72:ARG:NH1	2.45	0.50
3:L:143:GLU:O	3:L:144:ALA:HB2	2.12	0.50
1:E:143:ALA:HB2	1:E:193:SER:HA	1.94	0.50
3:G:116:PHE:HD2	3:G:135:LEU:HD23	1.76	0.49
3:G:147:GLN:HG2	3:G:195:GLU:HB3	1.93	0.49
2:H:109:GLU:HB3	2:H:113:LYS:NZ	2.27	0.49
2:K:90:MET:SD	2:K:170:ALA:HB2	2.52	0.49
2:F:164:MET:O	2:F:168:THR:HG23	2.12	0.49
3:G:106:ILE:O	3:G:166:GLN:NE2	2.33	0.49
2:F:91:PHE:CD2	2:F:99:THR:HG21	2.48	0.49
2:C:131:VAL:HG11	2:C:148:PHE:CZ	2.48	0.49
3:I:115:VAL:HA	3:I:135:LEU:O	2.13	0.49
2:K:88:PRO:HA	2:K:99:THR:HG23	1.93	0.49
1:E:17:SER:HA	1:E:83:MET:O	2.13	0.49
2:H:22:LEU:HD21	2:H:64:GLN:HA	1.94	0.49
1:B:137:SER:HA	3:D:116:PHE:CD1	2.48	0.49
2:C:42:TYR:O	2:C:132:ILE:HA	2.12	0.49
3:I:40:PRO:HB3	3:I:165:GLU:HG3	1.95	0.49
1:E:143:ALA:HB3	1:E:191:VAL:HG23	1.94	0.48
1:B:126:PRO:HB3	1:B:152:TYR:HB3	1.95	0.48
1:J:155:GLU:N	1:J:156:PRO:HD2	2.28	0.48
3:L:149:LYS:HD3	3:L:152:ASN:HA	1.95	0.48
1:A:51:ILE:HG13	1:A:58:ILE:HG12	1.94	0.48
1:A:83:MET:HE1	1:A:116:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:43:ILE:HB	2:H:46:ASN:HB2	1.94	0.48
3:L:40:PRO:HG3	3:L:165:GLU:OE1	2.14	0.48
1:A:145:LEU:HB2	1:A:218:VAL:HG11	1.94	0.48
2:H:109:GLU:O	2:H:113:LYS:HG3	2.14	0.48
3:D:183:LYS:HE3	3:D:187:GLU:OE2	2.13	0.48
3:I:31:THR:HA	3:I:71:PHE:HZ	1.79	0.48
1:A:136:LYS:HE2	3:G:209:PHE:HB3	1.96	0.48
1:B:83:MET:HB3	1:B:86:LEU:HD21	1.96	0.48
1:E:12:VAL:HB	1:E:18:LEU:HD21	1.96	0.48
1:J:138:THR:HG21	3:L:115:VAL:H	1.79	0.48
3:L:190:LYS:HA	3:L:211:ARG:HB2	1.94	0.48
2:F:91:PHE:HE1	2:F:166:LEU:HD11	1.79	0.47
2:H:76:TYR:HE1	2:H:87:VAL:HG21	1.79	0.47
1:J:97:ALA:HB1	1:J:107:PHE:HB3	1.96	0.47
1:J:136:LYS:HE2	1:J:136:LYS:HB2	1.55	0.47
2:K:100:SER:N	2:K:103:THR:OG1	2.43	0.47
2:H:144:THR:HG22	2:H:146:MET:HG3	1.96	0.47
3:L:151:ASP:OD2	3:L:189:HIS:HB3	2.13	0.47
2:F:91:PHE:HZ	2:F:108:PHE:HB2	1.78	0.47
2:H:76:TYR:OH	2:H:101:VAL:HG13	2.14	0.47
3:I:170:ASP:O	3:I:172:THR:HG23	2.15	0.47
1:J:61:ALA:O	1:J:65:LYS:HB2	2.14	0.47
1:J:4:LEU:HB3	1:J:22:CYS:SG	2.55	0.47
3:L:108:ARG:HG2	3:L:109:THR:O	2.15	0.47
1:A:142:THR:HG22	1:A:191:VAL:O	2.15	0.47
1:B:12:VAL:HG11	1:B:86:LEU:HD12	1.97	0.47
1:B:51:ILE:HG12	1:B:70:ILE:CD1	2.45	0.47
1:B:139:SER:HB3	3:D:114:SER:OG	2.15	0.47
1:J:134:SER:C	1:J:136:LYS:H	2.17	0.47
1:A:43:LYS:HE2	1:A:43:LYS:HB3	1.61	0.47
1:A:33:TYR:CD1	1:A:52:SER:HA	2.49	0.47
2:F:133:ILE:HG21	2:F:168:THR:HG21	1.96	0.47
3:G:160:GLN:O	3:G:178:THR:N	2.48	0.47
1:B:202:ILE:HD13	1:B:217:LYS:HA	1.96	0.47
3:D:150:VAL:HG22	3:D:192:TYR:CD2	2.50	0.46
1:E:83:MET:HB3	1:E:86:LEU:HD21	1.97	0.46
3:L:193:ALA:HA	3:L:208:SER:HB3	1.96	0.46
2:F:46:ASN:ND2	2:F:49:CYS:O	2.48	0.46
3:G:120:PRO:HD3	3:G:132:VAL:HG22	1.97	0.46
1:J:159:VAL:HG21	1:J:185:LEU:HD11	1.96	0.46
1:A:204:ASN:ND2	1:A:215:ASP:OD1	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:GLY:O	1:E:18:LEU:HD12	2.16	0.46
2:K:70:SER:O	2:K:74:GLU:HG3	2.15	0.46
2:F:116:CYS:HA	2:F:121:VAL:HG21	1.96	0.46
2:F:48:GLY:HA2	2:F:143:PRO:HB3	1.97	0.46
3:D:131:SER:HA	3:D:179:LEU:O	2.16	0.46
1:B:145:LEU:HD21	1:B:201:TYR:CD2	2.51	0.46
3:G:136:LEU:HB2	3:G:175:LEU:HB3	1.98	0.46
1:B:52:SER:HB3	1:B:57:THR:O	2.16	0.46
3:L:25:ALA:HB3	3:L:69:THR:HA	1.97	0.46
3:L:30:GLY:O	3:L:68:GLY:HA3	2.16	0.46
3:L:123:GLU:HA	3:L:126:LYS:HE2	1.96	0.46
3:L:133:VAL:HG22	3:L:178:THR:HG22	1.97	0.46
1:A:138:THR:HG21	3:G:115:VAL:HB	1.98	0.46
2:F:70:SER:O	2:F:74:GLU:HG3	2.16	0.46
2:K:8:GLN:O	2:K:11:VAL:HG22	2.15	0.46
1:B:105:TYR:OH	2:C:35:ASP:HA	2.16	0.45
1:A:36:TRP:HE1	1:A:79:LEU:HG	1.81	0.45
3:G:136:LEU:HD21	3:G:196:VAL:HG13	1.97	0.45
1:E:105:TYR:O	3:I:91:THR:OG1	2.34	0.45
1:E:148:LEU:HD12	1:E:185:LEU:O	2.16	0.45
1:J:103:SER:CB	1:J:108:ASP:OD1	2.64	0.45
2:F:117:ASN:OD1	2:F:155:LYS:HE3	2.17	0.45
2:C:91:PHE:CD2	2:C:99:THR:HG21	2.51	0.45
2:H:69:LEU:O	2:H:73:THR:HG23	2.16	0.45
2:K:51:ILE:HG12	2:K:146:MET:HB2	1.99	0.45
2:C:7:ILE:O	2:C:11:VAL:HG13	2.17	0.45
3:D:125:LEU:O	3:D:183:LYS:HD2	2.17	0.45
1:J:12:VAL:HG11	1:J:86:LEU:HD13	1.99	0.45
3:L:201:LEU:HD13	3:L:205:VAL:HG22	1.98	0.45
2:C:122:VAL:HG13	2:C:155:LYS:HD2	1.99	0.45
3:L:32:TRP:HB3	3:L:91:THR:OG1	2.16	0.45
3:L:207:LYS:HD2	3:L:207:LYS:HA	1.56	0.45
2:H:79:LEU:HD23	2:H:79:LEU:HA	1.77	0.45
2:H:109:GLU:HB3	2:H:113:LYS:HZ3	1.81	0.45
2:F:61:ALA:HB1	2:F:155:LYS:HD3	1.99	0.44
2:C:54:LYS:HB3	2:C:149:ILE:HD13	1.98	0.44
1:E:3:GLN:HA	1:E:109:TYR:HE2	1.81	0.44
3:L:48:ILE:HG22	3:L:49:SER:H	1.80	0.44
3:G:30:GLY:O	3:G:71:PHE:HZ	2.00	0.44
3:L:108:ARG:HG2	3:L:109:THR:N	2.33	0.44
1:A:53:ARG:HH11	1:A:101:ALA:HB1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:SER:CB	1:A:141:GLY:HA2	2.47	0.44
2:C:48:GLY:O	2:C:138:GLY:HA3	2.18	0.44
1:J:176:VAL:HG13	3:L:162:SER:OG	2.18	0.44
2:F:118:SER:O	2:F:122:VAL:HG23	2.16	0.44
3:G:72:THR:OG1	3:I:51:ALA:HB3	2.18	0.44
1:B:29:PHE:CE1	1:B:34:MET:HG3	2.53	0.44
3:D:145:LYS:HE3	3:D:147:GLN:CG	2.47	0.44
1:J:131:LEU:HB2	1:J:146:GLY:C	2.38	0.44
2:C:31:GLN:H	2:C:31:GLN:HG2	1.40	0.44
2:H:122:VAL:HG22	2:H:155:LYS:CG	2.48	0.44
1:J:22:CYS:HB3	1:J:79:LEU:HB3	2.00	0.44
2:F:38:ILE:HB	2:F:53:VAL:HG11	1.98	0.44
3:G:29:ILE:HG22	3:G:90:GLN:HE21	1.82	0.44
3:G:72:THR:OG1	1:E:104:ASN:ND2	2.51	0.44
1:J:40:ALA:HB1	1:J:41:PRO:CD	2.46	0.44
2:K:54:LYS:HA	2:K:54:LYS:HD3	1.85	0.44
2:K:76:TYR:O	2:K:79:LEU:HB2	2.18	0.44
2:K:118:SER:O	2:K:122:VAL:HG23	2.17	0.44
3:D:114:SER:HB3	3:D:116:PHE:CZ	2.53	0.44
3:I:207:LYS:HD3	3:I:207:LYS:HA	1.70	0.44
1:E:52:SER:HB2	2:H:37:GLU:OE1	2.18	0.43
3:I:155:GLN:HG3	3:I:158:ASN:OD1	2.17	0.43
3:L:31:THR:OG1	3:L:51:ALA:C	2.57	0.43
1:B:208:LYS:HB2	1:B:208:LYS:HE2	1.45	0.43
2:C:118:SER:O	2:C:122:VAL:HG23	2.18	0.43
3:D:40:PRO:HB3	3:D:165:GLU:HG3	2.00	0.43
1:J:207:HIS:CD2	1:J:209:PRO:HD2	2.53	0.43
3:L:31:THR:HA	3:L:71:PHE:HZ	1.83	0.43
1:B:18:LEU:HD12	1:B:18:LEU:HA	1.77	0.43
3:G:150:VAL:HG22	3:G:192:TYR:CD2	2.54	0.43
2:C:6:SER:OG	2:C:9:THR:HG23	2.18	0.43
2:C:134:ASP:N	2:C:134:ASP:OD1	2.51	0.43
3:I:31:THR:HG22	3:I:31:THR:O	2.19	0.43
2:K:20:SER:O	2:K:23:GLU:HG2	2.18	0.43
3:D:47:LEU:HD23	3:D:47:LEU:HA	1.75	0.43
3:D:74:THR:H	3:L:49:SER:HG	1.67	0.43
2:H:155:LYS:H	2:H:155:LYS:HD2	1.83	0.43
3:I:39:LYS:HE3	3:I:42:LYS:HD3	2.01	0.43
3:G:125:LEU:HA	3:G:125:LEU:HD23	1.63	0.43
2:F:54:LYS:HD3	2:F:54:LYS:HA	1.72	0.42
1:A:199:GLN:HG3	1:A:200:THR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:107:LYS:HG2	3:D:140:TYR:OH	2.18	0.42
1:J:177:LEU:HB2	1:J:183:TYR:CE1	2.53	0.42
1:A:188:VAL:HG21	3:G:135:LEU:HD22	2.00	0.42
1:B:8:GLY:O	1:B:18:LEU:HG	2.18	0.42
1:E:91:THR:HG23	1:E:117:THR:HA	2.02	0.42
1:A:148:LEU:HD12	1:A:185:LEU:O	2.19	0.42
3:I:89:GLN:HG2	3:I:90:GLN:O	2.20	0.42
3:D:169:LYS:HD2	3:D:169:LYS:HA	1.90	0.42
3:I:186:TYR:C	3:I:188:LYS:H	2.22	0.42
1:E:110:TRP:CD1	1:E:110:TRP:N	2.88	0.42
1:A:137:SER:HA	3:G:116:PHE:HD1	1.84	0.42
1:B:52:SER:OG	1:B:53:ARG:N	2.53	0.42
2:H:22:LEU:HD23	2:H:22:LEU:HA	1.88	0.42
1:A:100:GLU:OE1	1:A:103:SER:HB2	2.20	0.42
1:A:166:LEU:HD12	1:A:166:LEU:HA	1.91	0.42
2:F:91:PHE:HD2	2:F:99:THR:HG21	1.85	0.42
3:D:147:GLN:OE1	3:D:154:LEU:HD11	2.20	0.42
2:F:60:ASP:HB3	2:F:63:ALA:HB3	2.02	0.42
3:L:136:LEU:HD21	3:L:196:VAL:HG11	2.02	0.42
3:L:190:LYS:HG3	3:L:211:ARG:HB3	2.02	0.42
2:C:65:LEU:O	2:C:68:VAL:HG22	2.20	0.42
3:D:12:SER:HA	3:D:105:GLU:O	2.20	0.42
1:E:40:ALA:HB1	1:E:41:PRO:HD2	2.02	0.42
3:G:47:LEU:HD23	3:G:47:LEU:HA	1.81	0.41
1:B:28:THR:OG1	1:B:31:ASP:HB2	2.20	0.41
2:K:43:ILE:HA	2:K:133:ILE:O	2.20	0.41
1:A:149:VAL:HB	1:A:185:LEU:HB3	2.02	0.41
2:F:121:VAL:O	2:F:154:SER:OG	2.26	0.41
1:B:17:SER:HA	1:B:83:MET:O	2.20	0.41
1:B:91:THR:HG23	1:B:117:THR:HA	2.02	0.41
1:B:188:VAL:HG21	3:D:135:LEU:HD22	2.02	0.41
2:H:94:ALA:HB3	2:H:166:LEU:HD23	2.01	0.41
1:E:126:PRO:HD2	1:E:212:THR:OG1	2.20	0.41
2:H:91:PHE:CE2	2:H:97:ILE:HB	2.55	0.41
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.85	0.41
2:H:61:ALA:HB1	2:H:155:LYS:HD3	2.02	0.41
2:H:85:ALA:O	2:H:88:PRO:HD2	2.20	0.41
1:A:57:THR:HG21	2:F:55:ASN:ND2	2.36	0.41
1:J:166:LEU:HD12	1:J:166:LEU:HA	1.87	0.41
3:G:78:LEU:HD23	3:G:78:LEU:HA	1.85	0.41
2:C:65:LEU:HD11	2:C:112:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:LYS:HA	1:E:43:LYS:HD3	1.82	0.41
3:I:210:ASN:O	3:I:211:ARG:C	2.58	0.41
1:A:22:CYS:HB3	1:A:79:LEU:HB3	2.03	0.41
2:K:85:ALA:O	2:K:88:PRO:HD2	2.20	0.41
3:G:131:SER:HA	3:G:179:LEU:O	2.21	0.41
1:B:134:SER:HB3	1:B:136:LYS:HE3	2.03	0.41
1:E:33:TYR:CD1	1:E:52:SER:HA	2.56	0.41
3:I:108:ARG:HG3	3:I:171:SER:HB2	2.02	0.41
3:L:151:ASP:OD1	3:L:191:VAL:HB	2.20	0.41
3:D:19:VAL:O	3:D:74:THR:HA	2.21	0.40
3:L:166:GLN:HG3	3:L:171:SER:HA	2.02	0.40
3:G:186:TYR:HA	3:G:192:TYR:OH	2.21	0.40
2:C:17:ARG:HA	2:C:17:ARG:HD3	1.86	0.40
3:I:159:SER:HA	3:I:178:THR:O	2.21	0.40
2:F:61:ALA:HB1	2:F:155:LYS:CG	2.51	0.40
1:J:134:SER:C	1:J:136:LYS:N	2.75	0.40
1:B:35:SER:HA	1:B:50:SER:HA	2.04	0.40
2:H:135:GLU:O	2:H:168:THR:HB	2.22	0.40
2:F:57:CYS:SG	2:F:150:ASN:ND2	2.93	0.40
2:C:146:MET:HE1	2:C:167:THR:HG21	2.04	0.40
2:H:91:PHE:CD2	2:H:97:ILE:HB	2.56	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)
2:F:96:ASN:ND2	1:J:31:ASP:OD1[2_645]	1.88	0.32

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	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
1	B	216/218 (99%)	203 (94%)	12 (6%)	1 (0%)	25	59
1	E	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
1	J	215/218 (99%)	196 (91%)	17 (8%)	2 (1%)	14	49
2	C	165/187 (88%)	160 (97%)	5 (3%)	0	100	100
2	F	165/187 (88%)	159 (96%)	5 (3%)	1 (1%)	22	56
2	H	165/187 (88%)	159 (96%)	6 (4%)	0	100	100
2	K	165/187 (88%)	154 (93%)	8 (5%)	3 (2%)	7	35
3	D	195/213 (92%)	188 (96%)	7 (4%)	0	100	100
3	G	194/213 (91%)	188 (97%)	5 (3%)	1 (0%)	25	59
3	I	195/213 (92%)	190 (97%)	3 (2%)	2 (1%)	13	46
3	L	195/213 (92%)	180 (92%)	13 (7%)	2 (1%)	13	46
All	All	2302/2472 (93%)	2191 (95%)	99 (4%)	12 (0%)	25	59

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	140	PRO
2	F	44	ARG
3	G	138	ASN
1	B	51	ILE
3	I	68	GLY
3	I	211	ARG
1	J	41	PRO
1	J	156	PRO
3	L	142	ARG
2	K	143	PRO
3	L	144	ALA
2	K	142	SER

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	A	181/181 (100%)	176 (97%)	5 (3%)	38	65
1	B	178/181 (98%)	168 (94%)	10 (6%)	17	45
1	E	181/181 (100%)	173 (96%)	8 (4%)	24	53
1	J	179/181 (99%)	170 (95%)	9 (5%)	20	49
2	C	142/155 (92%)	133 (94%)	9 (6%)	15	42
2	F	141/155 (91%)	134 (95%)	7 (5%)	20	49
2	H	141/155 (91%)	133 (94%)	8 (6%)	17	45
2	K	140/155 (90%)	133 (95%)	7 (5%)	20	49
3	D	174/186 (94%)	168 (97%)	6 (3%)	32	60
3	G	173/186 (93%)	168 (97%)	5 (3%)	37	64
3	I	173/186 (93%)	170 (98%)	3 (2%)	56	75
3	L	173/186 (93%)	164 (95%)	9 (5%)	19	47
All	All	1976/2088 (95%)	1890 (96%)	86 (4%)	24	53

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	45	LEU
1	A	98	ARG
1	A	134	SER
1	A	198	THR
2	F	42	TYR
2	F	43	ILE
2	F	97	ILE
2	F	125	LYS
2	F	126	LEU
2	F	134	ASP
2	F	146	MET
3	G	42	LYS
3	G	45	LYS
3	G	48	ILE
3	G	49	SER
3	G	106	ILE
1	B	17	SER
1	B	18	LEU
1	B	35	SER
1	B	48	VAL
1	B	50	SER

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Mol	Chain	Res	Type
1	B	51	ILE
1	B	52	SER
1	B	57	THR
1	B	63	SER
1	B	208	LYS
2	C	31	GLN
2	C	36	ILE
2	C	125	LYS
2	C	131	VAL
2	C	132	ILE
2	C	137	TYR
2	C	142	SER
2	C	144	THR
2	C	146	MET
3	D	48	ILE
3	D	67	SER
3	D	72	THR
3	D	156	SER
3	D	158	ASN
3	D	159	SER
1	E	33	TYR
1	E	35	SER
1	E	100	GLU
1	E	134	SER
1	E	135	SER
1	E	136	LYS
1	E	142	THR
1	E	145	LEU
2	H	43	ILE
2	H	45	GLN
2	H	80	THR
2	H	84	LYS
2	H	95	LEU
2	H	153	SER
2	H	154	SER
2	H	155	LYS
3	I	188	LYS
3	I	190	LYS
3	I	207	LYS
1	J	38	ARG
1	J	135	SER
1	J	136	LYS

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Mol	Chain	Res	Type
1	J	138	THR
1	J	139	SER
1	J	142	THR
1	J	145	LEU
1	J	155	GLU
1	J	157	VAL
2	K	43	ILE
2	K	79	LEU
2	K	80	THR
2	K	96	ASN
2	K	142	SER
2	K	144	THR
2	K	155	LYS
3	L	53	SER
3	L	69	THR
3	L	114	SER
3	L	117	ILE
3	L	143	GLU
3	L	146	VAL
3	L	206	THR
3	L	207	LYS
3	L	208	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
2	F	129	GLN
2	H	64	GLN
2	H	83	GLN
3	I	137	ASN
1	J	104	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 [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

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	A	218/218 (100%)	-0.07	2 (0%) 81 64	28, 55, 80, 112	0
1	B	218/218 (100%)	0.05	4 (1%) 67 48	38, 63, 89, 115	0
1	E	218/218 (100%)	0.08	1 (0%) 87 75	38, 66, 121, 139	0
1	J	217/218 (99%)	0.18	1 (0%) 87 75	30, 66, 126, 149	0
2	C	167/187 (89%)	0.09	0 100 100	51, 75, 109, 139	0
2	F	167/187 (89%)	-0.06	1 (0%) 85 72	34, 57, 96, 130	0
2	H	167/187 (89%)	0.35	2 (1%) 76 57	51, 92, 131, 154	0
2	K	167/187 (89%)	0.12	0 100 100	41, 73, 115, 135	0
3	D	199/213 (93%)	0.04	2 (1%) 79 61	42, 66, 91, 99	0
3	G	198/213 (92%)	-0.00	4 (2%) 64 45	30, 56, 80, 89	0
3	I	199/213 (93%)	0.32	4 (2%) 64 45	41, 79, 118, 129	0
3	L	199/213 (93%)	0.45	8 (4%) 43 29	44, 88, 139, 157	0
All	All	2334/2472 (94%)	0.13	29 (1%) 76 57	28, 67, 121, 157	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	117	ILE	3.0
3	D	29	ILE	2.7
3	G	67	SER	2.6
3	I	90	GLN	2.6
1	B	33	TYR	2.5
2	H	142	SER	2.5
3	I	29	ILE	2.5
1	B	195	SER	2.4
3	I	209	PHE	2.3
3	L	134	CYS	2.3
3	L	29	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
3	L	153	ALA	2.3
2	H	170	ALA	2.3
3	G	127	SER	2.2
3	G	76	SER	2.2
3	D	67	SER	2.2
1	A	104	ASN	2.1
1	B	101	ALA	2.1
3	L	120	PRO	2.1
3	G	90	GLN	2.1
1	J	130	PRO	2.1
1	B	138	THR	2.1
1	E	141	GLY	2.1
3	L	113	PRO	2.1
3	I	148	TRP	2.0
2	F	119	SER	2.0
1	A	100	GLU	2.0
3	L	194	CYS	2.0
3	L	131	SER	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 monosaccharides 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.