



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:11 AM UTC

PDB ID : 2BM8 / pdb_00002bm8
Title : CmcI-N160 apo-structure
Authors : Oster, L.M.; Lester, D.R.; Terwisscha van Scheltinga, A.; Svenda, M.;
Genereux, C.; Andersson, I.
Deposited on : 2005-03-10
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

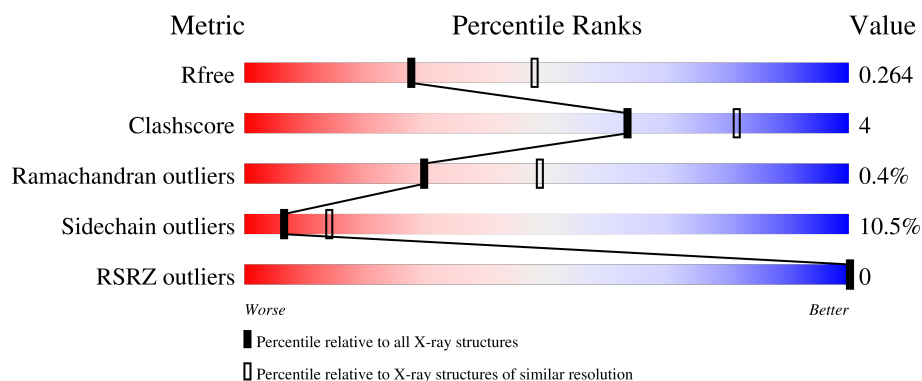
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	236	
1	B	236	
1	C	236	
1	D	236	
1	E	236	

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Mol	Chain	Length	Quality of chain
1	F	236	 82% 14% ..
1	G	236	 83% 12% ..
1	H	236	 83% 14% ..
1	I	236	 82% 15% ..
1	J	236	 83% 14% ..
1	K	236	 81% 15% ..
1	L	236	 81% 16% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23710 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 CEPHALOSPORIN HYDROXYLASE CMCI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	6	0	0
			1915	1219	331	353	12			
1	B	233	Total	C	N	O	S	0	0	0
			1920	1222	332	354	12			
1	C	232	Total	C	N	O	S	0	0	0
			1915	1219	331	353	12			
1	D	232	Total	C	N	O	S	0	0	0
			1915	1219	331	353	12			
1	E	233	Total	C	N	O	S	6	0	0
			1920	1222	332	354	12			
1	F	233	Total	C	N	O	S	0	0	0
			1920	1222	332	354	12			
1	G	232	Total	C	N	O	S	0	0	0
			1912	1218	330	352	12			
1	H	233	Total	C	N	O	S	0	0	0
			1920	1222	332	354	12			
1	I	232	Total	C	N	O	S	0	0	0
			1915	1219	331	353	12			
1	J	232	Total	C	N	O	S	0	0	0
			1915	1219	331	353	12			
1	K	231	Total	C	N	O	S	0	0	0
			1907	1215	329	351	12			
1	L	233	Total	C	N	O	S	0	0	0
			1919	1222	332	353	12			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLN	LEU	engineered mutation	UNP O85726
A	160	ASN	ASP	engineered mutation	UNP O85726
A	200	PHE	LEU	engineered mutation	UNP O85726
B	10	GLN	LEU	engineered mutation	UNP O85726
B	160	ASN	ASP	engineered mutation	UNP O85726

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Chain	Residue	Modelled	Actual	Comment	Reference
B	200	PHE	LEU	engineered mutation	UNP O85726
C	10	GLN	LEU	engineered mutation	UNP O85726
C	160	ASN	ASP	engineered mutation	UNP O85726
C	200	PHE	LEU	engineered mutation	UNP O85726
D	10	GLN	LEU	engineered mutation	UNP O85726
D	160	ASN	ASP	engineered mutation	UNP O85726
D	200	PHE	LEU	engineered mutation	UNP O85726
E	10	GLN	LEU	engineered mutation	UNP O85726
E	160	ASN	ASP	engineered mutation	UNP O85726
E	200	PHE	LEU	engineered mutation	UNP O85726
F	10	GLN	LEU	engineered mutation	UNP O85726
F	160	ASN	ASP	engineered mutation	UNP O85726
F	200	PHE	LEU	engineered mutation	UNP O85726
G	10	GLN	LEU	engineered mutation	UNP O85726
G	160	ASN	ASP	engineered mutation	UNP O85726
G	200	PHE	LEU	engineered mutation	UNP O85726
H	10	GLN	LEU	engineered mutation	UNP O85726
H	160	ASN	ASP	engineered mutation	UNP O85726
H	200	PHE	LEU	engineered mutation	UNP O85726
I	10	GLN	LEU	engineered mutation	UNP O85726
I	160	ASN	ASP	engineered mutation	UNP O85726
I	200	PHE	LEU	engineered mutation	UNP O85726
J	10	GLN	LEU	engineered mutation	UNP O85726
J	160	ASN	ASP	engineered mutation	UNP O85726
J	200	PHE	LEU	engineered mutation	UNP O85726
K	10	GLN	LEU	engineered mutation	UNP O85726
K	160	ASN	ASP	engineered mutation	UNP O85726
K	200	PHE	LEU	engineered mutation	UNP O85726
L	10	GLN	LEU	engineered mutation	UNP O85726
L	160	ASN	ASP	engineered mutation	UNP O85726
L	200	PHE	LEU	engineered mutation	UNP O85726

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	51	Total O 51 51	0	0
2	B	66	Total O 66 66	0	0
2	C	60	Total O 60 60	0	0
2	D	42	Total O 42 42	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	43	Total 43	O 43	0	0
2	F	60	Total 60	O 60	0	0
2	G	84	Total 84	O 84	0	0
2	H	74	Total 74	O 74	0	0
2	I	37	Total 37	O 37	0	0
2	J	65	Total 65	O 65	0	0
2	K	79	Total 79	O 79	0	0
2	L	56	Total 56	O 56	0	0

3 Residue-property plots

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.

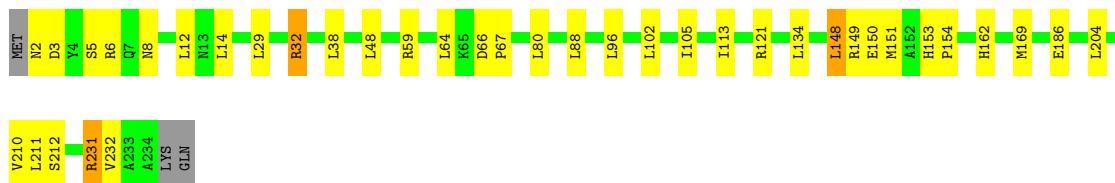
• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

Chain A: 



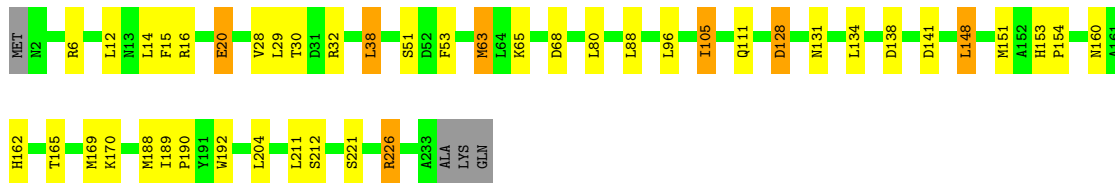
• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

Chain B: 



• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

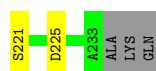
Chain C: 



• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

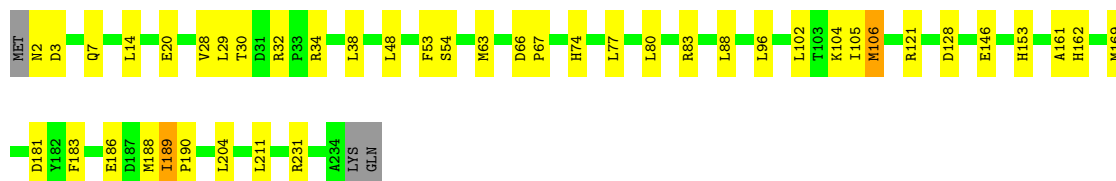
Chain D: 





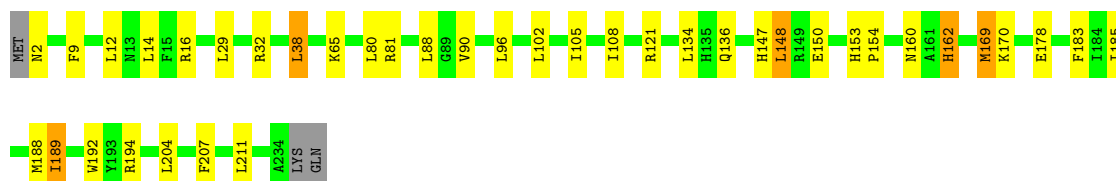
• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

Chain E: 81% 17% ..



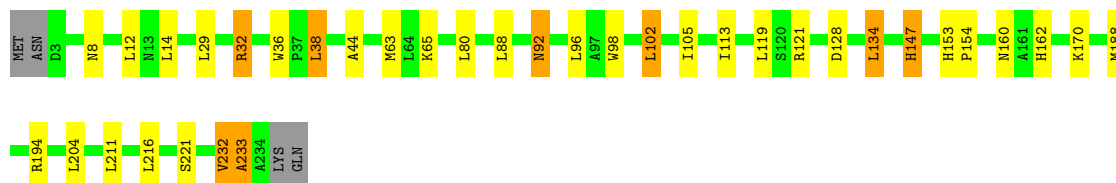
• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

Chain F: 82% 14% ..



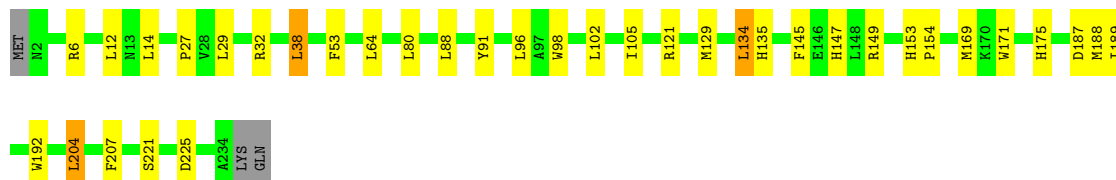
• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

Chain G: 83% 12% ..



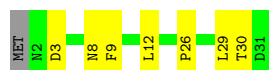
• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

Chain H: 83% 14% ..



• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

Chain I: 82% 15% ..





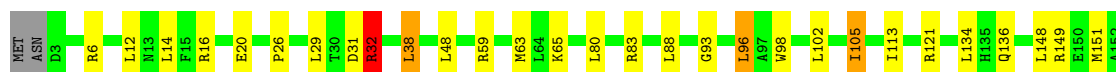
• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

Chain J: 83% 14% ..



• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

Chain K: 81% 15% ..



• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

Chain L: 81% 16% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.65Å 182.64Å 103.24Å 90.00° 91.05° 90.00°	Depositor
Resolution (Å)	95.35 – 2.50 95.35 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (95.35-2.50) 99.5 (95.35-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.192 , 0.245 (Not available) , 0.264	Depositor DCC
R_{free} test set	5962 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 14.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.125 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23710	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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	0.64	2/1970 (0.1%)	0.85	0/2679
1	B	0.66	0/1975	0.88	2/2686 (0.1%)
1	C	0.65	1/1970 (0.1%)	0.86	1/2679 (0.0%)
1	D	0.57	0/1970	0.80	0/2679
1	E	0.64	1/1975 (0.1%)	0.82	0/2686
1	F	0.66	0/1975	0.82	0/2686
1	G	0.70	0/1967	0.86	1/2675 (0.0%)
1	H	0.67	0/1975	0.82	0/2686
1	I	0.62	0/1970	0.86	3/2679 (0.1%)
1	J	0.64	0/1970	0.83	0/2679
1	K	0.69	0/1962	0.88	2/2668 (0.1%)
1	L	0.66	1/1974 (0.1%)	0.83	1/2685 (0.0%)
All	All	0.65	5/23653 (0.0%)	0.84	10/32167 (0.0%)

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
1	I	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	189	ILE	CA-CB	7.67	1.58	1.54
1	A	6	ARG	CB-CG	7.03	1.73	1.52
1	A	189	ILE	CA-CB	6.12	1.58	1.53
1	C	63	MET	SD-CE	-5.62	1.65	1.79
1	E	106	MET	SD-CE	-5.42	1.66	1.79

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	149	ARG	N-CA-C	10.66	126.10	112.89
1	K	32	ARG	N-CA-C	6.86	114.40	108.22
1	L	51	SER	N-CA-C	6.53	118.94	111.11
1	B	149	ARG	N-CA-C	-6.13	105.06	112.54
1	G	32	ARG	N-CA-C	5.62	113.07	108.07
1	C	128	ASP	N-CA-C	5.54	117.13	109.54
1	I	90	VAL	N-CA-C	5.46	116.26	111.56
1	B	32	ARG	N-CA-C	5.45	114.57	108.25
1	K	26	PRO	O-C-N	5.30	123.75	121.31
1	I	26	PRO	O-C-N	5.27	123.73	121.31

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	148	LEU	Peptide
1	I	148	LEU	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	A	1915	0	1816	21	0
1	B	1920	0	1821	20	0
1	C	1915	0	1816	15	0
1	D	1915	0	1816	17	0
1	E	1920	0	1821	20	0
1	F	1920	0	1821	18	0
1	G	1912	0	1815	16	0
1	H	1920	0	1821	19	0
1	I	1915	0	1816	13	0
1	J	1915	0	1816	14	0
1	K	1907	0	1810	14	0
1	L	1919	0	1821	20	0
2	A	51	0	0	0	0
2	B	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	60	0	0	2	0
2	D	42	0	0	1	0
2	E	43	0	0	1	0
2	F	60	0	0	1	0
2	G	84	0	0	1	0
2	H	74	0	0	0	0
2	I	37	0	0	0	0
2	J	65	0	0	0	0
2	K	79	0	0	0	0
2	L	56	0	0	0	0
All	All	23710	0	21810	178	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 4.

All (178) 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:A:162:HIS:HE1	1:A:186:GLU:O	1.60	0.83
1:A:105:ILE:HD11	1:B:105:ILE:CD1	2.12	0.80
1:D:58:TRP:HA	1:E:74:HIS:HE1	1.47	0.80
1:D:105:ILE:HG21	1:E:105:ILE:HD11	1.64	0.79
1:J:162:HIS:HE1	1:J:186:GLU:O	1.66	0.79
1:L:148:LEU:HD12	1:L:151:MET:HE2	1.66	0.77
1:G:105:ILE:HG12	1:H:105:ILE:HD11	1.68	0.75
1:L:162:HIS:HE1	1:L:186:GLU:O	1.70	0.75
1:F:162:HIS:CD2	1:F:188:MET:HB2	2.22	0.74
1:I:105:ILE:HG13	1:L:105:ILE:HD11	1.73	0.69
1:C:105:ILE:HG13	1:F:105:ILE:HD11	1.73	0.69
1:J:204:LEU:HD13	1:K:38:LEU:HG	1.76	0.68
1:I:117:ARG:O	1:I:136:GLN:NE2	2.27	0.67
1:H:171:TRP:CD1	1:H:175:HIS:HD1	2.12	0.67
1:A:46:ARG:HG2	1:A:46:ARG:HH11	1.60	0.67
1:H:135:HIS:ND1	1:H:147:HIS:CE1	2.65	0.65
1:E:128:ASP:HA	2:E:2029:HOH:O	1.95	0.65
1:K:98:TRP:CZ2	1:K:102:LEU:HD22	2.33	0.63
1:E:162:HIS:HE1	1:E:186:GLU:O	1.81	0.62
1:K:188:MET:HE3	1:K:191:TYR:HB2	1.80	0.62
1:F:90:VAL:O	2:F:2023:HOH:O	2.16	0.62
1:B:162:HIS:HE1	1:B:186:GLU:O	1.83	0.61
1:D:162:HIS:ND1	1:D:188:MET:HB2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:153:HIS:HD2	1:K:181:ASP:OD2	1.85	0.60
1:A:105:ILE:HD11	1:B:105:ILE:HD11	1.83	0.60
1:D:162:HIS:HE1	1:D:186:GLU:O	1.85	0.59
1:G:128:ASP:HA	2:G:2053:HOH:O	2.03	0.58
1:H:129:MET:HE1	1:H:134:LEU:HD22	1.86	0.58
1:B:148:LEU:HB3	1:B:151:MET:CG	2.34	0.57
1:A:101:ASP:O	1:A:105:ILE:HD12	2.05	0.56
1:D:5:SER:HA	1:F:170:LYS:HE3	1.86	0.56
1:D:162:HIS:CE1	1:D:188:MET:HB2	2.41	0.56
1:E:162:HIS:ND1	1:E:188:MET:HB2	2.21	0.56
1:A:161:ALA:C	1:A:162:HIS:CD2	2.84	0.55
1:L:169:MET:HE3	1:L:211:LEU:HD12	1.88	0.55
1:H:135:HIS:ND1	1:H:147:HIS:HE1	2.05	0.54
1:A:87:GLU:OE1	1:A:160:ASN:ND2	2.41	0.54
1:G:119:LEU:HD22	1:G:134:LEU:HG	1.90	0.54
1:J:105:ILE:HD11	1:K:105:ILE:HG21	1.89	0.54
1:G:38:LEU:HG	1:H:204:LEU:HD22	1.89	0.54
1:D:135:HIS:CD2	1:D:148:LEU:HD22	2.43	0.54
1:E:162:HIS:CE1	1:E:188:MET:HB2	2.42	0.53
1:A:38:LEU:HD22	1:B:211:LEU:O	2.07	0.53
1:K:31:ASP:C	1:K:32:ARG:HG3	2.34	0.53
1:F:162:HIS:N	1:F:162:HIS:ND1	2.55	0.53
1:C:65:LYS:NZ	1:C:160:ASN:HD21	2.07	0.52
1:F:81:ARG:HA	1:F:108:ILE:HD13	1.92	0.52
1:E:169:MET:HE3	1:E:211:LEU:HD12	1.91	0.52
1:G:147:HIS:C	1:G:147:HIS:CD2	2.87	0.52
1:B:148:LEU:HB3	1:B:151:MET:HG3	1.89	0.52
1:D:162:HIS:CE1	1:D:186:GLU:O	2.63	0.52
1:E:74:HIS:CD2	1:E:106:MET:CE	2.93	0.52
1:A:105:ILE:CD1	1:B:105:ILE:HD11	2.40	0.51
1:H:98:TRP:CZ2	1:H:102:LEU:HD22	2.46	0.51
1:D:66:ASP:HB2	1:D:67:PRO:CD	2.40	0.51
1:F:185:ILE:HD12	1:F:189:ILE:HD11	1.92	0.51
1:G:92:ASN:H	1:G:92:ASN:HD22	1.58	0.51
1:L:65:LYS:NZ	1:L:160:ASN:HD21	2.09	0.51
1:C:189:ILE:HB	1:C:190:PRO:HD3	1.93	0.50
1:E:169:MET:HE3	1:E:211:LEU:CD1	2.41	0.50
1:C:111:GLN:HE22	1:C:131:ASN:HA	1.76	0.50
2:D:2003:HOH:O	1:F:170:LYS:HE2	2.11	0.50
1:J:92:ASN:HD22	1:J:92:ASN:H	1.58	0.50
1:F:169:MET:HE2	1:F:207:PHE:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:161:ALA:C	1:L:162:HIS:CD2	2.90	0.50
1:E:153:HIS:HD2	1:E:181:ASP:OD2	1.94	0.50
1:I:153:HIS:HE1	1:I:176:LEU:O	1.95	0.50
1:B:151:MET:HA	1:B:151:MET:HE2	1.94	0.50
1:D:66:ASP:HB2	1:D:67:PRO:HD2	1.94	0.50
1:L:162:HIS:CE1	1:L:186:GLU:O	2.59	0.50
1:A:105:ILE:HD11	1:B:105:ILE:HG12	1.94	0.50
1:A:153:HIS:HB3	1:A:154:PRO:HA	1.94	0.49
1:E:66:ASP:HB2	1:E:67:PRO:HD2	1.94	0.49
1:L:205:GLY:O	1:L:208:ARG:HG2	2.13	0.49
1:L:117:ARG:O	1:L:136:GLN:NE2	2.45	0.49
1:A:105:ILE:HD11	1:B:105:ILE:CG1	2.42	0.49
1:L:65:LYS:HZ1	1:L:160:ASN:HD21	1.60	0.49
1:L:72:VAL:HG11	1:L:224:LEU:CD1	2.43	0.49
1:J:162:HIS:CE1	1:J:186:GLU:O	2.56	0.49
1:H:145:PHE:HB3	1:H:171:TRP:CH2	2.48	0.49
1:I:153:HIS:HA	1:I:154:PRO:C	2.38	0.48
1:K:113:ILE:HD11	1:K:151:MET:HE3	1.95	0.48
1:B:102:LEU:HA	1:B:105:ILE:HD12	1.94	0.48
1:H:169:MET:HE2	1:H:207:PHE:CE1	2.48	0.48
1:F:153:HIS:HA	1:F:154:PRO:C	2.39	0.48
1:E:74:HIS:HD2	1:E:106:MET:HE1	1.77	0.48
1:J:161:ALA:C	1:J:162:HIS:CD2	2.92	0.48
1:K:153:HIS:CD2	1:K:181:ASP:OD2	2.65	0.48
1:I:8:ASN:HD22	1:I:9:PHE:H	1.61	0.47
1:L:185:ILE:HD12	1:L:189:ILE:HD11	1.96	0.47
1:B:148:LEU:HB3	1:B:151:MET:HG2	1.96	0.47
1:B:210:VAL:O	1:B:231:ARG:HD3	2.14	0.47
1:G:162:HIS:CG	1:G:188:MET:HG3	2.49	0.47
1:K:93:GLY:HA2	1:K:96:LEU:HD22	1.95	0.47
1:G:105:ILE:HG21	1:H:105:ILE:HD11	1.97	0.47
1:B:212:SER:HB3	1:B:232:VAL:CG2	2.45	0.47
1:L:162:HIS:ND1	1:L:188:MET:HB2	2.29	0.47
1:I:59:ARG:HD3	1:L:105:ILE:HG22	1.96	0.46
1:H:153:HIS:HA	1:H:154:PRO:C	2.40	0.46
1:B:153:HIS:HA	1:B:154:PRO:C	2.39	0.46
1:J:12:LEU:HD22	1:L:166:PHE:HE1	1.80	0.46
1:L:153:HIS:HD2	1:L:181:ASP:OD2	1.98	0.46
1:D:53:PHE:HA	1:F:194:ARG:NH2	2.30	0.46
1:F:188:MET:HG3	1:F:192:TRP:CE2	2.51	0.46
1:K:188:MET:CE	1:K:191:TYR:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:149:ARG:N	1:I:150:GLU:HA	2.31	0.46
1:G:98:TRP:CZ2	1:G:102:LEU:HD22	2.51	0.46
1:C:38:LEU:HD22	1:F:211:LEU:O	2.16	0.46
1:L:169:MET:HE3	1:L:211:LEU:CD1	2.46	0.46
1:D:65:LYS:NZ	1:D:160:ASN:HD21	2.14	0.45
1:J:74:HIS:ND1	1:J:74:HIS:C	2.74	0.45
1:E:161:ALA:C	1:E:162:HIS:CD2	2.94	0.45
1:C:153:HIS:HA	1:C:154:PRO:C	2.41	0.45
1:C:128:ASP:HA	2:C:2045:HOH:O	2.15	0.45
1:C:15:PHE:CD2	1:C:20:GLU:HA	2.52	0.45
1:F:169:MET:HG3	1:F:183:PHE:CE2	2.52	0.45
1:G:216:LEU:HD11	1:H:27:PRO:HG2	1.98	0.45
1:H:188:MET:CE	1:H:192:TRP:NE1	2.80	0.45
1:A:164:ASN:OD1	1:A:167:ASN:ND2	2.43	0.44
1:G:153:HIS:HA	1:G:154:PRO:C	2.43	0.44
1:J:55:PRO:HD2	1:J:56:TYR:CD1	2.52	0.44
1:E:66:ASP:HB2	1:E:67:PRO:CD	2.47	0.44
1:A:162:HIS:CE1	1:A:186:GLU:O	2.52	0.44
1:E:74:HIS:CD2	1:E:74:HIS:C	2.95	0.44
1:A:162:HIS:ND1	1:A:188:MET:HB2	2.32	0.44
1:B:66:ASP:HB2	1:B:67:PRO:HD2	1.99	0.44
1:A:161:ALA:C	1:A:162:HIS:HD2	2.25	0.44
1:H:129:MET:CE	1:H:134:LEU:HD22	2.47	0.44
1:L:153:HIS:CD2	1:L:181:ASP:OD2	2.70	0.44
1:G:211:LEU:O	1:H:38:LEU:HD22	2.18	0.43
1:A:153:HIS:HA	1:A:154:PRO:C	2.43	0.43
1:B:66:ASP:HB2	1:B:67:PRO:CD	2.49	0.43
1:C:211:LEU:O	1:F:38:LEU:HD22	2.19	0.43
1:F:65:LYS:NZ	1:F:160:ASN:HD21	2.16	0.43
1:I:153:HIS:HB3	1:I:154:PRO:HA	2.01	0.43
1:A:105:ILE:HG22	1:B:59:ARG:HD2	2.00	0.43
1:A:189:ILE:HD12	1:A:227:GLY:HA2	2.00	0.43
1:H:153:HIS:HB3	1:H:154:PRO:HA	2.00	0.43
1:A:231:ARG:O	1:A:232:VAL:HG23	2.19	0.43
1:I:162:HIS:CD2	1:I:188:MET:HB2	2.54	0.43
1:E:53:PHE:CD2	1:E:53:PHE:C	2.96	0.43
1:K:153:HIS:HB3	1:K:154:PRO:HA	2.00	0.43
1:L:169:MET:HG3	1:L:183:PHE:CZ	2.54	0.43
1:L:31:ASP:C	1:L:32:ARG:HG3	2.44	0.42
1:E:153:HIS:CD2	1:E:181:ASP:OD2	2.71	0.42
1:I:66:ASP:HB2	1:I:67:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:MET:HG3	1:C:192:TRP:CE2	2.54	0.42
1:E:169:MET:HG3	1:E:183:PHE:CE2	2.54	0.42
1:C:63:MET:HE1	1:C:65:LYS:HB2	2.01	0.42
1:D:185:ILE:CD1	1:D:189:ILE:HD11	2.49	0.42
1:D:188:MET:HG2	1:D:192:TRP:CZ2	2.54	0.42
1:J:153:HIS:HA	1:J:154:PRO:C	2.45	0.42
1:C:162:HIS:HE1	2:C:2054:HOH:O	2.02	0.42
1:J:105:ILE:HD11	1:K:105:ILE:HG12	2.01	0.42
1:E:189:ILE:HB	1:E:190:PRO:HD3	2.02	0.42
1:B:162:HIS:CE1	1:B:186:GLU:O	2.69	0.42
1:H:64:LEU:HD11	1:H:91:TYR:CD2	2.55	0.41
1:J:74:HIS:CE1	1:K:59:ARG:H	2.38	0.41
1:J:179:GLU:HA	1:J:231:ARG:HB3	2.02	0.41
1:K:65:LYS:NZ	1:K:160:ASN:HD21	2.18	0.41
1:G:65:LYS:NZ	1:G:160:ASN:HD21	2.18	0.41
1:D:65:LYS:HZ1	1:D:160:ASN:HD21	1.69	0.41
1:D:2:ASN:HB3	1:D:3:ASP:H	1.77	0.41
1:C:53:PHE:CD2	1:C:53:PHE:C	2.99	0.41
1:H:53:PHE:CD2	1:H:53:PHE:C	2.97	0.41
1:C:148:LEU:HD23	1:C:151:MET:HE1	2.02	0.41
1:C:212:SER:HA	1:F:38:LEU:HD13	2.03	0.41
1:D:161:ALA:C	1:D:162:HIS:CD2	2.99	0.41
1:G:232:VAL:CG1	1:G:233:ALA:N	2.84	0.41
1:J:153:HIS:HE1	1:J:176:LEU:O	2.04	0.40
1:A:196:ALA:HA	1:E:20:GLU:HG3	2.03	0.40
1:B:113:ILE:CD1	1:B:148:LEU:HD13	2.51	0.40
1:G:105:ILE:CG2	1:H:105:ILE:HD11	2.52	0.40
1:I:169:MET:HE2	1:I:207:PHE:CE1	2.56	0.40
1:G:36:TRP:CZ2	1:G:44:ALA:HA	2.56	0.40
1:I:189:ILE:HD12	1:I:227:GLY:HA2	2.03	0.40
1:F:147:HIS:CD2	1:F:148:LEU:HD13	2.56	0.40
1:I:214:ASP:OD1	1:I:214:ASP:C	2.63	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	A	230/236 (98%)	217 (94%)	12 (5%)	1 (0%)	30	49
1	B	231/236 (98%)	218 (94%)	12 (5%)	1 (0%)	30	49
1	C	230/236 (98%)	217 (94%)	12 (5%)	1 (0%)	30	49
1	D	230/236 (98%)	218 (95%)	10 (4%)	2 (1%)	14	27
1	E	231/236 (98%)	217 (94%)	14 (6%)	0	100	100
1	F	231/236 (98%)	219 (95%)	11 (5%)	1 (0%)	30	49
1	G	230/236 (98%)	218 (95%)	11 (5%)	1 (0%)	30	49
1	H	231/236 (98%)	221 (96%)	8 (4%)	2 (1%)	14	27
1	I	230/236 (98%)	220 (96%)	10 (4%)	0	100	100
1	J	230/236 (98%)	218 (95%)	12 (5%)	0	100	100
1	K	229/236 (97%)	221 (96%)	7 (3%)	1 (0%)	30	49
1	L	231/236 (98%)	219 (95%)	11 (5%)	1 (0%)	30	49
All	All	2764/2832 (98%)	2623 (95%)	130 (5%)	11 (0%)	30	49

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	233	ALA
1	B	5	SER
1	D	141	ASP
1	K	208	ARG
1	A	53	PHE
1	H	225	ASP
1	D	225	ASP
1	L	225	ASP
1	C	226	ARG
1	F	9	PHE
1	H	187	ASP

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	204/207 (99%)	179 (88%)	25 (12%)	4	10
1	B	204/207 (99%)	184 (90%)	20 (10%)	7	16
1	C	204/207 (99%)	178 (87%)	26 (13%)	4	9
1	D	204/207 (99%)	186 (91%)	18 (9%)	9	20
1	E	204/207 (99%)	179 (88%)	25 (12%)	4	10
1	F	204/207 (99%)	183 (90%)	21 (10%)	7	14
1	G	203/207 (98%)	182 (90%)	21 (10%)	7	14
1	H	204/207 (99%)	189 (93%)	15 (7%)	13	27
1	I	204/207 (99%)	186 (91%)	18 (9%)	9	20
1	J	204/207 (99%)	179 (88%)	25 (12%)	4	10
1	K	203/207 (98%)	178 (88%)	25 (12%)	4	10
1	L	204/207 (99%)	185 (91%)	19 (9%)	8	18
All	All	2446/2484 (98%)	2188 (90%)	258 (10%)	6	14

All (258) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	6	ARG
1	A	7	GLN
1	A	14	LEU
1	A	20	GLU
1	A	28	VAL
1	A	29	LEU
1	A	30	THR
1	A	38	LEU
1	A	40	ARG
1	A	51	SER
1	A	59	ARG
1	A	88	LEU
1	A	96	LEU
1	A	117	ARG
1	A	121	ARG
1	A	130	GLU
1	A	140	SER
1	A	149	ARG

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Mol	Chain	Res	Type
1	A	150	GLU
1	A	162	HIS
1	A	169	MET
1	A	194	ARG
1	A	204	LEU
1	A	221	SER
1	B	2	ASN
1	B	3	ASP
1	B	6	ARG
1	B	8	ASN
1	B	12	LEU
1	B	14	LEU
1	B	29	LEU
1	B	32	ARG
1	B	38	LEU
1	B	48	LEU
1	B	64	LEU
1	B	80	LEU
1	B	88	LEU
1	B	96	LEU
1	B	121	ARG
1	B	134	LEU
1	B	150	GLU
1	B	169	MET
1	B	204	LEU
1	B	231	ARG
1	C	6	ARG
1	C	12	LEU
1	C	14	LEU
1	C	16	ARG
1	C	20	GLU
1	C	28	VAL
1	C	29	LEU
1	C	30	THR
1	C	32	ARG
1	C	38	LEU
1	C	51	SER
1	C	68	ASP
1	C	80	LEU
1	C	88	LEU
1	C	96	LEU
1	C	105	ILE

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Mol	Chain	Res	Type
1	C	134	LEU
1	C	138	ASP
1	C	141	ASP
1	C	148	LEU
1	C	165	THR
1	C	169	MET
1	C	170	LYS
1	C	204	LEU
1	C	221	SER
1	C	226	ARG
1	D	7	GLN
1	D	12	LEU
1	D	14	LEU
1	D	29	LEU
1	D	32	ARG
1	D	38	LEU
1	D	51	SER
1	D	80	LEU
1	D	88	LEU
1	D	96	LEU
1	D	104	LYS
1	D	121	ARG
1	D	134	LEU
1	D	135	HIS
1	D	141	ASP
1	D	143	THR
1	D	148	LEU
1	D	221	SER
1	E	2	ASN
1	E	3	ASP
1	E	7	GLN
1	E	14	LEU
1	E	28	VAL
1	E	29	LEU
1	E	30	THR
1	E	32	ARG
1	E	34	ARG
1	E	38	LEU
1	E	48	LEU
1	E	54	SER
1	E	63	MET
1	E	77	LEU

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Mol	Chain	Res	Type
1	E	80	LEU
1	E	83	ARG
1	E	88	LEU
1	E	96	LEU
1	E	102	LEU
1	E	104	LYS
1	E	121	ARG
1	E	146	GLU
1	E	189	ILE
1	E	204	LEU
1	E	231	ARG
1	F	2	ASN
1	F	12	LEU
1	F	14	LEU
1	F	16	ARG
1	F	29	LEU
1	F	32	ARG
1	F	38	LEU
1	F	80	LEU
1	F	88	LEU
1	F	96	LEU
1	F	102	LEU
1	F	121	ARG
1	F	134	LEU
1	F	136	GLN
1	F	148	LEU
1	F	150	GLU
1	F	162	HIS
1	F	169	MET
1	F	178	GLU
1	F	189	ILE
1	F	204	LEU
1	G	8	ASN
1	G	12	LEU
1	G	14	LEU
1	G	29	LEU
1	G	32	ARG
1	G	38	LEU
1	G	63	MET
1	G	80	LEU
1	G	88	LEU
1	G	92	ASN

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Mol	Chain	Res	Type
1	G	96	LEU
1	G	102	LEU
1	G	113	ILE
1	G	121	ARG
1	G	134	LEU
1	G	147	HIS
1	G	170	LYS
1	G	194	ARG
1	G	204	LEU
1	G	221	SER
1	G	232	VAL
1	H	6	ARG
1	H	12	LEU
1	H	14	LEU
1	H	29	LEU
1	H	32	ARG
1	H	38	LEU
1	H	80	LEU
1	H	88	LEU
1	H	96	LEU
1	H	121	ARG
1	H	134	LEU
1	H	149	ARG
1	H	189	ILE
1	H	204	LEU
1	H	221	SER
1	I	3	ASP
1	I	12	LEU
1	I	29	LEU
1	I	30	THR
1	I	32	ARG
1	I	46	ARG
1	I	80	LEU
1	I	88	LEU
1	I	96	LEU
1	I	102	LEU
1	I	105	ILE
1	I	117	ARG
1	I	121	ARG
1	I	134	LEU
1	I	146	GLU
1	I	151	MET

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Mol	Chain	Res	Type
1	I	204	LEU
1	I	221	SER
1	J	6	ARG
1	J	7	GLN
1	J	12	LEU
1	J	14	LEU
1	J	16	ARG
1	J	29	LEU
1	J	30	THR
1	J	32	ARG
1	J	38	LEU
1	J	40	ARG
1	J	46	ARG
1	J	63	MET
1	J	80	LEU
1	J	88	LEU
1	J	92	ASN
1	J	96	LEU
1	J	121	ARG
1	J	127	SER
1	J	134	LEU
1	J	146	GLU
1	J	150	GLU
1	J	189	ILE
1	J	204	LEU
1	J	221	SER
1	J	232	VAL
1	K	6	ARG
1	K	12	LEU
1	K	14	LEU
1	K	16	ARG
1	K	20	GLU
1	K	29	LEU
1	K	32	ARG
1	K	38	LEU
1	K	48	LEU
1	K	63	MET
1	K	80	LEU
1	K	83	ARG
1	K	88	LEU
1	K	96	LEU
1	K	105	ILE

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Mol	Chain	Res	Type
1	K	121	ARG
1	K	134	LEU
1	K	136	GLN
1	K	148	LEU
1	K	149	ARG
1	K	169	MET
1	K	204	LEU
1	K	208	ARG
1	K	221	SER
1	K	231	ARG
1	L	8	ASN
1	L	12	LEU
1	L	14	LEU
1	L	16	ARG
1	L	29	LEU
1	L	32	ARG
1	L	52	ASP
1	L	59	ARG
1	L	80	LEU
1	L	96	LEU
1	L	121	ARG
1	L	136	GLN
1	L	148	LEU
1	L	151	MET
1	L	179	GLU
1	L	198	GLN
1	L	204	LEU
1	L	221	SER
1	L	231	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	70	GLN
1	A	160	ASN
1	A	162	HIS
1	B	8	ASN
1	B	135	HIS
1	B	160	ASN
1	B	162	HIS
1	B	167	ASN

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Mol	Chain	Res	Type
1	B	175	HIS
1	C	70	GLN
1	C	111	GLN
1	C	136	GLN
1	C	160	ASN
1	C	175	HIS
1	D	10	GLN
1	D	111	GLN
1	D	135	HIS
1	D	160	ASN
1	D	162	HIS
1	E	7	GLN
1	E	74	HIS
1	E	135	HIS
1	E	136	GLN
1	E	153	HIS
1	E	162	HIS
1	E	167	ASN
1	F	2	ASN
1	F	160	ASN
1	G	7	GLN
1	G	92	ASN
1	G	147	HIS
1	G	153	HIS
1	G	160	ASN
1	G	167	ASN
1	G	175	HIS
1	H	136	GLN
1	H	147	HIS
1	H	160	ASN
1	I	2	ASN
1	I	7	GLN
1	I	8	ASN
1	I	25	HIS
1	I	135	HIS
1	I	160	ASN
1	J	7	GLN
1	J	25	HIS
1	J	70	GLN
1	J	92	ASN
1	J	160	ASN
1	J	162	HIS

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Mol	Chain	Res	Type
1	K	7	GLN
1	K	8	ASN
1	K	153	HIS
1	K	160	ASN
1	L	7	GLN
1	L	135	HIS
1	L	160	ASN
1	L	162	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, 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	232/236 (98%)	-1.42	0 100 100	15, 23, 42, 45	1 (0%)
1	B	233/236 (98%)	-1.58	0 100 100	10, 18, 38, 42	0
1	C	232/236 (98%)	-1.58	0 100 100	8, 20, 33, 43	0
1	D	232/236 (98%)	-1.42	0 100 100	11, 28, 49, 58	0
1	E	233/236 (98%)	-1.48	0 100 100	19, 27, 39, 42	1 (0%)
1	F	233/236 (98%)	-1.56	0 100 100	6, 17, 33, 42	0
1	G	232/236 (98%)	-1.64	0 100 100	5, 13, 32, 37	0
1	H	233/236 (98%)	-1.51	0 100 100	9, 19, 42, 47	0
1	I	232/236 (98%)	-1.31	0 100 100	16, 26, 46, 49	0
1	J	232/236 (98%)	-1.45	0 100 100	13, 21, 37, 40	0
1	K	231/236 (97%)	-1.60	0 100 100	9, 15, 35, 41	0
1	L	233/236 (98%)	-1.50	0 100 100	14, 20, 35, 45	0
All	All	2788/2832 (98%)	-1.51	0 100 100	5, 21, 38, 58	2 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.