



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 03:51 PM GMT

PDB ID : 3D19
Title : Crystal structure of a conserved metalloprotein from *Bacillus cereus*
Authors : Bonanno, J.B.; Patskovsky, Y.; Freeman, J.; Bain, K.T.; Chang, S.; Ozyurt, S.; Smith, D.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-05-05
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

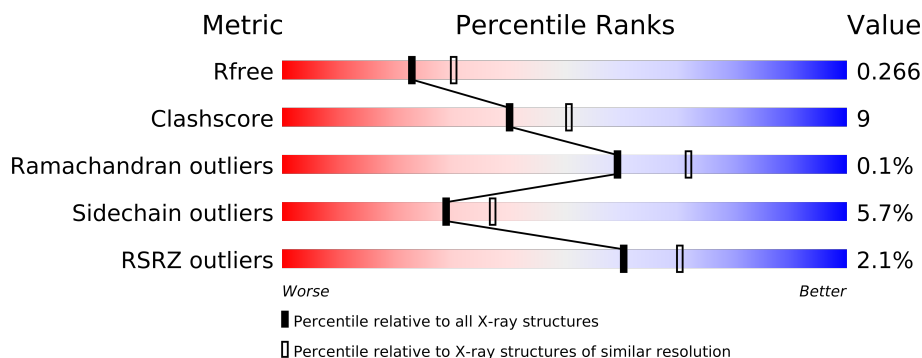
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	283	
1	B	283	
1	C	283	
1	D	283	
1	E	283	
1	F	283	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	C	301	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13109 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Conserved metalloprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2183	1393	381	400	9			
1	B	262	Total	C	N	O	S	0	3	0
			2181	1396	379	395	11			
1	C	258	Total	C	N	O	S	0	2	0
			2156	1380	375	391	10			
1	D	260	Total	C	N	O	S	0	1	0
			2160	1382	377	392	9			
1	E	257	Total	C	N	O	S	0	1	0
			2142	1371	374	388	9			
1	F	257	Total	C	N	O	S	0	1	0
			2146	1374	374	389	9			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	EXPRESSION TAG	UNP Q4MW04
A	9	SER	-	EXPRESSION TAG	UNP Q4MW04
A	10	LEU	-	EXPRESSION TAG	UNP Q4MW04
A	39	PHE	LEU	ENGINEERED	UNP Q4MW04
A	137	ILE	MET	ENGINEERED	UNP Q4MW04
A	138	GLN	GLU	ENGINEERED	UNP Q4MW04
A	193	GLU	ALA	ENGINEERED	UNP Q4MW04
A	211	ALA	VAL	ENGINEERED	UNP Q4MW04
A	283	GLU	-	EXPRESSION TAG	UNP Q4MW04
A	284	GLY	-	EXPRESSION TAG	UNP Q4MW04
A	285	HIS	-	EXPRESSION TAG	UNP Q4MW04
A	286	HIS	-	EXPRESSION TAG	UNP Q4MW04
A	287	HIS	-	EXPRESSION TAG	UNP Q4MW04
A	288	HIS	-	EXPRESSION TAG	UNP Q4MW04
A	289	HIS	-	EXPRESSION TAG	UNP Q4MW04
A	290	HIS	-	EXPRESSION TAG	UNP Q4MW04
B	8	MET	-	EXPRESSION TAG	UNP Q4MW04

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	SER	-	EXPRESSION TAG	UNP Q4MW04
B	10	LEU	-	EXPRESSION TAG	UNP Q4MW04
B	39	PHE	LEU	ENGINEERED	UNP Q4MW04
B	137	ILE	MET	ENGINEERED	UNP Q4MW04
B	138	GLN	GLU	ENGINEERED	UNP Q4MW04
B	193	GLU	ALA	ENGINEERED	UNP Q4MW04
B	211	ALA	VAL	ENGINEERED	UNP Q4MW04
B	283	GLU	-	EXPRESSION TAG	UNP Q4MW04
B	284	GLY	-	EXPRESSION TAG	UNP Q4MW04
B	285	HIS	-	EXPRESSION TAG	UNP Q4MW04
B	286	HIS	-	EXPRESSION TAG	UNP Q4MW04
B	287	HIS	-	EXPRESSION TAG	UNP Q4MW04
B	288	HIS	-	EXPRESSION TAG	UNP Q4MW04
B	289	HIS	-	EXPRESSION TAG	UNP Q4MW04
B	290	HIS	-	EXPRESSION TAG	UNP Q4MW04
C	8	MET	-	EXPRESSION TAG	UNP Q4MW04
C	9	SER	-	EXPRESSION TAG	UNP Q4MW04
C	10	LEU	-	EXPRESSION TAG	UNP Q4MW04
C	39	PHE	LEU	ENGINEERED	UNP Q4MW04
C	137	ILE	MET	ENGINEERED	UNP Q4MW04
C	138	GLN	GLU	ENGINEERED	UNP Q4MW04
C	193	GLU	ALA	ENGINEERED	UNP Q4MW04
C	211	ALA	VAL	ENGINEERED	UNP Q4MW04
C	283	GLU	-	EXPRESSION TAG	UNP Q4MW04
C	284	GLY	-	EXPRESSION TAG	UNP Q4MW04
C	285	HIS	-	EXPRESSION TAG	UNP Q4MW04
C	286	HIS	-	EXPRESSION TAG	UNP Q4MW04
C	287	HIS	-	EXPRESSION TAG	UNP Q4MW04
C	288	HIS	-	EXPRESSION TAG	UNP Q4MW04
C	289	HIS	-	EXPRESSION TAG	UNP Q4MW04
C	290	HIS	-	EXPRESSION TAG	UNP Q4MW04
D	8	MET	-	EXPRESSION TAG	UNP Q4MW04
D	9	SER	-	EXPRESSION TAG	UNP Q4MW04
D	10	LEU	-	EXPRESSION TAG	UNP Q4MW04
D	39	PHE	LEU	ENGINEERED	UNP Q4MW04
D	137	ILE	MET	ENGINEERED	UNP Q4MW04
D	138	GLN	GLU	ENGINEERED	UNP Q4MW04
D	193	GLU	ALA	ENGINEERED	UNP Q4MW04
D	211	ALA	VAL	ENGINEERED	UNP Q4MW04
D	283	GLU	-	EXPRESSION TAG	UNP Q4MW04
D	284	GLY	-	EXPRESSION TAG	UNP Q4MW04
D	285	HIS	-	EXPRESSION TAG	UNP Q4MW04

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Chain	Residue	Modelled	Actual	Comment	Reference
D	286	HIS	-	EXPRESSION TAG	UNP Q4MW04
D	287	HIS	-	EXPRESSION TAG	UNP Q4MW04
D	288	HIS	-	EXPRESSION TAG	UNP Q4MW04
D	289	HIS	-	EXPRESSION TAG	UNP Q4MW04
D	290	HIS	-	EXPRESSION TAG	UNP Q4MW04
E	8	MET	-	EXPRESSION TAG	UNP Q4MW04
E	9	SER	-	EXPRESSION TAG	UNP Q4MW04
E	10	LEU	-	EXPRESSION TAG	UNP Q4MW04
E	39	PHE	LEU	ENGINEERED	UNP Q4MW04
E	137	ILE	MET	ENGINEERED	UNP Q4MW04
E	138	GLN	GLU	ENGINEERED	UNP Q4MW04
E	193	GLU	ALA	ENGINEERED	UNP Q4MW04
E	211	ALA	VAL	ENGINEERED	UNP Q4MW04
E	283	GLU	-	EXPRESSION TAG	UNP Q4MW04
E	284	GLY	-	EXPRESSION TAG	UNP Q4MW04
E	285	HIS	-	EXPRESSION TAG	UNP Q4MW04
E	286	HIS	-	EXPRESSION TAG	UNP Q4MW04
E	287	HIS	-	EXPRESSION TAG	UNP Q4MW04
E	288	HIS	-	EXPRESSION TAG	UNP Q4MW04
E	289	HIS	-	EXPRESSION TAG	UNP Q4MW04
E	290	HIS	-	EXPRESSION TAG	UNP Q4MW04
F	8	MET	-	EXPRESSION TAG	UNP Q4MW04
F	9	SER	-	EXPRESSION TAG	UNP Q4MW04
F	10	LEU	-	EXPRESSION TAG	UNP Q4MW04
F	39	PHE	LEU	ENGINEERED	UNP Q4MW04
F	137	ILE	MET	ENGINEERED	UNP Q4MW04
F	138	GLN	GLU	ENGINEERED	UNP Q4MW04
F	193	GLU	ALA	ENGINEERED	UNP Q4MW04
F	211	ALA	VAL	ENGINEERED	UNP Q4MW04
F	283	GLU	-	EXPRESSION TAG	UNP Q4MW04
F	284	GLY	-	EXPRESSION TAG	UNP Q4MW04
F	285	HIS	-	EXPRESSION TAG	UNP Q4MW04
F	286	HIS	-	EXPRESSION TAG	UNP Q4MW04
F	287	HIS	-	EXPRESSION TAG	UNP Q4MW04
F	288	HIS	-	EXPRESSION TAG	UNP Q4MW04
F	289	HIS	-	EXPRESSION TAG	UNP Q4MW04
F	290	HIS	-	EXPRESSION TAG	UNP Q4MW04

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Fe	0	0
			1	1		
3	E	1	Total	Fe	0	0
			1	1		
3	B	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	A	1	Total	Fe	0	0
			1	1		
3	F	1	Total	Fe	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total	O	0	0
			25	25		
4	B	39	Total	O	0	0
			39	39		
4	C	37	Total	O	0	0
			37	37		
4	D	8	Total	O	0	0
			8	8		

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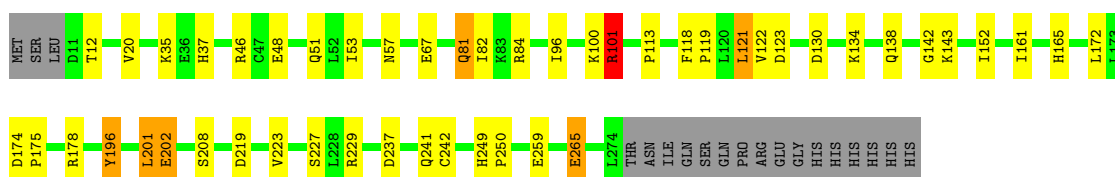
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	6	Total	O	0	0
			6	6		
4	F	14	Total	O	0	0
			14	14		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

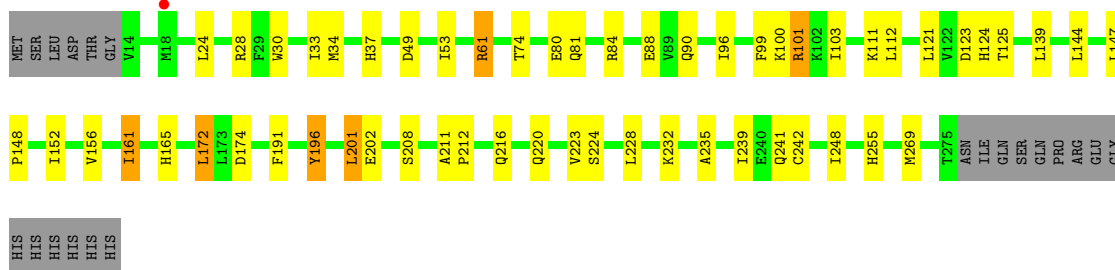
- Molecule 1: Conserved metalloprotein

Chain A:



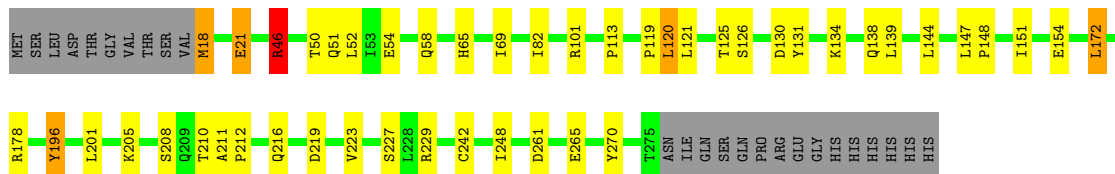
- Molecule 1: Conserved metalloprotein

Chain B:



- Molecule 1: Conserved metalloprotein

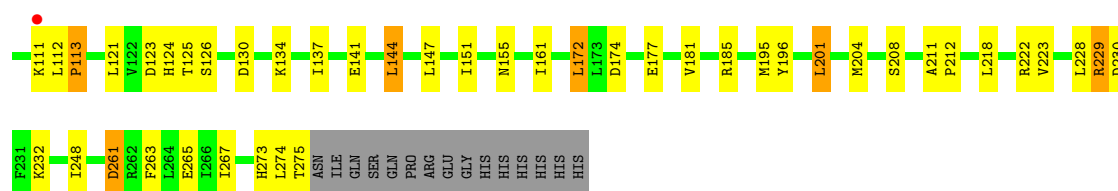
Chain C:



- Molecule 1: Conserved metalloprotein

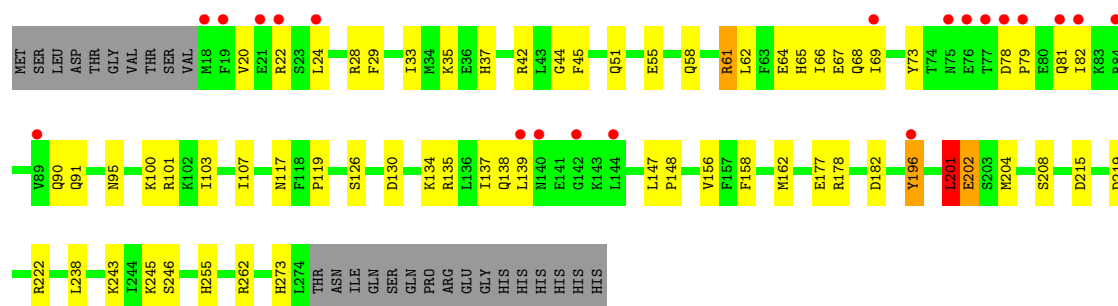
Chain D:





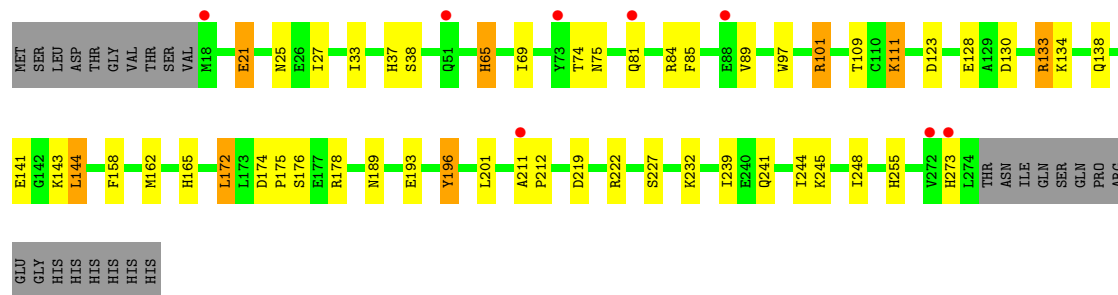
- Molecule 1: Conserved metalloprotein

Chain E:



- Molecule 1: Conserved metalloprotein

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.83Å 136.38Å 87.06Å 90.00° 102.84° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 40.07 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.30) 99.2 (40.07-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.206 , 0.268 0.207 , 0.266	Depositor DCC
R_{free} test set	3758 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 74864 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13109	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FE

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	0.83	0/2228	0.83	3/3004 (0.1%)
1	B	0.88	1/2236 (0.0%)	0.83	2/3014 (0.1%)
1	C	0.92	1/2208 (0.0%)	0.87	4/2976 (0.1%)
1	D	0.77	0/2209	0.77	0/2978
1	E	0.70	0/2191	0.76	3/2954 (0.1%)
1	F	0.75	0/2195	0.75	0/2958
All	All	0.81	2/13267 (0.0%)	0.80	12/17884 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	242	CYS	CB-SG	-6.69	1.70	1.82
1	B	88	GLU	CB-CG	5.27	1.62	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	A	101	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	B	101	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	E	222	ARG	NE-CZ-NH1	-6.49	117.05	120.30
1	C	178	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	C	46	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	C	178	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	E	101	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	E	201	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	121	LEU	CA-CB-CG	-5.14	103.48	115.30
1	C	46	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	B	161	ILE	CG1-CB-CG2	-5.11	100.16	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2183	0	2161	33	0
1	B	2181	0	2148	44	0
1	C	2156	0	2131	30	0
1	D	2160	0	2135	59	0
1	E	2142	0	2117	46	0
1	F	2146	0	2125	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	25	0	0	1	0
4	B	39	0	0	0	0
4	C	37	0	0	0	0
4	D	8	0	0	0	0
4	E	6	0	0	1	0
4	F	14	0	0	1	0
All	All	13109	0	12817	242	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (242) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:196[B]:TYR:CD2	1:C:196[B]:TYR:OH	1.66	1.46
1:D:81:GLN:OE1	1:D:84:ARG:NH2	1.66	1.27
1:E:61:ARG:HH11	1:E:61:ARG:HG2	1.00	1.11
1:D:229:ARG:NH1	1:D:230:ASP:OD1	1.87	1.05
1:D:22:ARG:NH2	1:D:144:LEU:HD23	1.69	1.05
1:B:196[B]:TYR:CE2	1:C:196[B]:TYR:OH	0.68	1.03
1:B:81:GLN:OE1	1:B:84:ARG:NH2	1.94	1.00
1:F:81:GLN:NE2	1:F:84:ARG:HH21	1.60	0.97
1:D:22:ARG:HH21	1:D:144:LEU:CD2	1.76	0.96
1:F:81:GLN:HE21	1:F:84:ARG:HH21	1.11	0.94
1:E:61:ARG:HG2	1:E:61:ARG:NH1	1.73	0.93
1:F:130:ASP:OD1	1:F:133:ARG:NH2	2.03	0.91
1:B:37:HIS:HD1	1:B:100:LYS:HZ3	1.18	0.85
1:D:22:ARG:NH2	1:D:144:LEU:CD2	2.37	0.84
1:C:130:ASP:OD2	1:C:134:LYS:HE3	1.77	0.84
1:D:22:ARG:HH21	1:D:144:LEU:HD23	1.35	0.83
1:D:106:LEU:HD23	1:D:111:LYS:HD2	1.58	0.83
1:F:81:GLN:NE2	1:F:84:ARG:NH2	2.29	0.81
1:D:18:MET:SD	1:D:22:ARG:HD2	2.20	0.81
1:B:165:HIS:HD1	1:B:232:LYS:HZ1	1.28	0.80
1:D:23:SER:O	1:D:27:ILE:HG13	1.81	0.80
1:C:54:GLU:O	1:C:58:GLN:HG3	1.82	0.79
1:F:165:HIS:HD1	1:F:232:LYS:HZ1	1.30	0.79
1:D:74:THR:HG23	1:D:76:GLU:H	1.46	0.79
1:C:261:ASP:O	1:C:265:GLU:HG3	1.85	0.77
1:A:81:GLN:OE1	1:A:84:ARG:NH2	2.16	0.77
1:F:81:GLN:HE22	1:F:84:ARG:HE	1.33	0.75
1:F:81:GLN:HE21	1:F:84:ARG:NH2	1.84	0.75
1:A:12:THR:HG23	1:A:265:GLU:OE2	1.85	0.75
1:D:81:GLN:OE1	1:D:84:ARG:CZ	2.33	0.75
1:B:61:ARG:HH11	1:B:61:ARG:HG2	1.51	0.74
1:D:106:LEU:CD2	1:D:111:LYS:HD2	2.16	0.74
1:A:178:ARG:NH2	1:C:196[A]:TYR:CD2	2.55	0.74
1:D:172:LEU:HB3	1:D:248:ILE:HG13	1.67	0.74
1:E:61:ARG:HH11	1:E:61:ARG:CG	1.90	0.73
1:A:196:TYR:HD1	1:A:196:TYR:O	1.72	0.72
1:E:42:ARG:HA	1:E:45:PHE:CD2	2.25	0.72
1:E:178:ARG:NH2	1:F:196[A]:TYR:CD2	2.58	0.72
1:B:61:ARG:HH11	1:B:61:ARG:CG	2.02	0.71
1:E:37:HIS:HD1	1:E:100:LYS:HZ3	1.37	0.71
1:D:42:ARG:HA	1:D:45:PHE:CD2	2.25	0.71
1:D:21:GLU:HG2	1:D:75:ASN:ND2	2.06	0.70
1:A:241:GLN:O	1:A:242:CYS:HB2	1.90	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:130:ASP:OD1	1:F:133:ARG:NE	2.25	0.70
1:B:228:LEU:HG	1:B:232:LYS:HD2	1.72	0.70
1:E:20:VAL:HG13	1:E:82:ILE:CD1	2.21	0.69
1:D:261:ASP:O	1:D:265:GLU:HG3	1.93	0.69
1:A:178:ARG:NH2	1:C:196[A]:TYR:CE2	2.61	0.69
1:A:20:VAL:HG13	1:A:82:ILE:HG13	1.75	0.68
1:A:46:ARG:HH12	1:A:113:PRO:HD2	1.59	0.68
1:D:18:MET:O	1:D:22:ARG:HD3	1.95	0.67
1:A:121:LEU:HD23	1:A:122:VAL:N	2.10	0.67
1:D:228:LEU:HG	1:D:232:LYS:HD2	1.78	0.66
1:E:135:ARG:HG2	1:E:135:ARG:HH11	1.61	0.65
1:D:112:LEU:O	1:D:113:PRO:C	2.35	0.65
1:E:90:GLN:OE1	1:E:137:ILE:HG12	1.97	0.64
1:D:21:GLU:HG2	1:D:75:ASN:HD21	1.61	0.64
1:D:263:PHE:CZ	1:D:267:ILE:HD11	2.33	0.64
1:A:152:ILE:HG21	1:A:202:GLU:HG2	1.80	0.63
1:E:178:ARG:NH2	1:F:196[A]:TYR:CE2	2.67	0.63
1:B:269[A]:MET:HA	1:B:269[A]:MET:CE	2.26	0.63
1:E:35:LYS:NZ	1:E:67:GLU:OE1	2.30	0.63
1:F:130:ASP:OD1	1:F:133:ARG:CZ	2.46	0.63
1:D:22:ARG:HH21	1:D:144:LEU:HD21	1.64	0.62
1:B:165:HIS:HD1	1:B:232:LYS:NZ	1.98	0.62
1:D:130:ASP:O	1:D:134:LYS:HG3	2.00	0.62
1:B:191:PHE:CE2	1:B:228:LEU:HD22	2.35	0.61
1:B:241:GLN:O	1:B:242:CYS:HB2	2.00	0.61
1:E:201:LEU:HD22	1:E:208:SER:HB2	1.82	0.60
1:A:121:LEU:C	1:A:121:LEU:HD23	2.22	0.60
1:C:134:LYS:O	1:C:138:GLN:HG3	2.01	0.60
1:D:18:MET:SD	1:D:22:ARG:CD	2.90	0.60
1:B:37:HIS:HD1	1:B:100:LYS:NZ	1.96	0.60
1:D:177:GLU:O	1:D:181:VAL:HG23	2.02	0.60
1:B:124:HIS:CE1	1:B:161:ILE:HG13	2.37	0.59
1:A:46:ARG:NH1	1:A:113:PRO:HD2	2.17	0.59
1:A:101:ARG:NH2	1:A:123:ASP:OD1	2.36	0.59
1:B:147:LEU:HB3	1:B:148:PRO:HD3	1.84	0.59
1:D:91:GLN:NE2	1:D:95:ASN:OD1	2.36	0.59
1:F:211:ALA:HB3	1:F:212:PRO:HD3	1.84	0.58
1:B:223:VAL:HG23	1:B:224:SER:H	1.68	0.58
1:E:20:VAL:HG13	1:E:82:ILE:HD12	1.84	0.58
1:A:35:LYS:NZ	1:A:67:GLU:OE1	2.32	0.58
1:A:37:HIS:HD1	1:A:100:LYS:HZ1	1.50	0.58
1:C:120:LEU:HD23	1:F:175:PRO:HB2	1.84	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:61:ARG:NH1	1:B:61:ARG:HG2	2.19	0.58
1:F:81:GLN:HE22	1:F:84:ARG:NE	2.03	0.57
1:B:30:TRP:O	1:B:34:MET:HG2	2.04	0.57
1:B:24:LEU:O	1:B:28:ARG:HG3	2.04	0.57
1:E:147:LEU:HB3	1:E:148:PRO:HD3	1.87	0.56
1:C:201:LEU:HD22	1:C:208:SER:HB2	1.87	0.56
1:D:84:ARG:O	1:D:88:GLU:HG3	2.05	0.56
1:D:61:ARG:HG2	1:D:61:ARG:HH11	1.70	0.56
1:E:158:PHE:O	1:E:162:MET:HG2	2.06	0.56
1:F:81:GLN:NE2	1:F:81:GLN:HA	2.19	0.56
1:F:239:ILE:HG13	1:F:244:ILE:HD11	1.87	0.56
1:D:174:ASP:OD1	1:E:119:PRO:HD2	2.06	0.56
1:C:130:ASP:O	1:C:134:LYS:HG3	2.04	0.56
1:F:85:PHE:O	1:F:89:VAL:HG23	2.07	0.55
1:E:91:GLN:NE2	1:E:95:ASN:OD1	2.40	0.55
1:D:263:PHE:CE1	1:D:267:ILE:HD11	2.41	0.55
1:B:223:VAL:HG23	1:B:224:SER:N	2.22	0.55
1:C:147:LEU:HB3	1:C:148:PRO:HD3	1.89	0.55
1:F:65:HIS:CE1	1:F:69:ILE:HD11	2.42	0.55
1:A:196:TYR:CD1	1:A:196:TYR:O	2.59	0.54
1:C:120:LEU:HD12	1:C:120:LEU:O	2.07	0.54
1:A:12:THR:CG2	1:A:265:GLU:OE2	2.54	0.53
1:E:90:GLN:OE1	1:E:137:ILE:CG1	2.56	0.53
1:A:142:GLY:C	1:A:143:LYS:HG3	2.28	0.53
1:E:177:GLU:OE2	1:E:245:LYS:NZ	2.42	0.53
1:D:211:ALA:HB3	1:D:212:PRO:HD3	1.90	0.53
1:A:119:PRO:HD2	1:B:174:ASP:OD1	2.08	0.52
1:D:62:LEU:O	1:D:62:LEU:HD12	2.10	0.52
1:C:147:LEU:O	1:C:151:ILE:HG13	2.10	0.52
1:C:154:GLU:HG3	1:C:270:TYR:OH	2.10	0.52
1:E:24:LEU:O	1:E:28:ARG:HG3	2.10	0.52
1:F:138:GLN:HG2	1:F:143:LYS:O	2.10	0.52
1:E:81:GLN:O	1:E:81:GLN:HG3	2.09	0.51
1:F:172:LEU:HB3	1:F:248:ILE:HG13	1.91	0.51
1:E:37:HIS:HD1	1:E:100:LYS:NZ	2.05	0.51
1:C:139:LEU:HD23	1:C:144:LEU:HD11	1.92	0.51
1:F:141:GLU:HB3	1:F:143:LYS:HD2	1.92	0.50
1:B:211:ALA:HB3	1:B:212:PRO:HD3	1.93	0.50
1:F:33:ILE:HD12	1:F:255:HIS:CE1	2.47	0.50
1:B:49:ASP:O	1:B:53:ILE:HG13	2.11	0.50
1:B:220:GLN:O	1:B:223:VAL:HG22	2.12	0.50
1:D:151:ILE:O	1:D:155:ASN:ND2	2.45	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:109:THR:OG1	1:F:111:LYS:HD3	2.12	0.50
1:B:121:LEU:O	1:B:125:THR:HG23	2.12	0.50
1:B:196[A]:TYR:CE2	1:F:178:ARG:NH2	2.80	0.50
1:D:81:GLN:CD	1:D:84:ARG:NH2	2.60	0.49
1:A:237:ASP:O	1:A:241:GLN:HG3	2.12	0.49
1:F:158:PHE:O	1:F:162:MET:HG2	2.12	0.49
1:B:152:ILE:O	1:B:156:VAL:HG23	2.12	0.49
1:D:21:GLU:CG	1:D:75:ASN:ND2	2.75	0.49
1:C:211:ALA:HB3	1:C:212:PRO:HD3	1.94	0.49
1:E:29:PHE:CE2	1:E:262:ARG:HD3	2.48	0.49
1:F:165:HIS:HD1	1:F:232:LYS:NZ	2.04	0.49
1:B:235:ALA:O	1:B:239:ILE:HD12	2.12	0.49
1:D:101:ARG:NH2	1:D:123:ASP:OD1	2.46	0.49
1:E:55:GLU:O	1:E:58:GLN:HB2	2.13	0.48
1:F:21:GLU:HG2	1:F:75:ASN:ND2	2.27	0.48
1:E:130:ASP:O	1:E:134:LYS:HG3	2.13	0.48
1:C:121:LEU:O	1:C:125:THR:HG23	2.13	0.48
1:B:172:LEU:HB3	1:B:248:ILE:CG1	2.43	0.48
1:E:134:LYS:O	1:E:138:GLN:HG3	2.14	0.48
1:B:99:PHE:CZ	1:B:103:ILE:HD11	2.49	0.48
1:E:135:ARG:HD3	1:E:135:ARG:O	2.13	0.48
1:E:44:GLY:HA3	1:E:117:ASN:OD1	2.14	0.48
1:A:96:ILE:HG12	1:A:100:LYS:HE3	1.96	0.48
1:E:22:ARG:HG2	1:E:139:LEU:HD21	1.95	0.48
1:F:176:SER:OG	1:F:245:LYS:NZ	2.42	0.47
1:B:111:LYS:O	1:B:112:LEU:HD23	2.14	0.47
1:D:137:ILE:O	1:D:141:GLU:HG3	2.14	0.47
1:B:196[A]:TYR:CD2	1:F:178:ARG:NH2	2.83	0.47
1:F:101:ARG:NH2	1:F:123:ASP:OD1	2.47	0.47
1:E:156:VAL:HG21	1:E:202:GLU:HG3	1.97	0.47
1:E:178:ARG:HD2	4:E:305:HOH:O	2.15	0.47
1:D:201:LEU:HD22	1:D:208:SER:HB2	1.97	0.47
1:F:97:TRP:CZ2	1:F:101:ARG:HD2	2.50	0.47
1:E:62:LEU:O	1:E:66:ILE:HG13	2.15	0.47
1:B:80:GLU:O	1:B:84:ARG:HG3	2.14	0.46
1:A:51:GLN:HB2	4:A:319:HOH:O	2.14	0.46
1:F:27:ILE:HD13	1:F:89:VAL:HG21	1.97	0.46
1:D:74:THR:CG2	1:D:76:GLU:H	2.23	0.46
1:D:195:MET:HE1	1:F:196[A]:TYR:CE2	2.51	0.46
1:F:21:GLU:HG2	1:F:75:ASN:HD21	1.81	0.46
1:E:238:LEU:HD23	1:E:243:LYS:HD3	1.98	0.46
1:E:204:MET:HB3	1:E:208:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:130:ASP:O	1:A:134:LYS:HG3	2.16	0.46
1:F:81:GLN:NE2	1:F:84:ARG:HE	2.09	0.46
1:B:96:ILE:HG12	1:B:100:LYS:HE3	1.97	0.46
1:A:118:PHE:HB3	1:B:174:ASP:OD1	2.16	0.45
1:D:103:ILE:O	1:D:107:ILE:HD12	2.15	0.45
1:C:18:MET:HB3	1:C:21:GLU:HB2	1.97	0.45
1:D:21:GLU:CG	1:D:75:ASN:HD21	2.29	0.45
1:D:50:THR:O	1:D:54:GLU:HG3	2.16	0.45
1:D:124:HIS:CE1	1:D:161:ILE:HG13	2.52	0.45
1:F:189:ASN:ND2	4:F:311:HOH:O	2.42	0.45
1:D:195:MET:CE	1:F:196[A]:TYR:CE2	2.99	0.45
1:C:65:HIS:CE1	1:C:69:ILE:HD11	2.52	0.45
1:A:165:HIS:CE1	1:A:259:GLU:OE1	2.69	0.45
1:A:121:LEU:C	1:A:121:LEU:CD2	2.84	0.44
1:D:121:LEU:HD23	1:D:125:THR:HG23	1.99	0.44
1:E:103:ILE:HG22	1:E:107:ILE:HD12	2.00	0.44
1:F:81:GLN:NE2	1:F:84:ARG:CZ	2.81	0.44
1:A:152:ILE:CG2	1:A:202:GLU:HG2	2.48	0.44
1:E:147:LEU:N	1:E:148:PRO:CD	2.80	0.44
1:D:147:LEU:O	1:D:151:ILE:HG13	2.18	0.44
1:E:42:ARG:NH1	1:E:42:ARG:HG2	2.33	0.44
1:D:274:LEU:O	1:D:275:THR:O	2.36	0.44
1:C:52:LEU:HD23	1:C:52:LEU:HA	1.81	0.44
1:E:65:HIS:NE2	1:E:69:ILE:HD11	2.33	0.44
1:D:17:VAL:O	1:D:20:VAL:HB	2.17	0.43
1:B:201:LEU:HD22	1:B:208:SER:HB2	2.00	0.43
1:B:33:ILE:HG23	1:B:255:HIS:CE1	2.53	0.43
1:B:61:ARG:HH11	1:B:61:ARG:CB	2.31	0.43
1:B:269[A]:MET:HE1	1:B:269[A]:MET:HA	1.99	0.43
1:E:135:ARG:NH1	1:E:135:ARG:HG2	2.31	0.43
1:D:112:LEU:O	1:D:113:PRO:O	2.35	0.43
1:D:147:LEU:HD23	1:D:274:LEU:HD12	2.01	0.43
1:A:249:HIS:ND1	1:A:250:PRO:HD2	2.34	0.43
1:C:46:ARG:HD2	1:C:46:ARG:HH11	1.66	0.43
1:D:112:LEU:N	1:D:113:PRO:CD	2.81	0.43
1:C:131:TYR:CD2	1:C:131:TYR:C	2.92	0.43
1:D:66:ILE:HD13	1:D:89:VAL:HG22	2.00	0.43
1:A:53:ILE:O	1:A:57:ASN:ND2	2.52	0.43
1:E:24:LEU:HD21	1:E:73:TYR:HB2	2.01	0.42
1:A:161:ILE:HG22	1:A:165:HIS:CE1	2.54	0.42
1:C:46:ARG:HD2	1:C:113:PRO:O	2.19	0.42
1:F:81:GLN:NE2	1:F:84:ARG:NE	2.66	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:172:LEU:HB3	1:C:248:ILE:HG13	2.02	0.42
1:C:82:ILE:HA	1:C:82:ILE:HD13	1.79	0.42
1:A:134:LYS:O	1:A:138:GLN:HG3	2.20	0.42
1:E:51:GLN:H	1:E:51:GLN:HG2	1.62	0.42
1:B:139:LEU:HD23	1:B:144:LEU:HD21	2.01	0.42
1:C:46:ARG:HE	1:C:46:ARG:HB2	1.77	0.42
1:F:37:HIS:HE1	1:F:128:GLU:OE1	2.02	0.42
1:D:151:ILE:HG23	1:D:218:LEU:HD21	2.01	0.42
1:D:204:MET:HB3	1:D:208:SER:HB3	2.01	0.42
1:E:33:ILE:HG23	1:E:255:HIS:CE1	2.55	0.42
1:D:46:ARG:HD3	1:D:113:PRO:O	2.20	0.41
1:E:64:GLU:O	1:E:68:GLN:HG3	2.20	0.41
1:E:78:ASP:HA	1:E:79:PRO:HD2	1.81	0.41
1:A:201:LEU:HD22	1:A:208:SER:HB2	2.01	0.41
1:C:210:THR:HB	1:C:212:PRO:HD2	2.02	0.41
1:A:174:ASP:HA	1:A:175:PRO:HD3	1.85	0.41
1:F:144:LEU:HD12	1:F:144:LEU:HA	1.77	0.41
1:B:172:LEU:HB3	1:B:248:ILE:HG12	2.01	0.41
1:C:119:PRO:HD2	1:F:174:ASP:OD1	2.20	0.41
1:D:61:ARG:CG	1:D:61:ARG:HH11	2.33	0.41
1:F:174:ASP:OD2	1:F:176:SER:OG	2.31	0.41
1:D:108:LEU:HA	1:D:108:LEU:HD23	1.74	0.41
1:B:101:ARG:NH2	1:B:123:ASP:OD1	2.53	0.41
1:D:82:ILE:HD13	1:D:82:ILE:HA	1.84	0.40
1:F:138:GLN:HB3	1:F:144:LEU:HD12	2.03	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	262/283 (93%)	255 (97%)	7 (3%)	0	100	100
1	B	263/283 (93%)	261 (99%)	2 (1%)	0	100	100
1	C	258/283 (91%)	254 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	259/283 (92%)	248 (96%)	10 (4%)	1 (0%)	43	52
1	E	256/283 (90%)	251 (98%)	5 (2%)	0	100	100
1	F	256/283 (90%)	251 (98%)	5 (2%)	0	100	100
All	All	1554/1698 (92%)	1520 (98%)	33 (2%)	1 (0%)	59	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	113	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	A	239/258 (93%)	227 (95%)	12 (5%)	34	45
1	B	236/258 (92%)	227 (96%)	9 (4%)	44	59
1	C	235/258 (91%)	218 (93%)	17 (7%)	21	25
1	D	235/258 (91%)	219 (93%)	16 (7%)	22	28
1	E	233/258 (90%)	222 (95%)	11 (5%)	36	47
1	F	234/258 (91%)	214 (92%)	20 (8%)	15	18
All	All	1412/1548 (91%)	1327 (94%)	85 (6%)	29	35

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	81	GLN
1	A	101	ARG
1	A	172	LEU
1	A	196	TYR
1	A	201	LEU
1	A	202	GLU
1	A	219	ASP
1	A	223	VAL

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Mol	Chain	Res	Type
1	A	227	SER
1	A	229	ARG
1	A	265	GLU
1	B	61	ARG
1	B	74	THR
1	B	90	GLN
1	B	172	LEU
1	B	196[A]	TYR
1	B	196[B]	TYR
1	B	201	LEU
1	B	202	GLU
1	B	216	GLN
1	C	18	MET
1	C	21	GLU
1	C	46	ARG
1	C	50	THR
1	C	51	GLN
1	C	101	ARG
1	C	120	LEU
1	C	126	SER
1	C	172	LEU
1	C	196[A]	TYR
1	C	196[B]	TYR
1	C	205	LYS
1	C	216	GLN
1	C	219	ASP
1	C	223	VAL
1	C	227	SER
1	C	229	ARG
1	D	19	PHE
1	D	51	GLN
1	D	61	ARG
1	D	74	THR
1	D	126	SER
1	D	144	LEU
1	D	172	LEU
1	D	185	ARG
1	D	196[A]	TYR
1	D	196[B]	TYR
1	D	201	LEU
1	D	222	ARG
1	D	223	VAL

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Mol	Chain	Res	Type
1	D	229	ARG
1	D	261	ASP
1	D	273	HIS
1	E	61	ARG
1	E	126	SER
1	E	182	ASP
1	E	196[A]	TYR
1	E	196[B]	TYR
1	E	201	LEU
1	E	202	GLU
1	E	215	ASP
1	E	219	ASP
1	E	246	SER
1	E	273	HIS
1	F	21	GLU
1	F	25	ASN
1	F	38	SER
1	F	65	HIS
1	F	74	THR
1	F	101	ARG
1	F	111	LYS
1	F	133	ARG
1	F	134	LYS
1	F	144	LEU
1	F	172	LEU
1	F	193	GLU
1	F	196[A]	TYR
1	F	196[B]	TYR
1	F	201	LEU
1	F	219	ASP
1	F	222	ARG
1	F	227	SER
1	F	241	GLN
1	F	273	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	ASN
1	A	216	GLN
1	B	90	GLN
1	B	189	ASN

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Mol	Chain	Res	Type
1	B	216	GLN
1	C	51	GLN
1	C	189	ASN
1	C	216	GLN
1	D	71	HIS
1	D	75	ASN
1	D	90	GLN
1	D	91	GLN
1	D	95	ASN
1	D	189	ASN
1	D	216	GLN
1	E	51	GLN
1	E	58	GLN
1	E	91	GLN
1	E	95	ASN
1	E	189	ASN
1	E	216	GLN
1	F	25	ASN
1	F	75	ASN
1	F	81	GLN
1	F	90	GLN
1	F	189	ASN
1	F	216	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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	264/283 (93%)	-0.11	0 100 100	29, 40, 53, 62	0
1	B	262/283 (92%)	-0.10	1 (0%) 90 95	28, 39, 53, 60	0
1	C	258/283 (91%)	-0.26	0 100 100	27, 37, 50, 59	0
1	D	260/283 (91%)	0.00	4 (1%) 70 78	31, 46, 62, 70	0
1	E	257/283 (90%)	0.36	20 (7%) 13 19	34, 51, 74, 86	0
1	F	257/283 (90%)	0.05	8 (3%) 47 56	29, 46, 62, 71	0
All	All	1558/1698 (91%)	-0.01	33 (2%) 60 70	27, 43, 62, 86	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	19	PHE	4.4
1	F	272	VAL	4.1
1	E	76	GLU	3.5
1	E	18	MET	3.5
1	B	18[A]	MET	3.4
1	E	75	ASN	3.3
1	E	82	ILE	3.2
1	E	78	ASP	3.0
1	E	144	LEU	2.9
1	D	73	TYR	2.8
1	F	273	HIS	2.7
1	F	88	GLU	2.7
1	F	51	GLN	2.7
1	E	21	GLU	2.7
1	E	140	ASN	2.6
1	E	81	GLN	2.6
1	E	77	THR	2.6
1	F	211	ALA	2.5
1	D	85	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	139	LEU	2.5
1	F	18	MET	2.4
1	E	142	GLY	2.4
1	E	69	ILE	2.4
1	E	196[A]	TYR	2.3
1	D	87	ALA	2.3
1	E	89	VAL	2.3
1	D	111	LYS	2.3
1	E	79	PRO	2.2
1	E	24	LEU	2.2
1	F	73	TYR	2.2
1	E	22	ARG	2.1
1	E	84	ARG	2.1
1	F	81	GLN	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	C	301	1/1	0.19	3.61	35,35,35,35	0
2	MG	B	301	1/1	0.14	0.37	37,37,37,37	0
2	MG	A	301	1/1	0.15	0.19	31,31,31,31	0
3	FE	B	302	1/1	0.13	-0.05	42,42,42,42	0
2	MG	F	301	1/1	0.12	-0.19	36,36,36,36	0
3	FE	F	302	1/1	0.11	-0.36	45,45,45,45	0
3	FE	A	302	1/1	0.14	-0.98	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	FE	C	302	1/1	0.10	-1.15	38,38,38,38	0
3	FE	E	302	1/1	0.12	-1.49	53,53,53,53	0
3	FE	D	302	1/1	0.08	-2.43	46,46,46,46	0
2	MG	D	301	1/1	0.06	-3.63	35,35,35,35	0
2	MG	E	301	1/1	0.05	-4.26	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.