

Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 01:33 PM JST

PDB ID	:	6J55
Title	:	Crystal structure of an iron superoxide dismutate (FeSOD) from a pathogenic
		Acanthamoeba castellanii
Authors	:	Lee, K.H.; Dao, T.O.; Asaithambi, K.; Na, B.K.
Deposited on	:	2019-01-10
Resolution	:	2.33 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 (i) 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 (1)) were used in the production of this report:

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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.33 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	$2096 \ (2.36-2.32)$
Clashscore	141614	$2193 \ (2.36-2.32)$
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	А	205	86%	12%	•
1	В	205	86%	12%	·
1	С	205	.% 88%	10%	·
1	D	205	83%	15%	·
1	Е	205	.% 80%	16%	·
1	F	205	82%	13%	·



Contr	nued fron	<i>i</i> previous	page		
Mol	Chain	Length	Quality of chain		
1	G	205	% • 770/	10%	
	u u	200	4%	19%	•
1	Н	205	73%	22%	•
1	Ι	205	% 	7%	• •
1	J	205	71%	24%	• •
1	K	205	2% 8 1%	14%	•
1	L	205	78%	21%	





2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20294 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	202	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	202	1637	1051	278	305	3	0	0	0
1	В	202	Total	С	Ν	Ο	S	0	1	0
1	D	202	1643	1056	279	305	3	0	I	0
1	С	202	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	U	202	1637	1051	278	305	3	0	0	0
1	Л	201	Total	С	Ν	Ο	S	0	0	0
1	D	201	1632	1048	277	304	3	0	0	0
1	F	107	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	Ľ	197	1602	1031	269	299	3	0	0 0	0
1	F	106	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	Ľ	190	1594	1026	268	298	2	0	0	U
1	С	106	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	G	190	1594	1026	268	298	2	0	0	0
1	Ц	107	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	11	197	1602	1031	269	299	3	0	0	0
1	т	107	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	1	197	1602	1031	269	299	3	0	0	0
1	Т	107	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	J	197	1602	1031	269	299	3	0	0	0
1	K	107	Total	С	Ν	Ο	S	0	0	0
		191	1602	1031	269	299	3	0	U	0
1	T	203	Total	С	Ν	0	S	0	0	0
		200	1653	1061	284	305	3	0	U	U

• Molecule 1 is a protein called Superoxide dismutase.

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-7	HIS	-	expression tag	UNP Q5IZD9
А	-6	HIS	-	expression tag	UNP Q5IZD9
А	-5	HIS	-	expression tag	UNP Q5IZD9
А	-4	HIS	-	expression tag	UNP Q5IZD9
А	-3	HIS	-	expression tag	UNP Q5IZD9



Chain	Residue	Modelled	Actual	Comment	Reference
А	-2	HIS	-	expression tag	UNP Q5IZD9
А	-1	GLY	_	expression tag	UNP Q5IZD9
А	0	SER	-	expression tag	UNP Q5IZD9
А	34	THR	ALA	conflict	UNP Q5IZD9
В	-7	HIS	-	expression tag	UNP Q5IZD9
В	-6	HIS	-	expression tag	UNP Q5IZD9
В	-5	HIS	-	expression tag	UNP Q5IZD9
В	-4	HIS	-	expression tag	UNP Q5IZD9
В	-3	HIS	-	expression tag	UNP Q5IZD9
В	-2	HIS	-	expression tag	UNP Q5IZD9
В	-1	GLY	-	expression tag	UNP Q5IZD9
В	0	SER	-	expression tag	UNP Q5IZD9
В	34	THR	ALA	conflict	UNP Q5IZD9
С	-7	HIS	-	expression tag	UNP Q5IZD9
С	-6	HIS	-	expression tag	UNP Q5IZD9
С	-5	HIS	-	expression tag	UNP Q5IZD9
С	-4	HIS	-	expression tag	UNP Q5IZD9
С	-3	HIS	-	expression tag	UNP Q5IZD9
С	-2	HIS	-	expression tag	UNP Q5IZD9
С	-1	GLY	-	expression tag	UNP Q5IZD9
С	0	SER	-	expression tag	UNP Q5IZD9
С	34	THR	ALA	conflict	UNP Q5IZD9
D	-7	HIS	-	expression tag	UNP Q5IZD9
D	-6	HIS	-	expression tag	UNP Q5IZD9
D	-5	HIS	-	expression tag	UNP Q5IZD9
D	-4	HIS	-	expression tag	UNP Q5IZD9
D	-3	HIS	-	expression tag	UNP Q5IZD9
D	-2	HIS	-	expression tag	UNP Q5IZD9
D	-1	GLY	-	expression tag	UNP Q5IZD9
D	0	SER	-	expression tag	UNP Q5IZD9
D	34	THR	ALA	conflict	UNP Q5IZD9
Е	-7	HIS	-	expression tag	UNP Q5IZD9
Е	-6	HIS	-	expression tag	UNP Q5IZD9
Е	-5	HIS	-	expression tag	UNP Q5IZD9
Е	-4	HIS	-	expression tag	UNP Q5IZD9
Е	-3	HIS	-	expression tag	UNP Q5IZD9
Е	-2	HIS	-	expression tag	UNP Q5IZD9
Е	-1	GLY	-	expression tag	UNP Q5IZD9
Е	0	SER	-	expression tag	UNP Q5IZD9
Е	34	THR	ALA	conflict	UNP Q5IZD9
F	-7	HIS	-	expression tag	UNP Q5IZD9
F	-6	HIS	-	expression tag	UNP Q5IZD9



Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	HIS	-	expression tag	UNP Q5IZD9
F	-4	HIS	-	expression tag	UNP Q5IZD9
F	-3	HIS	-	expression tag	UNP Q5IZD9
F	-2	HIS	-	expression tag	UNP Q5IZD9
F	-1	GLY	-	expression tag	UNP Q5IZD9
F	0	SER	-	expression tag	UNP Q5IZD9
F	34	THR	ALA	conflict	UNP Q5IZD9
G	-7	HIS	-	expression tag	UNP Q5IZD9
G	-6	HIS	-	expression tag	UNP Q5IZD9
G	-5	HIS	-	expression tag	UNP Q5IZD9
G	-4	HIS	-	expression tag	UNP Q5IZD9
G	-3	HIS	-	expression tag	UNP Q5IZD9
G	-2	HIS	-	expression tag	UNP Q5IZD9
G	-1	GLY	-	expression tag	UNP Q5IZD9
G	0	SER	-	expression tag	UNP Q5IZD9
G	34	THR	ALA	conflict	UNP Q5IZD9
Н	-7	HIS	-	expression tag	UNP Q5IZD9
Н	-6	HIS	-	expression tag	UNP Q5IZD9
Н	-5	HIS	_	expression tag	UNP Q5IZD9
Н	-4	HIS	-	expression tag	UNP Q5IZD9
Н	-3	HIS	-	expression tag	UNP Q5IZD9
Н	-2	HIS	-	expression tag	UNP Q5IZD9
Н	-1	GLY	-	expression tag	UNP Q5IZD9
Н	0	SER	-	expression tag	UNP Q5IZD9
Н	34	THR	ALA	conflict	UNP Q5IZD9
Ι	-7	HIS	-	expression tag	UNP Q5IZD9
Ι	-6	HIS	-	expression tag	UNP Q5IZD9
Ι	-5	HIS	-	expression tag	UNP Q5IZD9
Ι	-4	HIS	-	expression tag	UNP Q5IZD9
Ι	-3	HIS	-	expression tag	UNP Q5IZD9
Ι	-2	HIS	-	expression tag	UNP Q5IZD9
Ι	-1	GLY	-	expression tag	UNP Q5IZD9
Ι	0	SER	-	expression tag	UNP Q5IZD9
Ι	34	THR	ALA	conflict	UNP Q5IZD9
J	-7	HIS	-	expression tag	UNP Q5IZD9
J	-6	HIS	-	expression tag	UNP Q5IZD9
J	-5	HIS	-	expression tag	UNP Q5IZD9
J	-4	HIS	-	expression tag	UNP Q5IZD9
J	-3	HIS	-	expression tag	UNP Q5IZD9
J	-2	HIS	-	expression tag	UNP Q5IZD9
J	-1	GLY	-	expression tag	UNP Q5IZD9
J	0	SER	-	expression tag	UNP Q5IZD9

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Chain	Residue	Modelled	Actual Comment		Reference
J	34	THR	ALA	conflict	UNP Q5IZD9
K	-7	HIS	-	expression tag	UNP Q5IZD9
K	-6	HIS	-	expression tag	UNP Q5IZD9
K	-5	HIS	-	expression tag	UNP Q5IZD9
K	-4	HIS	-	expression tag	UNP Q5IZD9
K	-3	HIS	-	expression tag	UNP Q5IZD9
K	-2	HIS	-	expression tag	UNP Q5IZD9
K	-1	GLY	-	expression tag	UNP Q5IZD9
K	0	SER	-	expression tag	UNP Q5IZD9
K	34	THR	ALA	conflict	UNP Q5IZD9
L	-7	HIS	-	expression tag	UNP Q5IZD9
L	-6	HIS	-	expression tag	UNP Q5IZD9
L	-5	HIS	-	expression tag	UNP Q5IZD9
L	-4	HIS	-	expression tag	UNP Q5IZD9
L	-3	HIS	-	expression tag	UNP Q5IZD9
L	-2	HIS	-	expression tag	UNP Q5IZD9
L	-1	GLY	-	expression tag	UNP Q5IZD9
L	0	SER	-	expression tag	UNP Q5IZD9
L	34	THR	ALA	conflict	UNP Q5IZD9

• Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Fe 1 1	0	0
2	В	1	Total Fe 1 1	0	0
2	С	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	Е	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0
2	G	1	Total Fe 1 1	0	0
2	Н	1	Total Fe 1 1	0	0
2	Ι	1	Total Fe 1 1	0	0
2	J	1	Total Fe 1 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	1	Total Fe 1 1	0	0
2	L	1	Total Fe 1 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	121	Total O 121 121	0	0
3	В	82	TotalO8282	0	0
3	С	110	Total O 110 110	0	0
3	D	108	Total O 108 108	0	0
3	Е	71	Total O 71 71	0	0
3	F	54	$\begin{array}{ccc} \text{Total} & \text{O} \\ 54 & 54 \end{array}$	0	0
3	G	50	Total O 50 50	0	0
3	Н	62	$\begin{array}{cc} \text{Total} & \text{O} \\ 62 & 62 \end{array}$	0	0
3	Ι	57	Total O 57 57	0	0
3	J	42	$\begin{array}{cc} \text{Total} & \text{O} \\ 42 & 42 \end{array}$	0	0
3	K	55	$\begin{array}{cc} \text{Total} & \text{O} \\ 55 & 55 \end{array}$	0	0
3	L	70	Total O 70 70	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Superoxide dismutase













4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants	127.49Å 127.49Å 327.06Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
D ecolution $(\hat{\lambda})$	36.57 - 2.33	Depositor
Resolution (A)	36.80 - 2.33	EDS
% Data completeness	100.0 (36.57-2.33)	Depositor
(in resolution range)	99.9 (36.80 - 2.33)	EDS
R _{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$5.38 (at 2.31 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
P. P.	0.200 , 0.248	Depositor
n, n_{free}	0.200 , 0.248	DCC
R_{free} test set	6498 reflections $(5.07%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	37.6	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35 , 31.9	EDS
L-test for twinning ²	$< L > = 0.42, < L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.228 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20294	wwPDB-VP
Average B, all atoms $(Å^2)$	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2

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		Bo	nd lengths	Bond angles		
1VIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.47	0/1683	0.62	1/2292~(0.0%)	
1	В	0.45	0/1692	0.58	0/2303	
1	С	0.47	0/1683	0.61	1/2292~(0.0%)	
1	D	0.45	0/1678	0.58	0/2285	
1	Е	0.43	0/1646	0.60	0/2242	
1	F	0.42	0/1638	0.58	0/2232	
1	G	0.43	0/1638	0.62	1/2232~(0.0%)	
1	Н	0.42	0/1646	0.61	0/2242	
1	Ι	0.40	0/1646	0.58	1/2242~(0.0%)	
1	J	0.45	1/1646~(0.1%)	0.62	0/2242	
1	Κ	0.40	0/1646	0.58	0/2242	
1	L	0.40	0/1702	0.57	0/2318	
All	All	0.43	1/19944~(0.0%)	0.60	4/27164~(0.0%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	49	GLU	CD-OE2	7.91	1.34	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Ι	24	LEU	CB-CG-CD2	-7.55	98.16	111.00
1	А	2	LEU	CA-CB-CG	6.92	131.22	115.30
1	С	161	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	G	131	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.



5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1637	0	1585	20	0
1	В	1643	0	1598	16	0
1	С	1637	0	1585	15	0
1	D	1632	0	1583	23	0
1	Е	1602	0	1561	23	0
1	F	1594	0	1549	21	0
1	G	1594	0	1549	27	0
1	Н	1602	0	1561	44	0
1	Ι	1602	0	1561	17	0
1	J	1602	0	1561	43	0
1	K	1602	0	1561	23	0
1	L	1653	0	1596	33	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
2	Е	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	Н	1	0	0	0	0
2	Ι	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	А	121	0	0	6	0
3	В	82	0	0	2	0
3	С	110	0	0	6	0
3	D	108	0	0	7	0
3	Е	71	0	0	3	0
3	F	54	0	0	9	0
3	G	50	0	0	6	0
3	Н	62	0	0	17	0
3	Ι	57	0	0	0	0
3	J	42	0	0	3	0
3	К	55	0	0	1	0
3	L	70	0	0	8	0
All	All	20294	0	18850	294	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 8.

All (294) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:22:LYS:NZ	3:A:303:HOH:O	1.96	0.98
1:H:113:LYS:NZ	3:H:302:HOH:O	1.95	0.94
1:F:49:GLU:O	3:F:302:HOH:O	1.86	0.92
1:L:17:PRO:O	3:L:301:HOH:O	1.87	0.92
1:L:90:GLN:O	1:L:189:LYS:NZ	2.02	0.91
1:A:192:ASP:OD2	3:A:302:HOH:O	1.90	0.90
1:J:46:THR:HG23	1:J:48:LEU:H	1.35	0.89
1:K:38:LYS:HE2	1:K:71:ASN:OD1	1.72	0.89
1:A:155:THR:OG1	3:A:301:HOH:O	1.88	0.89
1:F:47:SER:OG	3:F:301:HOH:O	1.81	0.86
1:G:37:ASN:OD1	3:G:301:HOH:O	1.93	0.85
1:K:46:THR:HG23	1:K:48:LEU:H	1.42	0.84
1:F:99:GLU:OE2	3:F:303:HOH:O	1.95	0.83
1:L:172:GLN:OE1	1:L:174:ARG:NH2	2.12	0.82
1:A:54:GLU:OE2	3:A:304:HOH:O	1.98	0.82
1:G:17:PRO:HB2	1:G:181:LYS:HD3	1.60	0.81
1:J:5:LEU:HD21	1:J:75:LEU:HD11	1.62	0.81
1:J:29:ASN:HA	1:J:33:LYS:HE3	1.62	0.80
1:D:100:LYS:NZ	1:D:104:GLU:OE2	2.15	0.80
1:H:196:LYS:NZ	3:H:309:HOH:O	2.15	0.80
1:J:98:LEU:HD12	1:J:195:LEU:HD13	1.64	0.80
1:F:118:ASP:O	3:F:304:HOH:O	2.00	0.79
1:L:188:TRP:O	3:L:303:HOH:O	2.00	0.79
1:H:75:LEU:O	3:H:301:HOH:O	2.00	0.78
1:E:19:ILE:HG22	1:E:24:LEU:HD12	1.65	0.77
1:E:177:GLU:OE1	3:E:301:HOH:O	2.03	0.77
1:H:10:TYR:O	3:H:303:HOH:O	2.02	0.77
1:K:67:ALA:O	1:K:71:ASN:ND2	2.18	0.76
1:D:97:GLU:O	3:D:301:HOH:O	2.04	0.74
1:J:192:ASP:HA	1:J:195:LEU:HD22	1.69	0.74
1:F:2:LEU:N	3:F:306:HOH:O	2.19	0.74
1:H:14:GLY:N	3:H:303:HOH:O	2.21	0.74
1:A:97:GLU:OE1	1:A:196:LYS:NZ	2.19	0.73
1:H:9:ALA:O	3:H:304:HOH:O	2.06	0.73
1:G:94:ILE:HG23	1:G:98:LEU:HD12	1.70	0.73
1:H:147:GLU:OE2	3:H:305:HOH:O	2.07	0.72
1:D:94:ILE:HG23	1:D:98:LEU:HD23	1.72	0.71



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:J:25:ASP:OD1	1:J:29:ASN:ND2	2.23	0.71
1:A:2:LEU:HD22	1:A:44:LYS:HE3	1.72	0.71
1:H:197:GLN:OE1	1:H:197:GLN:C	2.30	0.70
1:H:10:TYR:HB2	3:H:303:HOH:O	1.91	0.70
1:L:54:GLU:OE2	3:L:304:HOH:O	2.10	0.69
1:D:180:ASN:HB2	3:D:385:HOH:O	1.92	0.69
1:I:94:ILE:HG23	1:I:98:LEU:HD23	1.75	0.69
1:B:115:LYS:HD3	3:B:323:HOH:O	1.90	0.69
1:G:18:ALA:HA	1:G:181:LYS:HG2	1.74	0.69
1:H:93:GLN:O	3:H:307:HOH:O	2.11	0.68
1:H:153:ARG:O	3:H:306:HOH:O	2.10	0.68
1:H:190:PHE:O	3:H:308:HOH:O	2.12	0.68
1:A:40:ASN:O	1:A:44:LYS:HG2	1.93	0.68
1:A:94:ILE:HG23	1:A:98:LEU:HD23	1.77	0.67
1:H:10:TYR:CE1	1:H:15:LEU:HD21	2.29	0.67
1:B:94:ILE:HG23	1:B:98:LEU:HD23	1.75	0.67
1:C:197:GLN:O	3:C:301:HOH:O	2.12	0.67
1:J:4:THR:O	3:J:302:HOH:O	2.13	0.66
1:L:93:GLN:NE2	3:L:305:HOH:O	2.12	0.66
1:G:16:GLU:OE1	3:G:302:HOH:O	2.13	0.66
1:G:7:ASP:OD1	3:G:303:HOH:O	2.13	0.66
1:A:2:LEU:CD2	1:A:44:LYS:HE3	2.26	0.65
1:L:110:ALA:O	1:L:114:LYS:NZ	2.29	0.65
1:H:93:GLN:NE2	3:H:310:HOH:O	2.15	0.65
1:D:6:ASN:OD1	3:D:302:HOH:O	2.14	0.65
1:L:90:GLN:OE1	3:L:306:HOH:O	2.14	0.65
1:K:134:ILE:HG12	1:K:154:VAL:HG12	1.78	0.65
1:H:189:LYS:HG2	1:H:193:GLN:HE21	1.61	0.64
1:I:168:TYR:HE1	1:J:169:LEU:HD21	1.62	0.64
1:J:15:LEU:HB2	1:J:19:ILE:HG23	1.80	0.63
1:F:137:LYS:NZ	1:F:139:GLU:OE2	2.31	0.63
1:K:94:ILE:HG23	1:K:98:LEU:HD23	1.81	0.62
1:C:14:GLY:HA2	1:C:24:LEU:HD12	1.81	0.62
1:C:94:ILE:HG23	1:C:98:LEU:HD23	1.82	0.61
1:H:19:ILE:HG22	1:H:24:LEU:HD12	1.82	0.61
1:E:25:ASP:OD2	1:E:29:ASN:ND2	2.28	0.61
1:A:137:LYS:HD2	1:E:51:LYS:HE3	1.82	0.61
1:J:137:LYS:NZ	1:J:139:GLU:OE1	2.33	0.61
1:H:188:TRP:HE3	1:H:191:VAL:HG21	1.64	0.61
1:I:172:GLN:NE2	1:I:174:ARG:HH22	1.98	0.61
1:K:17:PRO:HG2	1:K:181:LYS:HD2	1.83	0.60



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:G:61:LYS:NZ	1:G:147:GLU:OE2	2.30	0.60	
1:I:172:GLN:HE21	1:I:174:ARG:HH12	1.50	0.60	
1:L:41:ASP:O	3:L:308:HOH:O	2.17	0.60	
1:B:97:GLU:OE1	1:B:97:GLU:N	2.34	0.59	
1:C:60:ALA:HB2	1:C:68:LEU:HD23	1.84	0.59	
1:D:22:LYS:NZ	3:D:303:HOH:O	2.16	0.59	
1:K:34:THR:O	1:K:38:LYS:HD3	2.02	0.59	
1:G:14:GLY:HA2	1:G:24:LEU:HD12	1.84	0.59	
1:H:193:GLN:HB2	3:H:308:HOH:O	2.01	0.59	
1:L:97:GLU:OE1	1:L:97:GLU:N	2.36	0.59	
1:I:172:GLN:HG3	1:J:26:PHE:CE1	2.38	0.59	
1:C:100:LYS:NZ	3:C:308:HOH:O	2.35	0.58	
1:K:128:TRP:CZ3	1:K:161:ASP:HB2	2.38	0.58	
1:C:7:ASP:OD2	3:C:303:HOH:O	2.17	0.58	
1:D:6:ASN:O	3:D:304:HOH:O	2.17	0.58	
1:H:5:LEU:HD23	1:H:36:LEU:HD22	1.86	0.58	
1:H:15:LEU:HB3	1:H:185:VAL:HG11	1.85	0.58	
1:D:153:ARG:NH1	3:D:307:HOH:O	2.37	0.57	
1:H:49:GLU:HA	3:H:311:HOH:O	2.03	0.57	
1:C:132:VAL:HB	1:C:154:VAL:HG11	1.86	0.57	
1:C:-4:HIS:O	3:C:302:HOH:O	2.17	0.57	
1:J:46:THR:OG1	1:J:47:SER:N	2.35	0.56	
1:A:134:ILE:HG12	1:A:154:VAL:HG12	1.88	0.56	
1:G:133:ASN:HB3	1:G:155:THR:OG1	2.06	0.56	
1:A:147:GLU:OE1	3:A:305:HOH:O	2.18	0.56	
1:J:137:LYS:HD2	1:L:51:LYS:HE3	1.87	0.56	
1:I:20:SER:O	1:I:24:LEU:HD12	2.06	0.55	
1:E:192:ASP:HB2	3:E:322:HOH:O	2.07	0.55	
1:K:55:ASP:O	1:K:59:VAL:HG12	2.07	0.55	
1:C:132:VAL:HB	1:C:154:VAL:CG1	2.37	0.55	
1:F:94:ILE:HG23	1:F:98:LEU:HD23	1.89	0.55	
1:L:134:ILE:HG12	1:L:154:VAL:HG22	1.87	0.55	
1:B:130:TRP:CE3	1:B:159:THR:HB	2.43	0.54	
1:F:61:LYS:NZ	3:F:308:HOH:O	2.40	0.54	
1:G:128:TRP:CZ3	1:G:161:ASP:HB2	2.42	0.54	
1:J:29:ASN:HA	1:J:33:LYS:CE	2.36	0.54	
1:G:48:LEU:HD23	1:G:56:VAL:HG13	1.89	0.54	
1:H:189:LYS:CG	1:H:193:GLN:HE21	2.21	0.54	
1:J:25:ASP:O	1:J:29:ASN:HB2	2.08	0.53	
1:B:49:GLU:HG2	1:B:50:ASN:ND2	2.24	0.53	
1:G:37:ASN:HA	3:G:301:HOH:O	2.08	0.53	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:J:100:LYS:NZ	1:J:104:GLU:OE2	2.27	0.53	
1:J:180:ASN:OD1	1:J:181:LYS:N	2.42	0.53	
1:H:128:TRP:CZ3	1:H:161:ASP:HB2	2.44	0.53	
1:F:14:GLY:HA2	1:F:24:LEU:HD12	1.90	0.53	
1:H:94:ILE:HG23	1:H:98:LEU:HD23	1.91	0.53	
1:E:187:ASN:OD1	1:E:189:LYS:HG3	2.09	0.52	
1:A:58:LEU:HD22	1:E:154:VAL:HG13	1.91	0.52	
1:D:10:TYR:CE1	1:D:15:LEU:HD11	2.44	0.52	
1:K:43:VAL:O	1:K:46:THR:HG22	2.09	0.52	
1:J:48:LEU:HD21	1:J:59:VAL:HG11	1.92	0.52	
1:K:85:MET:HB3	1:K:185:VAL:HG22	1.91	0.52	
1:E:99:GLU:HG2	1:E:103:LYS:HE2	1.92	0.52	
1:F:144:SER:OG	3:F:305:HOH:O	2.09	0.52	
1:I:172:GLN:HE21	1:I:174:ARG:HH22	1.58	0.52	
1:D:128:TRP:CZ3	1:D:161:ASP:HB2	2.46	0.51	
1:L:1:MET:H	1:L:50:ASN:HD21	1.57	0.51	
1:J:94:ILE:HD11	3:J:332:HOH:O	2.09	0.51	
1:J:192:ASP:O	1:J:195:LEU:HD23	2.10	0.51	
1:L:1:MET:H	1:L:50:ASN:ND2	2.09	0.51	
1:E:19:ILE:CG2	1:E:24:LEU:HD12	2.40	0.51	
1:J:5:LEU:HD23	1:J:36:LEU:HD22	1.91	0.51	
1:K:14:GLY:HA2	1:K:24:LEU:HD12	1.91	0.51	
1:H:188:TRP:CE3	1:H:191:VAL:HG21	2.44	0.50	
1:A:44:LYS:NZ	3:A:312:HOH:O	2.44	0.50	
1:B:111:ASP:O	1:B:115:LYS:HG2	2.11	0.50	
1:K:86:ALA:O	1:K:185:VAL:HG23	2.10	0.50	
1:H:189:LYS:O	1:H:193:GLN:HG3	2.12	0.50	
1:L:126:SER:HB3	1:L:163:TRP:CD2	2.46	0.50	
1:H:79:SER:N	3:H:301:HOH:O	1.89	0.49	
1:L:192:ASP:HB2	3:L:303:HOH:O	2.12	0.49	
1:E:94:ILE:HG23	1:E:98:LEU:HD23	1.94	0.49	
1:K:192:ASP:HB2	3:K:315:HOH:O	2.11	0.49	
1:K:165:HIS:HB2	1:L:168:TYR:CZ	2.47	0.49	
1:C:10:TYR:CE1	1:C:15:LEU:HD11	2.47	0.49	
1:L:101:LEU:HD12	1:L:195:LEU:HD11	1.94	0.49	
1:L:132:VAL:HB	1:L:154:VAL:CG1	2.42	0.49	
1:I:164:GLU:OE1	1:J:165:HIS:ND1	2.34	0.49	
1:H:25:ASP:O	1:H:29:ASN:HB2	2.13	0.49	
1:H:46:THR:O	1:H:49:GLU:HG3	2.13	0.49	
1:J:3:PHE:HE2	1:J:43:VAL:HG21	1.78	0.48	
1:C:56:VAL:HG13	1:C:68:LEU:HD21	1.95	0.48	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:172:GLN:HE21	1:I:174:ARG:NH1	2.11	0.48
1:L:95:SER:OG	1:L:192:ASP:OD2	2.26	0.48
1:E:130:TRP:CE3	1:E:159:THR:HB	2.48	0.48
1:F:15:LEU:HD13	1:F:85:MET:HE2	1.94	0.48
1:A:153:ARG:HB2	1:E:58:LEU:HD11	1.95	0.48
1:A:152:LEU:HB2	1:A:154:VAL:HG22	1.95	0.48
1:J:134:ILE:HG12	1:J:154:VAL:HG12	1.95	0.48
1:D:152:LEU:HB2	1:D:154:VAL:HG22	1.96	0.47
1:G:28:PHE:CE2	1:G:33:LYS:HE3	2.48	0.47
1:C:25:ASP:OD1	3:C:304:HOH:O	2.20	0.47
1:G:115:LYS:HD3	1:G:115:LYS:HA	1.57	0.47
1:G:10:TYR:CE2	1:G:15:LEU:HD11	2.48	0.47
1:J:98:LEU:HD11	1:J:191:VAL:HG12	1.96	0.47
1:A:94:ILE:HD12	1:A:94:ILE:H	1.79	0.47
1:C:130:TRP:CE3	1:C:159:THR:HB	2.49	0.47
1:D:126:SER:HB3	1:D:163:TRP:CD2	2.49	0.47
1:J:46:THR:HG23	1:J:48:LEU:N	2.17	0.47
1:K:130:TRP:CE3	1:K:159:THR:HB	2.50	0.47
1:L:14:GLY:HA2	1:L:24:LEU:HD12	1.96	0.47
1:C:128:TRP:CZ3	1:C:161:ASP:HB2	2.50	0.47
1:G:46:THR:O	1:G:49:GLU:HG3	2.15	0.47
1:I:168:TYR:CE1	1:J:169:LEU:HD21	2.46	0.46
1:F:119:SER:OG	1:F:142:ASN:OD1	2.33	0.46
1:G:17:PRO:O	1:G:181:LYS:HD3	2.15	0.46
1:D:95:SER:OG	1:D:192:ASP:OD2	2.32	0.46
1:J:114:LYS:O	1:J:117:THR:HG22	2.15	0.46
1:B:189:LYS:HA	1:B:189:LYS:HD2	1.65	0.46
1:D:134:ILE:HG12	1:D:154:VAL:HG12	1.98	0.46
1:F:29:ASN:HA	1:F:33:LYS:HD2	1.98	0.46
1:H:19:ILE:CG2	1:H:24:LEU:HD12	2.45	0.46
1:E:44:LYS:HE2	1:E:44:LYS:HB3	1.68	0.46
1:F:48:LEU:HD13	1:F:56:VAL:HG13	1.98	0.46
1:K:15:LEU:HB3	1:K:185:VAL:HG21	1.97	0.46
1:D:15:LEU:HB3	1:D:185:VAL:HG11	1.97	0.46
1:H:45:GLY:N	1:H:49:GLU:OE1	2.44	0.46
1:J:95:SER:OG	1:J:192:ASP:OD1	2.21	0.46
1:J:152:LEU:HB2	1:J:154:VAL:HG22	1.97	0.46
1:E:2:LEU:HD22	1:E:40:ASN:HB3	1.99	0.45
1:G:133:ASN:HB3	1:G:155:THR:HG1	1.81	0.45
1:F:93:GLN:HA	3:F:309:HOH:O	2.16	0.45
1:G:95:SER:HB2	3:G:307:HOH:O	2.16	0.45



	lio us puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:14:GLY:HA2	1:B:24:LEU:HD12	1.98	0.45
1:A:126:SER:HB3	1:A:163:TRP:CD2	2.51	0.45
1:E:7:ASP:OD2	3:E:303:HOH:O	2.21	0.45
1:H:190:PHE:HA	1:H:193:GLN:NE2	2.32	0.45
1:G:94:ILE:HG23	1:G:98:LEU:CD1	2.43	0.45
1:F:99:GLU:O	1:F:103:LYS:HD3	2.17	0.45
1:B:89:ASN:OD1	1:B:89:ASN:N	2.49	0.45
1:E:187:ASN:HD21	1:E:189:LYS:HE3	1.81	0.45
1:I:172:GLN:HG3	1:J:26:PHE:CD1	2.51	0.45
1:L:137:LYS:HG2	1:L:138:LEU:N	2.32	0.45
1:H:14:GLY:C	1:H:15:LEU:HD22	2.37	0.45
1:J:139:GLU:OE2	3:J:303:HOH:O	2.21	0.45
1:B:128:TRP:CZ3	1:B:161:ASP:HB2	2.52	0.44
1:G:51:LYS:NZ	3:G:306:HOH:O	2.26	0.44
1:J:74:GLN:O	1:J:78:HIS:ND1	2.34	0.44
1:A:74:GLN:HG2	1:A:146:ALA:HB2	1.98	0.44
1:H:188:TRP:O	1:H:191:VAL:HG22	2.17	0.44
1:E:97:GLU:OE2	1:E:196:LYS:HE2	2.16	0.44
1:H:28:PHE:CE2	1:H:33:LYS:HE3	2.52	0.44
1:K:34:THR:HG22	1:K:38:LYS:HD2	1.99	0.44
1:B:-3:HIS:O	3:B:301:HOH:O	2.21	0.44
1:K:134:ILE:HG12	1:K:154:VAL:CG1	2.47	0.44
1:D:61:LYS:NZ	1:D:147:GLU:OE1	2.35	0.44
1:D:97:GLU:HB2	1:D:196:LYS:HZ3	1.83	0.44
1:J:192:ASP:O	1:J:195:LEU:CD2	2.66	0.44
1:L:90:GLN:NE2	3:L:316:HOH:O	2.48	0.44
1:H:192:ASP:O	1:H:195:LEU:HB3	2.18	0.44
1:D:1:MET:O	1:D:2:LEU:HD12	2.17	0.43
1:G:98:LEU:HD23	1:G:195:LEU:HD12	2.00	0.43
1:D:97:GLU:HB2	1:D:196:LYS:NZ	2.32	0.43
1:G:193:GLN:HA	1:G:196:LYS:HG2	1.99	0.43
1:J:8:PRO:HD3	1:J:28:PHE:CE2	2.53	0.43
1:H:2:LEU:HD23	1:H:2:LEU:HA	1.78	0.43
1:B:88:THR:HG22	1:B:184:GLU:O	2.18	0.43
1:J:85:MET:HA	1:J:185:VAL:O	2.18	0.43
1:J:180:ASN:OD1	1:J:181:LYS:HG2	2.19	0.43
1:K:83:ASP:HB3	1:K:190:PHE:CE2	2.53	0.43
1:L:15:LEU:HD22	1:L:185:VAL:HG13	1.99	0.43
1:E:83:ASP:HB3	1:E:190:PHE:CE1	2.54	0.43
1:I:23:THR:O	1:I:27:HIS:HB2	2.19	0.43
1:K:34:THR:HG22	1:K:38:LYS:CD	2.49	0.43



		Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance (Å)		
1:L:110:ALA:O	1:L:114:LYS:HG2	2.19	0.43	
1:B:126:SER:HB3	1:B:163:TRP:CD2	2.53	0.43	
1:L:2:LEU:HD22	1:L:40:ASN:HB3	2.00	0.43	
1:L:111:ASP:O	1:L:115:LYS:HG2	2.17	0.43	
1:L:128:TRP:CZ3	1:L:161:ASP:HB2	2.54	0.43	
1:F:130:TRP:CE3	1:F:159:THR:HB	2.54	0.42	
1:G:102:ILE:HG21	1:G:109:VAL:HA	2.01	0.42	
1:I:14:GLY:HA2	1:I:24:LEU:HD13	2.00	0.42	
1:B:44:LYS:HE3	1:B:49:GLU:OE2	2.18	0.42	
1:G:162:VAL:HG22	1:G:175:ARG:CZ	2.49	0.42	
1:H:78:HIS:N	3:H:301:HOH:O	2.51	0.42	
1:J:1:MET:HB3	1:J:2:LEU:H	1.64	0.42	
1:D:33:LYS:NZ	3:D:311:HOH:O	2.43	0.42	
1:H:2:LEU:HD13	1:H:40:ASN:HB3	2.01	0.42	
1:F:97:GLU:H	1:F:97:GLU:CD	2.23	0.42	
1:J:15:LEU:HB2	1:J:19:ILE:CG2	2.49	0.42	
1:L:94:ILE:HG22	1:L:99:GLU:HB2	2.01	0.42	
1:A:99:GLU:HG2	1:A:103:LYS:HE3	2.01	0.42	
1:H:115:LYS:HA	1:H:115:LYS:HD2	1.73	0.42	
1:J:14:GLY:HA2	1:J:24:LEU:HD12	2.01	0.42	
1:L:39:THR:O	1:L:43:VAL:HG13	2.19	0.42	
1:D:14:GLY:HA2	1:D:24:LEU:HD12	2.01	0.42	
1:E:95:SER:OG	1:E:192:ASP:OD1	2.30	0.42	
1:D:38:LYS:HA	1:D:38:LYS:HD2	1.74	0.42	
1:I:172:GLN:HE21	1:I:174:ARG:NH2	2.17	0.42	
1:L:61:LYS:HD2	1:L:61:LYS:HA	1.83	0.42	
1:K:196:LYS:HE2	1:K:196:LYS:HB3	1.86	0.42	
1:I:168:TYR:CG	1:I:172:GLN:HA	2.55	0.42	
1:E:70:ASN:HB3	1:H:124:PHE:CZ	2.55	0.41	
1:G:98:LEU:O	1:G:102:ILE:HD13	2.20	0.41	
1:G:16:GLU:OE1	1:G:16:GLU:N	2.53	0.41	
1:L:132:VAL:HB	1:L:154:VAL:HG13	2.02	0.41	
1:D:97:GLU:OE2	1:D:196:LYS:NZ	2.50	0.41	
1:E:85:MET:HA	1:E:185:VAL:O	2.21	0.41	
1:K:185:VAL:HG22	1:K:185:VAL:O	2.20	0.41	
1:C:33:LYS:NZ	3:C:314:HOH:O	2.54	0.41	
1:J:10:TYR:CE1	1:J:15:LEU:HD11	2.56	0.41	
1:H:12:LYS:HE2	3:H:312:HOH:O	2.21	0.41	
1:F:97:GLU:HG3	3:F:338:HOH:O	2.21	0.41	
1:I:128:TRP:HB2	1:I:130:TRP:NE1	2.35	0.41	
1:L:10:TYR:CE1	1:L:15:LEU:HD11	2.55	0.41	



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:E:10:TYR:CE1	1:E:15:LEU:HD11	2.56	0.41
1:E:115:LYS:HA	1:E:115:LYS:HD3	1.85	0.41
1:F:58:LEU:HD13	1:F:58:LEU:HA	1.95	0.41
1:J:83:ASP:HB3	1:J:190:PHE:CE1	2.55	0.41
1:B:10:TYR:CE1	1:B:15:LEU:HD11	2.56	0.41
1:I:167:TYR:HB3	1:I:178:TYR:CD1	2.57	0.41
1:J:23:THR:O	1:J:27:HIS:HB2	2.21	0.41
1:B:1:MET:N	1:B:50:ASN:OD1	2.53	0.40
1:F:2:LEU:HD12	1:F:40:ASN:OD1	2.21	0.40
1:H:85:MET:SD	1:H:182:TRP:NE1	2.94	0.40
1:H:133:ASN:HA	1:H:138:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

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	Perce	ntiles
1	А	200/205~(98%)	191 (96%)	9 (4%)	0	100	100
1	В	201/205~(98%)	194 (96%)	7 (4%)	0	100	100
1	С	200/205~(98%)	193 (96%)	7 (4%)	0	100	100
1	D	199/205~(97%)	191 (96%)	8 (4%)	0	100	100
1	Ε	195/205~(95%)	188 (96%)	7 (4%)	0	100	100
1	F	194/205~(95%)	186 (96%)	8 (4%)	0	100	100
1	G	194/205~(95%)	188 (97%)	6 (3%)	0	100	100
1	Η	195/205~(95%)	187 (96%)	7 (4%)	1 (0%)	29	31
1	Ι	195/205~(95%)	186 (95%)	9~(5%)	0	100	100
1	J	$19\overline{5/205}~(95\%)$	187 (96%)	8 (4%)	0	100	100
1	K	195/205~(95%)	187 (96%)	8 (4%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	L	201/205~(98%)	194 (96%)	7 (4%)	0	100	100
All	All	2364/2460~(96%)	2272 (96%)	91 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Н	50	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	179/183~(98%)	178~(99%)	1 (1%)	86	92
1	В	180/183~(98%)	179~(99%)	1 (1%)	86	92
1	С	179/183~(98%)	178~(99%)	1 (1%)	86	92
1	D	179/183~(98%)	179~(100%)	0	100	100
1	Ε	176/183~(96%)	174 (99%)	2(1%)	73	83
1	F	175/183~(96%)	174 (99%)	1 (1%)	86	92
1	G	175/183~(96%)	172~(98%)	3(2%)	60	72
1	Н	176/183~(96%)	174 (99%)	2(1%)	73	83
1	Ι	176/183~(96%)	174 (99%)	2(1%)	73	83
1	J	176/183~(96%)	172 (98%)	4 (2%)	50	61
1	Κ	176/183~(96%)	175 (99%)	1 (1%)	86	92
1	L	181/183~(99%)	180 (99%)	1 (1%)	86	92
All	All	2128/2196~(97%)	2109 (99%)	19 (1%)	78	87

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	144	SER
1	В	197	GLN
	a	7	



Mol	Chain	Res	Type
1	С	38	LYS
1	Е	144	SER
1	Е	189	LYS
1	F	61	LYS
1	G	44	LYS
1	G	89	ASN
1	G	100	LYS
1	Н	4	THR
1	Н	197	GLN
1	Ι	13	THR
1	Ι	172	GLN
1	J	27	HIS
1	J	98	LEU
1	J	195	LEU
1	J	196	LYS
1	К	59	VAL
1	L	-5	HIS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such side chains are listed below:

Mol	Chain	Res	Type
1	А	64	ASN
1	В	90	GLN
1	Е	197	GLN
1	Н	193	GLN
1	Ι	90	GLN
1	Ι	172	GLN
1	L	50	ASN
1	L	123	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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.

No monomer is involved in short contacts.

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, 95^{th} 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	А	202/205~(98%)	-0.19	3 (1%) 73 81	21, 31, 54, 69	0
1	В	202/205~(98%)	-0.20	1 (0%) 91 95	21, 34, 59, 74	0
1	С	202/205~(98%)	-0.27	2 (0%) 82 88	21, 31, 49, 77	0
1	D	201/205~(98%)	-0.26	1 (0%) 91 95	20, 32, 52, 63	0
1	Е	197/205~(96%)	-0.15	2 (1%) 82 88	27, 39, 55, 84	0
1	F	196/205~(95%)	-0.10	3 (1%) 73 81	29, 40, 55, 72	0
1	G	196/205~(95%)	0.02	2 (1%) 82 88	28, 44, 61, 85	0
1	Н	197/205~(96%)	0.13	8 (4%) 37 48	31, 44, 64, 83	0
1	Ι	197/205~(96%)	-0.02	3 (1%) 73 81	33, 46, 59, 65	0
1	J	197/205~(96%)	0.54	20 (10%) 6 11	39, 59, 88, 99	0
1	K	197/205~(96%)	-0.13	5 (2%) 57 66	33, 45, 63, 90	0
1	L	203/205~(99%)	-0.03	2 (0%) 82 88	35, 48, 66, 82	0
All	All	2387/2460~(97%)	-0.06	52 (2%) 62 71	20, 41, 66, 99	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	-6	HIS	6.3
1	Ι	2	LEU	5.8
1	Κ	1	MET	5.4
1	В	-4	HIS	4.9
1	С	-4	HIS	4.7
1	D	-3	HIS	4.3
1	J	1	MET	4.3
1	F	197	GLN	4.0
1	J	46	THR	4.0
1	J	197	GLN	3.9
1	А	197	GLN	3.8



6J	55

Mol	Chain	Res	Type	RSRZ	
1	Н	2	LEU	3.8	
1	А	-4	HIS	3.8	
1	J	3	PHE	3.7	
1	J	44	LYS	3.4	
1	Ι	49	GLU	3.4	
1	J	180	ASN	3.4	
1	J	93	GLN	3.3	
1	Н	9	ALA	3.1	
1	Н	197	GLN	3.0	
1	J	97	GLU	2.9	
1	Н	1	MET	2.9	
1	L	-5	HIS	2.8	
1	J	14	GLY	2.7	
1	Κ	43	VAL	2.7	
1	J	18	ALA	2.6	
1	J	107	GLY	2.6	
1	J	48	LEU	2.6	
1	F	196	LYS	2.6	
1	Κ	2	LEU	2.6	
1	J	45	GLY	2.5	
1	Е	1	MET	2.5	
1	G	197	GLN	2.5	
1	Κ	93	GLN	2.4	
1	Н	50	ASN	2.4	
1	Н	110	ALA	2.4	
1	J	89	ASN	2.3	
1	Н	188	TRP	2.3	
1	J	188	TRP	2.3	
1	J	99	GLU	2.2	
1	А	-3	HIS	2.1	
1	С	197	GLN	2.1	
1	G	193	GLN	2.1	
1	J	191	VAL	2.1	
1	F	4	THR	2.1	
1	J	50	ASN	2.1	
1	Н	10	TYR	2.1	
1	Е	197	GLN	2.1	
1	J	28	PHE	2.1	
1	J	96	PRO	2.0	
1	K	197	GLN	2.0	
1	Ι	196	LYS	2.0	

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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)

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. The B-factors column lists the minimum, median, 95^{th} 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	RSCC	RSR	${f B} ext{-factors}({ m \AA}^2)$	Q < 0.9
2	FE2	Н	201	1/1	0.98	0.17	38, 38, 38, 38	0
2	FE2	Ι	201	1/1	0.98	0.16	40,40,40,40	0
2	FE2	J	201	1/1	0.98	0.19	$51,\!51,\!51,\!51$	0
2	FE2	F	201	1/1	0.99	0.15	32,32,32,32	0
2	FE2	G	201	1/1	0.99	0.14	37,37,37,37	0
2	FE2	В	201	1/1	0.99	0.19	27,27,27,27	0
2	FE2	С	201	1/1	0.99	0.17	24,24,24,24	0
2	FE2	Е	201	1/1	0.99	0.15	30,30,30,30	0
2	FE2	K	201	1/1	0.99	0.15	40,40,40,40	0
2	FE2	L	201	1/1	0.99	0.15	40,40,40,40	0
2	FE2	A	201	1/1	1.00	0.18	23,23,23,23	0
2	FE2	D	201	1/1	1.00	0.16	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.

