



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 11:21 PM EDT

PDB ID : 7S8T
Title : M. xanthus ferritin-like protein EncC
Authors : Eren, E.
Deposited on : 2021-09-19
Resolution : 2.49 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

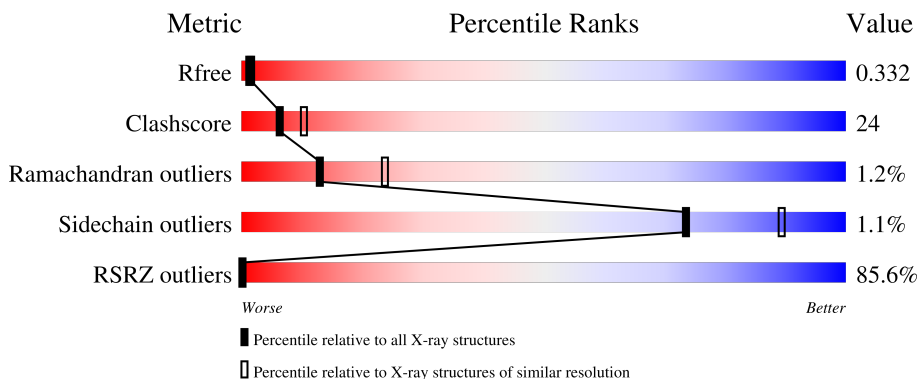
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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	137	
1	B	137	
1	C	137	
1	D	137	
1	E	137	

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Mol	Chain	Length	Quality of chain
1	F	137	
1	G	137	
1	H	137	
1	I	137	
1	J	137	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FE	A	201	-	-	-	X
2	FE	J	201	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6434 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 EncC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	82	Total 657	C 409	N 118	O 128	S 2	0	0	0
1	B	80	Total 634	C 395	N 113	O 125	S 1	0	0	0
1	C	80	Total 635	C 396	N 110	O 127	S 2	0	0	0
1	D	80	Total 637	C 396	N 112	O 127	S 2	0	0	0
1	E	78	Total 624	C 388	N 110	O 125	S 1	0	0	0
1	F	80	Total 637	C 396	N 112	O 127	S 2	0	0	0
1	G	80	Total 634	C 394	N 112	O 127	S 1	0	0	0
1	H	78	Total 618	C 385	N 107	O 125	S 1	0	0	0
1	I	79	Total 629	C 391	N 111	O 126	S 1	0	0	0
1	J	83	Total 636	C 396	N 112	O 127	S 1	0	0	0

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A4Y6CD88
A	2	HIS	-	expression tag	UNP A0A4Y6CD88
A	3	HIS	-	expression tag	UNP A0A4Y6CD88
A	4	HIS	-	expression tag	UNP A0A4Y6CD88
A	5	HIS	-	expression tag	UNP A0A4Y6CD88
A	6	HIS	-	expression tag	UNP A0A4Y6CD88
A	7	HIS	-	expression tag	UNP A0A4Y6CD88
B	1	MET	-	initiating methionine	UNP A0A4Y6CD88
B	2	HIS	-	expression tag	UNP A0A4Y6CD88

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	HIS	-	expression tag	UNP A0A4Y6CD88
B	4	HIS	-	expression tag	UNP A0A4Y6CD88
B	5	HIS	-	expression tag	UNP A0A4Y6CD88
B	6	HIS	-	expression tag	UNP A0A4Y6CD88
B	7	HIS	-	expression tag	UNP A0A4Y6CD88
C	1	MET	-	initiating methionine	UNP A0A4Y6CD88
C	2	HIS	-	expression tag	UNP A0A4Y6CD88
C	3	HIS	-	expression tag	UNP A0A4Y6CD88
C	4	HIS	-	expression tag	UNP A0A4Y6CD88
C	5	HIS	-	expression tag	UNP A0A4Y6CD88
C	6	HIS	-	expression tag	UNP A0A4Y6CD88
C	7	HIS	-	expression tag	UNP A0A4Y6CD88
D	1	MET	-	initiating methionine	UNP A0A4Y6CD88
D	2	HIS	-	expression tag	UNP A0A4Y6CD88
D	3	HIS	-	expression tag	UNP A0A4Y6CD88
D	4	HIS	-	expression tag	UNP A0A4Y6CD88
D	5	HIS	-	expression tag	UNP A0A4Y6CD88
D	6	HIS	-	expression tag	UNP A0A4Y6CD88
D	7	HIS	-	expression tag	UNP A0A4Y6CD88
E	1	MET	-	initiating methionine	UNP A0A4Y6CD88
E	2	HIS	-	expression tag	UNP A0A4Y6CD88
E	3	HIS	-	expression tag	UNP A0A4Y6CD88
E	4	HIS	-	expression tag	UNP A0A4Y6CD88
E	5	HIS	-	expression tag	UNP A0A4Y6CD88
E	6	HIS	-	expression tag	UNP A0A4Y6CD88
E	7	HIS	-	expression tag	UNP A0A4Y6CD88
F	1	MET	-	initiating methionine	UNP A0A4Y6CD88
F	2	HIS	-	expression tag	UNP A0A4Y6CD88
F	3	HIS	-	expression tag	UNP A0A4Y6CD88
F	4	HIS	-	expression tag	UNP A0A4Y6CD88
F	5	HIS	-	expression tag	UNP A0A4Y6CD88
F	6	HIS	-	expression tag	UNP A0A4Y6CD88
F	7	HIS	-	expression tag	UNP A0A4Y6CD88
G	1	MET	-	initiating methionine	UNP A0A4Y6CD88
G	2	HIS	-	expression tag	UNP A0A4Y6CD88
G	3	HIS	-	expression tag	UNP A0A4Y6CD88
G	4	HIS	-	expression tag	UNP A0A4Y6CD88
G	5	HIS	-	expression tag	UNP A0A4Y6CD88
G	6	HIS	-	expression tag	UNP A0A4Y6CD88
G	7	HIS	-	expression tag	UNP A0A4Y6CD88
H	1	MET	-	initiating methionine	UNP A0A4Y6CD88
H	2	HIS	-	expression tag	UNP A0A4Y6CD88

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Chain	Residue	Modelled	Actual	Comment	Reference
H	3	HIS	-	expression tag	UNP A0A4Y6CD88
H	4	HIS	-	expression tag	UNP A0A4Y6CD88
H	5	HIS	-	expression tag	UNP A0A4Y6CD88
H	6	HIS	-	expression tag	UNP A0A4Y6CD88
H	7	HIS	-	expression tag	UNP A0A4Y6CD88
I	1	MET	-	initiating methionine	UNP A0A4Y6CD88
I	2	HIS	-	expression tag	UNP A0A4Y6CD88
I	3	HIS	-	expression tag	UNP A0A4Y6CD88
I	4	HIS	-	expression tag	UNP A0A4Y6CD88
I	5	HIS	-	expression tag	UNP A0A4Y6CD88
I	6	HIS	-	expression tag	UNP A0A4Y6CD88
I	7	HIS	-	expression tag	UNP A0A4Y6CD88
J	1	MET	-	initiating methionine	UNP A0A4Y6CD88
J	2	HIS	-	expression tag	UNP A0A4Y6CD88
J	3	HIS	-	expression tag	UNP A0A4Y6CD88
J	4	HIS	-	expression tag	UNP A0A4Y6CD88
J	5	HIS	-	expression tag	UNP A0A4Y6CD88
J	6	HIS	-	expression tag	UNP A0A4Y6CD88
J	7	HIS	-	expression tag	UNP A0A4Y6CD88

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0
2	I	2	Total Fe 2 2	0	0
2	J	1	Total Fe 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0
3	B	7	Total O 7 7	0	0

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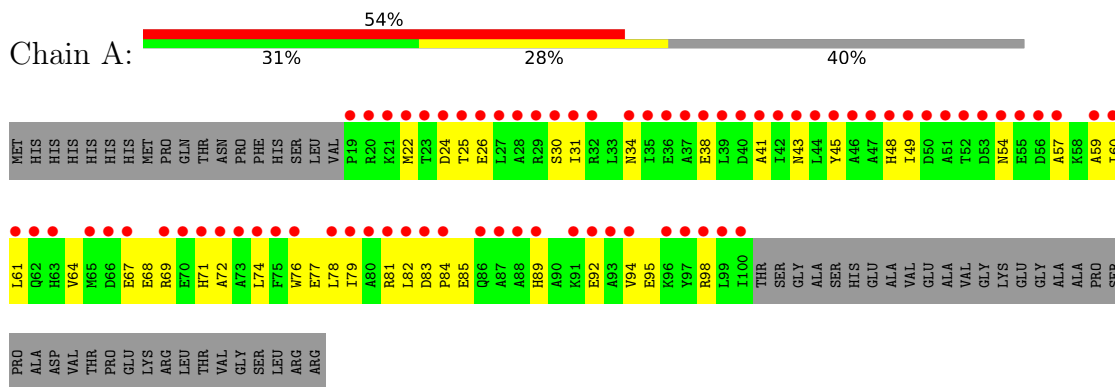
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	14	Total O 14 14	0	0
3	D	6	Total O 6 6	0	0
3	E	10	Total O 10 10	0	0
3	F	10	Total O 10 10	0	0
3	G	12	Total O 12 12	0	0
3	H	3	Total O 3 3	0	0
3	I	5	Total O 5 5	0	0
3	J	9	Total O 9 9	0	0

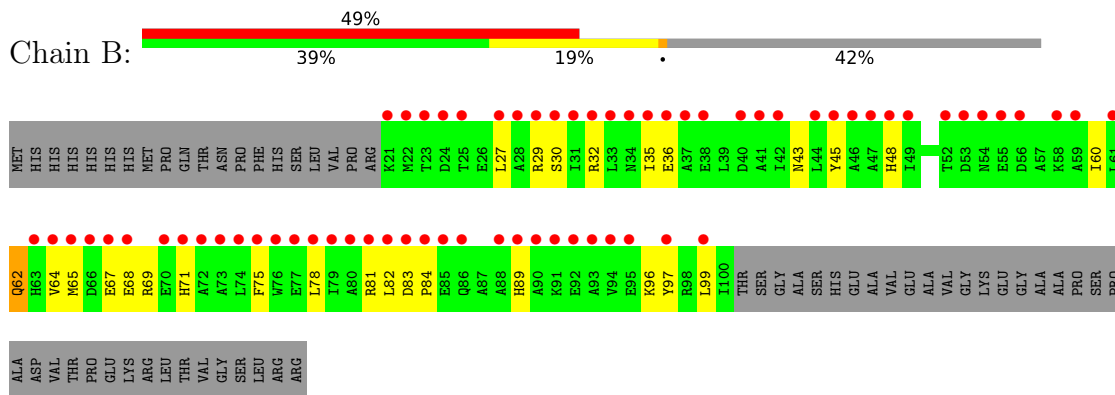
3 Residue-property plots i

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.

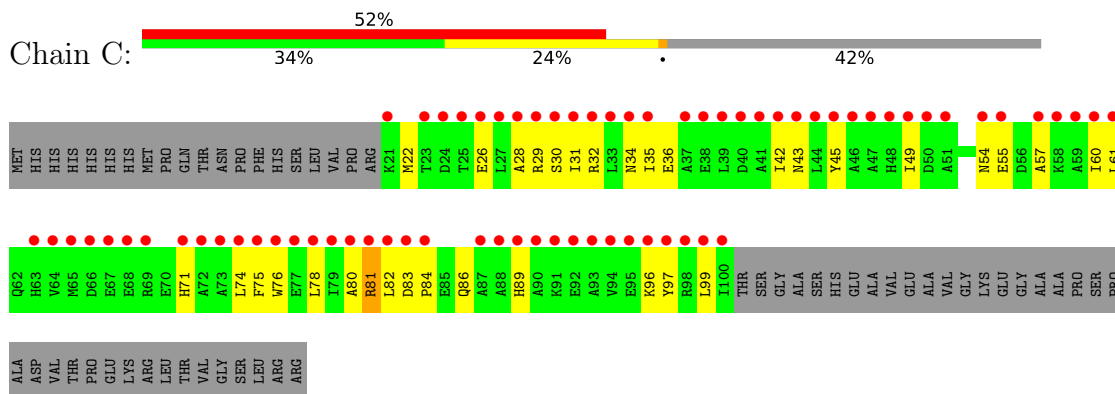
• Molecule 1: EncC



• Molecule 1: EncC

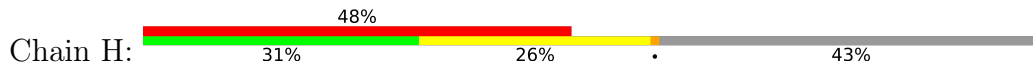


• Molecule 1: EncC



ALA
ASP
VAL
THR
PRO
GLU
LYS
ARG
MET
PRO
LEU
THR
VAL
GLY
SER
LEU
ARG
ARG

● Molecule 1: EncC

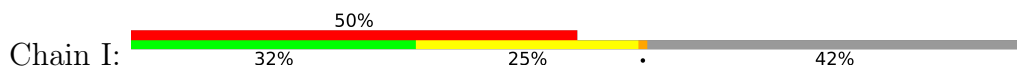


MET
HIS
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HIS
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ASN
PRO
PHE
HIS
SER
LEU
VAL
PRO
ARG
LYS
MET
T23
D24
T25
E26
L27
A28
R29
S30
I31
R32
L33
N34
I35
E36
A37
E38
L39
D40
A41
I42
N43
L44
Y45
A46
A47
H48
I49
D50
A51
T52
D53
N54
E55
D56
A57
K58
A59
I60

L61
Q62
H63
V64
M65
D66
E67
E68
R69
E70
H71
A72
A73
L74
F75
W76
E77
L78
I79
A80
R81
D82
D83
P84
E85
Q86
A87
A88
H89
S90
K91
E92
A93
V94
E95
K96
Y97
R98
L99
I100
THR
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● Molecule 1: EncC

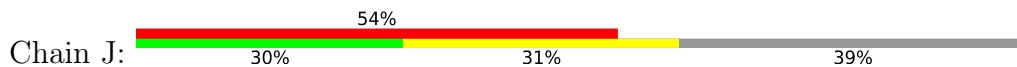


MET
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LYS
M22
T23
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T25
E26
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A28
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I31
R32
L33
N34
I35
E36
A37
E38
L39
D40
A41
I42
N43
L44
Y45
A46
A47
H48
I49
D50
A51
T52
D53
N54
E55
D56
A57
K58
A59
I60

L61
Q62
H63
V64
M65
D66
E67
E68
R69
E70
H71
A72
A73
L74
F75
W76
E77
L78
I79
A80
R81
D82
D83
P84
E85
Q86
A87
A88
H89
S90
K91
E92
A93
V94
E95
K96
Y97
R98
L99
I100
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● Molecule 1: EncC



MET
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A28
R29
S30
I31
R32
L33
N34
I35
E36
A37
E38
L39
D40
A41
I42
N43
L44
Y45
A46
A47
H48
I49
D50
A51
T52
D53
N54
E55
D56
A57
K58
A59
I60

L61
Q62
H63
V64
M65
D66
E67
E68
R69
E70
H71
A72
A73
L74
F75
W76
E77
L78
I79
A80
R81
D82
D83
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E85
Q86
A87
A88
H89
S90
K91
E92
A93
V94
E95
K96
Y97
R98
L99
I100
THR
SER
GLY
ALA
SER
HIS
GLU
ALA
VAL
GLU
ALA
VAL
GLU
ALA
VAL
GLY
LYS
GLY
GLY
ALA
ALA
PRO
SER

PRO
ALA
ASP
VAL
THR
PRO
GLU
LYS
ARG
MET
PRO
LEU
THR
VAL
GLY
SER
LEU
ARG

4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.70Å 47.80Å 135.33Å 90.00° 90.13° 90.00°	Depositor
Resolution (Å)	37.77 – 2.49 37.77 – 2.49	Depositor EDS
% Data completeness (in resolution range)	96.4 (37.77-2.49) 96.1 (37.77-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	95.48 (at 2.48Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.325 , 0.340 0.329 , 0.332	Depositor DCC
R_{free} test set	1994 reflections (6.13%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtrriage
Anisotropy	0.291	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.397 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6434	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.64% 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

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.33	0/667	0.63	0/901
1	B	0.34	0/643	0.64	0/871
1	C	0.31	0/644	0.66	0/872
1	D	0.33	0/646	0.55	0/875
1	E	0.37	0/633	0.57	0/858
1	F	0.34	0/646	0.56	0/875
1	G	0.30	0/643	0.55	0/872
1	H	0.34	0/627	0.57	0/851
1	I	0.31	0/638	0.55	0/865
1	J	0.32	0/645	0.52	0/878
All	All	0.33	0/6432	0.58	0/8718

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	657	0	636	47	0
1	B	634	0	609	31	0
1	C	635	0	609	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	637	0	609	42	0
1	E	624	0	598	40	0
1	F	637	0	609	34	0
1	G	634	0	602	43	0
1	H	618	0	587	34	0
1	I	629	0	600	44	0
1	J	636	0	598	47	0
2	A	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	0	0
2	I	2	0	0	0	0
2	J	1	0	0	0	0
3	A	10	0	0	2	0
3	B	7	0	0	1	0
3	C	14	0	0	1	0
3	D	6	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	1	0
3	G	12	0	0	2	0
3	H	3	0	0	0	0
3	I	5	0	0	0	0
3	J	9	0	0	0	0
All	All	6434	0	6057	300	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 24.

All (300) 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:J:68:GLU:HA	1:J:71:HIS:HD2	1.08	1.12
1:J:68:GLU:HA	1:J:71:HIS:CD2	1.98	0.99
1:I:82:LEU:HD23	1:I:83:ASP:H	1.42	0.82
1:E:74:LEU:HD21	1:F:60:ILE:HB	1.62	0.81
1:G:60:ILE:HD11	1:I:78:LEU:HD22	1.63	0.79
1:G:67:GLU:OE1	1:I:71:HIS:CE1	2.35	0.79
1:G:71:HIS:ND1	1:I:64:VAL:HG13	1.98	0.78
1:E:25:THR:HA	1:E:29:ARG:HB2	1.67	0.77
1:I:67:GLU:O	1:I:71:HIS:CD2	2.38	0.76
1:C:31:ILE:HG12	1:C:78:LEU:HD22	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:HIS:HB2	1:J:99:LEU:HD11	1.67	0.74
1:E:78:LEU:HD13	1:F:60:ILE:HD13	1.69	0.73
1:I:89:HIS:HA	1:I:92:GLU:HG2	1.71	0.72
1:E:67:GLU:OE1	1:F:71:HIS:NE2	2.21	0.72
1:C:89:HIS:ND1	1:C:89:HIS:O	2.22	0.72
1:F:77:GLU:HG3	1:G:96:LYS:HD3	1.70	0.72
1:B:71:HIS:HE1	1:D:71:HIS:HE1	1.38	0.72
1:A:69:ARG:NH1	3:A:301:HOH:O	2.22	0.71
1:J:49:ILE:O	1:J:58:LYS:NZ	2.23	0.71
1:B:78:LEU:HD13	1:D:60:ILE:HD13	1.72	0.71
1:G:71:HIS:ND1	1:I:64:VAL:HG22	2.06	0.71
1:C:78:LEU:HD12	1:H:60:ILE:HD11	1.72	0.70
1:E:60:ILE:HD11	1:F:78:LEU:HD22	1.72	0.69
1:I:56:ASP:O	1:I:60:ILE:HG12	1.92	0.69
1:I:88:ALA:O	1:I:92:GLU:HB3	1.93	0.68
1:J:68:GLU:CA	1:J:71:HIS:HD2	1.97	0.68
1:C:71:HIS:NE2	1:H:67:GLU:OE1	2.27	0.67
1:D:96:LYS:HZ1	1:I:78:LEU:HA	1.60	0.67
1:D:64:VAL:O	1:D:68:GLU:HG2	1.96	0.66
1:B:60:ILE:HD11	1:D:78:LEU:HD22	1.78	0.66
1:E:30:SER:HB3	1:F:48:HIS:CD2	2.31	0.65
1:D:43:ASN:OD1	1:I:32:ARG:NH2	2.27	0.65
1:B:64:VAL:O	1:B:68:GLU:HG2	1.97	0.65
1:B:43:ASN:OD1	1:J:32:ARG:NE	2.23	0.64
1:A:85:GLU:HG2	1:H:69:ARG:HH12	1.62	0.63
1:C:29:ARG:H	1:C:29:ARG:HD2	1.64	0.63
1:B:71:HIS:HE1	1:D:71:HIS:CE1	2.16	0.63
1:J:67:GLU:O	1:J:70:GLU:HG2	1.99	0.63
1:B:30:SER:HB2	1:D:48:HIS:CE1	2.33	0.62
1:A:94:VAL:O	1:A:98:ARG:N	2.31	0.62
1:F:66:ASP:OD1	1:F:69:ARG:NH1	2.33	0.62
1:G:32:ARG:HH11	1:G:84:PRO:HG3	1.65	0.62
1:G:35:ILE:HD12	1:G:79:ILE:HD12	1.80	0.62
1:B:89:HIS:O	1:B:89:HIS:ND1	2.33	0.61
1:A:89:HIS:HE1	1:H:76:TRP:HD1	1.49	0.61
1:B:67:GLU:OE1	1:D:71:HIS:NE2	2.34	0.61
1:H:25:THR:HG23	1:H:29:ARG:HD3	1.81	0.61
1:E:29:ARG:N	1:E:29:ARG:HD2	2.16	0.61
1:C:29:ARG:HD2	1:C:29:ARG:N	2.15	0.61
1:B:81:ARG:HE	1:J:96:LYS:HZ3	1.49	0.60
1:F:46:ALA:O	1:F:49:ILE:HG22	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:85:GLU:N	1:J:85:GLU:OE1	2.35	0.60
1:A:95:GLU:HA	1:A:98:ARG:HB2	1.84	0.59
1:G:71:HIS:CE1	1:I:64:VAL:HG13	2.37	0.59
1:A:71:HIS:NE2	1:J:67:GLU:OE1	2.23	0.59
1:E:34:ASN:HB3	1:E:75:PHE:CE2	2.37	0.59
1:F:86:GLN:OE1	1:G:69:ARG:NH1	2.31	0.59
1:E:27:LEU:HG	1:E:82:LEU:HD21	1.83	0.59
1:E:81:ARG:NH1	1:F:56:ASP:OD2	2.32	0.59
1:E:71:HIS:CD2	1:F:64:VAL:HG22	2.37	0.59
1:B:81:ARG:HE	1:J:96:LYS:NZ	2.00	0.59
1:D:46:ALA:O	1:D:49:ILE:HG22	2.02	0.59
1:C:45:TYR:O	1:C:49:ILE:HG13	2.03	0.58
1:D:32:ARG:HH22	1:D:84:PRO:HG2	1.68	0.58
1:D:27:LEU:O	1:D:31:ILE:HG12	2.03	0.58
1:E:35:ILE:HG12	1:E:75:PHE:HB3	1.85	0.58
1:I:95:GLU:OE2	1:I:98:ARG:NH1	2.37	0.58
1:C:22:MET:H	1:C:26:GLU:HB3	1.68	0.58
1:E:76:TRP:HE1	1:E:89:HIS:CD2	2.21	0.58
1:H:66:ASP:O	1:H:70:GLU:HG2	2.03	0.58
1:E:32:ARG:HH11	1:E:84:PRO:HG3	1.68	0.58
1:E:78:LEU:HD13	1:F:60:ILE:CD1	2.33	0.57
1:H:57:ALA:O	1:H:61:LEU:HB2	2.04	0.57
1:F:27:LEU:HB3	1:F:82:LEU:HD21	1.86	0.57
1:C:82:LEU:HG	1:C:83:ASP:H	1.70	0.57
1:D:54:ASN:OD1	1:D:55:GLU:N	2.38	0.57
1:G:67:GLU:O	1:G:71:HIS:CD2	2.58	0.57
1:B:65:MET:HG2	1:B:69:ARG:NH1	2.20	0.57
1:C:43:ASN:OD1	1:E:32:ARG:HD2	2.05	0.57
1:C:80:ALA:HB1	1:C:86:GLN:HB3	1.86	0.57
1:C:32:ARG:HD2	1:E:43:ASN:OD1	2.05	0.56
1:A:82:LEU:HB3	1:A:84:PRO:HD2	1.87	0.56
1:A:92:GLU:N	1:A:92:GLU:OE1	2.33	0.56
1:G:71:HIS:CE1	1:I:67:GLU:OE1	2.58	0.56
1:A:78:LEU:HD22	1:J:60:ILE:HD11	1.87	0.56
1:C:54:ASN:HD22	1:H:27:LEU:HD21	1.70	0.56
1:B:82:LEU:HB3	1:B:84:PRO:HD2	1.87	0.56
1:G:44:LEU:HD11	1:I:33:LEU:HD21	1.87	0.56
1:G:78:LEU:HD11	1:I:60:ILE:CD1	2.36	0.56
1:E:94:VAL:O	1:E:98:ARG:HD3	2.06	0.55
1:B:48:HIS:CE1	1:D:30:SER:HB2	2.42	0.55
1:H:64:VAL:O	1:H:68:GLU:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:TYR:CE2	1:A:64:VAL:HG12	2.42	0.55
1:A:74:LEU:HD21	1:H:95:GLU:HB3	1.87	0.55
1:I:85:GLU:OE1	1:I:85:GLU:N	2.40	0.55
1:J:94:VAL:O	1:J:98:ARG:HB2	2.06	0.55
1:C:30:SER:HB3	1:H:48:HIS:CD2	2.42	0.54
1:I:34:ASN:HB3	1:I:75:PHE:CE2	2.42	0.54
1:G:27:LEU:O	1:G:31:ILE:HG12	2.08	0.54
1:I:49:ILE:HG23	1:I:58:LYS:HG2	1.90	0.54
1:E:27:LEU:HD13	1:F:52:THR:HG21	1.90	0.54
1:A:67:GLU:OE1	1:J:71:HIS:CE1	2.62	0.53
1:G:27:LEU:HG	1:G:82:LEU:HD21	1.90	0.53
1:G:44:LEU:HD21	1:I:33:LEU:HG	1.90	0.53
1:A:82:LEU:HG	1:A:83:ASP:H	1.74	0.53
1:J:76:TRP:HE1	1:J:89:HIS:CE1	2.26	0.53
1:A:38:GLU:HB3	1:A:72:ALA:HB2	1.91	0.53
1:B:36:GLU:HG2	1:J:36:GLU:HA	1.90	0.53
1:D:55:GLU:O	1:D:58:LYS:HG3	2.09	0.53
1:B:78:LEU:HD13	1:D:60:ILE:CD1	2.36	0.53
1:J:76:TRP:O	1:J:79:ILE:HG22	2.08	0.53
1:C:29:ARG:HE	1:E:46:ALA:CB	2.22	0.52
1:E:27:LEU:O	1:E:31:ILE:HG12	2.09	0.52
1:A:49:ILE:HD11	1:A:61:LEU:HB3	1.92	0.52
1:A:89:HIS:CE1	1:H:76:TRP:HD1	2.27	0.52
1:A:30:SER:HB3	1:J:48:HIS:NE2	2.25	0.52
1:A:77:GLU:OE1	1:H:96:LYS:HD3	2.10	0.52
1:A:94:VAL:O	1:A:98:ARG:HG2	2.10	0.52
1:E:66:ASP:OD1	1:E:69:ARG:NH2	2.43	0.52
1:I:45:TYR:O	1:I:49:ILE:HG13	2.09	0.52
1:J:83:ASP:N	1:J:84:PRO:HD2	2.24	0.52
1:J:35:ILE:O	1:J:39:LEU:HG	2.10	0.51
1:C:54:ASN:OD1	1:C:55:GLU:N	2.43	0.51
1:D:29:ARG:HD2	1:D:29:ARG:N	2.25	0.51
1:H:24:ASP:O	1:H:28:ALA:N	2.29	0.51
1:H:32:ARG:CZ	1:H:79:ILE:HD11	2.40	0.51
1:H:38:GLU:O	1:H:42:ILE:HG13	2.10	0.51
1:D:96:LYS:HZ1	1:I:78:LEU:HD12	1.75	0.51
1:A:61:LEU:HD21	1:J:31:ILE:HD11	1.92	0.51
1:D:43:ASN:OD1	1:I:32:ARG:HD2	2.11	0.51
1:A:81:ARG:NH2	1:J:60:ILE:HD13	2.26	0.51
1:F:23:THR:HA	1:F:27:LEU:HD23	1.91	0.51
1:F:32:ARG:HE	1:F:79:ILE:HD11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:LEU:HD23	1:H:83:ASP:H	1.76	0.51
1:F:38:GLU:HB3	1:F:72:ALA:HB2	1.92	0.51
1:C:35:ILE:HD13	1:C:76:TRP:HE3	1.75	0.50
1:G:26:GLU:OE2	1:I:51:ALA:HB1	2.11	0.50
1:D:29:ARG:HD2	1:D:29:ARG:H	1.77	0.50
1:F:97:TYR:HE1	1:G:81:ARG:HH21	1.60	0.50
1:D:96:LYS:NZ	1:I:78:LEU:HA	2.26	0.50
1:G:64:VAL:O	1:G:68:GLU:HG3	2.11	0.50
1:I:38:GLU:OE1	1:I:71:HIS:HB2	2.12	0.50
1:I:57:ALA:O	1:I:61:LEU:HB2	2.11	0.50
1:J:18:VAL:O	1:J:20:ARG:N	2.45	0.50
1:B:71:HIS:CE1	1:D:71:HIS:HE1	2.26	0.50
1:D:75:PHE:O	1:D:79:ILE:HG22	2.12	0.50
1:G:79:ILE:CG2	1:G:84:PRO:HG2	2.42	0.50
1:F:39:LEU:HD22	1:G:32:ARG:HG2	1.94	0.49
1:G:35:ILE:CD1	1:G:79:ILE:HD12	2.41	0.49
1:I:32:ARG:O	1:I:36:GLU:HG3	2.12	0.49
1:D:25:THR:HA	1:D:29:ARG:HD3	1.95	0.49
1:G:71:HIS:NE2	1:I:67:GLU:OE1	2.46	0.49
1:C:76:TRP:HE1	1:C:89:HIS:HD2	1.59	0.49
1:F:76:TRP:HA	1:F:79:ILE:HG22	1.94	0.49
1:C:60:ILE:HD11	1:H:78:LEU:HD22	1.93	0.49
1:G:38:GLU:OE2	1:G:68:GLU:HB3	2.12	0.49
1:H:96:LYS:HG3	1:H:97:TYR:N	2.28	0.48
1:J:63:HIS:O	1:J:67:GLU:HG3	2.12	0.48
1:A:45:TYR:HE1	1:J:34:ASN:CG	2.17	0.48
1:B:62:GLN:HE21	1:B:62:GLN:HB3	1.51	0.48
1:I:54:ASN:OD1	1:I:55:GLU:N	2.46	0.48
1:F:22:MET:HB3	1:F:26:GLU:HB2	1.94	0.48
1:G:54:ASN:OD1	1:G:55:GLU:N	2.47	0.48
1:C:96:LYS:NZ	1:E:78:LEU:HD12	2.28	0.48
1:B:82:LEU:HG	1:B:83:ASP:H	1.79	0.48
1:J:46:ALA:O	1:J:49:ILE:HG22	2.13	0.48
1:B:99:LEU:O	3:B:201:HOH:O	2.20	0.47
1:F:27:LEU:O	1:F:31:ILE:HG12	2.14	0.47
1:D:82:LEU:HG	1:D:83:ASP:H	1.79	0.47
1:D:99:LEU:HD13	1:G:60:ILE:HG22	1.97	0.47
1:E:64:VAL:O	1:E:68:GLU:HG3	2.14	0.47
1:G:57:ALA:O	1:G:61:LEU:HB2	2.13	0.47
1:D:34:ASN:HB3	1:D:75:PHE:CE2	2.50	0.47
1:C:22:MET:H	1:C:26:GLU:CB	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:58:LYS:C	1:I:58:LYS:HD2	2.35	0.47
1:J:20:ARG:C	1:J:22:MET:H	2.18	0.47
1:J:31:ILE:HG21	1:J:78:LEU:HD22	1.96	0.47
1:E:32:ARG:HH11	1:E:84:PRO:CG	2.27	0.47
1:C:96:LYS:O	1:C:99:LEU:HG	2.15	0.46
1:E:67:GLU:O	1:E:70:GLU:HG2	2.16	0.46
1:H:93:ALA:HA	1:H:96:LYS:HG2	1.97	0.46
1:B:69:ARG:NH2	1:J:85:GLU:OE1	2.48	0.46
1:F:54:ASN:OD1	1:F:55:GLU:N	2.49	0.46
1:H:76:TRP:HE1	1:H:89:HIS:CD2	2.34	0.46
1:A:92:GLU:HG2	1:H:77:GLU:HB2	1.97	0.46
1:B:43:ASN:OD1	1:J:29:ARG:HA	2.16	0.46
1:E:46:ALA:HA	1:E:65:MET:HE1	1.97	0.46
1:A:60:ILE:CD1	1:J:78:LEU:HD13	2.46	0.46
1:C:32:ARG:NH1	1:C:84:PRO:HG3	2.31	0.46
1:C:35:ILE:HD13	1:C:76:TRP:CE3	2.50	0.46
1:J:67:GLU:O	1:J:71:HIS:CD2	2.69	0.46
1:C:22:MET:N	1:C:26:GLU:HB3	2.31	0.46
1:C:26:GLU:OE2	1:H:51:ALA:HB1	2.16	0.46
1:D:43:ASN:OD1	1:I:29:ARG:HA	2.16	0.46
1:F:77:GLU:HG2	1:G:92:GLU:O	2.16	0.46
1:A:41:ALA:HB1	1:A:68:GLU:OE1	2.16	0.45
1:E:24:ASP:OD1	1:E:25:THR:N	2.49	0.45
1:G:28:ALA:HB1	1:G:32:ARG:HH22	1.80	0.45
1:B:29:ARG:HA	1:J:43:ASN:OD1	2.16	0.45
1:C:34:ASN:HB3	1:C:75:PHE:CE2	2.51	0.45
1:G:78:LEU:HD11	1:I:60:ILE:HD12	1.97	0.45
1:B:68:GLU:HA	1:B:71:HIS:ND1	2.32	0.45
1:C:36:GLU:HG3	1:E:36:GLU:HG2	1.97	0.45
1:D:36:GLU:HG3	1:I:36:GLU:HG2	1.99	0.45
1:C:30:SER:HB3	1:H:48:HIS:NE2	2.30	0.45
1:F:42:ILE:HD11	1:F:69:ARG:HA	1.97	0.45
1:G:67:GLU:HB2	1:I:71:HIS:HE1	1.82	0.45
1:G:95:GLU:O	3:G:201:HOH:O	2.20	0.45
1:A:22:MET:HB3	1:A:26:GLU:HB3	1.99	0.45
1:D:91:LYS:O	1:D:95:GLU:HG2	2.17	0.45
1:C:74:LEU:HD12	1:C:74:LEU:HA	1.77	0.45
1:G:48:HIS:CD2	1:I:34:ASN:HD21	2.34	0.45
1:D:32:ARG:HD2	1:D:79:ILE:HD12	1.99	0.45
1:D:35:ILE:HG13	1:D:75:PHE:HB3	1.99	0.45
1:C:99:LEU:HD12	1:C:99:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:HD13	1:A:34:ASN:HD22	1.82	0.45
1:A:79:ILE:HG13	1:A:84:PRO:HG2	1.98	0.45
1:E:67:GLU:HG2	1:E:70:GLU:OE1	2.17	0.44
1:B:96:LYS:HG3	1:B:97:TYR:CD1	2.52	0.44
1:C:83:ASP:HB2	1:C:84:PRO:HD3	1.99	0.44
1:C:76:TRP:HB2	3:C:201:HOH:O	2.16	0.44
1:E:57:ALA:O	1:E:61:LEU:HD23	2.18	0.44
1:A:48:HIS:CD2	1:J:30:SER:HB3	2.53	0.44
1:B:45:TYR:OH	1:D:38:GLU:OE2	2.36	0.44
1:C:54:ASN:HB3	1:C:57:ALA:HB3	2.00	0.44
1:D:28:ALA:O	1:D:32:ARG:HD3	2.18	0.44
1:G:67:GLU:OE1	1:I:71:HIS:HE1	1.94	0.44
1:A:78:LEU:O	1:A:82:LEU:HB2	2.17	0.44
1:C:42:ILE:HG22	1:E:32:ARG:NH2	2.33	0.44
1:D:49:ILE:HG23	1:D:50:ASP:OD1	2.18	0.44
1:I:32:ARG:HH11	1:I:84:PRO:HG3	1.82	0.44
1:A:45:TYR:HE1	1:J:34:ASN:ND2	2.15	0.44
1:B:81:ARG:HH21	1:J:96:LYS:HE2	1.83	0.43
1:D:85:GLU:OE1	1:D:85:GLU:N	2.51	0.43
1:A:89:HIS:CE1	1:H:76:TRP:CD1	3.06	0.43
1:C:89:HIS:HA	1:E:73:ALA:HB1	1.99	0.43
1:A:77:GLU:O	1:A:81:ARG:HG2	2.17	0.43
1:B:32:ARG:HD2	1:J:43:ASN:OD1	2.17	0.43
1:F:29:ARG:HA	1:F:32:ARG:HD3	1.99	0.43
1:G:82:LEU:HB3	1:G:83:ASP:H	1.61	0.43
1:J:76:TRP:NE1	1:J:89:HIS:CE1	2.86	0.43
1:B:27:LEU:HD12	1:B:27:LEU:HA	1.65	0.43
1:F:25:THR:HG23	1:F:29:ARG:HG2	2.00	0.43
1:F:64:VAL:O	1:F:68:GLU:HG3	2.19	0.43
1:I:68:GLU:HA	1:I:71:HIS:HD2	1.83	0.43
1:J:23:THR:O	1:J:27:LEU:HD21	2.18	0.43
1:C:28:ALA:HB3	1:C:29:ARG:NH1	2.33	0.43
1:D:35:ILE:O	1:D:39:LEU:HG	2.19	0.43
1:F:29:ARG:HE	1:G:46:ALA:CB	2.32	0.43
1:A:67:GLU:HB2	1:J:71:HIS:HE1	1.84	0.43
1:H:96:LYS:HG3	1:H:97:TYR:H	1.84	0.43
1:G:74:LEU:O	1:G:78:LEU:HD13	2.19	0.43
1:A:59:ALA:HB1	1:B:99:LEU:HB3	2.00	0.43
1:F:43:ASN:OD1	1:G:32:ARG:HD2	2.19	0.43
1:H:34:ASN:O	1:H:38:GLU:HG2	2.19	0.43
1:A:81:ARG:HH21	1:J:60:ILE:HD13	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:TRP:O	1:A:79:ILE:HG22	2.19	0.42
1:A:64:VAL:HG13	1:J:71:HIS:ND1	2.34	0.42
1:A:74:LEU:HD21	1:H:95:GLU:CB	2.50	0.42
1:F:61:LEU:HA	3:F:304:HOH:O	2.18	0.42
1:A:43:ASN:HD21	1:H:32:ARG:CB	2.32	0.42
1:D:57:ALA:O	1:D:61:LEU:HB2	2.19	0.42
1:A:48:HIS:NE2	1:J:30:SER:HB3	2.35	0.42
1:A:61:LEU:HD21	1:J:31:ILE:CD1	2.49	0.42
1:A:22:MET:HG2	1:A:24:ASP:H	1.85	0.42
1:C:82:LEU:CG	1:C:83:ASP:H	2.31	0.42
1:E:79:ILE:O	1:E:84:PRO:HD2	2.20	0.42
1:H:54:ASN:O	1:H:58:LYS:HD3	2.19	0.42
1:A:22:MET:HB3	1:A:26:GLU:CB	2.49	0.42
1:C:81:ARG:HD3	1:C:86:GLN:OE1	2.20	0.42
1:C:82:LEU:HG	1:C:83:ASP:N	2.33	0.42
1:I:22:MET:HA	1:I:26:GLU:HB2	2.02	0.41
1:E:71:HIS:CG	1:F:64:VAL:HG13	2.55	0.41
1:G:79:ILE:HG23	1:G:84:PRO:HG2	2.02	0.41
1:B:35:ILE:HG12	1:B:75:PHE:HB3	2.01	0.41
1:F:29:ARG:HD2	1:F:29:ARG:N	2.36	0.41
1:I:89:HIS:CG	1:I:89:HIS:O	2.74	0.41
1:A:54:ASN:HB3	1:A:57:ALA:HB3	2.01	0.41
1:I:82:LEU:CD2	1:I:83:ASP:H	2.24	0.41
1:J:56:ASP:O	1:J:60:ILE:HG23	2.20	0.41
1:D:60:ILE:HG13	1:D:61:LEU:N	2.35	0.41
1:E:31:ILE:O	1:E:35:ILE:HG13	2.21	0.41
1:H:54:ASN:OD1	1:H:55:GLU:N	2.49	0.41
1:A:61:LEU:HD22	1:J:75:PHE:HE1	1.85	0.41
1:E:28:ALA:HB3	1:E:29:ARG:HH11	1.85	0.41
1:E:46:ALA:CA	1:E:65:MET:HE1	2.51	0.41
1:G:44:LEU:HD23	1:I:34:ASN:HD22	1.86	0.40
1:H:27:LEU:O	1:H:31:ILE:HG12	2.21	0.40
1:C:61:LEU:HD11	1:H:34:ASN:HD21	1.85	0.40
1:E:32:ARG:NH1	1:E:84:PRO:HG3	2.36	0.40
1:I:76:TRP:O	1:I:79:ILE:HG22	2.22	0.40
1:J:57:ALA:O	1:J:61:LEU:HD23	2.20	0.40
1:A:25:THR:HA	3:A:305:HOH:O	2.21	0.40
1:D:74:LEU:HD12	1:D:74:LEU:HA	1.91	0.40
1:F:29:ARG:HH21	1:G:46:ALA:CB	2.35	0.40
1:G:68:GLU:HA	1:G:71:HIS:HD2	1.85	0.40
1:H:58:LYS:O	1:H:62:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:GLU:HA	1:D:80:ALA:HB3	2.04	0.40
1:E:29:ARG:HG3	1:E:32:ARG:NH2	2.36	0.40
1:G:76:TRP:HB2	3:G:202:HOH:O	2.22	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	Percentiles	
1	A	80/137 (58%)	76 (95%)	4 (5%)	0	100	100
1	B	78/137 (57%)	73 (94%)	5 (6%)	0	100	100
1	C	78/137 (57%)	70 (90%)	7 (9%)	1 (1%)	12	21
1	D	78/137 (57%)	70 (90%)	8 (10%)	0	100	100
1	E	76/137 (56%)	72 (95%)	2 (3%)	2 (3%)	5	8
1	F	78/137 (57%)	74 (95%)	2 (3%)	2 (3%)	5	8
1	G	78/137 (57%)	74 (95%)	3 (4%)	1 (1%)	12	21
1	H	76/137 (56%)	72 (95%)	4 (5%)	0	100	100
1	I	77/137 (56%)	74 (96%)	3 (4%)	0	100	100
1	J	81/137 (59%)	73 (90%)	5 (6%)	3 (4%)	3	4
All	All	780/1370 (57%)	728 (93%)	43 (6%)	9 (1%)	13	24

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	97	TYR
1	G	26	GLU
1	E	25	THR
1	E	83	ASP

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Mol	Chain	Res	Type
1	F	82	LEU
1	F	83	ASP
1	J	21	LYS
1	J	25	THR
1	J	19	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	65/112 (58%)	65 (100%)	0	100	100
1	B	62/112 (55%)	61 (98%)	1 (2%)	62	84
1	C	63/112 (56%)	62 (98%)	1 (2%)	62	84
1	D	63/112 (56%)	62 (98%)	1 (2%)	62	84
1	E	62/112 (55%)	62 (100%)	0	100	100
1	F	63/112 (56%)	61 (97%)	2 (3%)	39	65
1	G	62/112 (55%)	62 (100%)	0	100	100
1	H	61/112 (54%)	60 (98%)	1 (2%)	62	84
1	I	62/112 (55%)	61 (98%)	1 (2%)	62	84
1	J	61/112 (54%)	61 (100%)	0	100	100
All	All	624/1120 (56%)	617 (99%)	7 (1%)	73	89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	62	GLN
1	C	81	ARG
1	D	58	LYS
1	F	26	GLU
1	F	55	GLU
1	H	82	LEU
1	I	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	62	GLN
1	C	48	HIS
1	D	34	ASN
1	G	34	ASN
1	G	48	HIS
1	G	86	GLN
1	H	34	ASN
1	I	34	ASN
1	I	71	HIS
1	J	71	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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, 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	82/137 (59%)	4.86	74 (90%)	0 0	51, 55, 65, 77	0
1	B	80/137 (58%)	4.61	67 (83%)	0 0	53, 58, 70, 78	0
1	C	80/137 (58%)	4.89	71 (88%)	0 0	50, 54, 65, 69	0
1	D	80/137 (58%)	4.75	71 (88%)	0 0	52, 58, 67, 68	0
1	E	78/137 (56%)	4.52	66 (84%)	0 0	45, 54, 62, 64	0
1	F	80/137 (58%)	4.52	68 (85%)	0 0	49, 53, 66, 68	0
1	G	80/137 (58%)	4.61	60 (75%)	0 0	51, 56, 61, 65	0
1	H	78/137 (56%)	4.54	66 (84%)	0 0	49, 54, 65, 73	0
1	I	79/137 (57%)	5.48	68 (86%)	0 0	54, 59, 72, 73	0
1	J	83/137 (60%)	5.59	74 (89%)	0 0	53, 58, 71, 82	0
All	All	800/1370 (58%)	4.84	685 (85%)	0 0	45, 56, 67, 82	0

All (685) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	18	VAL	21.4
1	F	97	TYR	19.5
1	J	24	ASP	19.0
1	I	60	ILE	16.2
1	G	56	ASP	16.0
1	A	56	ASP	15.9
1	D	79	ILE	15.8
1	B	97	TYR	15.5
1	I	51	ALA	15.4
1	J	44	LEU	15.3
1	E	77	GLU	14.8
1	G	78	LEU	14.8
1	A	52	THR	14.8

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Mol	Chain	Res	Type	RSRZ
1	I	80	ALA	14.6
1	H	98	ARG	14.5
1	C	25	THR	13.9
1	J	99	LEU	13.8
1	E	49	ILE	13.5
1	C	97	TYR	13.4
1	C	80	ALA	13.3
1	J	59	ALA	13.3
1	A	88	ALA	13.2
1	I	56	ASP	13.2
1	E	97	TYR	13.1
1	H	97	TYR	12.8
1	J	89	HIS	12.6
1	J	62	GLN	12.4
1	E	61	LEU	12.4
1	J	66	ASP	12.3
1	I	35	ILE	12.3
1	D	25	THR	12.3
1	D	22	MET	12.1
1	I	71	HIS	12.0
1	G	99	LEU	11.7
1	B	59	ALA	11.7
1	G	30	SER	11.7
1	A	96	LYS	11.6
1	D	86	GLN	11.6
1	F	51	ALA	11.5
1	G	87	ALA	11.4
1	F	74	LEU	11.4
1	J	35	ILE	11.3
1	A	87	ALA	11.2
1	D	83	ASP	11.2
1	C	33	LEU	11.1
1	E	33	LEU	11.1
1	D	88	ALA	11.0
1	J	22	MET	11.0
1	H	34	ASN	11.0
1	B	40	ASP	10.9
1	C	49	ILE	10.9
1	J	75	PHE	10.9
1	D	94	VAL	10.9
1	J	92	GLU	10.9
1	H	37	ALA	10.8

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Mol	Chain	Res	Type	RSRZ
1	C	75	PHE	10.8
1	H	89	HIS	10.7
1	I	64	VAL	10.6
1	J	23	THR	10.6
1	A	43	ASN	10.5
1	A	89	HIS	10.4
1	I	34	ASN	10.4
1	C	42	ILE	10.3
1	J	87	ALA	10.3
1	H	80	ALA	10.2
1	I	92	GLU	10.2
1	B	86	GLN	10.1
1	F	98	ARG	10.1
1	J	55	GLU	10.1
1	D	97	TYR	10.0
1	F	81	ARG	10.0
1	I	90	ALA	9.8
1	C	99	LEU	9.8
1	A	26	GLU	9.8
1	J	71	HIS	9.7
1	B	65	MET	9.6
1	I	87	ALA	9.5
1	H	50	ASP	9.5
1	G	64	VAL	9.4
1	I	39	LEU	9.4
1	I	61	LEU	9.3
1	D	74	LEU	9.3
1	J	48	HIS	9.2
1	B	33	LEU	9.2
1	A	32	ARG	9.1
1	G	89	HIS	9.1
1	J	46	ALA	9.0
1	I	70	GLU	9.0
1	G	73	ALA	9.0
1	A	91	LYS	9.0
1	E	31	ILE	8.9
1	C	94	VAL	8.8
1	A	41	ALA	8.8
1	I	75	PHE	8.6
1	H	24	ASP	8.6
1	F	54	ASN	8.5
1	B	79	ILE	8.5

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Mol	Chain	Res	Type	RSRZ
1	B	88	ALA	8.5
1	H	83	ASP	8.5
1	H	36	GLU	8.4
1	B	42	ILE	8.3
1	H	100	ILE	8.3
1	J	79	ILE	8.2
1	I	99	LEU	8.2
1	E	88	ALA	8.1
1	A	19	PRO	8.1
1	J	73	ALA	8.1
1	B	66	ASP	8.1
1	E	25	THR	8.1
1	F	87	ALA	8.1
1	E	35	ILE	8.1
1	A	79	ILE	8.0
1	E	42	ILE	8.0
1	B	83	ASP	8.0
1	F	25	THR	8.0
1	F	67	GLU	8.0
1	B	25	THR	8.0
1	A	86	GLN	7.9
1	F	88	ALA	7.9
1	B	27	LEU	7.9
1	B	94	VAL	7.8
1	I	62	GLN	7.8
1	G	37	ALA	7.8
1	C	92	GLU	7.8
1	D	81	ARG	7.7
1	C	77	GLU	7.7
1	D	40	ASP	7.6
1	F	49	ILE	7.6
1	A	22	MET	7.6
1	E	95	GLU	7.6
1	A	36	GLU	7.6
1	H	60	ILE	7.5
1	E	68	GLU	7.5
1	C	45	TYR	7.5
1	G	80	ALA	7.4
1	G	32	ARG	7.3
1	J	40	ASP	7.3
1	G	44	LEU	7.3
1	G	100	ILE	7.3

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Mol	Chain	Res	Type	RSRZ
1	I	76	TRP	7.3
1	C	35	ILE	7.3
1	H	25	THR	7.3
1	C	73	ALA	7.3
1	D	90	ALA	7.3
1	E	23	THR	7.3
1	C	81	ARG	7.2
1	B	53	ASP	7.2
1	J	68	GLU	7.2
1	G	76	TRP	7.2
1	J	42	ILE	7.2
1	I	32	ARG	7.2
1	E	51	ALA	7.2
1	I	44	LEU	7.1
1	B	24	ASP	7.1
1	C	83	ASP	7.1
1	H	52	THR	7.1
1	A	98	ARG	7.1
1	H	47	ALA	7.1
1	F	61	LEU	7.1
1	G	50	ASP	7.0
1	A	60	ILE	7.0
1	G	72	ALA	7.0
1	F	34	ASN	6.9
1	G	63	HIS	6.9
1	C	40	ASP	6.9
1	D	99	LEU	6.8
1	F	22	MET	6.8
1	G	86	GLN	6.8
1	D	89	HIS	6.8
1	H	41	ALA	6.8
1	F	63	HIS	6.7
1	B	31	ILE	6.7
1	B	47	ALA	6.7
1	D	41	ALA	6.7
1	E	87	ALA	6.6
1	B	52	THR	6.6
1	I	42	ILE	6.6
1	J	60	ILE	6.6
1	H	38	GLU	6.6
1	I	69	ARG	6.5
1	I	73	ALA	6.5

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Mol	Chain	Res	Type	RSRZ
1	J	33	LEU	6.5
1	G	93	ALA	6.5
1	I	37	ALA	6.5
1	H	43	ASN	6.5
1	E	47	ALA	6.5
1	E	44	LEU	6.4
1	C	88	ALA	6.4
1	A	81	ARG	6.4
1	G	74	LEU	6.4
1	D	47	ALA	6.4
1	F	100	ILE	6.4
1	E	99	LEU	6.3
1	C	90	ALA	6.3
1	J	72	ALA	6.3
1	G	24	ASP	6.3
1	I	58	LYS	6.3
1	C	84	PRO	6.2
1	F	65	MET	6.2
1	B	75	PHE	6.2
1	D	45	TYR	6.2
1	A	78	LEU	6.2
1	E	82	LEU	6.2
1	D	49	ILE	6.2
1	G	45	TYR	6.2
1	I	66	ASP	6.2
1	J	76	TRP	6.2
1	I	96	LYS	6.2
1	E	76	TRP	6.2
1	I	23	THR	6.2
1	G	71	HIS	6.1
1	E	94	VAL	6.1
1	G	34	ASN	6.1
1	D	23	THR	6.1
1	D	27	LEU	6.1
1	C	66	ASP	6.0
1	J	84	PRO	6.0
1	C	69	ARG	6.0
1	G	51	ALA	6.0
1	C	46	ALA	6.0
1	J	63	HIS	6.0
1	J	50	ASP	6.0
1	F	90	ALA	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	92	GLU	5.9
1	I	48	HIS	5.9
1	B	49	ILE	5.9
1	C	100	ILE	5.9
1	E	26	GLU	5.9
1	H	78	LEU	5.9
1	D	57	ALA	5.9
1	F	41	ALA	5.9
1	E	30	SER	5.8
1	H	51	ALA	5.8
1	I	65	MET	5.8
1	G	75	PHE	5.8
1	D	63	HIS	5.8
1	C	68	GLU	5.8
1	G	60	ILE	5.8
1	G	96	LYS	5.7
1	B	76	TRP	5.7
1	F	99	LEU	5.7
1	D	42	ILE	5.7
1	I	91	LYS	5.7
1	D	66	ASP	5.7
1	F	95	GLU	5.7
1	E	40	ASP	5.7
1	B	56	ASP	5.7
1	D	31	ILE	5.6
1	J	83	ASP	5.6
1	F	29	ARG	5.6
1	J	94	VAL	5.6
1	G	43	ASN	5.6
1	G	84	PRO	5.6
1	J	39	LEU	5.6
1	B	58	LYS	5.6
1	B	99	LEU	5.5
1	F	83	ASP	5.5
1	D	38	GLU	5.5
1	E	80	ALA	5.5
1	A	45	TYR	5.5
1	G	23	THR	5.5
1	D	61	LEU	5.5
1	C	61	LEU	5.5
1	F	93	ALA	5.5
1	C	87	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	F	94	VAL	5.4
1	I	57	ALA	5.4
1	I	97	TYR	5.4
1	I	22	MET	5.4
1	E	84	PRO	5.4
1	A	34	ASN	5.4
1	F	55	GLU	5.4
1	D	43	ASN	5.4
1	I	30	SER	5.3
1	I	94	VAL	5.3
1	G	52	THR	5.3
1	I	55	GLU	5.2
1	D	95	GLU	5.2
1	H	65	MET	5.2
1	I	93	ALA	5.2
1	B	93	ALA	5.2
1	A	63	HIS	5.2
1	C	89	HIS	5.2
1	J	86	GLN	5.1
1	I	67	GLU	5.1
1	A	49	ILE	5.1
1	E	45	TYR	5.1
1	H	91	LYS	5.1
1	B	55	GLU	5.1
1	A	61	LEU	5.1
1	F	36	GLU	5.1
1	F	80	ALA	5.1
1	A	24	ASP	5.1
1	I	50	ASP	5.1
1	J	56	ASP	5.1
1	C	21	LYS	5.0
1	C	64	VAL	5.0
1	I	24	ASP	5.0
1	D	72	ALA	5.0
1	E	75	PHE	5.0
1	B	23	THR	5.0
1	F	57	ALA	5.0
1	A	37	ALA	5.0
1	A	93	ALA	5.0
1	A	76	TRP	5.0
1	B	35	ILE	5.0
1	F	79	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	44	LEU	4.9
1	C	30	SER	4.9
1	A	27	LEU	4.9
1	H	56	ASP	4.9
1	D	36	GLU	4.9
1	B	63	HIS	4.9
1	J	49	ILE	4.9
1	B	92	GLU	4.8
1	G	41	ALA	4.8
1	A	82	LEU	4.8
1	I	28	ALA	4.8
1	A	94	VAL	4.8
1	I	98	ARG	4.8
1	F	35	ILE	4.8
1	B	71	HIS	4.8
1	F	42	ILE	4.8
1	I	72	ALA	4.8
1	D	82	LEU	4.7
1	I	77	GLU	4.7
1	H	63	HIS	4.7
1	H	75	PHE	4.7
1	J	78	LEU	4.7
1	H	27	LEU	4.7
1	B	91	LYS	4.7
1	F	38	GLU	4.6
1	G	98	ARG	4.6
1	J	69	ARG	4.6
1	E	54	ASN	4.6
1	H	49	ILE	4.6
1	D	54	ASN	4.6
1	H	30	SER	4.5
1	E	57	ALA	4.5
1	J	37	ALA	4.5
1	E	98	ARG	4.5
1	B	70	GLU	4.5
1	E	83	ASP	4.5
1	G	69	ARG	4.5
1	H	31	ILE	4.5
1	H	99	LEU	4.5
1	C	98	ARG	4.5
1	C	57	ALA	4.4
1	C	24	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	89	HIS	4.4
1	C	39	LEU	4.4
1	E	27	LEU	4.4
1	G	48	HIS	4.4
1	H	53	ASP	4.4
1	F	76	TRP	4.4
1	C	37	ALA	4.4
1	B	85	GLU	4.4
1	G	67	GLU	4.4
1	B	36	GLU	4.4
1	H	92	GLU	4.4
1	F	64	VAL	4.4
1	A	100	ILE	4.3
1	I	26	GLU	4.3
1	A	39	LEU	4.3
1	E	53	ASP	4.3
1	C	23	THR	4.3
1	A	73	ALA	4.3
1	B	41	ALA	4.3
1	A	97	TYR	4.3
1	D	29	ARG	4.3
1	C	76	TRP	4.2
1	D	44	LEU	4.2
1	B	45	TYR	4.2
1	H	86	GLN	4.2
1	A	67	GLU	4.2
1	H	48	HIS	4.2
1	E	72	ALA	4.2
1	B	54	ASN	4.2
1	F	68	GLU	4.2
1	E	64	VAL	4.2
1	G	25	THR	4.2
1	J	80	ALA	4.2
1	D	85	GLU	4.2
1	G	26	GLU	4.2
1	D	50	ASP	4.2
1	D	35	ILE	4.1
1	H	71	HIS	4.1
1	F	24	ASP	4.1
1	D	30	SER	4.1
1	D	51	ALA	4.1
1	C	50	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	79	ILE	4.1
1	H	76	TRP	4.1
1	B	84	PRO	4.1
1	B	73	ALA	4.1
1	I	89	HIS	4.1
1	A	21	LYS	4.0
1	I	100	ILE	4.0
1	G	97	TYR	4.0
1	C	47	ALA	4.0
1	C	54	ASN	4.0
1	A	25	THR	4.0
1	C	28	ALA	4.0
1	E	59	ALA	4.0
1	A	71	HIS	4.0
1	F	75	PHE	4.0
1	D	33	LEU	4.0
1	A	80	ALA	4.0
1	A	57	ALA	3.9
1	G	28	ALA	3.9
1	C	82	LEU	3.9
1	E	55	GLU	3.9
1	F	27	LEU	3.9
1	J	26	GLU	3.9
1	J	77	GLU	3.9
1	A	46	ALA	3.9
1	C	78	LEU	3.9
1	C	60	ILE	3.9
1	A	83	ASP	3.9
1	I	78	LEU	3.9
1	F	31	ILE	3.8
1	H	67	GLU	3.8
1	G	92	GLU	3.8
1	D	32	ARG	3.8
1	H	62	GLN	3.8
1	A	62	GLN	3.8
1	C	79	ILE	3.8
1	I	46	ALA	3.8
1	C	65	MET	3.8
1	D	75	PHE	3.8
1	B	61	LEU	3.8
1	F	82	LEU	3.8
1	H	81	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	J	57	ALA	3.7
1	A	74	LEU	3.7
1	H	39	LEU	3.7
1	F	23	THR	3.7
1	D	67	GLU	3.7
1	I	74	LEU	3.7
1	I	33	LEU	3.7
1	G	95	GLU	3.7
1	D	21	LYS	3.6
1	D	92	GLU	3.6
1	H	85	GLU	3.6
1	A	72	ALA	3.6
1	B	22	MET	3.6
1	F	47	ALA	3.6
1	J	58	LYS	3.6
1	G	65	MET	3.6
1	C	67	GLU	3.6
1	F	89	HIS	3.6
1	D	76	TRP	3.6
1	C	31	ILE	3.6
1	G	42	ILE	3.6
1	E	71	HIS	3.6
1	G	33	LEU	3.6
1	B	90	ALA	3.6
1	B	81	ARG	3.5
1	B	48	HIS	3.5
1	H	61	LEU	3.5
1	B	38	GLU	3.5
1	F	84	PRO	3.5
1	C	96	LYS	3.5
1	H	54	ASN	3.5
1	D	64	VAL	3.5
1	E	81	ARG	3.5
1	C	58	LYS	3.5
1	C	32	ARG	3.5
1	J	34	ASN	3.5
1	J	31	ILE	3.5
1	H	82	LEU	3.5
1	F	71	HIS	3.5
1	H	26	GLU	3.5
1	A	30	SER	3.4
1	D	70	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	91	LYS	3.4
1	H	93	ALA	3.4
1	C	72	ALA	3.4
1	D	53	ASP	3.4
1	J	30	SER	3.3
1	E	34	ASN	3.3
1	F	77	GLU	3.3
1	F	86	GLN	3.3
1	I	31	ILE	3.3
1	D	55	GLU	3.3
1	I	95	GLU	3.3
1	D	39	LEU	3.3
1	A	99	LEU	3.3
1	G	82	LEU	3.3
1	F	59	ALA	3.3
1	D	60	ILE	3.3
1	G	61	LEU	3.2
1	C	48	HIS	3.2
1	J	70	GLU	3.2
1	F	33	LEU	3.2
1	F	37	ALA	3.2
1	G	49	ILE	3.2
1	B	29	ARG	3.2
1	C	74	LEU	3.2
1	E	78	LEU	3.2
1	F	91	LYS	3.2
1	J	65	MET	3.2
1	B	44	LEU	3.2
1	J	20	ARG	3.2
1	A	48	HIS	3.2
1	A	38	GLU	3.2
1	I	59	ALA	3.1
1	J	45	TYR	3.1
1	E	50	ASP	3.1
1	H	96	LYS	3.1
1	B	28	ALA	3.1
1	B	77	GLU	3.1
1	J	32	ARG	3.1
1	J	51	ALA	3.1
1	F	45	TYR	3.1
1	D	48	HIS	3.1
1	J	96	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	70	GLU	3.0
1	E	93	ALA	3.0
1	I	68	GLU	3.0
1	A	65	MET	3.0
1	E	65	MET	3.0
1	J	100	ILE	3.0
1	D	37	ALA	3.0
1	E	73	ALA	3.0
1	B	74	LEU	3.0
1	A	59	ALA	3.0
1	C	27	LEU	3.0
1	F	32	ARG	3.0
1	A	23	THR	2.9
1	C	59	ALA	2.9
1	A	31	ILE	2.9
1	A	44	LEU	2.9
1	F	78	LEU	2.9
1	H	35	ILE	2.9
1	H	28	ALA	2.9
1	B	78	LEU	2.9
1	H	72	ALA	2.9
1	C	55	GLU	2.9
1	G	46	ALA	2.9
1	D	91	LYS	2.9
1	A	35	ILE	2.9
1	E	92	GLU	2.9
1	I	79	ILE	2.9
1	H	95	GLU	2.8
1	I	84	PRO	2.8
1	J	25	THR	2.8
1	J	64	VAL	2.8
1	G	21	LYS	2.8
1	H	94	VAL	2.8
1	F	44	LEU	2.8
1	B	32	ARG	2.8
1	D	34	ASN	2.8
1	H	84	PRO	2.8
1	F	43	ASN	2.8
1	D	84	PRO	2.8
1	J	29	ARG	2.8
1	A	75	PHE	2.8
1	F	73	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	29	ARG	2.8
1	I	43	ASN	2.8
1	I	27	LEU	2.8
1	C	34	ASN	2.7
1	C	63	HIS	2.7
1	A	20	ARG	2.7
1	G	55	GLU	2.7
1	E	32	ARG	2.7
1	I	45	TYR	2.7
1	E	48	HIS	2.7
1	J	82	LEU	2.7
1	B	95	GLU	2.7
1	I	40	ASP	2.7
1	J	93	ALA	2.7
1	A	51	ALA	2.6
1	B	34	ASN	2.6
1	J	19	PRO	2.6
1	A	50	ASP	2.6
1	A	28	ALA	2.6
1	J	47	ALA	2.6
1	D	68	GLU	2.6
1	F	69	ARG	2.6
1	J	88	ALA	2.6
1	J	91	LYS	2.6
1	E	66	ASP	2.6
1	H	74	LEU	2.6
1	H	32	ARG	2.6
1	A	55	GLU	2.6
1	G	31	ILE	2.6
1	D	80	ALA	2.5
1	I	41	ALA	2.5
1	C	95	GLU	2.5
1	J	27	LEU	2.5
1	C	38	GLU	2.5
1	G	91	LYS	2.5
1	H	87	ALA	2.5
1	E	39	LEU	2.5
1	A	54	ASN	2.5
1	E	29	ARG	2.5
1	E	46	ALA	2.5
1	B	82	LEU	2.5
1	D	96	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	64	VAL	2.5
1	E	62	GLN	2.5
1	D	98	ARG	2.5
1	B	37	ALA	2.5
1	E	43	ASN	2.5
1	F	39	LEU	2.5
1	H	45	TYR	2.5
1	J	98	ARG	2.5
1	E	100	ILE	2.5
1	A	66	ASP	2.5
1	F	53	ASP	2.5
1	B	80	ALA	2.5
1	A	69	ARG	2.4
1	J	74	LEU	2.4
1	C	51	ALA	2.4
1	D	28	ALA	2.4
1	E	28	ALA	2.4
1	E	41	ALA	2.4
1	B	21	LYS	2.4
1	F	52	THR	2.4
1	A	42	ILE	2.4
1	I	53	ASP	2.4
1	G	54	ASN	2.4
1	G	27	LEU	2.4
1	D	59	ALA	2.4
1	I	25	THR	2.4
1	J	28	ALA	2.4
1	E	60	ILE	2.4
1	H	68	GLU	2.4
1	A	47	ALA	2.4
1	C	93	ALA	2.4
1	F	50	ASP	2.4
1	D	78	LEU	2.4
1	H	40	ASP	2.4
1	J	53	ASP	2.4
1	G	39	LEU	2.4
1	D	52	THR	2.4
1	F	30	SER	2.3
1	B	64	VAL	2.3
1	B	46	ALA	2.3
1	H	69	ARG	2.3
1	D	58	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	41	ALA	2.3
1	E	38	GLU	2.3
1	E	63	HIS	2.3
1	H	70	GLU	2.3
1	J	54	ASN	2.2
1	D	65	MET	2.2
1	B	30	SER	2.2
1	A	84	PRO	2.2
1	J	52	THR	2.2
1	F	96	LYS	2.2
1	A	29	ARG	2.2
1	H	59	ALA	2.2
1	A	40	ASP	2.2
1	I	54	ASN	2.2
1	E	52	THR	2.2
1	G	35	ILE	2.2
1	A	70	GLU	2.2
1	B	68	GLU	2.2
1	D	77	GLU	2.2
1	I	82	LEU	2.1
1	F	40	ASP	2.1
1	J	97	TYR	2.1
1	H	88	ALA	2.1
1	E	67	GLU	2.1
1	B	67	GLU	2.1
1	C	43	ASN	2.1
1	F	60	ILE	2.1
1	A	53	ASP	2.1
1	E	74	LEU	2.1
1	J	81	ARG	2.1
1	E	89	HIS	2.1
1	D	46	ALA	2.1
1	G	38	GLU	2.1
1	C	71	HIS	2.1
1	C	26	GLU	2.1
1	G	85	GLU	2.1
1	B	72	ALA	2.0
1	I	63	HIS	2.0
1	J	67	GLU	2.0
1	D	71	HIS	2.0
1	E	79	ILE	2.0
1	H	42	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FE	A	201	1/1	0.26	0.58	57,57,57,57	1
2	FE	F	201	1/1	0.43	0.30	58,58,58,58	1
2	FE	H	201	1/1	0.50	0.25	54,54,54,54	1
2	FE	J	201	1/1	0.63	0.52	55,55,55,55	1
2	FE	E	201	1/1	0.64	0.39	65,65,65,65	1
2	FE	I	201	1/1	0.73	0.25	59,59,59,59	1
2	FE	I	202	1/1	0.75	0.20	59,59,59,59	1

6.5 Other polymers [i](#)

There are no such residues in this entry.