



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:48 PM UTC

PDB ID : 5XBQ / pdb_00005xbq
Title : Peroxiredoxin from *Pyrococcus horikoshii* (6m mutant)
Authors : Nakamura, T.; Uegaki, K.
Deposited on : 2017-03-21
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

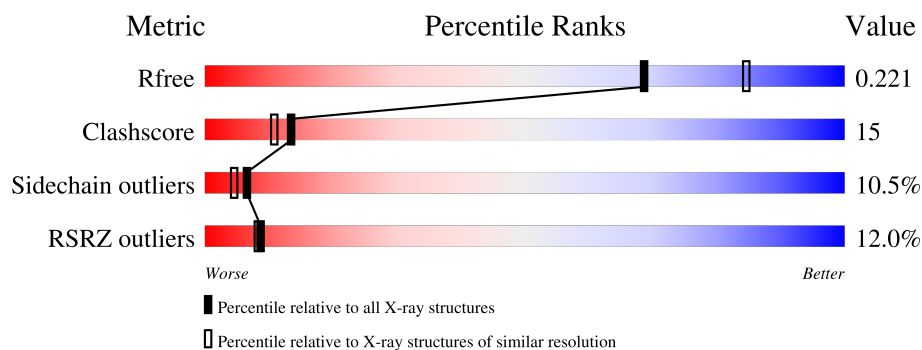
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	216	9% 64% 30% • •
1	B	216	12% 58% 31% 9% • •
1	C	216	10% 56% 36% 6% •
1	D	216	12% 65% 25% 8% •
1	E	216	12% 61% 34% • •
1	F	216	13% 65% 29% 5% •

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Mol	Chain	Length	Quality of chain
1	G	216	
1	H	216	
1	I	216	
1	J	216	
1	K	216	
1	L	216	

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
1	OCS	F	46	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20842 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 Peroxiredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	B	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	C	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	D	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	E	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	F	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	G	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	H	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	I	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	J	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	K	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	L	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ARG	VAL	engineered mutation	UNP O58966
A	76	GLU	PHE	engineered mutation	UNP O58966
A	77	ASP	SER	engineered mutation	UNP O58966
A	79	SER	ILE	engineered mutation	UNP O58966
A	80	ALA	LYS	engineered mutation	UNP O58966

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Chain	Residue	Modelled	Actual	Comment	Reference
A	208	SER	TRP	engineered mutation	UNP O58966
B	19	ARG	VAL	engineered mutation	UNP O58966
B	76	GLU	PHE	engineered mutation	UNP O58966
B	77	ASP	SER	engineered mutation	UNP O58966
B	79	SER	ILE	engineered mutation	UNP O58966
B	80	ALA	LYS	engineered mutation	UNP O58966
B	208	SER	TRP	engineered mutation	UNP O58966
C	19	ARG	VAL	engineered mutation	UNP O58966
C	76	GLU	PHE	engineered mutation	UNP O58966
C	77	ASP	SER	engineered mutation	UNP O58966
C	79	SER	ILE	engineered mutation	UNP O58966
C	80	ALA	LYS	engineered mutation	UNP O58966
C	208	SER	TRP	engineered mutation	UNP O58966
D	19	ARG	VAL	engineered mutation	UNP O58966
D	76	GLU	PHE	engineered mutation	UNP O58966
D	77	ASP	SER	engineered mutation	UNP O58966
D	79	SER	ILE	engineered mutation	UNP O58966
D	80	ALA	LYS	engineered mutation	UNP O58966
D	208	SER	TRP	engineered mutation	UNP O58966
E	19	ARG	VAL	engineered mutation	UNP O58966
E	76	GLU	PHE	engineered mutation	UNP O58966
E	77	ASP	SER	engineered mutation	UNP O58966
E	79	SER	ILE	engineered mutation	UNP O58966
E	80	ALA	LYS	engineered mutation	UNP O58966
E	208	SER	TRP	engineered mutation	UNP O58966
F	19	ARG	VAL	engineered mutation	UNP O58966
F	76	GLU	PHE	engineered mutation	UNP O58966
F	77	ASP	SER	engineered mutation	UNP O58966
F	79	SER	ILE	engineered mutation	UNP O58966
F	80	ALA	LYS	engineered mutation	UNP O58966
F	208	SER	TRP	engineered mutation	UNP O58966
G	19	ARG	VAL	engineered mutation	UNP O58966
G	76	GLU	PHE	engineered mutation	UNP O58966
G	77	ASP	SER	engineered mutation	UNP O58966
G	79	SER	ILE	engineered mutation	UNP O58966
G	80	ALA	LYS	engineered mutation	UNP O58966
G	208	SER	TRP	engineered mutation	UNP O58966
H	19	ARG	VAL	engineered mutation	UNP O58966
H	76	GLU	PHE	engineered mutation	UNP O58966
H	77	ASP	SER	engineered mutation	UNP O58966
H	79	SER	ILE	engineered mutation	UNP O58966
H	80	ALA	LYS	engineered mutation	UNP O58966

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Chain	Residue	Modelled	Actual	Comment	Reference
H	208	SER	TRP	engineered mutation	UNP O58966
I	19	ARG	VAL	engineered mutation	UNP O58966
I	76	GLU	PHE	engineered mutation	UNP O58966
I	77	ASP	SER	engineered mutation	UNP O58966
I	79	SER	ILE	engineered mutation	UNP O58966
I	80	ALA	LYS	engineered mutation	UNP O58966
I	208	SER	TRP	engineered mutation	UNP O58966
J	19	ARG	VAL	engineered mutation	UNP O58966
J	76	GLU	PHE	engineered mutation	UNP O58966
J	77	ASP	SER	engineered mutation	UNP O58966
J	79	SER	ILE	engineered mutation	UNP O58966
J	80	ALA	LYS	engineered mutation	UNP O58966
J	208	SER	TRP	engineered mutation	UNP O58966
K	19	ARG	VAL	engineered mutation	UNP O58966
K	76	GLU	PHE	engineered mutation	UNP O58966
K	77	ASP	SER	engineered mutation	UNP O58966
K	79	SER	ILE	engineered mutation	UNP O58966
K	80	ALA	LYS	engineered mutation	UNP O58966
K	208	SER	TRP	engineered mutation	UNP O58966
L	19	ARG	VAL	engineered mutation	UNP O58966
L	76	GLU	PHE	engineered mutation	UNP O58966
L	77	ASP	SER	engineered mutation	UNP O58966
L	79	SER	ILE	engineered mutation	UNP O58966
L	80	ALA	LYS	engineered mutation	UNP O58966
L	208	SER	TRP	engineered mutation	UNP O58966

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total O 9 9	0	0
2	B	16	Total O 16 16	0	0
2	C	17	Total O 17 17	0	0
2	D	6	Total O 6 6	0	0
2	E	15	Total O 15 15	0	0
2	F	10	Total O 10 10	0	0
2	G	11	Total O 11 11	0	0

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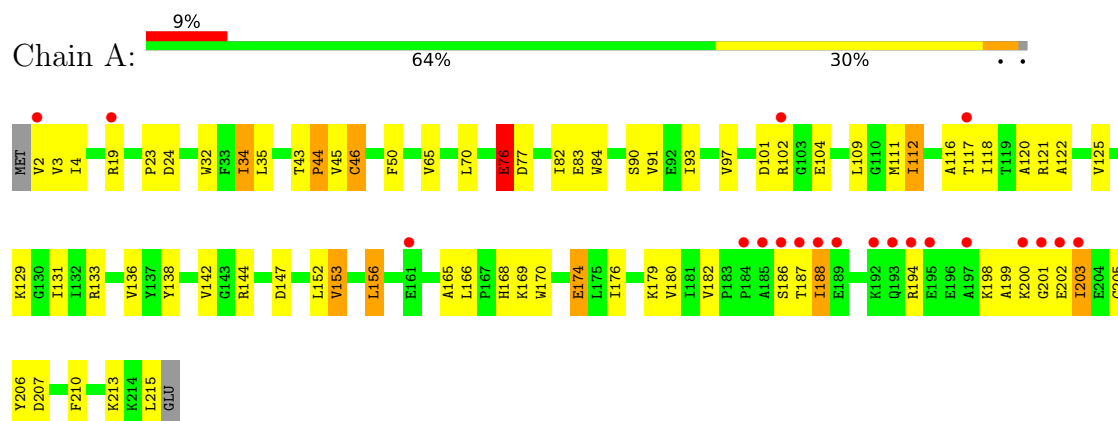
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	11	Total 11	O 11	0	0
2	I	18	Total 18	O 18	0	0
2	J	11	Total 11	O 11	0	0
2	K	9	Total 9	O 9	0	0
2	L	9	Total 9	O 9	0	0

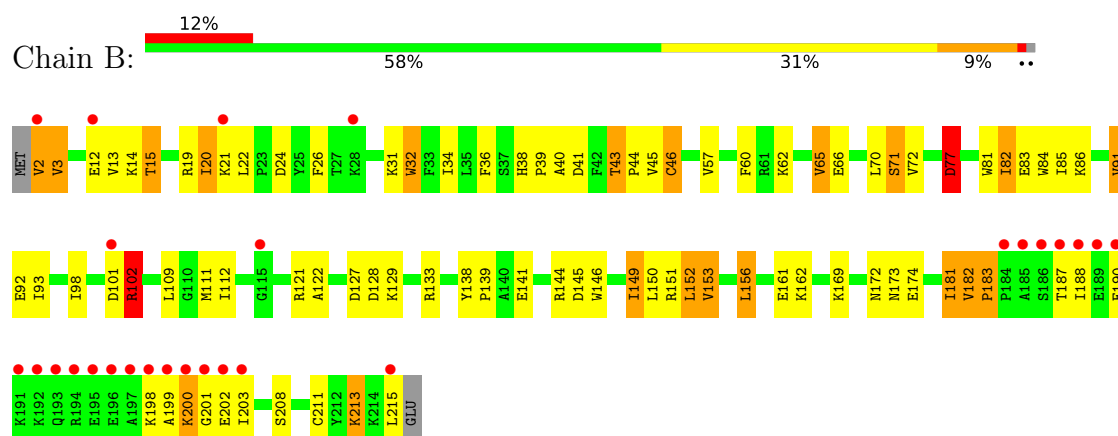
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

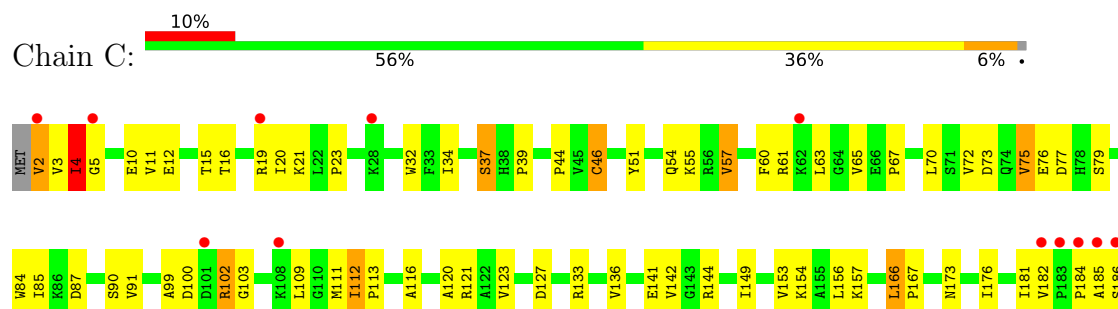
• Molecule 1: Peroxiredoxin

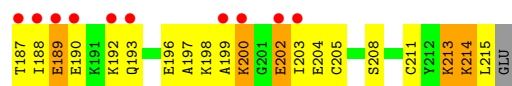


• Molecule 1: Peroxiredoxin

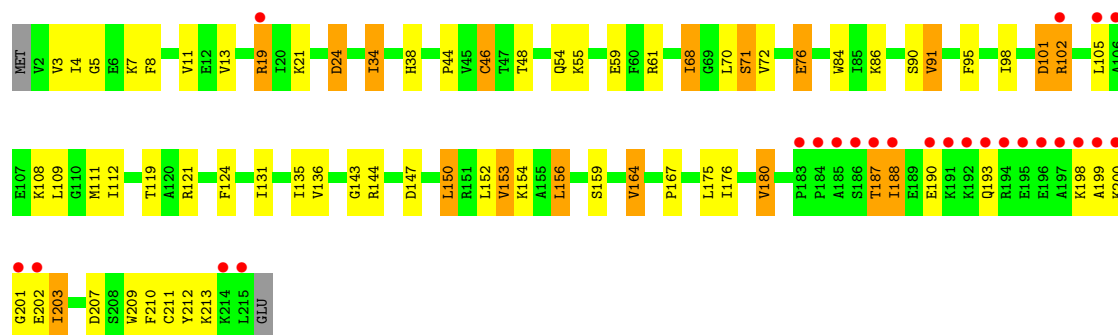


• Molecule 1: Peroxiredoxin

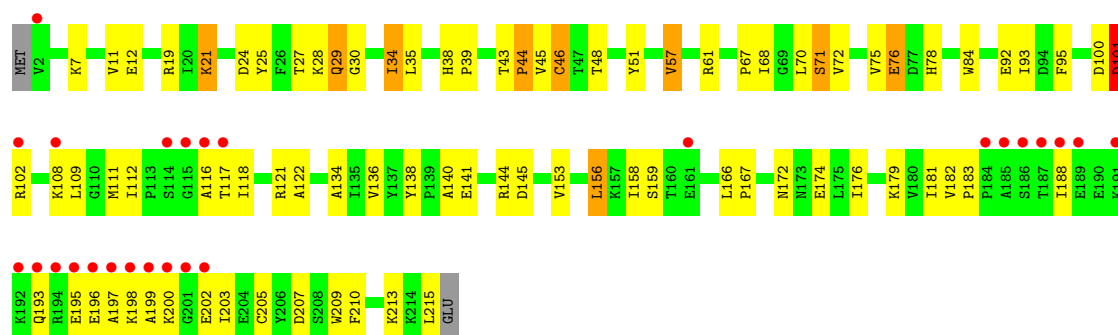




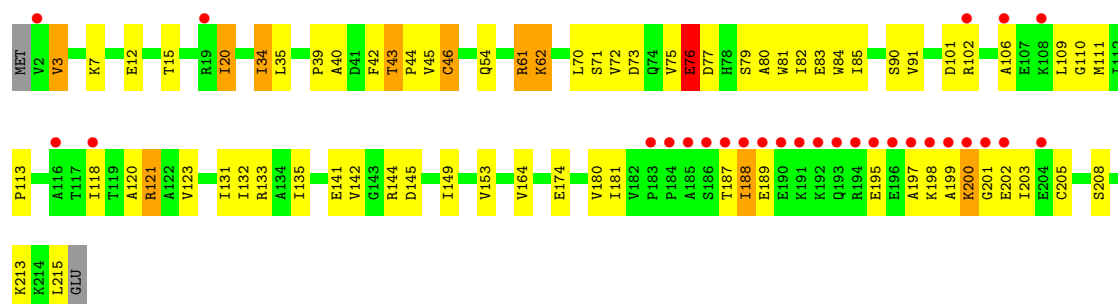
● Molecule 1: Peroxiredoxin



● Molecule 1: Peroxiredoxin

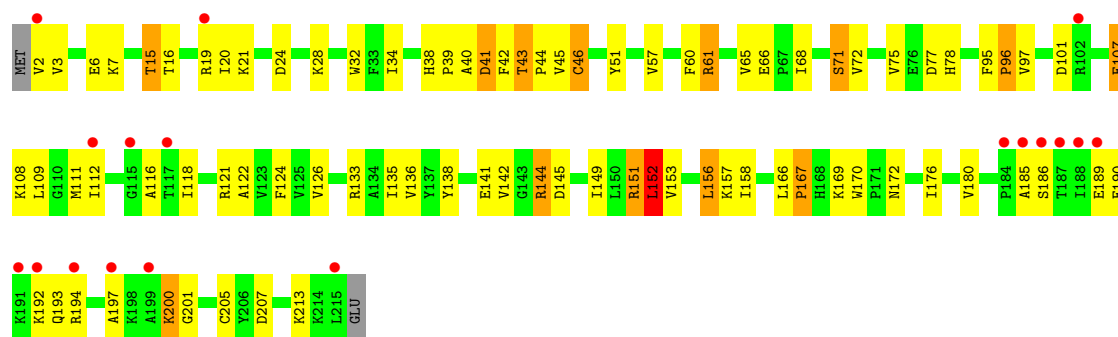


● Molecule 1: Peroxiredoxin

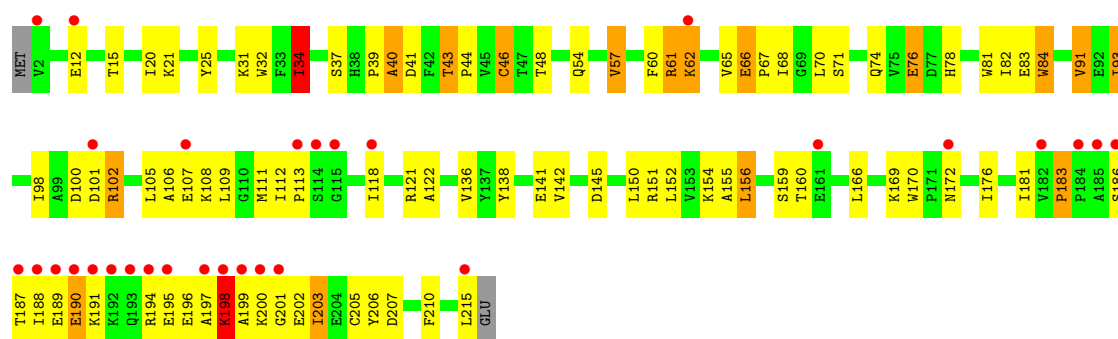


● Molecule 1: Peroxiredoxin

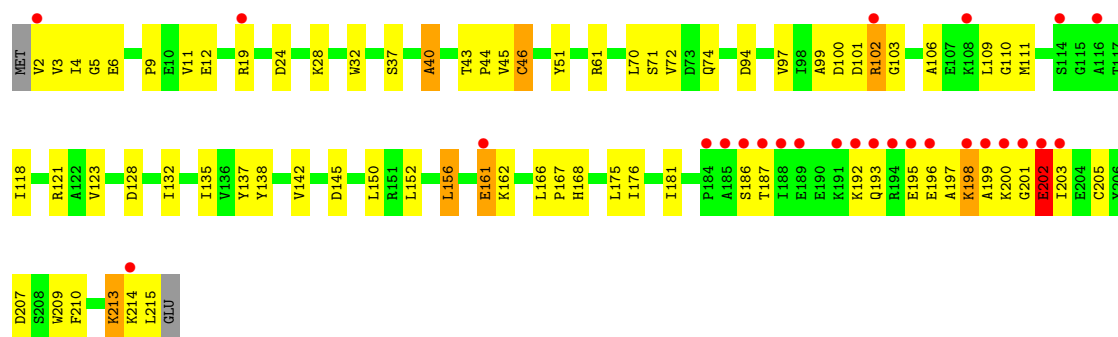




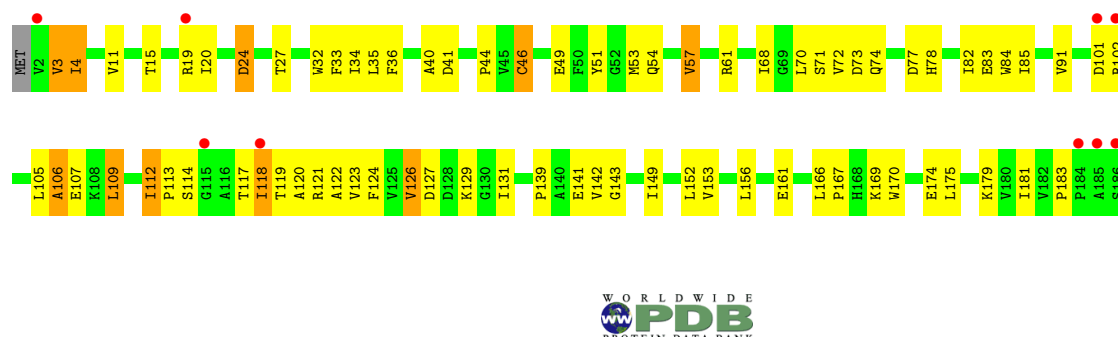
• Molecule 1: Peroxiredoxin

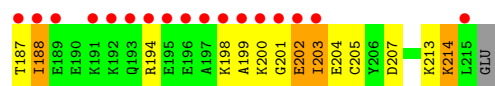


• Molecule 1: Peroxiredoxin

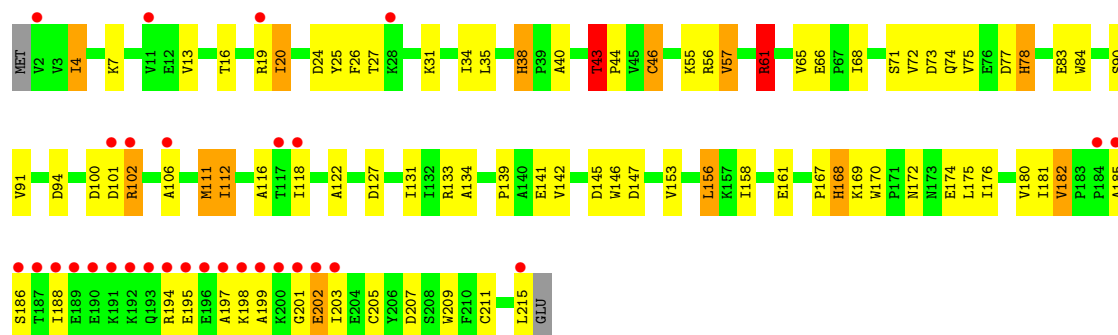


• Molecule 1: Peroxiredoxin

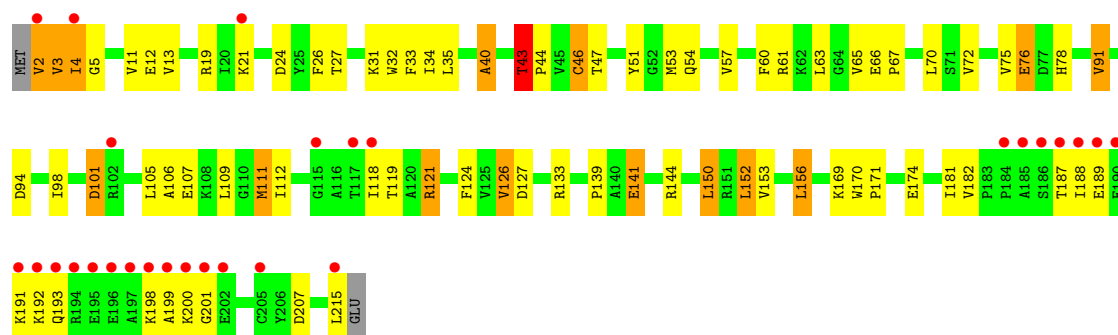




● Molecule 1: Peroxiredoxin



● Molecule 1: Peroxiredoxin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.58Å 98.60Å 137.57Å 90.00° 119.95° 90.00°	Depositor
Resolution (Å)	39.73 – 2.25 39.73 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.73-2.25) 99.9 (39.73-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	678.50 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.193 , 0.232 (Not available) , 0.221	Depositor DCC
R_{free} test set	7632 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.046 for l,k,-h-l 0.046 for -h-l,k,h 0.000 for -h-l,-k,l 0.000 for h,-k,-h-l 0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20842	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0440e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.34	9/1758 (0.5%)	1.31	7/2380 (0.3%)
1	B	1.36	8/1758 (0.5%)	1.40	18/2380 (0.8%)
1	C	1.33	5/1758 (0.3%)	1.38	6/2380 (0.3%)
1	D	1.24	3/1758 (0.2%)	1.31	10/2380 (0.4%)
1	E	1.38	10/1758 (0.6%)	1.37	16/2380 (0.7%)
1	F	1.30	5/1758 (0.3%)	1.35	10/2380 (0.4%)
1	G	1.36	9/1758 (0.5%)	1.34	13/2380 (0.5%)
1	H	1.27	8/1758 (0.5%)	1.40	15/2380 (0.6%)
1	I	1.33	6/1758 (0.3%)	1.31	6/2380 (0.3%)
1	J	1.30	5/1758 (0.3%)	1.35	8/2380 (0.3%)
1	K	1.31	8/1758 (0.5%)	1.31	11/2380 (0.5%)
1	L	1.27	4/1758 (0.2%)	1.32	15/2380 (0.6%)
All	All	1.32	80/21096 (0.4%)	1.34	135/28560 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
1	E	0	1
1	G	0	1
1	H	0	1
1	K	0	1
1	L	0	1
All	All	0	8

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	183	PRO	C-O	-12.76	1.10	1.24
1	E	93	ILE	C-O	-10.05	1.14	1.24
1	I	97	VAL	C-O	-8.14	1.15	1.24
1	F	77	ASP	N-CA	7.25	1.55	1.46
1	C	123	VAL	C-O	-7.24	1.16	1.24
1	K	172	ASN	CG-ND2	-7.17	1.18	1.33
1	G	151	ARG	C-O	-7.08	1.15	1.24
1	A	174	GLU	C-O	-6.88	1.15	1.24
1	C	90	SER	CB-OG	-6.85	1.28	1.42
1	A	180	VAL	C-O	-6.82	1.15	1.23
1	A	153	VAL	C-O	-6.68	1.16	1.24
1	E	138	TYR	CA-C	-6.61	1.43	1.52
1	K	182	VAL	C-O	-6.58	1.16	1.24
1	E	183	PRO	CA-C	6.47	1.58	1.52
1	E	43	THR	CB-CG2	-6.46	1.31	1.52
1	I	123	VAL	C-O	-6.42	1.17	1.24
1	L	152	LEU	CA-C	6.39	1.61	1.52
1	H	34	ILE	CA-C	-6.26	1.45	1.52
1	B	112	ILE	CA-C	6.22	1.58	1.53
1	H	82	ILE	CA-CB	6.17	1.61	1.54
1	E	44	PRO	CA-C	6.15	1.61	1.52
1	G	152	LEU	CA-C	6.07	1.60	1.52
1	J	123	VAL	C-O	6.06	1.30	1.24
1	H	84	TRP	N-CA	6.05	1.53	1.46
1	H	61	ARG	CD-NE	-5.95	1.38	1.46
1	A	182	VAL	CA-C	-5.92	1.46	1.52
1	K	40	ALA	CA-C	-5.90	1.44	1.52
1	F	3	VAL	CA-C	5.89	1.60	1.52
1	C	87	ASP	C-O	-5.88	1.17	1.24
1	B	41	ASP	C-O	-5.88	1.16	1.23
1	E	172	ASN	C-O	5.84	1.30	1.23
1	A	76	GLU	N-CA	5.79	1.53	1.46
1	B	181	ILE	N-CA	-5.72	1.39	1.46
1	G	144	ARG	CA-C	-5.69	1.45	1.53
1	G	167	PRO	N-CA	-5.69	1.40	1.47
1	E	134	ALA	N-CA	5.67	1.52	1.46
1	H	93	ILE	C-O	-5.65	1.18	1.24
1	H	183	PRO	C-O	-5.64	1.18	1.24
1	C	79	SER	CA-C	-5.61	1.45	1.52
1	G	172	ASN	CA-C	5.59	1.60	1.52
1	L	43	THR	CB-CG2	-5.59	1.34	1.52
1	A	206	TYR	N-CA	5.52	1.53	1.46
1	K	38	HIS	C-O	-5.52	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	PRO	CA-C	5.51	1.60	1.52
1	J	112	ILE	CA-C	5.48	1.57	1.53
1	D	68	ILE	N-CA	-5.48	1.39	1.46
1	F	77	ASP	C-O	-5.47	1.17	1.24
1	I	94	ASP	N-CA	5.46	1.52	1.46
1	K	168	HIS	C-O	-5.46	1.17	1.24
1	G	41	ASP	CA-C	-5.45	1.46	1.52
1	F	84	TRP	C-O	-5.44	1.17	1.24
1	I	166	LEU	CA-C	5.43	1.59	1.52
1	G	51	TYR	C-O	5.43	1.30	1.24
1	G	124	PHE	CA-C	-5.41	1.46	1.52
1	J	106	ALA	C-O	5.40	1.30	1.24
1	K	111	MET	N-CA	5.36	1.53	1.46
1	D	164	VAL	C-O	-5.36	1.17	1.24
1	L	141	GLU	CA-C	5.34	1.60	1.52
1	A	170	TRP	N-CA	5.33	1.51	1.45
1	H	82	ILE	C-O	5.33	1.30	1.24
1	E	140	ALA	N-CA	-5.32	1.39	1.46
1	J	82	ILE	CA-CB	5.32	1.60	1.54
1	E	70	LEU	CA-C	-5.30	1.45	1.52
1	J	106	ALA	N-CA	5.25	1.52	1.46
1	G	167	PRO	C-O	5.24	1.29	1.23
1	I	40	ALA	N-CA	5.23	1.52	1.46
1	L	112	ILE	CA-C	5.22	1.57	1.53
1	F	43	THR	CB-CG2	-5.21	1.35	1.52
1	A	118	ILE	C-O	5.20	1.30	1.24
1	B	139	PRO	C-O	-5.18	1.18	1.23
1	B	77	ASP	CA-C	5.13	1.59	1.52
1	I	61	ARG	C-O	-5.11	1.18	1.24
1	B	82	ILE	CA-CB	5.07	1.60	1.54
1	B	145	ASP	C-O	5.04	1.30	1.23
1	D	112	ILE	N-CA	-5.03	1.40	1.46
1	B	172	ASN	CA-C	-5.03	1.46	1.52
1	C	173	ASN	N-CA	-5.02	1.39	1.46
1	K	43	THR	CA-C	5.02	1.57	1.52
1	K	147	ASP	CA-C	-5.02	1.46	1.52
1	H	206	TYR	CA-C	-5.00	1.46	1.52

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	144	ARG	N-CA-C	10.69	124.13	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	34	ILE	CB-CA-C	-10.10	99.10	111.32
1	G	95	PHE	CA-C-N	9.74	130.13	119.90
1	G	95	PHE	C-N-CA	9.74	130.13	119.90
1	L	112	ILE	N-CA-C	9.61	116.30	107.56
1	C	90	SER	CB-CA-C	8.98	124.48	111.73
1	E	183	PRO	N-CA-C	8.95	121.62	110.70
1	J	153	VAL	N-CA-CB	8.77	121.79	110.57
1	H	66	GLU	CA-C-N	-8.57	111.20	119.85
1	H	66	GLU	C-N-CA	-8.57	111.20	119.85
1	E	61	ARG	NE-CZ-NH2	8.47	126.82	119.20
1	D	76	GLU	CA-CB-CG	8.17	130.44	114.10
1	H	61	ARG	NE-CZ-NH1	-8.06	113.44	121.50
1	B	183	PRO	N-CA-C	7.84	120.26	110.70
1	G	200	LYS	N-CA-C	7.65	122.38	112.89
1	B	149	ILE	N-CA-C	-7.65	102.67	111.00
1	B	112	ILE	N-CA-C	7.64	116.33	107.77
1	F	34	ILE	CB-CA-C	-7.63	100.59	111.19
1	F	153	VAL	N-CA-CB	7.54	120.22	110.57
1	F	123	VAL	CB-CA-C	-7.54	98.37	110.28
1	H	203	ILE	N-CA-C	7.49	119.50	108.65
1	E	61	ARG	NE-CZ-NH1	-7.48	114.02	121.50
1	G	65	VAL	CB-CA-C	-7.21	102.19	110.41
1	K	43	THR	CB-CA-C	7.11	119.89	108.87
1	L	182	VAL	CA-C-N	-7.09	113.08	120.38
1	L	182	VAL	C-N-CA	-7.09	113.08	120.38
1	H	206	TYR	N-CA-C	-7.08	104.79	113.50
1	A	112	ILE	N-CA-C	7.02	114.50	107.55
1	B	101	ASP	N-CA-C	-6.89	99.84	110.10
1	J	112	ILE	N-CA-C	6.77	114.45	108.63
1	F	144	ARG	N-CA-C	6.75	119.04	110.33
1	A	84	TRP	N-CA-C	-6.73	103.87	111.14
1	B	183	PRO	CB-CA-C	-6.69	102.76	110.92
1	K	61	ARG	NE-CZ-NH2	6.69	125.22	119.20
1	G	101	ASP	N-CA-C	6.68	118.57	111.28
1	C	4	ILE	CB-CA-C	-6.65	102.10	111.28
1	E	182	VAL	CA-C-N	6.52	127.09	120.38
1	E	182	VAL	C-N-CA	6.52	127.09	120.38
1	I	198	LYS	N-CA-C	6.51	118.35	109.11
1	L	111	MET	CA-C-N	6.46	126.99	122.60
1	L	111	MET	C-N-CA	6.46	126.99	122.60
1	E	61	ARG	CD-NE-CZ	6.42	133.38	124.40
1	L	32	TRP	N-CA-C	-6.35	101.58	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	61	ARG	NE-CZ-NH2	6.28	124.85	119.20
1	E	166	LEU	CA-C-N	6.23	126.19	120.21
1	E	166	LEU	C-N-CA	6.23	126.19	120.21
1	K	91	VAL	N-CA-C	-6.21	99.53	108.48
1	A	50	PHE	N-CA-C	-6.16	104.12	111.69
1	J	61	ARG	NE-CZ-NH1	-6.12	115.38	121.50
1	B	32	TRP	N-CA-C	-6.07	101.78	110.59
1	E	51	TYR	N-CA-C	-6.04	104.61	111.07
1	B	91	VAL	N-CA-C	-6.02	100.41	108.35
1	C	32	TRP	N-CA-C	-6.01	102.78	110.53
1	B	127	ASP	N-CA-C	5.99	119.21	110.17
1	K	43	THR	CA-C-N	-5.97	112.34	118.85
1	K	43	THR	C-N-CA	-5.97	112.34	118.85
1	B	183	PRO	CA-C-N	5.95	127.28	119.84
1	B	183	PRO	C-N-CA	5.95	127.28	119.84
1	E	158	ILE	N-CA-C	5.95	116.69	110.62
1	G	96	PRO	CB-CA-C	-5.94	104.27	111.46
1	A	77	ASP	N-CA-C	-5.93	104.39	111.69
1	B	102	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	J	3	VAL	N-CA-C	-5.91	100.49	107.70
1	L	126	VAL	CB-CA-C	-5.91	101.41	110.50
1	F	149	ILE	N-CA-C	-5.87	103.58	111.44
1	D	147	ASP	N-CA-C	-5.83	104.51	111.69
1	F	76	GLU	CA-CB-CG	5.80	125.70	114.10
1	L	66	GLU	CA-C-N	-5.76	114.33	120.03
1	L	66	GLU	C-N-CA	-5.76	114.33	120.03
1	D	61	ARG	NE-CZ-NH1	-5.74	115.76	121.50
1	H	176	ILE	N-CA-C	5.74	117.96	111.88
1	K	61	ARG	NE-CZ-NH1	-5.73	115.77	121.50
1	L	152	LEU	N-CA-C	5.70	117.95	111.11
1	G	116	ALA	N-CA-C	5.70	117.63	109.14
1	C	202	GLU	CA-C-N	-5.70	115.75	123.10
1	C	202	GLU	C-N-CA	-5.70	115.75	123.10
1	D	84	TRP	N-CA-C	-5.69	105.07	111.28
1	B	112	ILE	CA-C-O	5.68	123.34	119.20
1	F	61	ARG	NE-CZ-NH2	5.67	124.30	119.20
1	H	154	LYS	N-CA-C	5.64	117.88	111.11
1	K	142	VAL	CB-CA-C	-5.62	102.75	110.96
1	E	78	HIS	N-CA-C	-5.61	104.85	110.97
1	E	101	ASP	N-CA-CB	5.61	118.27	109.69
1	I	150	LEU	N-CA-C	-5.60	105.25	111.36
1	K	78	HIS	N-CA-C	-5.57	104.85	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	76	GLU	CB-CG-CD	5.55	122.03	112.60
1	B	15	THR	N-CA-C	5.52	117.81	109.41
1	H	60	PHE	N-CA-C	-5.49	105.38	111.36
1	F	40	ALA	N-CA-C	5.48	117.43	108.55
1	D	143	GLY	N-CA-C	5.48	117.77	111.36
1	E	61	ARG	CB-CG-CD	5.45	123.84	111.30
1	E	138	TYR	N-CA-C	-5.40	102.29	110.50
1	D	76	GLU	N-CA-CB	5.40	118.65	110.28
1	K	158	ILE	N-CA-C	5.40	116.12	110.62
1	A	34	ILE	CB-CA-C	-5.39	104.80	111.32
1	A	206	TYR	N-CA-C	-5.38	106.72	113.28
1	D	61	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	H	83	GLU	N-CA-C	-5.37	105.43	111.28
1	D	101	ASP	N-CA-C	-5.36	102.12	110.10
1	J	126	VAL	CB-CA-C	-5.35	102.71	110.63
1	K	66	GLU	CA-C-N	-5.32	114.50	120.14
1	K	66	GLU	C-N-CA	-5.32	114.50	120.14
1	G	66	GLU	CA-C-N	-5.32	114.50	120.14
1	G	66	GLU	C-N-CA	-5.32	114.50	120.14
1	H	40	ALA	N-CA-C	5.32	117.33	108.99
1	I	202	GLU	CA-C-O	-5.31	115.33	121.07
1	I	32	TRP	N-CA-C	-5.31	102.60	110.46
1	B	213	LYS	N-CA-C	5.30	116.90	108.79
1	G	3	VAL	CA-C-N	5.29	127.78	120.49
1	G	3	VAL	C-N-CA	5.29	127.78	120.49
1	L	101	ASP	N-CA-C	-5.27	102.59	110.23
1	L	121	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	L	76	GLU	N-CA-CB	5.25	117.62	110.01
1	B	182	VAL	CA-C-N	5.22	125.76	120.38
1	B	182	VAL	C-N-CA	5.22	125.76	120.38
1	I	102	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	G	142	VAL	CB-CA-C	-5.21	104.53	110.73
1	L	40	ALA	N-CA-C	5.20	117.08	108.13
1	B	84	TRP	N-CA-C	-5.18	105.71	111.36
1	E	25	TYR	N-CA-C	5.18	117.60	111.33
1	J	40	ALA	N-CA-C	5.18	117.80	108.48
1	L	4	ILE	CB-CA-C	-5.17	102.81	111.29
1	E	95	PHE	CB-CA-C	5.15	115.64	109.31
1	D	95	PHE	CB-CA-C	5.14	117.38	109.15
1	H	151	ARG	N-CA-C	-5.14	105.57	111.07
1	J	32	TRP	N-CA-C	-5.10	103.19	110.59
1	H	68	ILE	CA-C-N	5.09	127.06	120.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	68	ILE	C-N-CA	5.09	127.06	120.64
1	B	41	ASP	N-CA-C	-5.08	103.45	110.35
1	J	143	GLY	N-CA-C	-5.07	106.75	112.33
1	I	142	VAL	CB-CA-C	-5.07	104.14	111.19
1	A	43	THR	CB-CA-C	5.07	116.26	109.42
1	C	85	ILE	CB-CA-C	5.06	119.20	112.22
1	F	62	LYS	N-CA-C	5.05	117.45	111.33
1	G	138	TYR	N-CA-C	-5.05	103.79	110.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	183	PRO	Peptide
1	B	2	VAL	Peptide
1	C	196	GLU	Peptide
1	E	202	GLU	Peptide
1	G	200	LYS	Peptide
1	H	198	LYS	Peptide
1	K	202	GLU	Peptide
1	L	2	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1725	0	1727	51	0
1	B	1725	0	1728	54	0
1	C	1725	0	1727	71	0
1	D	1725	0	1728	55	0
1	E	1725	0	1728	44	0
1	F	1725	0	1727	56	0
1	G	1725	0	1727	48	0
1	H	1725	0	1728	73	0
1	I	1725	0	1727	55	0
1	J	1725	0	1728	63	0
1	K	1725	0	1728	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1725	0	1727	57	0
2	A	9	0	0	0	0
2	B	16	0	0	1	0
2	C	17	0	0	0	0
2	D	6	0	0	1	0
2	E	15	0	0	0	0
2	F	10	0	0	0	0
2	G	11	0	0	0	0
2	H	11	0	0	0	0
2	I	18	0	0	0	0
2	J	11	0	0	0	0
2	K	9	0	0	0	0
2	L	9	0	0	2	0
All	All	20842	0	20730	610	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 15.

All (610) 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:179:LYS:HE2	1:J:204:GLU:OE2	1.37	1.20
1:H:109:LEU:HD12	1:H:111:MET:HE2	1.29	1.12
1:C:185:ALA:HB3	1:C:186:SER:HA	1.41	1.02
1:J:179:LYS:CE	1:J:204:GLU:OE2	2.14	0.95
1:F:43:THR:HG21	1:F:46:OCS:OD3	1.66	0.94
1:H:106:ALA:HA	1:H:111:MET:HE3	1.50	0.91
1:H:46:OCS:OD2	1:H:121:ARG:NH2	2.03	0.89
1:E:156:LEU:HD13	1:F:142:VAL:HG21	1.51	0.89
1:C:16:THR:HG22	1:C:75:VAL:HG23	1.53	0.88
1:J:105:LEU:O	1:J:109:LEU:HD22	1.72	0.88
1:F:43:THR:CG2	1:F:46:OCS:OD3	2.23	0.85
1:J:102:ARG:NH2	1:K:102:ARG:O	2.11	0.84
1:B:77:ASP:OD1	1:C:77:ASP:CG	2.21	0.83
1:D:203:ILE:CD1	1:D:211:CYS:HB3	2.10	0.82
1:C:46:OCS:OD2	1:C:121:ARG:NH2	2.13	0.82
1:A:46:OCS:OD2	1:A:121:ARG:NH2	2.11	0.81
1:F:109:LEU:HD12	1:F:111:MET:CE	2.10	0.81
1:C:185:ALA:CB	1:C:186:SER:HA	2.09	0.81
1:E:72:VAL:HG22	1:E:72:VAL:O	1.79	0.81
1:H:54:GLN:O	1:H:57:VAL:HG12	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:HD11	1:A:153:VAL:HG11	1.62	0.80
1:H:199:ALA:O	1:H:201:GLY:N	2.16	0.79
1:H:74:GLN:HE22	1:I:118:ILE:HG21	1.47	0.79
1:H:109:LEU:CD1	1:H:111:MET:HE2	2.11	0.78
1:J:105:LEU:O	1:J:109:LEU:CD2	2.32	0.78
1:A:2:VAL:HG11	1:A:109:LEU:HD23	1.65	0.78
1:C:203:ILE:CD1	1:C:211:CYS:HB3	2.14	0.77
1:F:109:LEU:HD12	1:F:111:MET:HE3	1.67	0.77
1:K:44:PRO:HB2	1:L:181:ILE:HD13	1.65	0.77
1:F:164:VAL:HG11	1:F:180:VAL:HG21	1.67	0.76
1:D:201:GLY:O	1:D:202:GLU:C	2.29	0.75
1:J:198:LYS:N	1:J:199:ALA:HB3	2.01	0.75
1:D:34:ILE:HD11	1:D:153:VAL:HG11	1.69	0.74
1:E:44:PRO:HB2	1:F:181:ILE:HD13	1.69	0.74
1:L:200:LYS:NZ	2:L:301:HOH:O	2.20	0.74
1:H:74:GLN:NE2	1:I:118:ILE:HG21	2.02	0.73
1:G:46:OCS:OD3	1:G:121:ARG:NH2	2.20	0.73
1:C:185:ALA:HB1	1:C:190:GLU:OE1	1.88	0.73
1:D:5:GLY:O	1:D:131:ILE:HG23	1.89	0.73
1:I:156:LEU:HD13	1:J:142:VAL:HG21	1.69	0.72
1:D:111:MET:HE2	1:D:124:PHE:CE1	2.23	0.72
1:A:174:GLU:N	1:A:174:GLU:OE1	2.22	0.72
1:K:209:TRP:O	1:L:44:PRO:HG3	1.90	0.72
1:K:72:VAL:HG11	1:K:118:ILE:HG22	1.71	0.71
1:K:141:GLU:OE1	1:L:133:ARG:NH2	2.21	0.71
1:E:12:GLU:HG2	1:E:21:LYS:HE2	1.73	0.70
1:G:72:VAL:HG11	1:G:118:ILE:HG22	1.73	0.70
1:E:72:VAL:HG11	1:E:118:ILE:HG22	1.73	0.70
1:C:188:ILE:HA	1:C:189:GLU:C	2.17	0.69
1:B:198:LYS:N	1:B:199:ALA:HB3	2.08	0.69
1:G:34:ILE:HD11	1:G:153:VAL:HG11	1.74	0.69
1:E:156:LEU:HD13	1:F:142:VAL:CG2	2.21	0.68
1:I:24:ASP:O	1:I:28:LYS:HG3	1.92	0.68
1:A:101:ASP:O	1:A:104:GLU:HG3	1.93	0.68
1:D:201:GLY:O	1:D:202:GLU:O	2.11	0.68
1:D:24:ASP:OD1	1:D:24:ASP:N	2.23	0.68
1:B:149:ILE:O	1:B:153:VAL:HG12	1.93	0.68
1:C:149:ILE:O	1:C:153:VAL:HG13	1.94	0.68
1:L:43:THR:HG23	2:L:305:HOH:O	1.93	0.67
1:G:156:LEU:HD13	1:H:142:VAL:HG21	1.76	0.67
1:B:77:ASP:OD1	1:C:77:ASP:OD2	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:54:GLN:HG2	1:L:91:VAL:HG13	1.75	0.67
1:G:152:LEU:HG	1:H:138:TYR:CZ	2.30	0.67
1:E:34:ILE:HD11	1:E:153:VAL:HG11	1.76	0.67
1:F:113:PRO:HG3	1:F:120:ALA:HB2	1.76	0.67
1:H:46:OCS:HD2	1:H:121:ARG:HH22	1.39	0.67
1:A:202:GLU:HG3	1:A:213:LYS:HB2	1.77	0.66
1:L:57:VAL:HG22	1:L:67:PRO:HG2	1.78	0.66
1:C:12:GLU:HG2	1:C:21:LYS:HE2	1.77	0.66
1:F:39:PRO:O	1:F:118:ILE:HD11	1.95	0.66
1:L:35:LEU:HD21	1:L:111:MET:HE1	1.78	0.66
1:K:38:HIS:CE1	1:K:71:SER:HB3	2.31	0.66
1:L:54:GLN:HG2	1:L:91:VAL:CG1	2.26	0.65
1:A:112:ILE:HD11	1:A:117:THR:HA	1.77	0.65
1:D:198:LYS:N	1:D:199:ALA:HB3	2.11	0.65
1:E:198:LYS:N	1:E:199:ALA:HB3	2.11	0.65
1:E:46:OCS:OD3	1:E:121:ARG:NH2	2.29	0.65
1:D:101:ASP:O	1:D:102:ARG:HB2	1.96	0.64
1:I:197:ALA:C	1:I:199:ALA:HB3	2.22	0.64
1:K:61:ARG:NH2	1:K:94:ASP:OD1	2.30	0.64
1:H:197:ALA:O	1:H:198:LYS:HB2	1.98	0.64
1:J:53:MET:O	1:J:57:VAL:HG12	1.98	0.63
1:A:166:LEU:HD22	1:A:166:LEU:N	2.13	0.63
1:A:198:LYS:HG2	1:A:203:ILE:HD11	1.79	0.63
1:D:46:OCS:OD3	1:D:121:ARG:NH2	2.31	0.63
1:H:198:LYS:HG3	1:H:203:ILE:HD11	1.81	0.63
1:D:70:LEU:C	1:D:70:LEU:HD23	2.23	0.63
1:F:15:THR:HG21	1:F:20:ILE:HD11	1.79	0.63
1:G:24:ASP:O	1:G:28:LYS:HG2	1.98	0.62
1:D:55:LYS:NZ	2:D:301:HOH:O	2.27	0.62
1:J:85:ILE:HG22	1:J:85:ILE:O	1.99	0.62
1:C:100:ASP:OD2	1:C:103:GLY:HA2	2.00	0.62
1:C:112:ILE:CD1	1:C:116:ALA:O	2.48	0.62
1:L:53:MET:O	1:L:57:VAL:HG23	1.98	0.62
1:J:46:OCS:OD1	1:J:121:ARG:NH2	2.32	0.62
1:H:34:ILE:HD12	1:H:67:PRO:HA	1.81	0.62
1:E:193:GLN:HA	1:E:196:GLU:HB2	1.81	0.61
1:E:193:GLN:O	1:E:197:ALA:N	2.32	0.61
1:G:68:ILE:HG13	1:G:96:PRO:HG2	1.82	0.61
1:I:9:PRO:O	1:I:11:VAL:HG12	2.00	0.61
1:G:185:ALA:O	1:G:190:GLU:OE1	2.18	0.61
1:J:202:GLU:HG3	1:J:213:LYS:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:185:ALA:O	1:K:186:SER:HB2	2.00	0.61
1:B:102:ARG:O	1:C:102:ARG:HD2	2.02	0.60
1:K:168:HIS:O	1:K:169:LYS:HB3	2.01	0.60
1:C:84:TRP:O	1:C:84:TRP:CE3	2.54	0.60
1:L:189:GLU:C	1:L:191:LYS:H	2.10	0.60
1:E:145:ASP:OD2	1:E:145:ASP:C	2.43	0.60
1:B:198:LYS:HA	1:B:199:ALA:C	2.27	0.60
1:D:167:PRO:HG3	1:D:176:ILE:HD11	1.82	0.60
1:H:189:GLU:N	1:H:190:GLU:HB3	2.17	0.60
1:J:36:PHE:HA	1:J:122:ALA:O	2.01	0.60
1:D:203:ILE:HD13	1:D:211:CYS:HB3	1.83	0.60
1:E:112:ILE:HD11	1:E:116:ALA:O	2.02	0.60
1:L:40:ALA:O	1:L:43:THR:HB	2.02	0.60
1:E:174:GLU:OE1	1:E:174:GLU:N	2.29	0.60
1:G:109:LEU:HD12	1:G:111:MET:HE3	1.84	0.60
1:J:101:ASP:O	1:J:102:ARG:HB2	2.01	0.60
1:C:54:GLN:HG2	1:C:91:VAL:CG1	2.32	0.59
1:L:34:ILE:HG13	1:L:65:VAL:CG1	2.32	0.59
1:H:199:ALA:O	1:H:200:LYS:C	2.46	0.59
1:K:100:ASP:O	1:K:101:ASP:C	2.44	0.59
1:B:111:MET:HE2	1:B:122:ALA:HB3	1.84	0.59
1:F:35:LEU:HD21	1:F:111:MET:HE1	1.85	0.59
1:K:24:ASP:HA	1:K:27:THR:OG1	2.02	0.59
1:C:136:VAL:HG22	1:D:136:VAL:HG13	1.85	0.59
1:C:189:GLU:O	1:C:192:LYS:N	2.36	0.58
1:A:125:VAL:HG11	1:A:156:LEU:HD23	1.85	0.58
1:D:8:PHE:CZ	1:D:109:LEU:HD11	2.38	0.58
1:I:156:LEU:HD13	1:J:142:VAL:CG2	2.33	0.58
1:G:41:ASP:OD1	1:G:78:HIS:ND1	2.35	0.58
1:H:39:PRO:O	1:H:118:ILE:HG21	2.03	0.58
1:J:74:GLN:NE2	1:K:118:ILE:HG21	2.18	0.58
1:B:86:LYS:HG3	1:B:92:GLU:HG2	1.86	0.58
1:D:164:VAL:HG11	1:D:180:VAL:HG21	1.85	0.58
1:I:197:ALA:O	1:I:202:GLU:O	2.22	0.58
1:H:102:ARG:O	1:I:102:ARG:HG3	2.03	0.58
1:I:3:VAL:HG11	1:J:112:ILE:O	2.03	0.58
1:J:105:LEU:HG	1:J:109:LEU:HD21	1.84	0.58
1:I:209:TRP:O	1:J:44:PRO:HG3	2.03	0.58
1:C:203:ILE:HD13	1:C:211:CYS:HB3	1.85	0.57
1:K:127:ASP:OD1	1:K:131:ILE:N	2.27	0.57
1:D:109:LEU:HD12	1:D:111:MET:HE3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:THR:O	1:E:30:GLY:N	2.38	0.57
1:D:11:VAL:HG11	1:D:105:LEU:HD13	1.86	0.57
1:C:11:VAL:HG22	1:C:12:GLU:O	2.03	0.57
1:H:70:LEU:HD23	1:H:71:SER:N	2.19	0.57
1:H:197:ALA:O	1:H:198:LYS:CB	2.53	0.57
1:J:201:GLY:O	1:J:202:GLU:C	2.47	0.57
1:D:152:LEU:O	1:D:156:LEU:HB2	2.04	0.57
1:D:7:LYS:HD3	1:D:131:ILE:HD13	1.87	0.56
1:I:46:OCS:OD3	1:I:121:ARG:NH2	2.38	0.56
1:A:112:ILE:HD11	1:A:116:ALA:O	2.05	0.56
1:C:39:PRO:HD2	1:C:46:OCS:OD2	2.05	0.56
1:C:70:LEU:HD21	1:C:100:ASP:HB2	1.87	0.56
1:C:2:VAL:HG22	1:C:109:LEU:HA	1.88	0.56
1:F:70:LEU:C	1:F:70:LEU:HD23	2.30	0.56
1:F:132:ILE:HG21	1:F:135:ILE:HD11	1.87	0.56
1:C:70:LEU:C	1:C:70:LEU:HD23	2.31	0.56
1:C:166:LEU:N	1:C:166:LEU:HD22	2.19	0.56
1:E:167:PRO:HG3	1:E:176:ILE:HD11	1.87	0.56
1:E:34:ILE:HD11	1:E:153:VAL:CG1	2.36	0.56
1:F:83:GLU:OE1	1:H:207:ASP:OD1	2.24	0.56
1:H:44:PRO:O	1:H:48:THR:HG23	2.06	0.56
1:I:207:ASP:OD2	1:J:84:TRP:NE1	2.35	0.56
1:A:83:GLU:OE2	1:K:207:ASP:OD1	2.24	0.55
1:B:20:ILE:HD11	1:B:22:LEU:HD21	1.88	0.55
1:J:70:LEU:HD23	1:J:71:SER:N	2.21	0.55
1:J:141:GLU:HG2	1:J:142:VAL:HG23	1.89	0.55
1:A:203:ILE:CD1	1:A:205:CYS:SG	2.95	0.55
1:J:33:PHE:CZ	1:J:126:VAL:HG21	2.41	0.55
1:L:121:ARG:HB3	1:L:144:ARG:CZ	2.36	0.55
1:E:39:PRO:HD2	1:E:46:OCS:OD3	2.07	0.55
1:B:201:GLY:O	1:B:202:GLU:C	2.50	0.55
1:C:34:ILE:HD11	1:C:60:PHE:CD2	2.42	0.55
1:C:203:ILE:HD11	1:C:211:CYS:HB3	1.86	0.55
1:I:161:GLU:HG3	1:I:162:LYS:HG2	1.88	0.55
1:A:44:PRO:O	1:A:45:VAL:C	2.46	0.54
1:A:129:LYS:HB2	1:A:131:ILE:HG12	1.89	0.54
1:F:145:ASP:OD2	1:F:145:ASP:C	2.48	0.54
1:H:196:GLU:O	1:H:199:ALA:CB	2.56	0.54
1:I:100:ASP:OD2	1:I:103:GLY:HA2	2.07	0.54
1:B:2:VAL:HG11	1:B:109:LEU:HD23	1.89	0.54
1:F:198:LYS:N	1:F:199:ALA:HB3	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:85:ILE:O	1:J:85:ILE:CG2	2.55	0.54
1:A:199:ALA:O	1:A:201:GLY:CA	2.56	0.54
1:C:2:VAL:CG2	1:C:109:LEU:HA	2.38	0.54
1:C:189:GLU:O	1:C:190:GLU:C	2.51	0.54
1:E:159:SER:OG	1:F:141:GLU:HG3	2.08	0.54
1:F:198:LYS:HA	1:F:199:ALA:C	2.32	0.54
1:B:38:HIS:CE1	1:B:71:SER:HB3	2.42	0.54
1:J:54:GLN:HA	1:J:57:VAL:CG1	2.38	0.54
1:K:84:TRP:CE3	1:K:84:TRP:C	2.86	0.54
1:B:83:GLU:OE2	1:D:207:ASP:OD1	2.26	0.54
1:C:84:TRP:CE3	1:C:84:TRP:C	2.85	0.54
1:A:70:LEU:C	1:A:70:LEU:HD23	2.33	0.54
1:C:167:PRO:HG3	1:C:176:ILE:HD11	1.90	0.54
1:E:100:ASP:O	1:E:101:ASP:C	2.47	0.54
1:G:45:VAL:HG22	1:H:181:ILE:HD12	1.90	0.54
1:F:72:VAL:HG12	1:F:118:ILE:CD1	2.37	0.53
1:I:198:LYS:HB3	1:I:203:ILE:O	2.08	0.53
1:I:109:LEU:HD12	1:I:111:MET:HE3	1.91	0.53
1:K:133:ARG:NH2	1:L:141:GLU:OE1	2.41	0.53
1:J:113:PRO:HG3	1:J:120:ALA:HB2	1.91	0.53
1:K:111:MET:HG2	1:K:122:ALA:HB3	1.90	0.53
1:L:198:LYS:HA	1:L:199:ALA:C	2.34	0.53
1:J:167:PRO:HD2	1:J:170:TRP:HB2	1.91	0.53
1:L:111:MET:HE2	1:L:124:PHE:CE1	2.44	0.53
1:K:180:VAL:HG11	1:K:215:LEU:HD21	1.91	0.53
1:L:54:GLN:CG	1:L:91:VAL:HG13	2.39	0.53
1:C:10:GLU:OE2	1:C:23:PRO:HD2	2.08	0.53
1:D:203:ILE:HD12	1:D:211:CYS:HB3	1.91	0.53
1:J:70:LEU:HD23	1:J:70:LEU:C	2.34	0.53
1:L:26:PHE:O	1:L:31:LYS:HB2	2.09	0.53
1:C:112:ILE:HD11	1:C:116:ALA:O	2.09	0.52
1:H:54:GLN:NE2	1:H:57:VAL:HG11	2.23	0.52
1:C:73:ASP:O	1:C:99:ALA:HB1	2.09	0.52
1:C:184:PRO:O	1:C:185:ALA:CB	2.57	0.52
1:E:109:LEU:HD12	1:E:111:MET:HE3	1.91	0.52
1:A:198:LYS:CG	1:A:203:ILE:HD11	2.39	0.52
1:E:75:VAL:HG12	1:E:76:GLU:OE1	2.09	0.52
1:B:121:ARG:HB3	1:B:144:ARG:CZ	2.39	0.52
1:H:183:PRO:O	1:H:194:ARG:NH2	2.43	0.52
1:J:203:ILE:HD13	1:J:205:CYS:SG	2.50	0.52
1:L:109:LEU:HD12	1:L:111:MET:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:24:ASP:OD1	1:J:24:ASP:N	2.41	0.52
1:K:106:ALA:HB1	1:K:111:MET:HB2	1.91	0.52
1:G:107:GLU:OE2	1:G:112:ILE:HD13	2.08	0.51
1:I:167:PRO:HG3	1:I:176:ILE:HD11	1.92	0.51
1:A:120:ALA:HB1	1:A:138:TYR:O	2.09	0.51
1:F:80:ALA:HB2	1:G:42:PHE:CG	2.45	0.51
1:F:109:LEU:O	1:F:111:MET:N	2.43	0.51
1:H:166:LEU:HD12	1:H:170:TRP:CD2	2.44	0.51
1:H:102:ARG:O	1:I:102:ARG:CG	2.58	0.51
1:C:57:VAL:HG22	1:C:67:PRO:HG2	1.92	0.51
1:G:190:GLU:O	1:G:194:ARG:HG2	2.10	0.51
1:A:202:GLU:O	1:A:203:ILE:O	2.29	0.51
1:L:94:ASP:OD1	1:L:94:ASP:C	2.54	0.51
1:H:57:VAL:CG2	1:H:61:ARG:CZ	2.89	0.51
1:K:194:ARG:O	1:K:198:LYS:HG2	2.11	0.51
1:B:12:GLU:HG2	1:B:21:LYS:CD	2.41	0.51
1:E:35:LEU:HA	1:E:68:ILE:HG23	1.92	0.51
1:H:57:VAL:HG21	1:H:61:ARG:NH2	2.26	0.51
1:F:80:ALA:CB	1:G:42:PHE:CG	2.94	0.50
1:H:34:ILE:HG13	1:H:65:VAL:HG12	1.93	0.50
1:H:102:ARG:C	1:I:102:ARG:HG3	2.37	0.50
1:H:70:LEU:HD13	1:H:111:MET:HE1	1.92	0.50
1:J:109:LEU:HD22	1:J:109:LEU:H	1.76	0.50
1:F:109:LEU:O	1:F:110:GLY:C	2.54	0.50
1:H:39:PRO:O	1:H:118:ILE:CG2	2.60	0.50
1:I:203:ILE:HG22	1:I:213:LYS:HB3	1.94	0.50
1:B:2:VAL:O	1:B:3:VAL:HG23	2.12	0.50
1:D:190:GLU:HA	1:D:193:GLN:CG	2.41	0.50
1:D:198:LYS:H	1:D:199:ALA:HB3	1.77	0.50
1:J:74:GLN:HE22	1:K:118:ILE:HD13	1.75	0.50
1:F:109:LEU:HD12	1:F:111:MET:HE2	1.88	0.50
1:D:90:SER:O	1:D:90:SER:OG	2.28	0.50
1:H:187:THR:HG22	1:H:188:ILE:O	2.11	0.50
1:H:191:LYS:O	1:H:195:GLU:N	2.45	0.50
1:I:72:VAL:O	1:I:72:VAL:HG22	2.11	0.50
1:D:190:GLU:HA	1:D:193:GLN:HG2	1.93	0.50
1:G:145:ASP:C	1:G:145:ASP:OD2	2.55	0.50
1:I:197:ALA:O	1:I:199:ALA:HB3	2.11	0.50
1:E:198:LYS:HA	1:E:199:ALA:O	2.12	0.50
1:J:105:LEU:O	1:J:106:ALA:C	2.55	0.50
1:I:200:LYS:HD3	1:I:201:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:198:LYS:N	1:L:199:ALA:HB3	2.27	0.49
1:C:121:ARG:HB3	1:C:144:ARG:CZ	2.42	0.49
1:C:127:ASP:OD2	1:C:133:ARG:HD3	2.12	0.49
1:F:81:TRP:O	1:F:85:ILE:HG13	2.11	0.49
1:H:62:LYS:O	1:H:62:LYS:HG2	2.13	0.49
1:F:200:LYS:HA	1:F:201:GLY:O	2.12	0.49
1:H:34:ILE:HD12	1:H:67:PRO:CA	2.41	0.49
1:I:214:LYS:HG2	1:I:215:LEU:N	2.27	0.49
1:C:213:LYS:CG	1:C:214:LYS:O	2.60	0.49
1:I:2:VAL:HG11	1:I:109:LEU:HD23	1.93	0.49
1:L:13:VAL:HB	1:L:98:ILE:HG23	1.94	0.49
1:C:4:ILE:HG22	1:C:5:GLY:N	2.27	0.49
1:H:40:ALA:O	1:H:43:THR:OG1	2.29	0.49
1:L:2:VAL:O	1:L:3:VAL:HG23	2.13	0.49
1:C:199:ALA:CA	1:C:200:LYS:C	2.85	0.49
1:D:209:TRP:CE3	1:D:210:PHE:HB2	2.48	0.49
1:J:183:PRO:O	1:J:194:ARG:NH1	2.44	0.49
1:H:15:THR:HG22	1:H:98:ILE:HA	1.94	0.49
1:E:45:VAL:O	1:E:48:THR:OG1	2.29	0.49
1:F:202:GLU:HB3	1:F:213:LYS:HB2	1.93	0.49
1:I:203:ILE:C	1:I:203:ILE:HD12	2.37	0.49
1:E:205:CYS:HB3	1:E:207:ASP:O	2.13	0.48
1:F:72:VAL:CG1	1:F:118:ILE:HD13	2.43	0.48
1:I:181:ILE:HD13	1:J:44:PRO:HB2	1.95	0.48
1:F:73:ASP:OD2	1:G:77:ASP:OD1	2.31	0.48
1:J:109:LEU:HD22	1:J:109:LEU:N	2.28	0.48
1:G:32:TRP:HB3	1:G:126:VAL:O	2.12	0.48
1:B:86:LYS:HE2	2:B:313:HOH:O	2.12	0.48
1:C:198:LYS:O	1:C:199:ALA:CB	2.61	0.48
1:F:198:LYS:HB3	1:F:203:ILE:O	2.13	0.48
1:I:202:GLU:HG3	1:I:213:LYS:HB2	1.95	0.48
1:C:184:PRO:O	1:C:185:ALA:HB2	2.14	0.48
1:H:34:ILE:HG13	1:H:65:VAL:CG1	2.43	0.48
1:B:13:VAL:HB	1:B:98:ILE:HG23	1.95	0.48
1:B:141:GLU:OE2	1:B:141:GLU:N	2.42	0.48
1:E:112:ILE:HD11	1:E:117:THR:HA	1.94	0.48
1:E:176:ILE:O	1:E:179:LYS:HD3	2.13	0.48
1:G:149:ILE:O	1:G:153:VAL:HG13	2.14	0.48
1:B:46:OCS:OD1	1:B:121:ARG:NH1	2.38	0.48
1:C:200:LYS:O	1:C:202:GLU:N	2.45	0.48
1:H:37:SER:HA	1:H:70:LEU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASP:O	1:A:104:GLU:CG	2.61	0.48
1:C:112:ILE:HD12	1:C:116:ALA:O	2.13	0.48
1:D:198:LYS:HA	1:D:199:ALA:C	2.39	0.48
1:L:78:HIS:NE2	1:L:98:ILE:O	2.43	0.48
1:A:23:PRO:O	1:A:24:ASP:C	2.55	0.47
1:A:152:LEU:HD13	1:B:138:TYR:CE2	2.49	0.47
1:A:186:SER:O	1:A:187:THR:C	2.57	0.47
1:F:83:GLU:OE2	1:H:207:ASP:OD1	2.33	0.47
1:G:121:ARG:HB3	1:G:144:ARG:CZ	2.44	0.47
1:G:141:GLU:HG3	1:H:159:SER:OG	2.14	0.47
1:L:109:LEU:CD1	1:L:111:MET:HE3	2.44	0.47
1:E:203:ILE:HD12	1:E:203:ILE:C	2.38	0.47
1:H:31:LYS:NZ	1:H:66:GLU:OE1	2.46	0.47
1:D:180:VAL:O	1:D:212:TYR:HA	2.14	0.47
1:G:2:VAL:HA	1:G:6:GLU:OE1	2.14	0.47
1:I:175:LEU:HD21	1:J:51:TYR:CE2	2.49	0.47
1:E:72:VAL:O	1:E:72:VAL:CG2	2.50	0.47
1:F:72:VAL:CG1	1:F:118:ILE:CD1	2.92	0.47
1:H:76:GLU:HG3	1:I:43:THR:CG2	2.43	0.47
1:H:203:ILE:HD13	1:H:205:CYS:SG	2.54	0.47
1:F:42:PHE:CZ	1:F:81:TRP:HA	2.50	0.47
1:H:205:CYS:HA	1:H:210:PHE:O	2.13	0.47
1:I:145:ASP:C	1:I:145:ASP:OD2	2.58	0.47
1:K:167:PRO:HG3	1:K:176:ILE:HD11	1.96	0.47
1:F:7:LYS:HG3	1:F:131:ILE:CD1	2.45	0.47
1:H:155:ALA:HB1	1:H:166:LEU:HG	1.95	0.47
1:K:34:ILE:HD11	1:K:153:VAL:HG11	1.97	0.47
1:L:106:ALA:HB1	1:L:119:THR:HG22	1.97	0.47
1:A:76:GLU:H	1:A:76:GLU:CD	2.21	0.47
1:E:24:ASP:HB3	1:E:28:LYS:HD2	1.96	0.47
1:H:100:ASP:O	1:H:101:ASP:C	2.58	0.47
1:H:109:LEU:HD12	1:H:111:MET:CE	2.21	0.47
1:L:4:ILE:HG22	1:L:5:GLY:N	2.29	0.47
1:L:13:VAL:HG21	1:L:98:ILE:HG12	1.96	0.47
1:B:12:GLU:HG2	1:B:21:LYS:HD3	1.96	0.47
1:C:203:ILE:HD12	1:C:204:GLU:N	2.29	0.47
1:D:150:LEU:HD22	1:D:154:LYS:HE3	1.96	0.47
1:E:121:ARG:HB3	1:E:144:ARG:CZ	2.44	0.47
1:J:41:ASP:OD1	1:J:78:HIS:ND1	2.48	0.47
1:B:2:VAL:HG11	1:B:109:LEU:CD2	2.45	0.47
1:G:133:ARG:NH2	1:H:141:GLU:OE1	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:74:GLN:NE2	1:I:118:ILE:CG2	2.76	0.47
1:H:188:ILE:HD12	1:H:188:ILE:N	2.29	0.47
1:I:132:ILE:HG21	1:I:135:ILE:HD11	1.97	0.47
1:H:70:LEU:HD23	1:H:70:LEU:C	2.39	0.47
1:K:174:GLU:OE1	1:K:174:GLU:N	2.46	0.47
1:L:200:LYS:CD	1:L:201:GLY:HA2	2.45	0.47
1:F:195:GLU:HA	1:F:198:LYS:HG3	1.97	0.46
1:L:170:TRP:CD1	1:L:171:PRO:HA	2.50	0.46
1:B:82:ILE:HG23	1:B:93:ILE:HB	1.96	0.46
1:E:122:ALA:HA	1:E:136:VAL:O	2.15	0.46
1:I:4:ILE:CG2	1:I:5:GLY:N	2.76	0.46
1:C:213:LYS:HG2	1:C:214:LYS:O	2.14	0.46
1:G:15:THR:HG21	1:G:20:ILE:HD11	1.97	0.46
1:E:174:GLU:H	1:E:174:GLU:CD	2.17	0.46
1:I:168:HIS:HB2	1:J:49:GLU:HG2	1.97	0.46
1:B:188:ILE:C	1:B:190:GLU:N	2.70	0.46
1:J:77:ASP:OD2	1:K:73:ASP:OD2	2.34	0.46
1:L:150:LEU:HD12	1:L:150:LEU:HA	1.78	0.46
1:C:37:SER:OG	1:C:120:ALA:O	2.33	0.46
1:I:205:CYS:HA	1:I:210:PHE:O	2.14	0.46
1:K:26:PHE:O	1:K:31:LYS:HB2	2.15	0.46
1:K:43:THR:HG22	1:K:46:OCS:HB3	1.97	0.46
1:K:156:LEU:HD11	1:L:139:PRO:HG3	1.97	0.46
1:B:12:GLU:CD	1:B:21:LYS:HD3	2.40	0.46
1:D:19:ARG:O	1:D:19:ARG:HG2	2.15	0.46
1:D:54:GLN:HG2	1:D:91:VAL:HG13	1.98	0.46
1:F:121:ARG:HD2	1:F:142:VAL:O	2.16	0.46
1:A:168:HIS:NE2	1:B:146:TRP:CD1	2.84	0.46
1:F:43:THR:HG22	1:F:46:OCS:OD3	2.10	0.46
1:B:44:PRO:O	1:B:45:VAL:C	2.58	0.46
1:A:138:TYR:CZ	1:B:152:LEU:HD13	2.51	0.46
1:A:202:GLU:O	1:A:203:ILE:C	2.59	0.46
1:F:76:GLU:HG2	1:G:40:ALA:HB1	1.98	0.46
1:I:44:PRO:HG2	1:J:181:ILE:HG21	1.98	0.46
1:L:70:LEU:HD12	1:L:98:ILE:CD1	2.46	0.46
1:C:153:VAL:O	1:C:157:LYS:HG2	2.16	0.45
1:F:7:LYS:HG3	1:F:131:ILE:HD13	1.97	0.45
1:F:70:LEU:HD23	1:F:71:SER:N	2.31	0.45
1:L:192:LYS:O	1:L:193:GLN:C	2.57	0.45
1:E:84:TRP:CE3	1:E:84:TRP:C	2.95	0.45
1:K:25:TYR:CD2	1:K:25:TYR:C	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:VAL:HG22	1:B:181:ILE:HD12	1.99	0.45
1:A:198:LYS:HG2	1:A:203:ILE:CD1	2.44	0.45
1:H:122:ALA:HA	1:H:136:VAL:O	2.15	0.45
1:K:175:LEU:HD21	1:L:51:TYR:CZ	2.51	0.45
1:B:70:LEU:HD23	1:B:70:LEU:C	2.41	0.45
1:C:166:LEU:N	1:C:166:LEU:CD2	2.80	0.45
1:H:32:TRP:HB2	1:H:65:VAL:HG22	1.99	0.45
1:I:100:ASP:O	1:I:101:ASP:C	2.59	0.45
1:I:156:LEU:HD11	1:J:139:PRO:CG	2.46	0.45
1:J:127:ASP:OD1	1:J:131:ILE:N	2.41	0.45
1:C:57:VAL:CG2	1:C:67:PRO:HG2	2.46	0.45
1:H:105:LEU:HD11	1:H:109:LEU:HD11	1.97	0.45
1:I:192:LYS:O	1:I:196:GLU:HB2	2.16	0.45
1:J:203:ILE:HG22	1:J:213:LYS:HB3	1.98	0.45
1:L:61:ARG:O	1:L:63:LEU:N	2.50	0.45
1:A:168:HIS:O	1:A:169:LYS:HB3	2.17	0.45
1:A:199:ALA:O	1:A:201:GLY:HA3	2.16	0.45
1:A:202:GLU:CG	1:A:213:LYS:HB2	2.44	0.45
1:G:122:ALA:HA	1:G:136:VAL:O	2.16	0.45
1:L:34:ILE:HD11	1:L:65:VAL:HG11	1.99	0.45
1:L:35:LEU:CD2	1:L:111:MET:HE1	2.45	0.45
1:G:158:ILE:HD12	1:G:170:TRP:CH2	2.52	0.45
1:L:34:ILE:CD1	1:L:60:PHE:CE2	2.99	0.45
1:A:166:LEU:N	1:A:166:LEU:CD2	2.80	0.45
1:A:210:PHE:C	1:A:210:PHE:CD2	2.95	0.45
1:G:34:ILE:CD1	1:G:60:PHE:CE2	2.99	0.45
1:G:167:PRO:HG3	1:G:176:ILE:HD11	1.98	0.45
1:K:20:ILE:HG21	1:K:25:TYR:CD1	2.52	0.45
1:K:56:ARG:O	1:K:57:VAL:C	2.59	0.45
1:A:176:ILE:O	1:A:179:LYS:HG3	2.17	0.45
1:C:200:LYS:HA	1:C:200:LYS:NZ	2.32	0.45
1:D:86:LYS:O	1:D:90:SER:HA	2.16	0.45
1:D:187:THR:OG1	1:D:188:ILE:N	2.49	0.45
1:G:72:VAL:HG22	1:G:72:VAL:O	2.16	0.45
1:A:205:CYS:HB3	1:A:207:ASP:O	2.17	0.45
1:C:54:GLN:HG2	1:C:91:VAL:HG12	1.99	0.45
1:F:106:ALA:HB1	1:F:111:MET:HB2	1.98	0.45
1:J:109:LEU:HB3	1:J:124:PHE:CZ	2.52	0.45
1:K:139:PRO:HB2	1:K:141:GLU:OE2	2.16	0.45
1:A:187:THR:HG22	1:A:188:ILE:HD12	1.98	0.44
1:B:81:TRP:O	1:B:85:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:VAL:CG1	1:G:118:ILE:HG22	2.45	0.44
1:K:111:MET:HG2	1:K:122:ALA:CB	2.47	0.44
1:C:205:CYS:HA	1:C:211:CYS:HA	2.00	0.44
1:K:197:ALA:C	1:K:199:ALA:HB3	2.42	0.44
1:L:70:LEU:HD12	1:L:98:ILE:HD12	1.99	0.44
1:C:199:ALA:HA	1:C:200:LYS:C	2.43	0.44
1:K:201:GLY:O	1:K:202:GLU:C	2.61	0.44
1:L:174:GLU:CD	1:L:174:GLU:H	2.26	0.44
1:B:150:LEU:O	1:B:151:ARG:C	2.58	0.44
1:H:152:LEU:O	1:H:156:LEU:HB2	2.17	0.44
1:C:70:LEU:HD21	1:C:100:ASP:CB	2.46	0.44
1:F:203:ILE:HD12	1:F:205:CYS:SG	2.58	0.44
1:H:189:GLU:N	1:H:190:GLU:CB	2.81	0.44
1:B:40:ALA:H	1:B:46:OCS:HD2	1.64	0.44
1:B:65:VAL:HG21	1:B:153:VAL:HG21	2.00	0.44
1:C:63:LEU:HD11	1:C:154:LYS:HG2	2.00	0.44
1:D:210:PHE:C	1:D:210:PHE:CD2	2.96	0.44
1:F:46:OCS:OD2	1:F:121:ARG:NH2	2.50	0.44
1:F:54:GLN:HG2	1:F:91:VAL:CG1	2.48	0.44
1:G:38:HIS:CE1	1:G:71:SER:HB3	2.53	0.44
1:G:16:THR:HG23	1:G:97:VAL:O	2.17	0.44
1:K:169:LYS:O	1:K:170:TRP:C	2.58	0.44
1:D:34:ILE:CD1	1:D:153:VAL:HG11	2.45	0.43
1:I:152:LEU:HD12	1:I:156:LEU:HD22	2.00	0.43
1:A:35:LEU:HD21	1:A:111:MET:HE1	2.00	0.43
1:B:32:TRP:HB2	1:B:65:VAL:HG13	2.01	0.43
1:B:40:ALA:O	1:B:43:THR:HB	2.18	0.43
1:C:55:LYS:HD3	1:C:55:LYS:HA	1.78	0.43
1:C:198:LYS:HG3	1:C:203:ILE:HG13	1.99	0.43
1:K:44:PRO:CG	1:L:181:ILE:HG21	2.48	0.43
1:L:33:PHE:CZ	1:L:126:VAL:HG21	2.52	0.43
1:L:43:THR:CG2	1:L:46:OCS:OD1	2.66	0.43
1:A:121:ARG:HB2	1:A:138:TYR:HB2	2.00	0.43
1:H:54:GLN:HG2	1:H:91:VAL:HG13	2.00	0.43
1:B:200:LYS:HA	1:B:201:GLY:HA2	1.80	0.43
1:F:83:GLU:CD	1:H:207:ASP:OD1	2.61	0.43
1:F:197:ALA:O	1:F:202:GLU:O	2.37	0.43
1:G:39:PRO:HD2	1:G:46:OCS:OD3	2.19	0.43
1:D:13:VAL:HB	1:D:98:ILE:HG23	1.99	0.43
1:D:124:PHE:CE2	1:D:135:ILE:HG23	2.54	0.43
1:F:187:THR:HG22	1:F:188:ILE:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:151:ARG:NH2	1:H:145:ASP:HB2	2.33	0.43
1:I:3:VAL:O	1:I:6:GLU:HB3	2.18	0.43
1:L:169:LYS:O	1:L:170:TRP:C	2.59	0.43
1:B:173:ASN:O	1:B:174:GLU:C	2.59	0.43
1:G:189:GLU:O	1:G:190:GLU:C	2.62	0.43
1:G:189:GLU:O	1:G:192:LYS:N	2.52	0.43
1:J:24:ASP:HA	1:J:27:THR:OG1	2.18	0.43
1:K:198:LYS:HB3	1:K:203:ILE:O	2.18	0.43
1:L:61:ARG:C	1:L:63:LEU:H	2.26	0.43
1:A:147:ASP:OD2	1:B:169:LYS:NZ	2.47	0.43
1:B:39:PRO:HD2	1:B:46:OCS:OD3	2.19	0.43
1:D:44:PRO:O	1:D:48:THR:HG23	2.18	0.43
1:E:24:ASP:O	1:E:28:LYS:HG3	2.18	0.43
1:C:44:PRO:HB3	1:D:210:PHE:CD2	2.53	0.43
1:D:190:GLU:O	1:D:193:GLN:HB2	2.19	0.43
1:J:187:THR:O	1:J:188:ILE:HG23	2.17	0.43
1:C:141:GLU:HG3	1:D:159:SER:OG	2.19	0.43
1:J:35:LEU:HA	1:J:68:ILE:HG23	2.01	0.43
1:D:70:LEU:C	1:D:70:LEU:CD2	2.92	0.43
1:D:152:LEU:HD12	1:D:156:LEU:HD22	2.01	0.43
1:H:198:LYS:N	1:H:199:ALA:HB3	2.34	0.43
1:L:152:LEU:O	1:L:156:LEU:HD22	2.19	0.43
1:H:76:GLU:HG3	1:I:43:THR:HG23	2.01	0.42
1:I:106:ALA:O	1:I:110:GLY:N	2.52	0.42
1:K:34:ILE:HD11	1:K:65:VAL:HG11	2.01	0.42
1:A:133:ARG:HD2	1:A:133:ARG:HA	1.83	0.42
1:F:141:GLU:HG2	1:F:142:VAL:HG23	2.01	0.42
1:G:19:ARG:O	1:G:20:ILE:HG23	2.18	0.42
1:H:54:GLN:OE1	1:H:93:ILE:HA	2.19	0.42
1:B:34:ILE:HD11	1:B:60:PHE:CD2	2.54	0.42
1:B:133:ARG:NH2	1:B:156:LEU:HD12	2.34	0.42
1:H:15:THR:HG22	1:H:98:ILE:HG12	2.01	0.42
1:I:137:TYR:O	1:J:4:ILE:HD11	2.19	0.42
1:L:54:GLN:CG	1:L:91:VAL:CG1	2.96	0.42
1:L:61:ARG:C	1:L:63:LEU:N	2.77	0.42
1:G:185:ALA:O	1:G:186:SER:HB3	2.19	0.42
1:H:169:LYS:O	1:H:170:TRP:C	2.59	0.42
1:I:40:ALA:O	1:I:43:THR:OG1	2.34	0.42
1:J:34:ILE:CD1	1:J:149:ILE:HG21	2.49	0.42
1:J:118:ILE:HG12	1:K:74:GLN:NE2	2.33	0.42
1:D:38:HIS:O	1:D:119:THR:OG1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:PRO:HB2	1:B:181:ILE:HG21	2.01	0.42
1:F:199:ALA:O	1:F:200:LYS:C	2.63	0.42
1:K:202:GLU:HA	1:K:203:ILE:HA	1.75	0.42
1:C:16:THR:CG2	1:C:75:VAL:HG23	2.38	0.42
1:J:34:ILE:HD11	1:J:149:ILE:HG21	2.02	0.42
1:A:82:ILE:HG12	1:A:93:ILE:HB	2.01	0.42
1:C:142:VAL:CG2	1:D:156:LEU:HD13	2.50	0.42
1:E:193:GLN:HG3	1:E:197:ALA:HB2	2.02	0.42
1:H:81:TRP:O	1:H:84:TRP:HB3	2.20	0.42
1:I:138:TYR:CE2	1:J:152:LEU:HD13	2.55	0.42
1:I:37:SER:HA	1:I:70:LEU:O	2.20	0.42
1:K:182:VAL:HG22	1:K:211:CYS:O	2.20	0.42
1:F:109:LEU:CD1	1:F:111:MET:HE2	2.48	0.42
1:H:20:ILE:HG22	1:H:25:TYR:CE1	2.55	0.42
1:K:43:THR:CG2	1:K:46:OCS:OD3	2.68	0.42
1:K:55:LYS:HD3	1:K:55:LYS:HA	1.80	0.42
1:B:24:ASP:O	1:B:26:PHE:N	2.53	0.41
1:C:37:SER:HB2	1:C:111:MET:CE	2.49	0.41
1:C:197:ALA:O	1:C:200:LYS:O	2.38	0.41
1:C:213:LYS:HG3	1:C:214:LYS:O	2.19	0.41
1:F:76:GLU:HG2	1:G:40:ALA:CB	2.50	0.41
1:I:51:TYR:CZ	1:J:175:LEU:HD21	2.55	0.41
1:K:198:LYS:HA	1:K:199:ALA:C	2.44	0.41
1:F:72:VAL:HG11	1:F:118:ILE:HD13	2.03	0.41
1:J:70:LEU:HD23	1:J:71:SER:CA	2.50	0.41
1:L:11:VAL:HG11	1:L:105:LEU:HD22	2.01	0.41
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.79	0.41
1:D:202:GLU:HA	1:D:203:ILE:HA	1.78	0.41
1:G:40:ALA:O	1:G:43:THR:OG1	2.39	0.41
1:G:57:VAL:O	1:G:61:ARG:HB2	2.19	0.41
1:J:83:GLU:OE1	1:L:207:ASP:OD1	2.38	0.41
1:K:34:ILE:HG13	1:K:65:VAL:CG1	2.49	0.41
1:K:34:ILE:CD1	1:K:65:VAL:HG11	2.51	0.41
1:B:203:ILE:HG22	1:B:213:LYS:HB3	2.01	0.41
1:G:166:LEU:CD1	1:G:180:VAL:HG12	2.50	0.41
1:B:31:LYS:HD3	1:B:66:GLU:CG	2.51	0.41
1:H:41:ASP:OD1	1:H:78:HIS:ND1	2.48	0.41
1:K:75:VAL:O	1:K:78:HIS:HB2	2.20	0.41
1:C:34:ILE:HG13	1:C:65:VAL:CG1	2.50	0.41
1:E:38:HIS:CE1	1:E:71:SER:HB2	2.55	0.41
1:F:79:SER:HA	1:F:82:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:CYS:HB3	1:G:207:ASP:O	2.21	0.41
1:J:169:LYS:O	1:J:170:TRP:C	2.64	0.41
1:J:213:LYS:HG3	1:J:214:LYS:O	2.20	0.41
1:L:24:ASP:HA	1:L:27:THR:OG1	2.21	0.41
1:A:32:TRP:HB2	1:A:65:VAL:HG22	2.02	0.41
1:J:24:ASP:HA	1:J:27:THR:HG1	1.85	0.41
1:J:70:LEU:C	1:J:70:LEU:CD2	2.94	0.41
1:A:165:ALA:HB1	1:B:45:VAL:HG21	2.03	0.41
1:A:210:PHE:C	1:A:210:PHE:HD2	2.28	0.41
1:B:161:GLU:HG2	1:B:162:LYS:HD3	2.02	0.41
1:E:57:VAL:HG22	1:E:67:PRO:HG2	2.02	0.41
1:E:209:TRP:CE3	1:E:210:PHE:HB2	2.55	0.41
1:H:196:GLU:O	1:H:197:ALA:C	2.62	0.41
1:A:121:ARG:HB3	1:A:144:ARG:CZ	2.51	0.41
1:A:122:ALA:HA	1:A:136:VAL:O	2.21	0.41
1:B:36:PHE:HA	1:B:122:ALA:O	2.20	0.41
1:C:51:TYR:CZ	1:D:175:LEU:HD21	2.55	0.41
1:D:38:HIS:CE1	1:D:71:SER:HB3	2.56	0.41
1:D:200:LYS:HA	1:D:201:GLY:HA2	1.83	0.41
1:D:202:GLU:CG	1:D:213:LYS:HB2	2.51	0.41
1:I:44:PRO:O	1:I:45:VAL:C	2.60	0.41
1:K:35:LEU:HA	1:K:68:ILE:O	2.21	0.41
1:K:203:ILE:CD1	1:K:205:CYS:SG	3.09	0.41
1:L:127:ASP:OD2	1:L:133:ARG:HD3	2.20	0.41
1:L:189:GLU:C	1:L:191:LYS:N	2.75	0.41
1:C:198:LYS:HE3	1:C:205:CYS:SG	2.61	0.41
1:I:74:GLN:HA	1:I:99:ALA:HB1	2.01	0.41
1:I:198:LYS:HA	1:I:199:ALA:O	2.21	0.41
1:J:166:LEU:N	1:J:166:LEU:HD22	2.36	0.41
1:B:198:LYS:HB3	1:B:203:ILE:O	2.22	0.40
1:E:11:VAL:HG22	1:E:12:GLU:O	2.21	0.40
1:F:44:PRO:O	1:F:45:VAL:C	2.64	0.40
1:H:112:ILE:HG22	1:H:113:PRO:O	2.21	0.40
1:K:44:PRO:HG2	1:L:181:ILE:HG21	2.03	0.40
1:K:145:ASP:O	1:K:146:TRP:C	2.62	0.40
1:B:111:MET:HE2	1:B:122:ALA:CB	2.48	0.40
1:G:44:PRO:O	1:G:45:VAL:C	2.62	0.40
1:K:112:ILE:HD11	1:K:116:ALA:O	2.21	0.40
1:D:68:ILE:O	1:D:68:ILE:HG23	2.22	0.40
1:I:156:LEU:CD1	1:J:139:PRO:HG2	2.52	0.40
1:A:121:ARG:HD2	1:A:142:VAL:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ILE:O	1:A:203:ILE:HG13	2.21	0.40
1:B:203:ILE:HD13	1:B:211:CYS:HB3	2.03	0.40
1:D:210:PHE:C	1:D:210:PHE:HD2	2.29	0.40
1:E:141:GLU:OE1	1:F:133:ARG:NH2	2.41	0.40
1:J:73:ASP:OD2	1:K:77:ASP:OD2	2.39	0.40
1:K:4:ILE:HD11	1:K:134:ALA:HA	2.04	0.40
1:L:34:ILE:CD1	1:L:65:VAL:HG11	2.51	0.40
1:C:112:ILE:HA	1:C:113:PRO:HD2	1.85	0.40
1:C:181:ILE:HG21	1:D:44:PRO:HG2	2.04	0.40
1:E:24:ASP:HB3	1:E:28:LYS:CD	2.51	0.40
1:E:27:THR:O	1:E:29:GLN:N	2.54	0.40
1:G:71:SER:OG	1:G:72:VAL:N	2.54	0.40
1:G:169:LYS:O	1:G:170:TRP:C	2.65	0.40
1:G:197:ALA:O	1:G:201:GLY:HA2	2.21	0.40
1:I:197:ALA:O	1:I:199:ALA:O	2.40	0.40
1:K:215:LEU:HD23	1:K:215:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

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	185/187 (99%)	171 (92%)	14 (8%)	12	10
1	B	185/187 (99%)	162 (88%)	23 (12%)	4	3
1	C	179/187 (96%)	154 (86%)	25 (14%)	3	2
1	D	185/187 (99%)	165 (89%)	20 (11%)	6	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	185/187 (99%)	166 (90%)	19 (10%)	7	5
1	F	157/187 (84%)	139 (88%)	18 (12%)	5	3
1	G	185/187 (99%)	170 (92%)	15 (8%)	11	9
1	H	185/187 (99%)	165 (89%)	20 (11%)	6	4
1	I	185/187 (99%)	173 (94%)	12 (6%)	15	14
1	J	185/187 (99%)	159 (86%)	26 (14%)	3	2
1	K	185/187 (99%)	167 (90%)	18 (10%)	8	6
1	L	185/187 (99%)	166 (90%)	19 (10%)	7	5
All	All	2186/2244 (97%)	1957 (90%)	229 (10%)	6	4

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	4	ILE
1	A	19	ARG
1	A	76	GLU
1	A	90	SER
1	A	91	VAL
1	A	97	VAL
1	A	102	ARG
1	A	156	LEU
1	A	188	ILE
1	A	194	ARG
1	A	200	LYS
1	A	203	ILE
1	A	215	LEU
1	B	3	VAL
1	B	14	LYS
1	B	15	THR
1	B	19	ARG
1	B	20	ILE
1	B	43	THR
1	B	57	VAL
1	B	62	LYS
1	B	65	VAL
1	B	71	SER
1	B	72	VAL
1	B	77	ASP

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Mol	Chain	Res	Type
1	B	91	VAL
1	B	102	ARG
1	B	128	ASP
1	B	129	LYS
1	B	152	LEU
1	B	153	VAL
1	B	156	LEU
1	B	182	VAL
1	B	187	THR
1	B	200	LYS
1	B	208	SER
1	C	2	VAL
1	C	3	VAL
1	C	4	ILE
1	C	15	THR
1	C	19	ARG
1	C	20	ILE
1	C	37	SER
1	C	57	VAL
1	C	61	ARG
1	C	72	VAL
1	C	75	VAL
1	C	76	GLU
1	C	102	ARG
1	C	112	ILE
1	C	156	LEU
1	C	166	LEU
1	C	182	VAL
1	C	187	THR
1	C	189	GLU
1	C	193	GLN
1	C	200	LYS
1	C	208	SER
1	C	213	LYS
1	C	214	LYS
1	C	215	LEU
1	D	3	VAL
1	D	4	ILE
1	D	19	ARG
1	D	21	LYS
1	D	24	ASP
1	D	34	ILE

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Mol	Chain	Res	Type
1	D	59	GLU
1	D	71	SER
1	D	72	VAL
1	D	76	GLU
1	D	91	VAL
1	D	102	ARG
1	D	108	LYS
1	D	150	LEU
1	D	153	VAL
1	D	156	LEU
1	D	180	VAL
1	D	187	THR
1	D	188	ILE
1	D	203	ILE
1	E	7	LYS
1	E	19	ARG
1	E	21	LYS
1	E	29	GLN
1	E	34	ILE
1	E	57	VAL
1	E	71	SER
1	E	76	GLU
1	E	92	GLU
1	E	101	ASP
1	E	102	ARG
1	E	108	LYS
1	E	156	LEU
1	E	181	ILE
1	E	188	ILE
1	E	195	GLU
1	E	200	LYS
1	E	213	LYS
1	E	215	LEU
1	F	3	VAL
1	F	12	GLU
1	F	20	ILE
1	F	34	ILE
1	F	61	ARG
1	F	62	LYS
1	F	75	VAL
1	F	76	GLU
1	F	90	SER

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Mol	Chain	Res	Type
1	F	101	ASP
1	F	102	ARG
1	F	121	ARG
1	F	174	GLU
1	F	188	ILE
1	F	189	GLU
1	F	200	LYS
1	F	208	SER
1	F	215	LEU
1	G	7	LYS
1	G	15	THR
1	G	21	LYS
1	G	43	THR
1	G	61	ARG
1	G	71	SER
1	G	75	VAL
1	G	107	GLU
1	G	108	LYS
1	G	135	ILE
1	G	152	LEU
1	G	156	LEU
1	G	157	LYS
1	G	193	GLN
1	G	213	LYS
1	H	12	GLU
1	H	21	LYS
1	H	34	ILE
1	H	43	THR
1	H	57	VAL
1	H	62	LYS
1	H	76	GLU
1	H	91	VAL
1	H	102	ARG
1	H	107	GLU
1	H	108	LYS
1	H	150	LEU
1	H	156	LEU
1	H	160	THR
1	H	172	ASN
1	H	186	SER
1	H	190	GLU
1	H	198	LYS

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Mol	Chain	Res	Type
1	H	202	GLU
1	H	215	LEU
1	I	12	GLU
1	I	19	ARG
1	I	71	SER
1	I	128	ASP
1	I	156	LEU
1	I	161	GLU
1	I	186	SER
1	I	187	THR
1	I	193	GLN
1	I	195	GLU
1	I	202	GLU
1	I	213	LYS
1	J	3	VAL
1	J	4	ILE
1	J	11	VAL
1	J	15	THR
1	J	19	ARG
1	J	20	ILE
1	J	24	ASP
1	J	57	VAL
1	J	72	VAL
1	J	91	VAL
1	J	107	GLU
1	J	109	LEU
1	J	114	SER
1	J	117	THR
1	J	118	ILE
1	J	119	THR
1	J	129	LYS
1	J	156	LEU
1	J	161	GLU
1	J	174	GLU
1	J	188	ILE
1	J	200	LYS
1	J	202	GLU
1	J	203	ILE
1	J	207	ASP
1	J	214	LYS
1	K	4	ILE
1	K	7	LYS

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Mol	Chain	Res	Type
1	K	13	VAL
1	K	16	THR
1	K	19	ARG
1	K	20	ILE
1	K	43	THR
1	K	57	VAL
1	K	61	ARG
1	K	83	GLU
1	K	90	SER
1	K	102	ARG
1	K	112	ILE
1	K	156	LEU
1	K	161	GLU
1	K	181	ILE
1	K	188	ILE
1	K	195	GLU
1	L	3	VAL
1	L	12	GLU
1	L	19	ARG
1	L	21	LYS
1	L	43	THR
1	L	47	THR
1	L	72	VAL
1	L	75	VAL
1	L	76	GLU
1	L	91	VAL
1	L	101	ASP
1	L	107	GLU
1	L	118	ILE
1	L	150	LEU
1	L	153	VAL
1	L	156	LEU
1	L	187	THR
1	L	188	ILE
1	L	215	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	74	GLN
1	B	38	HIS

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Mol	Chain	Res	Type
1	B	74	GLN
1	C	74	GLN
1	C	88	ASN
1	D	17	HIS
1	D	74	GLN
1	E	88	ASN
1	F	74	GLN
1	H	17	HIS
1	H	74	GLN
1	I	74	GLN
1	I	88	ASN
1	I	193	GLN
1	J	17	HIS
1	J	74	GLN
1	K	74	GLN
1	K	193	GLN
1	L	88	ASN
1	L	172	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	OCS	E	46	1	6,8,9	2.61	3 (50%)	7,11,13	3.12	2 (28%)
1	OCS	G	46	1	6,8,9	2.23	1 (16%)	7,11,13	2.11	3 (42%)
1	OCS	L	46	1	6,8,9	3.39	1 (16%)	7,11,13	3.69	4 (57%)
1	OCS	C	46	1	6,8,9	3.63	3 (50%)	7,11,13	2.75	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OCS	D	46	1	6,8,9	1.97	1 (16%)	7,11,13	3.83	6 (85%)
1	OCS	I	46	1	6,8,9	3.29	2 (33%)	7,11,13	1.68	2 (28%)
1	OCS	J	46	1	6,8,9	1.98	1 (16%)	7,11,13	3.90	6 (85%)
1	OCS	H	46	1	6,8,9	1.84	1 (16%)	7,11,13	2.12	2 (28%)
1	OCS	K	46	1	6,8,9	1.80	1 (16%)	7,11,13	1.85	3 (42%)
1	OCS	B	46	1	6,8,9	2.21	3 (50%)	7,11,13	7.95	6 (85%)
1	OCS	F	46	1	6,8,9	2.83	1 (16%)	7,11,13	2.96	4 (57%)
1	OCS	A	46	1	6,8,9	3.24	3 (50%)	7,11,13	3.34	6 (85%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OCS	E	46	1	-	0/4/7/9	-
1	OCS	G	46	1	-	0/4/7/9	-
1	OCS	L	46	1	-	0/4/7/9	-
1	OCS	C	46	1	-	0/4/7/9	-
1	OCS	D	46	1	-	0/4/7/9	-
1	OCS	I	46	1	-	0/4/7/9	-
1	OCS	J	46	1	-	0/4/7/9	-
1	OCS	H	46	1	-	0/4/7/9	-
1	OCS	K	46	1	-	0/4/7/9	-
1	OCS	B	46	1	-	1/4/7/9	-
1	OCS	F	46	1	-	0/4/7/9	-
1	OCS	A	46	1	-	0/4/7/9	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	OCS	OD3-SG	8.01	1.67	1.45
1	L	46	OCS	OD1-SG	7.95	1.67	1.45
1	I	46	OCS	OD1-SG	7.32	1.65	1.45
1	A	46	OCS	OD3-SG	7.05	1.65	1.45
1	F	46	OCS	OD3-SG	6.33	1.63	1.45
1	G	46	OCS	OD3-SG	5.05	1.59	1.45
1	E	46	OCS	OD2-SG	4.47	1.64	1.47
1	D	46	OCS	OD2-SG	3.84	1.61	1.47
1	J	46	OCS	OD2-SG	3.82	1.61	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	46	OCS	OD2-SG	3.64	1.60	1.47
1	H	46	OCS	OD2-SG	3.63	1.60	1.47
1	E	46	OCS	CB-CA	3.21	1.55	1.53
1	B	46	OCS	OD2-SG	3.13	1.58	1.47
1	B	46	OCS	OD1-SG	-3.06	1.36	1.45
1	E	46	OCS	OD3-SG	-2.68	1.37	1.45
1	C	46	OCS	CB-CA	-2.54	1.51	1.53
1	I	46	OCS	OD2-SG	-2.40	1.38	1.47
1	B	46	OCS	CB-CA	-2.29	1.52	1.53
1	C	46	OCS	OD2-SG	-2.27	1.38	1.47
1	A	46	OCS	OD2-SG	-2.09	1.39	1.47
1	A	46	OCS	OD1-SG	-2.04	1.39	1.45

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	OCS	OD1-SG-CB	14.62	128.58	106.76
1	B	46	OCS	OD2-SG-OD3	-9.46	87.74	111.40
1	B	46	OCS	OD3-SG-OD1	-8.13	87.39	113.82
1	E	46	OCS	OD3-SG-CB	7.03	117.26	106.76
1	D	46	OCS	OD2-SG-CB	6.75	119.00	105.97
1	J	46	OCS	OD3-SG-CB	6.71	116.77	106.76
1	L	46	OCS	OD3-SG-CB	6.41	116.32	106.76
1	J	46	OCS	OD1-SG-CB	6.06	115.81	106.76
1	B	46	OCS	OD2-SG-CB	6.05	117.66	105.97
1	F	46	OCS	OD3-SG-CB	5.81	115.42	106.76
1	A	46	OCS	OD1-SG-CB	5.58	115.09	106.76
1	B	46	OCS	OD3-SG-CB	-5.57	98.45	106.76
1	L	46	OCS	OD2-SG-CB	5.09	115.80	105.97
1	C	46	OCS	OD2-SG-CB	5.04	115.71	105.97
1	D	46	OCS	OD3-SG-CB	4.65	113.69	106.76
1	G	46	OCS	OD1-SG-CB	4.31	113.19	106.76
1	L	46	OCS	OD3-SG-OD1	-4.30	99.85	113.82
1	A	46	OCS	OD2-SG-OD3	-4.12	101.10	111.40
1	H	46	OCS	OD2-SG-CB	4.02	113.74	105.97
1	A	46	OCS	OD2-SG-CB	3.91	113.52	105.97
1	C	46	OCS	CA-CB-SG	-3.68	108.14	113.61
1	I	46	OCS	OD1-SG-CB	3.66	112.22	106.76
1	F	46	OCS	OD2-SG-OD3	-3.56	102.50	111.40
1	D	46	OCS	OD2-SG-OD1	-3.38	102.95	111.40
1	C	46	OCS	OD2-SG-OD1	-3.28	103.19	111.40
1	E	46	OCS	OD3-SG-OD1	-2.94	104.25	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	46	OCS	OD3-SG-OD1	-2.90	104.40	113.82
1	J	46	OCS	OD2-SG-OD3	-2.85	104.28	111.40
1	D	46	OCS	CA-CB-SG	-2.81	109.43	113.61
1	D	46	OCS	OD3-SG-OD1	-2.67	105.15	113.82
1	F	46	OCS	OD1-SG-CB	2.66	110.73	106.76
1	K	46	OCS	OD3-SG-CB	2.57	110.60	106.76
1	K	46	OCS	OD2-SG-CB	2.52	110.83	105.97
1	G	46	OCS	OD3-SG-CB	2.51	110.51	106.76
1	J	46	OCS	OD2-SG-OD1	-2.47	105.23	111.40
1	D	46	OCS	OD2-SG-OD3	-2.42	105.34	111.40
1	J	46	OCS	OD3-SG-OD1	-2.34	106.20	113.82
1	L	46	OCS	OD2-SG-OD3	-2.34	105.55	111.40
1	B	46	OCS	CA-CB-SG	2.32	117.05	113.61
1	A	46	OCS	CA-CB-SG	2.27	116.98	113.61
1	H	46	OCS	CA-CB-SG	-2.26	110.25	113.61
1	I	46	OCS	OD3-SG-OD1	-2.26	106.48	113.82
1	J	46	OCS	CA-CB-SG	2.15	116.81	113.61
1	A	46	OCS	OD3-SG-OD1	-2.11	106.95	113.82
1	A	46	OCS	OD3-SG-CB	2.06	109.83	106.76
1	F	46	OCS	OD2-SG-CB	2.03	109.90	105.97
1	G	46	OCS	OD2-SG-OD1	-2.00	106.39	111.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	46	OCS	CA-CB-SG-OD1

There are no ring outliers.

12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	46	OCS	2	0
1	G	46	OCS	2	0
1	L	46	OCS	1	0
1	C	46	OCS	2	0
1	D	46	OCS	1	0
1	I	46	OCS	1	0
1	J	46	OCS	1	0
1	H	46	OCS	2	0
1	K	46	OCS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	46	OCS	3	0
1	F	46	OCS	4	0
1	A	46	OCS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	213/216 (98%)	0.34	20 (9%) 14 13	11, 23, 84, 100	0
1	B	213/216 (98%)	0.65	27 (12%) 8 7	13, 25, 111, 125	0
1	C	213/216 (98%)	0.68	22 (10%) 12 11	15, 26, 80, 112	0
1	D	213/216 (98%)	0.71	25 (11%) 9 9	15, 27, 109, 146	0
1	E	213/216 (98%)	0.74	26 (12%) 8 8	15, 25, 105, 141	0
1	F	213/216 (98%)	0.74	28 (13%) 7 6	14, 25, 119, 165	0
1	G	213/216 (98%)	0.42	18 (8%) 16 15	14, 24, 71, 93	0
1	H	213/216 (98%)	0.61	30 (14%) 6 5	14, 25, 84, 108	0
1	I	213/216 (98%)	0.69	26 (12%) 8 8	13, 25, 97, 149	0
1	J	213/216 (98%)	0.62	26 (12%) 8 8	13, 24, 109, 142	0
1	K	213/216 (98%)	0.78	30 (14%) 6 5	14, 27, 109, 132	0
1	L	213/216 (98%)	0.77	28 (13%) 7 6	14, 28, 108, 129	0
All	All	2556/2592 (98%)	0.65	306 (11%) 9 8	11, 25, 100, 165	0

All (306) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	185	ALA	9.2
1	F	188	ILE	8.1
1	K	188	ILE	8.0
1	E	188	ILE	8.0
1	J	188	ILE	7.9
1	F	185	ALA	7.7
1	I	188	ILE	7.5
1	A	185	ALA	7.1
1	J	185	ALA	6.8
1	B	188	ILE	6.8
1	D	188	ILE	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	200	LYS	6.7
1	B	185	ALA	6.7
1	E	192	LYS	6.7
1	D	193	GLN	6.5
1	F	202	GLU	6.5
1	I	200	LYS	6.4
1	D	200	LYS	6.3
1	E	185	ALA	6.2
1	F	186	SER	6.1
1	I	185	ALA	6.1
1	G	188	ILE	6.0
1	I	186	SER	6.0
1	F	187	THR	6.0
1	D	184	PRO	6.0
1	E	186	SER	5.9
1	K	199	ALA	5.7
1	J	200	LYS	5.7
1	B	184	PRO	5.7
1	F	184	PRO	5.7
1	J	187	THR	5.7
1	C	188	ILE	5.6
1	E	201	GLY	5.6
1	C	185	ALA	5.6
1	K	185	ALA	5.6
1	K	187	THR	5.5
1	E	187	THR	5.5
1	K	200	LYS	5.4
1	E	197	ALA	5.4
1	H	194	ARG	5.3
1	E	200	LYS	5.3
1	J	199	ALA	5.3
1	I	187	THR	5.2
1	L	197	ALA	5.2
1	F	200	LYS	5.2
1	D	202	GLU	5.2
1	J	193	GLN	5.2
1	E	194	ARG	5.1
1	D	185	ALA	5.1
1	E	199	ALA	5.1
1	F	197	ALA	5.1
1	A	188	ILE	5.0
1	H	192	LYS	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	201	GLY	5.0
1	H	188	ILE	5.0
1	A	200	LYS	5.0
1	L	2	VAL	4.9
1	D	187	THR	4.9
1	F	201	GLY	4.9
1	A	203	ILE	4.9
1	C	187	THR	4.9
1	L	188	ILE	4.7
1	J	202	GLU	4.7
1	A	187	THR	4.6
1	K	2	VAL	4.6
1	L	194	ARG	4.5
1	D	199	ALA	4.5
1	B	194	ARG	4.5
1	K	184	PRO	4.4
1	J	196	GLU	4.4
1	I	194	ARG	4.4
1	C	2	VAL	4.4
1	B	197	ALA	4.4
1	D	198	LYS	4.4
1	I	203	ILE	4.4
1	H	185	ALA	4.3
1	L	198	LYS	4.3
1	A	186	SER	4.3
1	J	186	SER	4.3
1	C	199	ALA	4.3
1	I	201	GLY	4.3
1	B	195	GLU	4.3
1	D	194	ARG	4.3
1	G	192	LYS	4.3
1	L	191	LYS	4.2
1	L	200	LYS	4.2
1	J	194	ARG	4.2
1	D	192	LYS	4.2
1	B	203	ILE	4.1
1	F	194	ARG	4.1
1	E	202	GLU	4.1
1	H	199	ALA	4.1
1	L	199	ALA	4.1
1	E	191	LYS	4.1
1	H	2	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	187	THR	4.0
1	K	192	LYS	4.0
1	C	186	SER	4.0
1	B	192	LYS	4.0
1	D	197	ALA	4.0
1	F	192	LYS	3.9
1	F	198	LYS	3.9
1	B	2	VAL	3.9
1	K	189	GLU	3.9
1	H	107	GLU	3.9
1	J	189	GLU	3.9
1	K	198	LYS	3.9
1	L	202	GLU	3.9
1	B	198	LYS	3.9
1	I	19	ARG	3.8
1	I	199	ALA	3.8
1	J	198	LYS	3.8
1	J	2	VAL	3.8
1	D	196	GLU	3.8
1	K	186	SER	3.8
1	J	201	GLY	3.8
1	D	195	GLU	3.7
1	B	193	GLN	3.7
1	H	197	ALA	3.7
1	I	202	GLU	3.7
1	F	118	ILE	3.7
1	D	215	LEU	3.7
1	K	106	ALA	3.7
1	J	192	LYS	3.7
1	C	189	GLU	3.6
1	E	184	PRO	3.6
1	B	115	GLY	3.6
1	G	185	ALA	3.6
1	D	186	SER	3.6
1	K	201	GLY	3.6
1	H	198	LYS	3.6
1	H	200	LYS	3.6
1	H	187	THR	3.5
1	C	182	VAL	3.5
1	K	196	GLU	3.5
1	H	62	LYS	3.5
1	D	201	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	J	203	ILE	3.5
1	F	189	GLU	3.5
1	C	193	GLN	3.5
1	K	193	GLN	3.5
1	F	199	ALA	3.4
1	I	193	GLN	3.4
1	D	191	LYS	3.4
1	B	186	SER	3.4
1	B	202	GLU	3.4
1	E	195	GLU	3.4
1	H	215	LEU	3.4
1	E	198	LYS	3.4
1	H	114	SER	3.4
1	A	184	PRO	3.4
1	C	192	LYS	3.4
1	L	201	GLY	3.4
1	B	199	ALA	3.3
1	C	200	LYS	3.3
1	E	115	GLY	3.3
1	L	187	THR	3.3
1	C	19	ARG	3.3
1	K	197	ALA	3.2
1	H	184	PRO	3.2
1	F	102	ARG	3.2
1	I	192	LYS	3.2
1	L	189	GLU	3.2
1	K	194	ARG	3.2
1	I	195	GLU	3.2
1	I	184	PRO	3.2
1	L	215	LEU	3.2
1	H	101	ASP	3.1
1	H	182	VAL	3.1
1	L	193	GLN	3.1
1	E	189	GLU	3.1
1	F	2	VAL	3.1
1	E	193	GLN	3.1
1	F	193	GLN	3.1
1	J	195	GLU	3.1
1	G	191	LYS	3.1
1	G	199	ALA	3.1
1	I	191	LYS	3.1
1	K	203	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	186	SER	3.0
1	G	197	ALA	3.0
1	J	184	PRO	3.0
1	L	190	GLU	3.0
1	D	183	PRO	3.0
1	H	113	PRO	3.0
1	C	190	GLU	3.0
1	H	118	ILE	3.0
1	B	187	THR	3.0
1	A	195	GLU	3.0
1	B	196	GLU	3.0
1	J	118	ILE	3.0
1	B	28	LYS	3.0
1	H	201	GLY	3.0
1	J	115	GLY	3.0
1	C	202	GLU	3.0
1	I	198	LYS	2.9
1	E	102	ARG	2.9
1	C	203	ILE	2.9
1	H	115	GLY	2.9
1	H	172	ASN	2.9
1	A	194	ARG	2.9
1	F	191	LYS	2.9
1	L	192	LYS	2.9
1	E	116	ALA	2.9
1	I	2	VAL	2.9
1	H	186	SER	2.9
1	C	62	LYS	2.8
1	E	196	GLU	2.8
1	H	161	GLU	2.8
1	K	190	GLU	2.8
1	H	191	LYS	2.8
1	C	184	PRO	2.8
1	F	195	GLU	2.8
1	K	195	GLU	2.8
1	J	197	ALA	2.8
1	B	21	LYS	2.7
1	K	28	LYS	2.7
1	A	197	ALA	2.7
1	L	118	ILE	2.7
1	J	191	LYS	2.7
1	K	191	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	19	ARG	2.7
1	B	191	LYS	2.6
1	D	214	LYS	2.6
1	G	189	GLU	2.6
1	L	4	ILE	2.6
1	B	215	LEU	2.6
1	K	202	GLU	2.6
1	D	19	ARG	2.6
1	L	184	PRO	2.6
1	A	117	THR	2.5
1	I	214	LYS	2.5
1	F	106	ALA	2.5
1	E	114	SER	2.5
1	A	161	GLU	2.5
1	I	102	ARG	2.5
1	J	19	ARG	2.5
1	K	117	THR	2.5
1	I	108	LYS	2.5
1	L	196	GLU	2.4
1	G	186	SER	2.4
1	G	194	ARG	2.4
1	D	190	GLU	2.4
1	A	189	GLU	2.4
1	F	19	ARG	2.4
1	A	193	GLN	2.4
1	D	106	ALA	2.3
1	J	102	ARG	2.3
1	J	215	LEU	2.3
1	A	202	GLU	2.3
1	I	196	GLU	2.3
1	C	108	LYS	2.3
1	G	184	PRO	2.3
1	A	201	GLY	2.3
1	H	195	GLU	2.3
1	C	28	LYS	2.3
1	G	115	GLY	2.3
1	E	117	THR	2.3
1	L	195	GLU	2.3
1	G	215	LEU	2.3
1	J	101	ASP	2.3
1	I	161	GLU	2.3
1	A	19	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	102	ARG	2.2
1	G	19	ARG	2.2
1	F	190	GLU	2.2
1	F	196	GLU	2.2
1	H	189	GLU	2.2
1	I	189	GLU	2.2
1	C	101	ASP	2.2
1	L	115	GLY	2.2
1	D	102	ARG	2.2
1	F	108	LYS	2.2
1	L	102	ARG	2.1
1	A	2	VAL	2.1
1	B	101	ASP	2.1
1	E	161	GLU	2.1
1	L	205	CYS	2.1
1	G	102	ARG	2.1
1	B	12	GLU	2.1
1	H	193	GLN	2.1
1	B	189	GLU	2.1
1	H	12	GLU	2.1
1	H	190	GLU	2.1
1	K	101	ASP	2.1
1	K	118	ILE	2.1
1	K	215	LEU	2.1
1	G	2	VAL	2.1
1	K	11	VAL	2.1
1	C	5	GLY	2.1
1	G	117	THR	2.1
1	L	117	THR	2.1
1	B	190	GLU	2.1
1	F	204	GLU	2.1
1	F	183	PRO	2.1
1	A	192	LYS	2.0
1	L	21	LYS	2.0
1	I	116	ALA	2.0
1	D	105	LEU	2.0
1	G	112	ILE	2.0
1	C	183	PRO	2.0
1	E	2	VAL	2.0
1	E	108	LYS	2.0
1	I	114	SER	2.0
1	F	116	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	K	102	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	OCS	C	46	9/10	0.95	0.13	19,21,36,38	0
1	OCS	B	46	9/10	0.96	0.09	20,21,33,34	0
1	OCS	F	46	9/10	0.96	0.09	18,19,39,48	0
1	OCS	H	46	9/10	0.96	0.09	19,23,43,45	0
1	OCS	I	46	9/10	0.96	0.10	20,24,39,39	0
1	OCS	L	46	9/10	0.96	0.08	17,19,35,39	0
1	OCS	G	46	9/10	0.97	0.08	20,22,40,42	0
1	OCS	D	46	9/10	0.97	0.09	15,16,31,38	0
1	OCS	E	46	9/10	0.97	0.09	19,19,35,40	0
1	OCS	K	46	9/10	0.97	0.08	20,22,38,42	0
1	OCS	A	46	9/10	0.97	0.08	17,21,37,40	0
1	OCS	J	46	9/10	0.98	0.06	14,18,41,41	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.