



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:41 am BST

PDB ID : 5XBQ
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

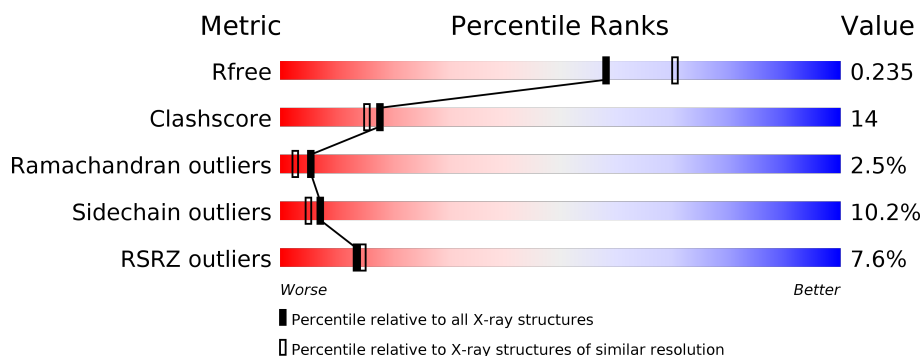
1 Overall quality at a glance i

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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (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 on 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	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>• •</div> </div> </div>
1	B	216	<div> <div>9%</div> <div> <div></div> <div>61%</div> <div>31%</div> <div>7%</div> <div>• •</div> </div> </div>
1	C	216	<div> <div>6%</div> <div> <div></div> <div>58%</div> <div>30%</div> <div>11%</div> <div>•</div> </div> </div>
1	D	216	<div> <div>10%</div> <div> <div></div> <div>66%</div> <div>26%</div> <div>7%</div> <div>•</div> </div> </div>
1	E	216	<div> <div>8%</div> <div> <div></div> <div>67%</div> <div>26%</div> <div>6%</div> <div>•</div> </div> </div>
1	F	216	<div> <div>9%</div> <div> <div></div> <div>65%</div> <div>31%</div> <div>• •</div> </div> </div>

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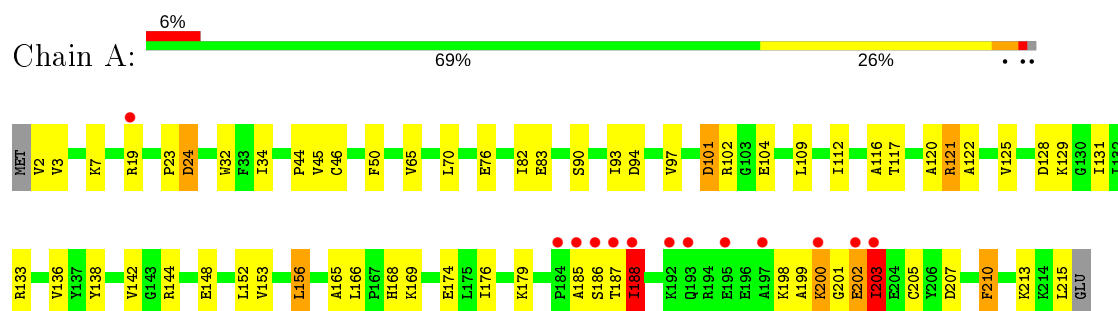
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	11	Total 11	O 11	0	0
2	I	18	Total 18	O 18	0	0
2	J	11	Total 11	O 11	0	0
2	K	9	Total 9	O 9	0	0
2	L	9	Total 9	O 9	0	0

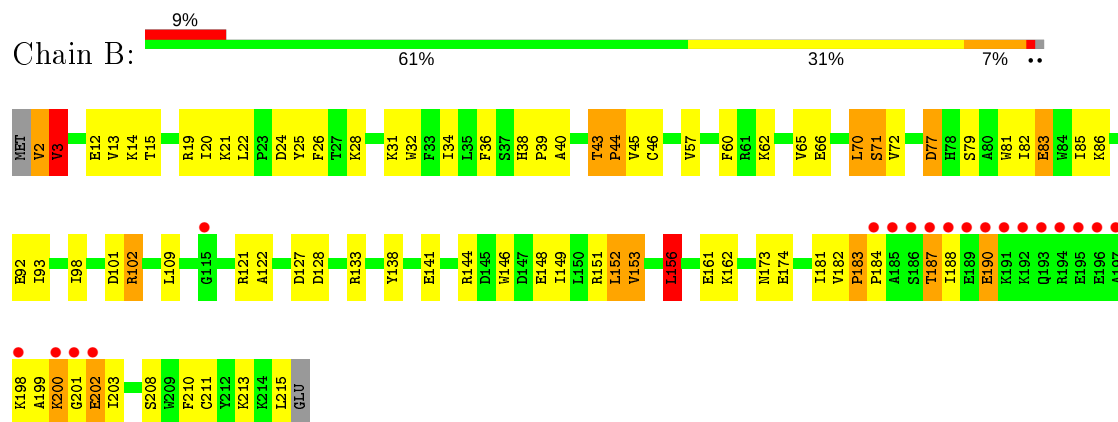
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

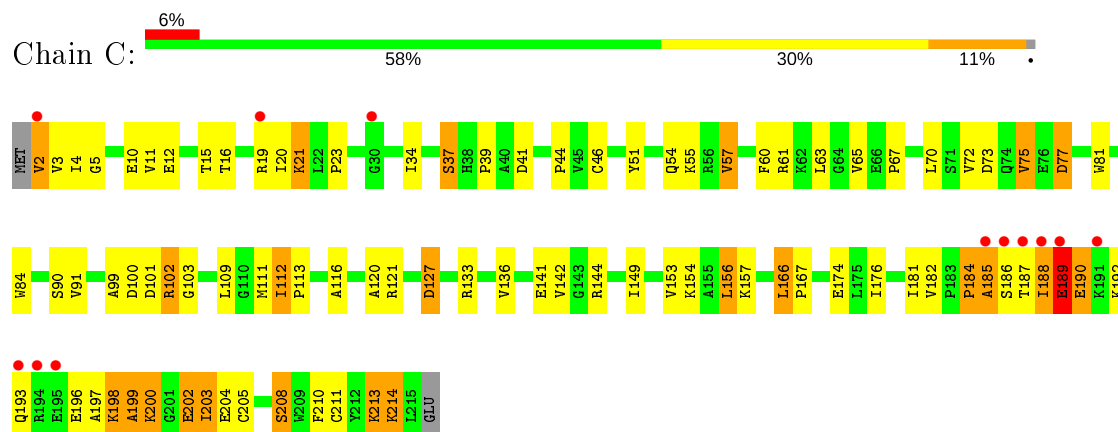
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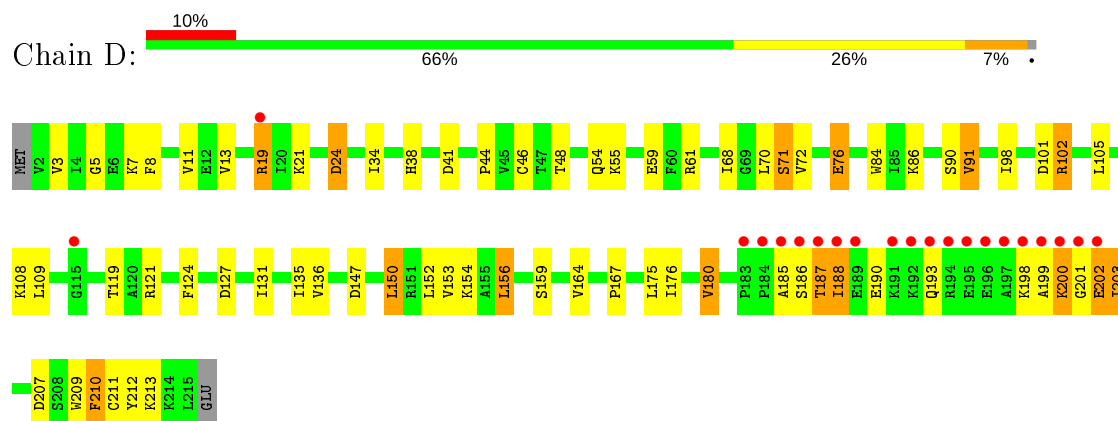
• Molecule 1: Peroxiredoxin



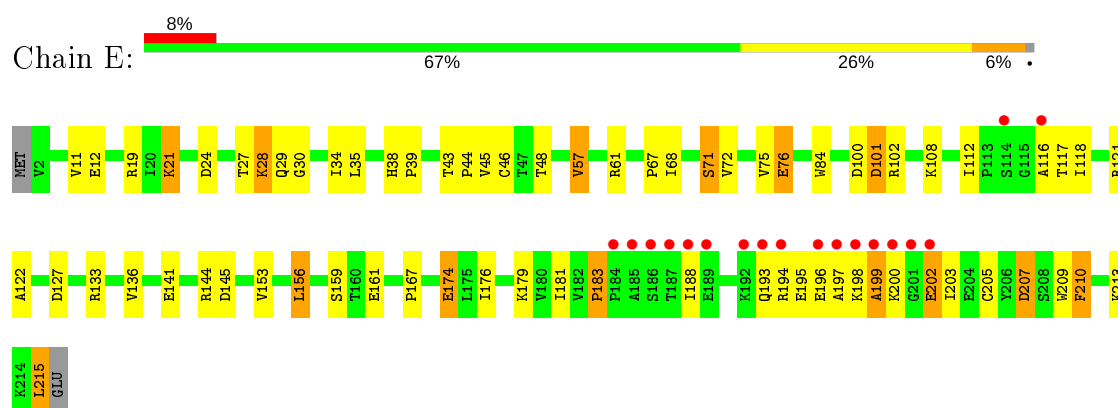
• Molecule 1: Peroxiredoxin



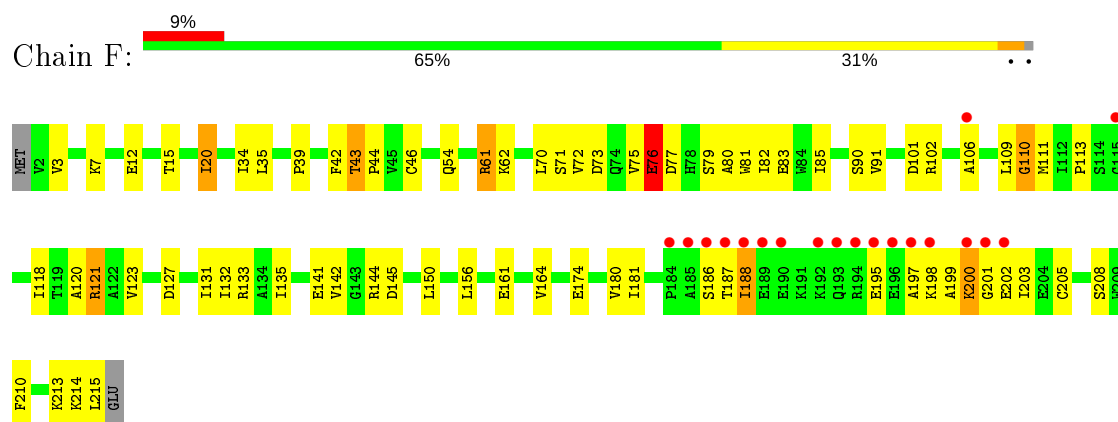
- Molecule 1: Peroxiredoxin



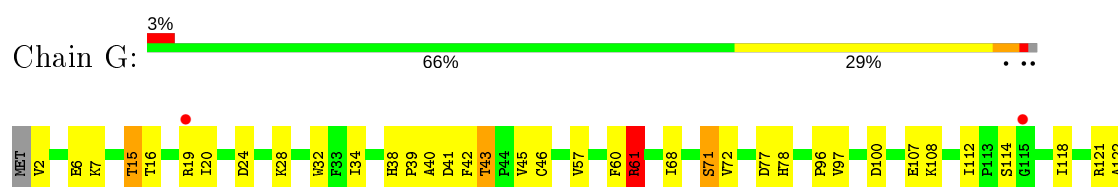
- Molecule 1: Peroxiredoxin



- Molecule 1: Peroxiredoxin

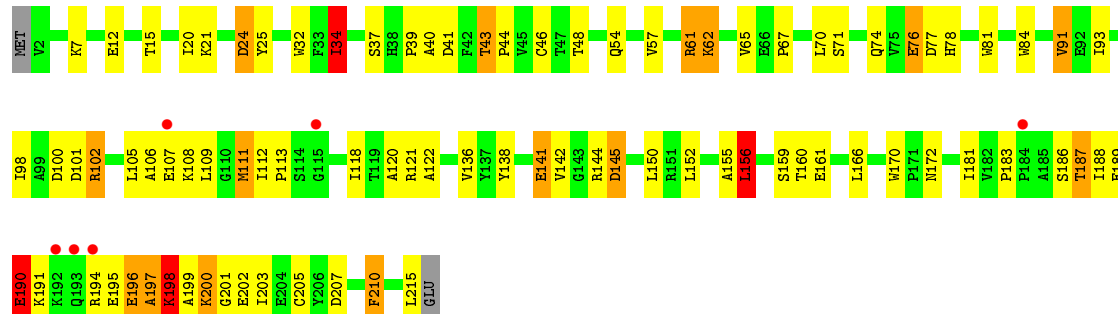


- Molecule 1: Peroxiredoxin

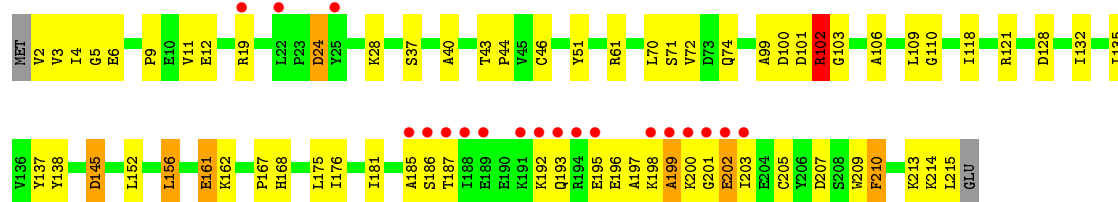




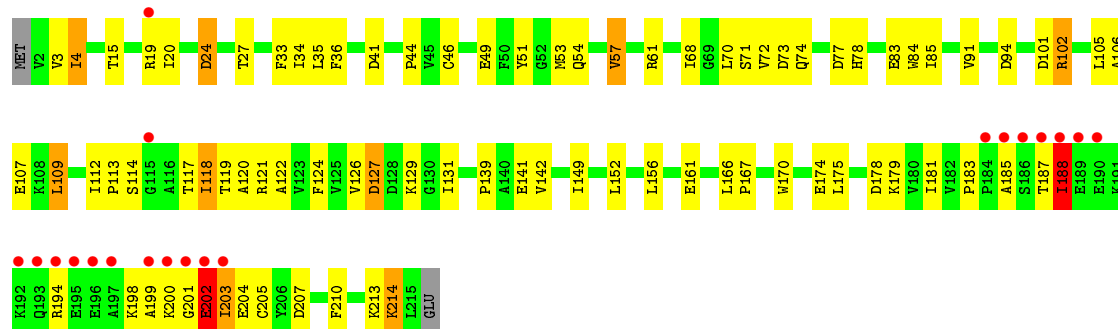
• Molecule 1: Peroxiredoxin



• Molecule 1: Peroxiredoxin

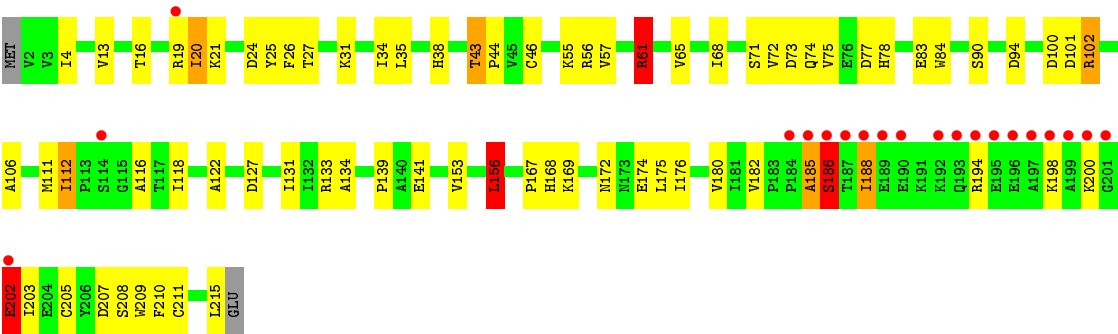


• Molecule 1: Peroxiredoxin

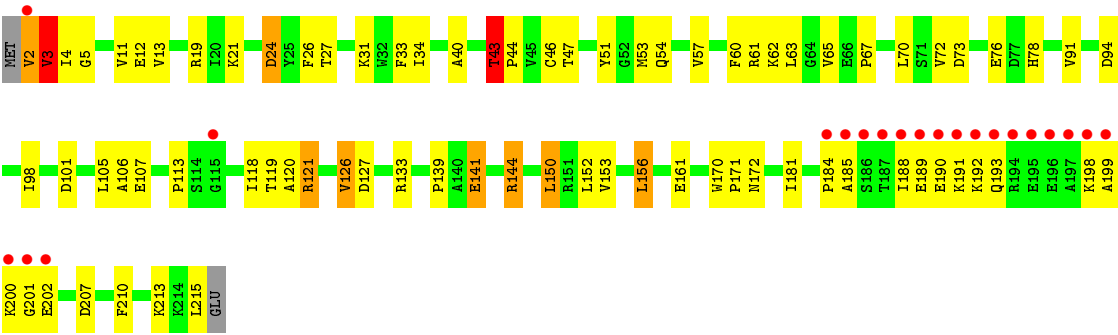


• Molecule 1: Peroxiredoxin





● 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	137.58 Å 98.60 Å 137.57 Å 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) 99.7 (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 2.24 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.193 , 0.232 0.198 , 0.235	Depositor DCC
R_{free} test set	7632 reflections (5.04%)	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)	0.36 , 49.7	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 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	1.00	1/1758 (0.1%)	1.06	4/2380 (0.2%)
1	B	1.01	3/1758 (0.2%)	1.13	9/2380 (0.4%)
1	C	1.02	2/1758 (0.1%)	1.13	8/2380 (0.3%)
1	D	0.94	1/1758 (0.1%)	1.05	7/2380 (0.3%)
1	E	1.05	3/1758 (0.2%)	1.13	9/2380 (0.4%)
1	F	0.97	1/1758 (0.1%)	1.09	9/2380 (0.4%)
1	G	1.05	3/1758 (0.2%)	1.07	5/2380 (0.2%)
1	H	0.98	2/1758 (0.1%)	1.16	10/2380 (0.4%)
1	I	0.97	0/1758	1.07	4/2380 (0.2%)
1	J	0.99	0/1758	1.11	5/2380 (0.2%)
1	K	0.98	1/1758 (0.1%)	1.06	5/2380 (0.2%)
1	L	0.98	3/1758 (0.2%)	1.01	4/2380 (0.2%)
All	All	1.00	20/21096 (0.1%)	1.09	79/28560 (0.3%)

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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	90	SER	CB-OG	-10.62	1.28	1.42
1	E	174	GLU	CD-OE2	-8.69	1.16	1.25
1	G	141	GLU	CD-OE2	-7.30	1.17	1.25
1	H	141	GLU	CD-OE2	-6.83	1.18	1.25
1	E	183	PRO	C-O	-6.53	1.10	1.23
1	E	43	THR	CB-CG2	-6.40	1.31	1.52
1	G	138	TYR	CE1-CZ	-6.07	1.30	1.38
1	K	172	ASN	CG-ND2	-5.87	1.18	1.32
1	G	148	GLU	CD-OE1	-5.59	1.19	1.25
1	L	43	THR	CB-CG2	-5.53	1.34	1.52
1	B	83	GLU	CD-OE2	5.37	1.31	1.25
1	A	148	GLU	CD-OE1	-5.36	1.19	1.25
1	L	144	ARG	CZ-NH1	-5.36	1.26	1.33
1	D	84	TRP	CB-CG	-5.35	1.40	1.50
1	L	141	GLU	CD-OE1	-5.20	1.20	1.25
1	F	43	THR	CB-CG2	-5.15	1.35	1.52
1	C	81	TRP	CB-CG	-5.11	1.41	1.50
1	B	148	GLU	CD-OE1	-5.03	1.20	1.25
1	H	61	ARG	CD-NE	-5.02	1.38	1.46
1	B	79	SER	CB-OG	5.01	1.48	1.42

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	61	ARG	NE-CZ-NH1	-13.71	113.44	120.30
1	E	61	ARG	NE-CZ-NH2	13.05	126.82	120.30
1	E	61	ARG	NE-CZ-NH1	-12.55	114.02	120.30
1	J	61	ARG	NE-CZ-NH1	-9.84	115.38	120.30
1	K	61	ARG	NE-CZ-NH2	9.84	125.22	120.30
1	G	127	ASP	CB-CG-OD1	9.64	126.98	118.30
1	B	127	ASP	CB-CG-OD1	9.17	126.55	118.30
1	H	61	ARG	NE-CZ-NH2	9.10	124.85	120.30
1	D	61	ARG	NE-CZ-NH1	-9.09	115.76	120.30
1	H	77	ASP	CB-CG-OD1	-9.08	110.13	118.30
1	K	61	ARG	NE-CZ-NH1	-9.05	115.77	120.30
1	G	61	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	B	102	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	F	144	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	F	61	ARG	NE-CZ-NH2	8.00	124.30	120.30
1	H	145	ASP	CB-CG-OD2	7.80	125.32	118.30
1	D	76	GLU	CA-CB-CG	7.75	130.44	113.40
1	C	77	ASP	CB-CG-OD1	-7.66	111.41	118.30
1	C	90	SER	CB-CA-C	7.57	124.48	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ASP	CB-CG-OD2	7.49	125.04	118.30
1	D	61	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	E	215	LEU	CA-CB-CG	7.39	132.29	115.30
1	L	121	ARG	NE-CZ-NH2	7.27	123.94	120.30
1	I	102	ARG	NE-CZ-NH2	7.19	123.90	120.30
1	L	121	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	E	61	ARG	CD-NE-CZ	6.99	133.38	123.60
1	C	101	ASP	CB-CG-OD2	6.98	124.58	118.30
1	I	102	ARG	NE-CZ-NH1	-6.97	116.81	120.30
1	F	123	VAL	CB-CA-C	-6.86	98.37	111.40
1	E	127	ASP	CB-CG-OD1	6.85	124.47	118.30
1	A	128	ASP	CB-CG-OD2	6.71	124.34	118.30
1	H	111	MET	CG-SD-CE	6.56	110.70	100.20
1	C	41	ASP	CB-CG-OD2	6.54	124.18	118.30
1	K	156	LEU	CA-CB-CG	6.47	130.18	115.30
1	D	127	ASP	CB-CG-OD1	6.29	123.96	118.30
1	B	70	LEU	CA-CB-CG	-6.28	100.86	115.30
1	F	77	ASP	CB-CG-OD1	-6.26	112.67	118.30
1	H	34	ILE	CB-CA-C	-6.25	99.10	111.60
1	E	133	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	F	61	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	I	61	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	H	77	ASP	CB-CG-OD2	6.17	123.85	118.30
1	H	141	GLU	OE1-CD-OE2	-6.13	115.94	123.30
1	G	152	LEU	CA-CB-CG	6.08	129.29	115.30
1	D	147	ASP	CB-CG-OD1	6.04	123.73	118.30
1	F	127	ASP	CB-CG-OD1	5.97	123.68	118.30
1	D	127	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	E	207	ASP	CB-CG-OD2	5.87	123.59	118.30
1	J	61	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	B	102	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	B	101	ASP	CB-CG-OD2	5.77	123.50	118.30
1	A	94	ASP	CB-CG-OD1	5.77	123.49	118.30
1	B	70	LEU	CB-CG-CD2	5.75	120.78	111.00
1	B	127	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	I	145	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	C	156	LEU	CA-CB-CG	5.60	128.19	115.30
1	F	76	GLU	CA-CB-CG	5.59	125.70	113.40
1	G	127	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	A	121	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	B	156	LEU	CA-CB-CG	5.55	128.06	115.30
1	C	174	GLU	OE1-CD-OE2	-5.55	116.64	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	34	ILE	CB-CA-C	-5.50	100.59	111.60
1	J	178	ASP	CB-CG-OD2	5.48	123.23	118.30
1	L	73	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	H	156	LEU	CB-CG-CD1	5.36	120.12	111.00
1	F	214	LYS	CD-CE-NZ	-5.33	99.45	111.70
1	L	126	VAL	CB-CA-C	-5.26	101.41	111.40
1	B	151	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	41	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	J	127	ASP	CB-CG-OD1	5.20	122.98	118.30
1	J	94	ASP	CB-CG-OD1	5.18	122.96	118.30
1	D	41	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	K	102	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	E	215	LEU	CB-CG-CD2	5.14	119.74	111.00
1	C	77	ASP	CB-CG-OD2	5.12	122.91	118.30
1	G	100	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	K	156	LEU	CB-CG-CD1	5.09	119.66	111.00
1	H	144	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	E	61	ARG	CG-CD-NE	-5.06	101.18	111.80

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	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1725	0	1728	50	0
1	C	1725	0	1727	70	0
1	D	1725	0	1728	50	0
1	E	1725	0	1728	43	0
1	F	1725	0	1727	51	0
1	G	1725	0	1727	44	0
1	H	1725	0	1728	69	0
1	I	1725	0	1727	53	0
1	J	1725	0	1728	60	0
1	K	1725	0	1728	52	0
1	L	1725	0	1727	47	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	565	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 14.

All (565) 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: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:F:109:LEU:HD12	1:F:111:MET:HE3	1.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:102:ARG:NH2	1:K:102:ARG:O	2.11	0.84
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:O	1:E:72:VAL:HG22	1.79	0.81
1:H:54:GLN:O	1:H:57:VAL:HG12	1.79	0.81
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:B:77:ASP:OD1	1:C:77:ASP:CG	2.21	0.79
1:H:74:GLN:HE22	1:I:118:ILE:HG21	1.47	0.79
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: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: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:109:LEU:HD12	1:H:111:MET:HE2	1.70	0.73
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: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:D:201:GLY:O	1:D:202:GLU:C	2.29	0.70
1:H:109:LEU:HD12	1:H:111:MET:CE	2.21	0.70
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:55:LYS:NZ	2:D:301:HOH:O	2.27	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: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:C:188:ILE:HA	1:C:189:GLU:C	2.17	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: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:N	1:A:166:LEU:HD22	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: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:J:85:ILE:O	1:J:85:ILE:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:CE3	1:C:84:TRP:O	2.54	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:N	1:E:174:GLU:OE1	2.29	0.60
1:J:101:ASP:O	1:J:102:ARG:HB2	2.01	0.60
1:I:197:ALA:C	1:I:199:ALA:HB3	2.22	0.59
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: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:D:70:LEU:C	1:D:70:LEU:HD23	2.23	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:J:105:LEU:HG	1:J:109:LEU:HD21	1.84	0.58
1:I:3:VAL:HG11	1:J:112:ILE:O	2.03	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:70:LEU:HD21	1:C:100:ASP:HB2	1.87	0.56
1:C:39:PRO:HD2	1:C:46:OCS:OD2	2.05	0.56
1:C:2:VAL:HG22	1:C:109:LEU:HA	1.88	0.56
1:F:132:ILE:HG21	1:F:135:ILE:HD11	1.87	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:B:198:LYS:HA	1:B:199:ALA:C	2.27	0.55
1:B:20:ILE:HD11	1:B:22:LEU:HD21	1.88	0.55
1:A:83:GLU:OE2	1:K:207:ASP:OD1	2.24	0.55
1:J:70:LEU:HD23	1:J:71:SER:N	2.21	0.55
1:L:189:GLU:C	1:L:191:LYS:H	2.10	0.55
1:E:145:ASP:C	1:E:145:ASP:OD2	2.43	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: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:H:199:ALA:O	1:H:200:LYS:C	2.46	0.55
1:I:161:GLU:HG3	1:I:162:LYS:HG2	1.88	0.55
1:K:100:ASP:O	1:K:101:ASP:C	2.44	0.55
1:A:129:LYS:HB2	1:A:131:ILE:HG12	1.89	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:SER:OG	1:F:141:GLU:HG3	2.08	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:B:83:GLU:OE2	1:D:207:ASP:OD1	2.26	0.54
1:C:167:PRO:HG3	1:C:176:ILE:HD11	1.90	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: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:J:167:PRO:HD2	1:J:170:TRP:HB2	1.91	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: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:184:PRO:O	1:C:185:ALA:CB	2.57	0.52
1:C:73:ASP:O	1:C:99:ALA:HB1	2.09	0.52
1:A:198:LYS:CG	1:A:203:ILE:HD11	2.39	0.52
1:J:201:GLY:O	1:J:202:GLU:C	2.47	0.52
1:E:75:VAL:HG12	1:E:76:GLU:OE1	2.09	0.52
1:F:70:LEU:HD23	1:F:70:LEU:C	2.30	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:H:106:ALA:HA	1:H:111:MET:CE	2.39	0.52
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:109:LEU:O	1:F:111:MET:N	2.43	0.51
1:F:80:ALA:HB2	1:G:42:PHE:CG	2.45	0.51
1:H:166:LEU:HD12	1:H:170:TRP:CD2	2.44	0.51
1:C:70:LEU:C	1:C:70:LEU:HD23	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLU:O	1:A:203:ILE:O	2.29	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:I:197:ALA:O	1:I:199:ALA:HB3	2.11	0.51
1:D:90:SER:OG	1:D:90:SER:O	2.28	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:J:109:LEU:H	1:J:109:LEU:HD22	1.76	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:B:201:GLY:O	1:B:202:GLU:C	2.50	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:A:44:PRO:O	1:A:45:VAL:C	2.46	0.50
1:E:198:LYS:HA	1:E:199:ALA:O	2.12	0.50
1:F:145:ASP:C	1:F:145:ASP:OD2	2.48	0.49
1:I:200:LYS:HD3	1:I:201:GLY:HA2	1.94	0.49
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:C:189:GLU:O	1:C:190:GLU:C	2.51	0.49
1:C:84:TRP:C	1:C:84:TRP:CE3	2.85	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:K:84:TRP:C	1:K:84:TRP:CE3	2.86	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:A:70:LEU:C	1:A:70:LEU:HD23	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:100:ASP:O	1:E:101:ASP:C	2.47	0.49
1:H:15:THR:HG22	1:H:98:ILE:HA	1.94	0.49
1:I:4:ILE:CG2	1:I:5:GLY:N	2.76	0.49
1:F:202:GLU:HB3	1:F:213:LYS:HB2	1.93	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:N	1:J:109:LEU:HD22	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:HA	1:F:199:ALA:C	2.32	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:J:70:LEU:C	1:J:70:LEU:HD23	2.34	0.48
1:L:198:LYS:HA	1:L:199:ALA:C	2.34	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
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:L:78:HIS:NE2	1:L:98:ILE:O	2.43	0.48
1:A:152:LEU:HD13	1:B:138:TYR:CE2	2.49	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:F:83:GLU:OE2	1:H:207:ASP:OD1	2.33	0.47
1:H:109:LEU:HD12	1:H:111:MET:HE1	1.97	0.47
1:D:180:VAL:O	1:D:212:TYR:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG2	1:E:72:VAL:O	2.50	0.47
1:F:72:VAL:CG1	1:F:118:ILE:CD1	2.92	0.47
1:H:203:ILE:HD13	1:H:205:CYS:SG	2.54	0.47
1:H:76:GLU:HG3	1:I:43:THR:CG2	2.43	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: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:E:24:ASP:HB3	1:E:28:LYS:HD2	1.96	0.47
1:L:13:VAL:HG21	1:L:98:ILE:HG12	1.96	0.47
1:L:4:ILE:HG22	1:L:5:GLY:N	2.29	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
1:H:188:ILE:HD12	1:H:188:ILE:N	2.29	0.47
1:H:74:GLN:NE2	1:I:118:ILE:CG2	2.76	0.47
1:I:132:ILE:HG21	1:I:135:ILE:HD11	1.97	0.47
1:K:174:GLU:N	1:K:174:GLU:OE1	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: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:L:94:ASP:OD1	1:L:94:ASP:C	2.54	0.46
1:I:168:HIS:HB2	1:J:49:GLU:HG2	1.97	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:156:LEU:HD11	1:L:139:PRO:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:102:ARG:C	1:I:102:ARG:HG3	2.37	0.46
1:A:138:TYR:CZ	1:B:152:LEU:HD13	2.51	0.46
1:F:109:LEU:O	1:F:110:GLY:C	2.54	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:70:LEU:HD23	1:F:71:SER:N	2.31	0.45
1:F:7:LYS:HG3	1:F:131:ILE:HD13	1.97	0.45
1:A:198:LYS:HG2	1:A:203:ILE:CD1	2.44	0.45
1:A:45:VAL:HG22	1:B:181:ILE:HD12	1.99	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:C:166:LEU:N	1:C:166:LEU:CD2	2.80	0.45
1:G:145:ASP:OD2	1:G:145:ASP:C	2.55	0.45
1:H:32:TRP:HB2	1:H:65:VAL:HG22	1.99	0.45
1:J:127:ASP:OD1	1:J:131:ILE:N	2.41	0.45
1:I:156:LEU:HD11	1:J:139:PRO:CG	2.46	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:J:105:LEU:O	1:J:106:ALA:C	2.55	0.45
1:L:34:ILE:HD11	1:L:65:VAL:HG11	1.99	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:G:167:PRO:HG3	1:G:176:ILE:HD11	1.98	0.45
1:G:34:ILE:CD1	1:G:60:PHE:CE2	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:20:ILE:HG21	1:K:25:TYR:CD1	2.52	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:187:THR:OG1	1:D:188:ILE:N	2.49	0.45
1:D:86:LYS:O	1:D:90:SER:HA	2.16	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
1:C:199:ALA:CA	1:C:200:LYS:C	2.85	0.44
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:L:70:LEU:HD12	1:L:98:ILE:HD12	1.99	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:35:LEU:HD21	1:F:111:MET:HE1	2.00	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:I:203:ILE:C	1:I:203:ILE:HD12	2.37	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: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: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:B:40:ALA:O	1:B:43:THR:HB	2.18	0.43
1:B:32:TRP:HB2	1:B:65:VAL:HG13	2.01	0.43
1:C:198:LYS:HG3	1:C:203:ILE:HG13	1.99	0.43
1:C:55:LYS:HD3	1:C:55:LYS:HA	1.78	0.43
1:L:33:PHE:CZ	1:L:126:VAL:HG21	2.52	0.43
1:K:44:PRO:CG	1:L:181:ILE:HG21	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:124:PHE:CE2	1:D:135:ILE:HG23	2.54	0.43
1:D:13:VAL:HB	1:D:98:ILE:HG23	1.99	0.43
1:F:187:THR:HG22	1:F:188:ILE:H	1.82	0.43
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: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:B:39:PRO:HD2	1:B:46:OCS:OD3	2.19	0.43
1:D:198:LYS:HA	1:D:199:ALA:C	2.39	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:E:45:VAL:O	1:E:48:THR:OG1	2.29	0.43
1:A:186:SER:O	1:A:187:THR:C	2.57	0.43
1:A:23:PRO:O	1:A:24:ASP:C	2.55	0.43
1:D:190:GLU:O	1:D:193:GLN:HB2	2.19	0.43
1:C:44:PRO:HB3	1:D:210:PHE:CD2	2.53	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:E:203:ILE:C	1:E:203:ILE:HD12	2.38	0.43
1:J:35:LEU:HA	1:J:68:ILE:HG23	2.01	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:B:188:ILE:C	1:B:190:GLU:N	2.70	0.42
1:I:106:ALA:O	1:I:110:GLY:N	2.52	0.42
1:H:76:GLU:HG3	1:I:43:THR:HG23	2.01	0.42
1:K:34:ILE:HD11	1:K:65:VAL:HG11	2.01	0.42
1:A:133:ARG:HA	1:A:133:ARG:HD2	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:I:145:ASP:OD2	1:I:145:ASP:C	2.58	0.42
1:B:133:ARG:NH2	1:B:156:LEU:HD12	2.34	0.42
1:B:34:ILE:HD11	1:B:60:PHE:CD2	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:54:GLN:CG	1:L:91:VAL:CG1	2.96	0.42
1:G:185:ALA:O	1:G:186:SER:HB3	2.19	0.42
1:H:100:ASP:O	1:H:101:ASP:C	2.58	0.42
1:I:40:ALA:O	1:I:43:THR:OG1	2.34	0.42
1:J:118:ILE:HG12	1:K:74:GLN:NE2	2.33	0.42
1:J:34:ILE:CD1	1:J:149:ILE:HG21	2.49	0.42
1:D:38:HIS:O	1:D:119:THR:OG1	2.38	0.42
1:A:44:PRO:HB2	1:B:181:ILE:HG21	2.01	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:H:70:LEU:C	1:H:70:LEU:HD23	2.39	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: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:HA	1:K:55:LYS:HD3	1.80	0.42
1:B:24:ASP:O	1:B:26:PHE:N	2.53	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:C:37:SER:HB2	1:C:111:MET:CE	2.49	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:A:76:GLU:CD	1:A:76:GLU:H	2.21	0.41
1:E:174:GLU:CD	1:E:174:GLU:H	2.17	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:12:GLU:CD	1:B:21:LYS:HD3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:205:CYS:HB3	1:G:207:ASP:O	2.21	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:A:165:ALA:HB1	1:B:45:VAL:HG21	2.03	0.41
1:A:202:GLU:O	1:A:203:ILE:C	2.59	0.41
1:B:161:GLU:HG2	1:B:162:LYS:HD3	2.02	0.41
1:B:44:PRO:O	1:B:45:VAL:C	2.58	0.41
1:E:209:TRP:CE3	1:E:210:PHE:HB2	2.55	0.41
1:E:57:VAL:HG22	1:E:67:PRO:HG2	2.02	0.41
1:B:36:PHE:HA	1:B:122:ALA:O	2.20	0.41
1:D:38:HIS:CE1	1:D:71:SER:HB3	2.56	0.41
1:K:203:ILE:CD1	1:K:205:CYS:SG	3.09	0.41
1:L:192:LYS:O	1:L:193:GLN:C	2.57	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:C:51:TYR:CZ	1:D:175:LEU:HD21	2.55	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:E:84:TRP:CE3	1:E:84:TRP:C	2.95	0.41
1:K:25:TYR:CD2	1:K:25:TYR:C	2.94	0.41
1:K:35:LEU:HA	1:K:68:ILE:O	2.21	0.41
1:L:127:ASP:OD2	1:L:133:ARG:HD3	2.20	0.41
1:A:210:PHE:CD2	1:A:210:PHE:C	2.95	0.41
1:B:70:LEU:C	1:B:70:LEU:HD23	2.41	0.41
1:C:198:LYS:HE3	1:C:205:CYS:SG	2.61	0.41
1:I:198:LYS:HA	1:I:199:ALA:O	2.21	0.41
1:I:74:GLN:HA	1:I:99:ALA:HB1	2.01	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:H:112:ILE:HG22	1:H:113:PRO:O	2.21	0.40
1:I:100:ASP:O	1:I:101:ASP:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:44:PRO:HG2	1:L:181:ILE:HG21	2.03	0.40
1:K:112:ILE:HD11	1:K:116:ALA:O	2.21	0.40
1:D:68:ILE:HG23	1:D:68:ILE:O	2.22	0.40
1:H:106:ALA:HA	1:H:111:MET:HE2	2.04	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
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:E:141:GLU:OE1	1:F:133:ARG:NH2	2.41	0.40
1:K:4:ILE:HD11	1:K:134:ALA:HA	2.04	0.40
1:J:73:ASP:OD2	1:K:77:ASP:OD2	2.39	0.40
1:L:34:ILE:CD1	1:L:65:VAL:HG11	2.51	0.40
1:B:173:ASN:O	1:B:174:GLU:C	2.59	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:197:ALA:O	1:G:201:GLY:HA2	2.21	0.40
1:G:71:SER:OG	1:G:72:VAL:N	2.54	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
1:K:56:ARG:O	1:K:57:VAL:C	2.59	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	211/216 (98%)	191 (90%)	14 (7%)	6 (3%)	5 2
1	B	211/216 (98%)	179 (85%)	23 (11%)	9 (4%)	2 0
1	C	211/216 (98%)	181 (86%)	21 (10%)	9 (4%)	2 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	211/216 (98%)	185 (88%)	23 (11%)	3 (1%)	11	7
1	E	211/216 (98%)	189 (90%)	17 (8%)	5 (2%)	6	3
1	F	211/216 (98%)	192 (91%)	16 (8%)	3 (1%)	11	7
1	G	211/216 (98%)	194 (92%)	16 (8%)	1 (0%)	29	29
1	H	211/216 (98%)	191 (90%)	12 (6%)	8 (4%)	3	1
1	I	211/216 (98%)	193 (92%)	16 (8%)	2 (1%)	17	14
1	J	211/216 (98%)	183 (87%)	25 (12%)	3 (1%)	11	7
1	K	211/216 (98%)	183 (87%)	22 (10%)	6 (3%)	5	2
1	L	211/216 (98%)	188 (89%)	15 (7%)	8 (4%)	3	1
All	All	2532/2592 (98%)	2249 (89%)	220 (9%)	63 (2%)	5	3

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	LYS
1	A	203	ILE
1	B	184	PRO
1	B	190	GLU
1	C	185	ALA
1	C	199	ALA
1	D	202	GLU
1	E	28	LYS
1	E	202	GLU
1	H	24	ASP
1	H	198	LYS
1	H	200	LYS
1	J	185	ALA
1	K	185	ALA
1	K	186	SER
1	L	184	PRO
1	A	24	ASP
1	A	185	ALA
1	B	202	GLU
1	C	198	LYS
1	F	110	GLY
1	F	186	SER
1	G	185	ALA
1	J	188	ILE
1	J	202	GLU

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Mol	Chain	Res	Type
1	K	202	GLU
1	K	208	SER
1	L	3	VAL
1	L	161	GLU
1	B	28	LYS
1	B	183	PRO
1	C	189	GLU
1	C	190	GLU
1	C	208	SER
1	E	161	GLU
1	H	187	THR
1	I	185	ALA
1	L	190	GLU
1	L	202	GLU
1	A	202	GLU
1	B	25	TYR
1	B	187	THR
1	D	185	ALA
1	D	186	SER
1	E	199	ALA
1	H	120	ALA
1	I	199	ALA
1	L	185	ALA
1	C	127	ASP
1	C	188	ILE
1	E	183	PRO
1	H	190	GLU
1	K	188	ILE
1	K	200	LYS
1	L	62	LYS
1	L	120	ALA
1	H	196	GLU
1	H	197	ALA
1	B	44	PRO
1	C	184	PRO
1	A	188	ILE
1	B	3	VAL
1	F	44	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/187 (99%)	172 (93%)	13 (7%)	15	13
1	B	185/187 (99%)	166 (90%)	19 (10%)	7	5
1	C	185/187 (99%)	159 (86%)	26 (14%)	3	2
1	D	185/187 (99%)	166 (90%)	19 (10%)	7	5
1	E	185/187 (99%)	168 (91%)	17 (9%)	9	7
1	F	185/187 (99%)	165 (89%)	20 (11%)	6	4
1	G	185/187 (99%)	172 (93%)	13 (7%)	15	13
1	H	185/187 (99%)	162 (88%)	23 (12%)	4	3
1	I	185/187 (99%)	171 (92%)	14 (8%)	13	12
1	J	185/187 (99%)	158 (85%)	27 (15%)	3	1
1	K	185/187 (99%)	171 (92%)	14 (8%)	13	12
1	L	185/187 (99%)	164 (89%)	21 (11%)	5	3
All	All	2220/2244 (99%)	1994 (90%)	226 (10%)	7	5

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	7	LYS
1	A	19	ARG
1	A	50	PHE
1	A	90	SER
1	A	97	VAL
1	A	102	ARG
1	A	156	LEU
1	A	188	ILE
1	A	200	LYS
1	A	203	ILE
1	A	210	PHE
1	A	215	LEU
1	B	3	VAL

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Mol	Chain	Res	Type
1	B	14	LYS
1	B	15	THR
1	B	19	ARG
1	B	43	THR
1	B	57	VAL
1	B	62	LYS
1	B	71	SER
1	B	72	VAL
1	B	77	ASP
1	B	128	ASP
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	B	210	PHE
1	C	2	VAL
1	C	3	VAL
1	C	15	THR
1	C	19	ARG
1	C	20	ILE
1	C	21	LYS
1	C	37	SER
1	C	57	VAL
1	C	61	ARG
1	C	72	VAL
1	C	75	VAL
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	202	GLU
1	C	203	ILE
1	C	208	SER
1	C	210	PHE

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Mol	Chain	Res	Type
1	C	213	LYS
1	C	214	LYS
1	D	3	VAL
1	D	19	ARG
1	D	21	LYS
1	D	24	ASP
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	156	LEU
1	D	180	VAL
1	D	187	THR
1	D	188	ILE
1	D	200	LYS
1	D	203	ILE
1	D	210	PHE
1	E	19	ARG
1	E	21	LYS
1	E	57	VAL
1	E	71	SER
1	E	76	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	194	ARG
1	E	195	GLU
1	E	200	LYS
1	E	210	PHE
1	E	213	LYS
1	E	215	LEU
1	F	3	VAL
1	F	12	GLU
1	F	20	ILE
1	F	61	ARG

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Mol	Chain	Res	Type
1	F	62	LYS
1	F	75	VAL
1	F	76	GLU
1	F	90	SER
1	F	101	ASP
1	F	102	ARG
1	F	121	ARG
1	F	150	LEU
1	F	156	LEU
1	F	161	GLU
1	F	174	GLU
1	F	188	ILE
1	F	200	LYS
1	F	208	SER
1	F	210	PHE
1	F	215	LEU
1	G	7	LYS
1	G	15	THR
1	G	43	THR
1	G	61	ARG
1	G	71	SER
1	G	108	LYS
1	G	114	SER
1	G	152	LEU
1	G	156	LEU
1	G	157	LYS
1	G	192	LYS
1	G	210	PHE
1	G	213	LYS
1	H	7	LYS
1	H	12	GLU
1	H	21	LYS
1	H	24	ASP
1	H	34	ILE
1	H	43	THR
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

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Mol	Chain	Res	Type
1	H	156	LEU
1	H	160	THR
1	H	161	GLU
1	H	172	ASN
1	H	186	SER
1	H	190	GLU
1	H	198	LYS
1	H	202	GLU
1	H	210	PHE
1	H	215	LEU
1	I	12	GLU
1	I	19	ARG
1	I	24	ASP
1	I	71	SER
1	I	102	ARG
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	210	PHE
1	J	3	VAL
1	J	4	ILE
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	102	ARG
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

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Mol	Chain	Res	Type
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	210	PHE
1	J	214	LYS
1	K	13	VAL
1	K	16	THR
1	K	19	ARG
1	K	20	ILE
1	K	21	LYS
1	K	43	THR
1	K	61	ARG
1	K	83	GLU
1	K	90	SER
1	K	112	ILE
1	K	156	LEU
1	K	186	SER
1	K	188	ILE
1	K	210	PHE
1	L	3	VAL
1	L	12	GLU
1	L	19	ARG
1	L	21	LYS
1	L	24	ASP
1	L	43	THR
1	L	47	THR
1	L	72	VAL
1	L	76	GLU
1	L	101	ASP
1	L	107	GLU
1	L	113	PRO
1	L	118	ILE
1	L	150	LEU
1	L	153	VAL
1	L	156	LEU
1	L	172	ASN
1	L	188	ILE
1	L	210	PHE

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Mol	Chain	Res	Type
1	L	213	LYS
1	L	215	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	B	38	HIS
1	B	74	GLN
1	D	74	GLN
1	E	74	GLN
1	F	74	GLN
1	H	74	GLN
1	I	74	GLN
1	I	193	GLN
1	J	74	GLN
1	K	74	GLN
1	K	193	GLN
1	L	74	GLN
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	G	46	1	7,8,9	2.23	2 (28%)	6,11,13	2.66	2 (33%)
1	OCS	K	46	1	7,8,9	1.83	2 (28%)	6,11,13	2.18	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OCS	A	46	1	7,8,9	3.08	3 (42%)	6,11,13	4.06	5 (83%)
1	OCS	E	46	1	7,8,9	2.37	3 (42%)	6,11,13	3.94	2 (33%)
1	OCS	C	46	1	7,8,9	3.47	4 (57%)	6,11,13	3.03	3 (50%)
1	OCS	J	46	1	7,8,9	1.87	1 (14%)	6,11,13	4.91	5 (83%)
1	OCS	H	46	1	7,8,9	1.88	2 (28%)	6,11,13	2.44	1 (16%)
1	OCS	L	46	1	7,8,9	3.14	2 (28%)	6,11,13	4.57	4 (66%)
1	OCS	B	46	1	7,8,9	2.15	3 (42%)	6,11,13	9.93	5 (83%)
1	OCS	F	46	1	7,8,9	2.68	2 (28%)	6,11,13	3.75	4 (66%)
1	OCS	D	46	1	7,8,9	2.09	2 (28%)	6,11,13	4.65	6 (100%)
1	OCS	I	46	1	7,8,9	3.02	2 (28%)	6,11,13	2.08	2 (33%)

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	G	46	1	-	0/4/7/9	-
1	OCS	K	46	1	-	0/4/7/9	-
1	OCS	A	46	1	-	0/4/7/9	-
1	OCS	E	46	1	-	0/4/7/9	-
1	OCS	C	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	L	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	D	46	1	-	0/4/7/9	-
1	OCS	I	46	1	-	0/4/7/9	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	OCS	OD3-SG	7.69	1.67	1.45
1	L	46	OCS	OD1-SG	7.62	1.67	1.45
1	I	46	OCS	OD1-SG	7.03	1.65	1.45
1	A	46	OCS	OD3-SG	6.77	1.65	1.45
1	F	46	OCS	OD3-SG	6.08	1.63	1.45
1	G	46	OCS	OD3-SG	4.86	1.59	1.45
1	E	46	OCS	OD2-SG	4.64	1.64	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	46	OCS	OD2-SG	3.97	1.61	1.47
1	J	46	OCS	OD2-SG	3.95	1.61	1.47
1	K	46	OCS	OD2-SG	3.75	1.60	1.47
1	H	46	OCS	OD2-SG	3.74	1.60	1.47
1	C	46	OCS	CB-SG	-3.39	1.64	1.77
1	B	46	OCS	OD2-SG	3.20	1.58	1.47
1	B	46	OCS	OD1-SG	-2.89	1.36	1.45
1	A	46	OCS	CB-SG	-2.80	1.67	1.77
1	D	46	OCS	CB-SG	-2.76	1.67	1.77
1	I	46	OCS	OD2-SG	-2.74	1.38	1.47
1	G	46	OCS	CB-SG	-2.68	1.67	1.77
1	C	46	OCS	OD2-SG	-2.61	1.38	1.47
1	E	46	OCS	OD3-SG	-2.53	1.37	1.45
1	B	46	OCS	CB-SG	-2.41	1.68	1.77
1	A	46	OCS	OD2-SG	-2.41	1.39	1.47
1	F	46	OCS	CB-SG	-2.33	1.68	1.77
1	E	46	OCS	CB-CA	2.27	1.55	1.53
1	L	46	OCS	CB-SG	-2.23	1.69	1.77
1	K	46	OCS	CB-SG	-2.16	1.69	1.77
1	H	46	OCS	CB-SG	-2.08	1.69	1.77
1	C	46	OCS	CB-CA	-2.03	1.51	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	OCS	OD1-SG-CB	18.21	128.58	106.94
1	B	46	OCS	OD2-SG-OD3	-9.63	87.74	111.27
1	E	46	OCS	OD3-SG-CB	8.68	117.26	106.94
1	D	46	OCS	OD2-SG-CB	8.32	119.00	105.74
1	J	46	OCS	OD3-SG-CB	8.27	116.77	106.94
1	L	46	OCS	OD3-SG-CB	7.89	116.32	106.94
1	B	46	OCS	OD3-SG-OD1	-7.67	87.39	113.95
1	B	46	OCS	OD2-SG-CB	7.48	117.66	105.74
1	J	46	OCS	OD1-SG-CB	7.46	115.81	106.94
1	B	46	OCS	OD3-SG-CB	-7.15	98.45	106.94
1	F	46	OCS	OD3-SG-CB	7.14	115.42	106.94
1	A	46	OCS	OD1-SG-CB	6.85	115.09	106.94
1	L	46	OCS	OD2-SG-CB	6.31	115.80	105.74
1	C	46	OCS	OD2-SG-CB	6.26	115.71	105.74
1	D	46	OCS	OD3-SG-CB	5.68	113.69	106.94
1	G	46	OCS	OD1-SG-CB	5.26	113.19	106.94
1	H	46	OCS	OD2-SG-CB	5.02	113.74	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	OCS	OD2-SG-CB	4.88	113.52	105.74
1	I	46	OCS	OD1-SG-CB	4.45	112.22	106.94
1	A	46	OCS	OD2-SG-OD3	-4.16	101.10	111.27
1	L	46	OCS	OD3-SG-OD1	-4.07	99.85	113.95
1	F	46	OCS	OD2-SG-OD3	-3.59	102.50	111.27
1	D	46	OCS	OD2-SG-OD1	-3.41	102.95	111.27
1	C	46	OCS	OD2-SG-OD1	-3.31	103.19	111.27
1	K	46	OCS	OD2-SG-CB	3.20	110.83	105.74
1	F	46	OCS	OD1-SG-CB	3.19	110.73	106.94
1	K	46	OCS	OD3-SG-CB	3.08	110.60	106.94
1	G	46	OCS	OD3-SG-CB	3.01	110.51	106.94
1	J	46	OCS	OD2-SG-OD3	-2.86	104.28	111.27
1	E	46	OCS	OD3-SG-OD1	-2.80	104.25	113.95
1	K	46	OCS	OD3-SG-OD1	-2.76	104.40	113.95
1	F	46	OCS	OD2-SG-CB	2.61	109.90	105.74
1	D	46	OCS	OD3-SG-OD1	-2.54	105.15	113.95
1	J	46	OCS	OD2-SG-OD1	-2.47	105.23	111.27
1	A	46	OCS	OD3-SG-CB	2.44	109.83	106.94
1	D	46	OCS	OD2-SG-OD3	-2.43	105.34	111.27
1	L	46	OCS	OD2-SG-OD3	-2.34	105.55	111.27
1	J	46	OCS	OD3-SG-OD1	-2.24	106.20	113.95
1	I	46	OCS	OD3-SG-OD1	-2.16	106.48	113.95
1	C	46	OCS	OD1-SG-CB	-2.10	104.44	106.94
1	D	46	OCS	OD1-SG-CB	2.05	109.38	106.94
1	A	46	OCS	OD3-SG-OD1	-2.02	106.95	113.95

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	G	46	OCS	2	0
1	K	46	OCS	2	0
1	A	46	OCS	1	0
1	E	46	OCS	2	0
1	C	46	OCS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	46	OCS	1	0
1	H	46	OCS	2	0
1	L	46	OCS	1	0
1	B	46	OCS	3	0
1	F	46	OCS	4	0
1	D	46	OCS	1	0
1	I	46	OCS	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	213/216 (98%)	0.03	13 (6%) 21 23	11, 23, 84, 100	0
1	B	213/216 (98%)	0.24	19 (8%) 9 10	13, 25, 111, 125	0
1	C	213/216 (98%)	0.19	12 (5%) 24 26	15, 26, 80, 112	0
1	D	213/216 (98%)	0.35	21 (9%) 7 7	15, 27, 109, 146	0
1	E	213/216 (98%)	0.33	18 (8%) 10 12	15, 25, 105, 141	0
1	F	213/216 (98%)	0.53	19 (8%) 9 10	14, 25, 119, 165	0
1	G	213/216 (98%)	0.00	7 (3%) 46 48	14, 24, 71, 93	0
1	H	213/216 (98%)	0.10	6 (2%) 53 55	14, 25, 84, 108	0
1	I	213/216 (98%)	0.35	19 (8%) 9 10	13, 25, 97, 149	0
1	J	213/216 (98%)	0.41	20 (9%) 8 9	13, 24, 109, 142	0
1	K	213/216 (98%)	0.41	20 (9%) 8 9	14, 27, 109, 132	0
1	L	213/216 (98%)	0.44	21 (9%) 7 7	14, 28, 108, 129	0
All	All	2556/2592 (98%)	0.28	195 (7%) 13 15	11, 25, 100, 165	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	185	ALA	22.0
1	I	188	ILE	12.2
1	F	188	ILE	11.2
1	E	186	SER	10.6
1	J	185	ALA	10.2
1	I	186	SER	9.7
1	J	188	ILE	9.1
1	K	188	ILE	9.0
1	J	193	GLN	8.6
1	K	197	ALA	8.5
1	J	187	THR	8.3

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Mol	Chain	Res	Type	RSRZ
1	I	187	THR	8.3
1	D	187	THR	8.1
1	L	185	ALA	8.0
1	D	185	ALA	7.9
1	F	186	SER	7.9
1	J	200	LYS	7.6
1	J	186	SER	7.6
1	D	200	LYS	7.5
1	F	202	GLU	7.3
1	C	185	ALA	7.2
1	E	193	GLN	7.1
1	F	193	GLN	7.1
1	E	188	ILE	7.0
1	K	200	LYS	7.0
1	A	185	ALA	7.0
1	K	185	ALA	6.9
1	B	185	ALA	6.9
1	K	192	LYS	6.9
1	J	201	GLY	6.8
1	E	187	THR	6.6
1	J	202	GLU	6.4
1	L	200	LYS	6.3
1	F	192	LYS	6.3
1	L	191	LYS	6.3
1	F	187	THR	6.2
1	L	202	GLU	6.2
1	E	197	ALA	6.0
1	E	201	GLY	6.0
1	E	192	LYS	6.0
1	L	197	ALA	6.0
1	D	192	LYS	5.9
1	B	188	ILE	5.8
1	K	201	GLY	5.8
1	K	187	THR	5.7
1	F	197	ALA	5.7
1	F	201	GLY	5.7
1	D	193	GLN	5.7
1	B	201	GLY	5.7
1	F	194	ARG	5.7
1	E	185	ALA	5.6
1	E	200	LYS	5.6
1	F	200	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	K	194	ARG	5.5
1	B	200	LYS	5.4
1	L	201	GLY	5.4
1	D	196	GLU	5.4
1	B	194	ARG	5.3
1	I	202	GLU	5.3
1	J	196	GLU	5.2
1	K	189	GLU	5.2
1	D	198	LYS	5.2
1	K	196	GLU	5.2
1	L	186	SER	5.1
1	I	194	ARG	5.1
1	B	193	GLN	5.1
1	B	192	LYS	5.1
1	B	195	GLU	5.1
1	D	195	GLU	5.1
1	B	184	PRO	5.0
1	D	188	ILE	5.1
1	A	186	SER	5.0
1	I	192	LYS	4.8
1	H	194	ARG	4.8
1	B	202	GLU	4.7
1	J	197	ALA	4.7
1	B	187	THR	4.7
1	I	201	GLY	4.6
1	I	185	ALA	4.6
1	D	199	ALA	4.6
1	F	198	LYS	4.6
1	I	19	ARG	4.6
1	I	195	GLU	4.5
1	F	189	GLU	4.5
1	L	193	GLN	4.4
1	A	197	ALA	4.4
1	A	188	ILE	4.4
1	F	196	GLU	4.2
1	K	202	GLU	4.1
1	I	199	ALA	4.0
1	J	195	GLU	4.0
1	L	192	LYS	4.0
1	L	196	GLU	4.0
1	J	115	GLY	3.9
1	L	199	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	192	LYS	3.9
1	D	184	PRO	3.9
1	C	19	ARG	3.9
1	D	186	SER	3.9
1	K	193	GLN	3.8
1	K	199	ALA	3.8
1	L	194	ARG	3.8
1	B	196	GLU	3.7
1	E	202	GLU	3.7
1	D	197	ALA	3.7
1	D	202	GLU	3.7
1	E	194	ARG	3.7
1	J	189	GLU	3.6
1	J	194	ARG	3.6
1	G	187	THR	3.5
1	L	2	VAL	3.4
1	G	188	ILE	3.4
1	C	186	SER	3.4
1	L	195	GLU	3.4
1	A	200	LYS	3.4
1	C	187	THR	3.4
1	A	195	GLU	3.4
1	E	199	ALA	3.3
1	G	192	LYS	3.3
1	E	189	GLU	3.3
1	L	190	GLU	3.3
1	C	195	GLU	3.3
1	F	184	PRO	3.3
1	D	191	LYS	3.2
1	E	198	LYS	3.2
1	E	116	ALA	3.2
1	K	190	GLU	3.1
1	L	198	LYS	3.1
1	E	196	GLU	3.1
1	L	189	GLU	3.1
1	I	191	LYS	3.1
1	H	107	GLU	3.0
1	K	184	PRO	3.0
1	H	115	GLY	3.0
1	J	184	PRO	3.0
1	D	201	GLY	3.0
1	K	186	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	183	PRO	2.9
1	A	187	THR	2.9
1	F	195	GLU	2.9
1	A	184	PRO	2.9
1	D	115	GLY	2.9
1	C	188	ILE	2.8
1	C	194	ARG	2.8
1	G	185	ALA	2.8
1	B	115	GLY	2.8
1	E	184	PRO	2.8
1	I	203	ILE	2.8
1	B	197	ALA	2.7
1	F	190	GLU	2.7
1	J	19	ARG	2.7
1	L	188	ILE	2.7
1	A	202	GLU	2.7
1	H	193	GLN	2.7
1	D	194	ARG	2.6
1	K	114	SER	2.6
1	L	187	THR	2.6
1	L	115	GLY	2.6
1	J	199	ALA	2.6
1	A	193	GLN	2.6
1	D	19	ARG	2.6
1	I	193	GLN	2.5
1	J	190	GLU	2.5
1	I	198	LYS	2.5
1	I	189	GLU	2.5
1	C	193	GLN	2.5
1	J	192	LYS	2.5
1	B	186	SER	2.4
1	C	30	GLY	2.4
1	G	199	ALA	2.4
1	G	19	ARG	2.4
1	K	195	GLU	2.3
1	B	191	LYS	2.3
1	A	19	ARG	2.3
1	K	19	ARG	2.3
1	G	115	GLY	2.3
1	C	191	LYS	2.3
1	A	192	LYS	2.3
1	C	2	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	189	GLU	2.2
1	F	106	ALA	2.2
1	A	203	ILE	2.2
1	B	198	LYS	2.2
1	I	200	LYS	2.2
1	I	25	TYR	2.1
1	L	184	PRO	2.1
1	B	189	GLU	2.1
1	B	190	GLU	2.1
1	E	114	SER	2.1
1	K	198	LYS	2.1
1	F	115	GLY	2.1
1	H	184	PRO	2.1
1	D	189	GLU	2.0
1	I	22	LEU	2.0
1	J	203	ILE	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	0.96	0.11	19,21,36,38	0
1	OCS	H	46	9/10	0.96	0.15	19,23,43,45	0
1	OCS	L	46	9/10	0.96	0.12	17,19,35,39	0
1	OCS	A	46	9/10	0.97	0.11	17,21,37,40	0
1	OCS	B	46	9/10	0.97	0.12	20,21,33,34	0
1	OCS	F	46	9/10	0.97	0.11	18,19,39,48	0
1	OCS	D	46	9/10	0.97	0.13	15,16,31,38	0
1	OCS	I	46	9/10	0.97	0.10	20,24,39,39	0
1	OCS	G	46	9/10	0.98	0.14	20,22,40,42	0
1	OCS	E	46	9/10	0.98	0.09	19,19,35,40	0
1	OCS	K	46	9/10	0.98	0.09	20,22,38,42	0
1	OCS	J	46	9/10	0.99	0.13	14,18,41,41	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.