Full wwPDB X-ray Structure Validation Report (i)

Dec 6, 2023 – 04:13 am GMT

PDB ID	:	2JD7
Title	:	Crystal Structure of the Fe-soaked Ferritin from the Hyperthermophilic Archaeal Anaerobe Pyrococcus furiosus
Authors	:	Tatur, J.; Hagen, W.R.; Matias, P.M.
Deposited on	:	2007-01-05
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

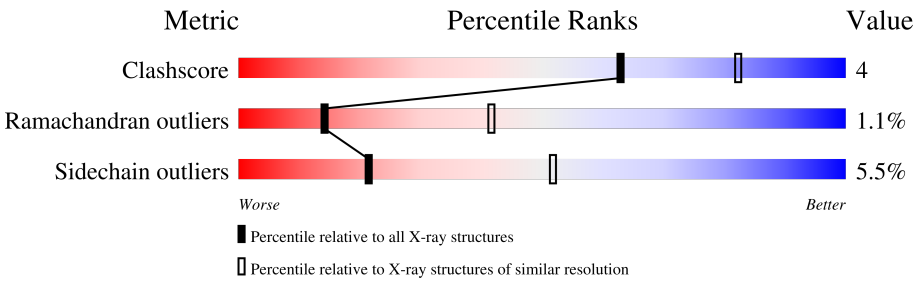
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	174	79% 16% • •
1	1	174	79% 17% •
1	2	174	81% 12% • •
1	3	174	82% 12% • •
1	4	174	83% 12% • •
1	5	174	90% 6% • •
1	6	174	85% 10% • •
1	7	174	79% 13% • •

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Mol	Chain	Length	Quality of chain
1	8	174	83% 11%
1	9	174	80% 14%
1	A	174	84% 10%
1	B	174	82% 12%
1	C	174	84% 11%
1	D	174	84% 10%
1	E	174	82% 12%
1	F	174	81% 13%
1	G	174	88% 7%
1	H	174	76% 17%
1	I	174	78% 15%
1	J	174	90% 5%
1	K	174	85% 10%
1	L	174	87% 9%
1	M	174	75% 21%
1	N	174	83% 10%
1	O	174	74% 20%
1	P	174	76% 18%
1	Q	174	82% 13%
1	R	174	84% 10%
1	S	174	84% 11%
1	T	174	85% 10%
1	U	174	88% 7%
1	V	174	82% 11%
1	W	174	84% 10%

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Mol	Chain	Length	Quality of chain
1	X	174	87% 9%
1	Y	174	81% 14%
1	Z	174	80% 16%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 50409 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 FERRITIN HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	0	167	1383	897	220	261	5	0	0	0
1	1	167	1383	897	220	261	5	0	0	0
1	2	167	1383	897	220	261	5	0	0	0
1	3	167	1383	897	220	261	5	0	0	0
1	4	167	1383	897	220	261	5	0	0	0
1	5	167	1383	897	220	261	5	0	0	0
1	6	167	1383	897	220	261	5	0	0	0
1	7	167	1383	897	220	261	5	0	0	0
1	8	167	1383	897	220	261	5	0	0	0
1	9	167	1383	897	220	261	5	0	0	0
1	A	167	1383	897	220	261	5	0	0	0
1	B	167	1383	897	220	261	5	0	0	0
1	C	167	1383	897	220	261	5	0	0	0
1	D	167	1383	897	220	261	5	0	0	0
1	E	167	1383	897	220	261	5	0	0	0
1	F	167	1383	897	220	261	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	167	1388	900	221	262	5	0	1	0
			Total	C	N	O	S			
1	H	167	1383	897	220	261	5	0	0	0
			Total	C	N	O	S			
1	I	167	1383	897	220	261	5	0	0	0
			Total	C	N	O	S			
1	J	167	1383	897	220	261	5	0	0	0
			Total	C	N	O	S			
1	K	167	1383	897	220	261	5	0	0	0
			Total	C	N	O	S			
1	L	167	1383	897	220	261	5	0	0	0
			Total	C	N	O	S			
1	M	167	1383	897	220	261	5	0	0	0
			Total	C	N	O	S			
1	N	167	1383	897	220	261	5	0	0	0
			Total	C	N	O	S			
1	O	167	1383	897	220	261	5	0	0	0
			Total	C	N	O	S			
1	P	167	1383	897	220	261	5	0	0	0
			Total	C	N	O	S			
1	Q	167	1383	897	220	261	5	0	0	0
			Total	C	N	O	S			
1	R	167	1383	897	220	261	5	0	0	0
			Total	C	N	O	S			
1	S	167	1383	897	220	261	5	0	0	0
			Total	C	N	O	S			
1	T	167	1388	900	221	262	5	0	1	0
			Total	C	N	O	S			
1	U	167	1383	897	220	261	5	0	0	0
			Total	C	N	O	S			
1	V	167	1383	897	220	261	5	0	0	0
			Total	C	N	O	S			
1	W	167	1388	900	221	262	5	0	1	0
			Total	C	N	O	S			
1	X	167	1383	897	220	261	5	0	0	0
			Total	C	N	O	S			
1	Y	167	1383	897	220	261	5	0	0	0
			Total	C	N	O	S			
1	Z	167	1383	897	220	261	5	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	0	3	3	3	0	0
2	1	3	3	3	0	0
2	2	3	3	3	0	0
2	3	3	3	3	0	0
2	4	3	3	3	0	0
2	5	3	3	3	0	0
2	6	3	3	3	0	0
2	7	3	3	3	0	0
2	8	3	3	3	0	0
2	9	3	3	3	0	0
2	A	3	3	3	0	0
2	B	3	3	3	0	0
2	C	3	3	3	0	0
2	D	3	3	3	0	0
2	E	3	3	3	0	0
2	F	3	3	3	0	0
2	G	3	3	3	0	0
2	H	3	3	3	0	0
2	I	3	3	3	0	0
2	J	3	3	3	0	0
2	K	3	3	3	0	0
2	L	3	3	3	0	0

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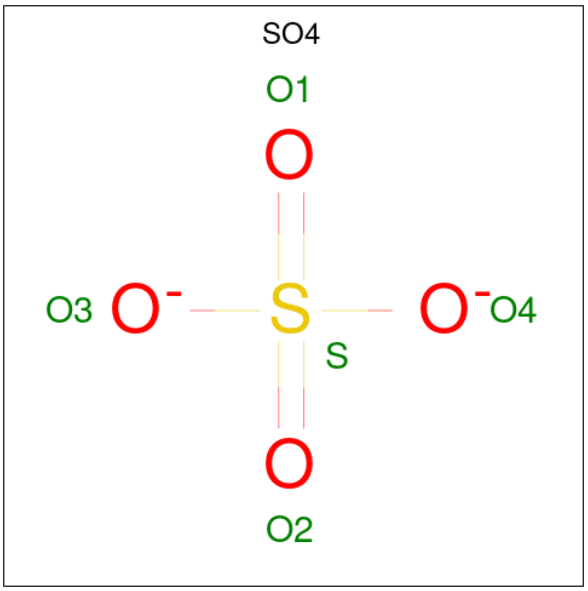
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	M	3	3	3	0	0
2	N	3	3	3	0	0
2	O	3	3	3	0	0
2	P	3	3	3	0	0
2	Q	3	3	3	0	0
2	R	3	3	3	0	0
2	S	3	3	3	0	0
2	T	3	3	3	0	0
2	U	3	3	3	0	0
2	V	3	3	3	0	0
2	W	3	3	3	0	0
2	X	3	3	3	0	0
2	Y	3	3	3	0	0
2	Z	3	3	3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1	1	Total O S 5 4 1	0	0
3	2	1	Total O S 5 4 1	0	0
3	3	1	Total O S 5 4 1	0	0
3	3	1	Total O S 5 4 1	0	0
3	8	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	O	1	Total O S 5 4 1	0	0
3	R	1	Total O S 5 4 1	0	0
3	S	1	Total O S 5 4 1	0	0
3	T	1	Total O S 5 4 1	0	0
3	V	1	Total O S 5 4 1	0	0
3	V	1	Total O S 5 4 1	0	0
3	W	1	Total O S 5 4 1	0	0
3	Y	1	Total O S 5 4 1	0	0
3	Y	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	0	7	Total O 7 7	0	0
4	1	10	Total O 10 10	0	0
4	2	7	Total O 7 7	0	0
4	3	15	Total O 15 15	0	0
4	4	8	Total O 8 8	0	0
4	5	5	Total O 5 5	0	0
4	6	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	7	11	11	11	0	0
			Total	O		
4	8	9	9	9	0	0
			Total	O		
4	9	7	7	7	0	0
			Total	O		
4	A	13	13	13	0	0
			Total	O		
4	B	17	17	17	0	0
			Total	O		
4	C	8	8	8	0	0
			Total	O		
4	D	16	16	16	0	0
			Total	O		
4	E	18	18	18	0	0
			Total	O		
4	F	21	21	21	0	0
			Total	O		
4	G	14	14	14	0	0
			Total	O		
4	H	2	2	2	0	0
			Total	O		
4	I	5	5	5	0	0
			Total	O		
4	J	16	16	16	0	0
			Total	O		
4	K	4	4	4	0	0
			Total	O		
4	L	9	9	9	0	0
			Total	O		
4	M	11	11	11	0	0
			Total	O		
4	N	3	3	3	0	0
			Total	O		
4	O	5	5	5	0	0
			Total	O		
4	P	5	5	5	0	0
			Total	O		
4	Q	9	9	9	0	0
			Total	O		
4	R	5	5	5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	S	17	17	17	0	0
			Total	O		
4	T	13	13	13	0	0
			Total	O		
4	U	18	18	18	0	0
			Total	O		
4	V	13	13	13	0	0
			Total	O		
4	W	9	9	9	0	0
			Total	O		
4	X	14	14	14	0	0
			Total	O		
4	Y	11	11	11	0	0
			Total	O		
4	Z	5	5	5	0	0

3 Residue-property plots (i)

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

Note EDS was not executed.

• Molecule 1: FERRITIN HOMOLOG

Chain 0:

• Molecule 1: FERRITIN HOMOLOG

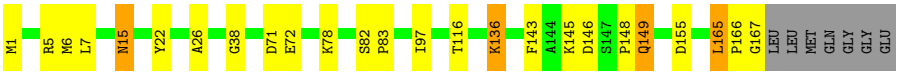
Chain 1:

• Molecule 1: FERRITIN HOMOLOG

Chain 2:

• Molecule 1: FERRITIN HOMOLOG

Chain 3:



• Molecule 1: FERRITIN HOMOLOG

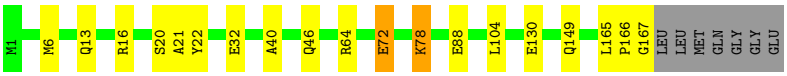
Chain 4:

• Molecule 1: FERRITIN HOMOLOG

Chain 5:

• Molecule 1: FERRITIN HOMOLOG

Chain 6:

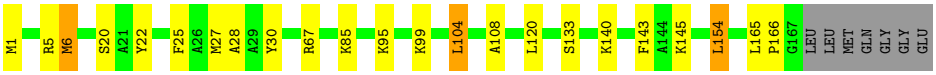


• Molecule 1: FERRITIN HOMOLOG

Chain 7:

• Molecule 1: FERRITIN HOMOLOG

Chain 8:

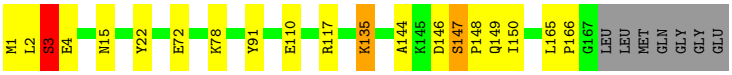


• Molecule 1: FERRITIN HOMOLOG

Chain 9:

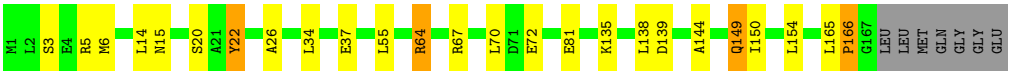
• Molecule 1: FERRITIN HOMOLOG

Chain A:



• Molecule 1: FERRITIN HOMOLOG

Chain B:



• Molecule 1: FERRITIN HOMOLOG

Chain C:

• Molecule 1: FERRITIN HOMOLOG

Chain D:

• Molecule 1: FERRITIN HOMOLOG

Chain E:

• Molecule 1: FERRITIN HOMOLOG

Chain F:

• Molecule 1: FERRITIN HOMOLOG

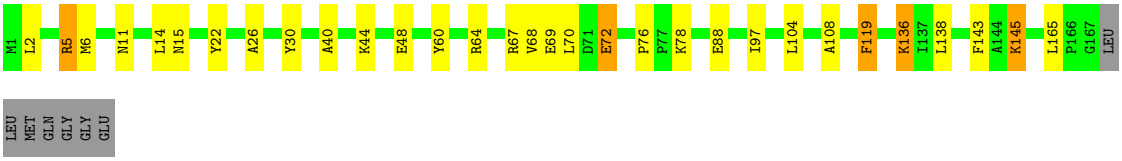
Chain G:

• Molecule 1: FERRITIN HOMOLOG

Chain H:

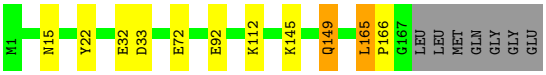
• Molecule 1: FERRITIN HOMOLOG

Chain I:



• Molecule 1: FERRITIN HOMOLOG

Chain J:



• Molecule 1: FERRITIN HOMOLOG

Chain K:

• Molecule 1: FERRITIN HOMOLOG

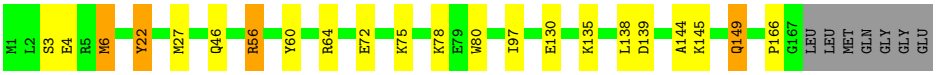
Chain L:

• Molecule 1: FERRITIN HOMOLOG

Chain M:

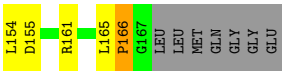
• Molecule 1: FERRITIN HOMOLOG

Chain N:



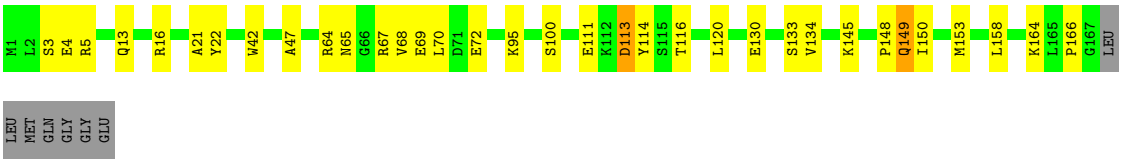
• Molecule 1: FERRITIN HOMOLOG

Chain O:



• Molecule 1: FERRITIN HOMOLOG

Chain P:



• Molecule 1: FERRITIN HOMOLOG

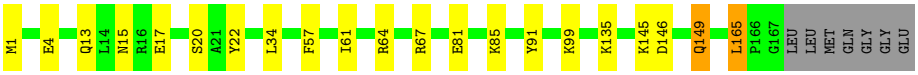
Chain Q:

• Molecule 1: FERRITIN HOMOLOG

Chain R:

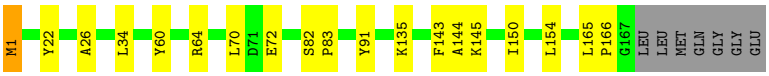
• Molecule 1: FERRITIN HOMOLOG

Chain S:



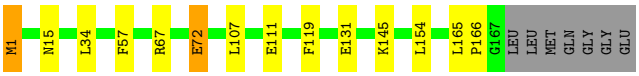
• Molecule 1: FERRITIN HOMOLOG

Chain T:



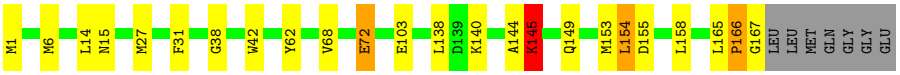
• Molecule 1: FERRITIN HOMOLOG

Chain U:



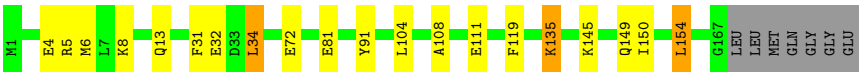
• Molecule 1: FERRITIN HOMOLOG

Chain V:



• Molecule 1: FERRITIN HOMOLOG

Chain W:



• Molecule 1: FERRITIN HOMOLOG

Chain X:

• Molecule 1: FERRITIN HOMOLOG

Chain Y:

• Molecule 1: FERRITIN HOMOLOG

Chain Z:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	254.30Å 342.88Å 266.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	204.12 – 2.80	Depositor
% Data completeness (in resolution range)	99.1 (204.12-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.3.0021	Depositor
R, R_{free}	0.199 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	50409	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

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: SO4, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	0	0.69	0/1417	0.72	0/1908
1	1	0.70	0/1417	0.70	0/1908
1	2	0.68	0/1417	0.69	0/1908
1	3	0.74	0/1417	0.76	0/1908
1	4	0.73	0/1417	0.72	0/1908
1	5	0.68	0/1417	0.67	0/1908
1	6	0.67	0/1417	0.68	0/1908
1	7	0.71	0/1417	0.69	0/1908
1	8	0.74	0/1417	0.72	0/1908
1	9	0.68	0/1417	0.68	0/1908
1	A	0.77	0/1417	0.75	0/1908
1	B	0.82	1/1417 (0.1%)	0.80	2/1908 (0.1%)
1	C	0.78	0/1417	0.76	0/1908
1	D	0.76	0/1417	0.80	1/1908 (0.1%)
1	E	0.74	0/1417	0.74	0/1908
1	F	0.78	0/1417	0.73	0/1908
1	G	0.77	0/1425	0.76	1/1919 (0.1%)
1	H	0.68	0/1417	0.69	0/1908
1	I	0.75	1/1417 (0.1%)	0.75	0/1908
1	J	0.74	1/1417 (0.1%)	0.71	0/1908
1	K	0.67	0/1417	0.71	0/1908
1	L	0.71	0/1417	0.71	0/1908
1	M	0.71	0/1417	0.73	0/1908
1	N	0.69	0/1417	0.69	0/1908
1	O	0.72	0/1417	0.72	0/1908
1	P	0.72	0/1417	0.73	2/1908 (0.1%)
1	Q	0.75	1/1417 (0.1%)	0.71	0/1908
1	R	0.65	0/1417	0.65	0/1908
1	S	0.76	1/1417 (0.1%)	0.75	0/1908
1	T	0.79	0/1425	0.75	0/1919
1	U	0.80	0/1417	0.74	0/1908
1	V	0.78	0/1417	0.78	0/1908

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	W	0.84	0/1425	0.80	0/1919
1	X	0.73	0/1417	0.73	0/1908
1	Y	0.77	0/1417	0.78	1/1908 (0.1%)
1	Z	0.65	0/1417	0.69	0/1908
All	All	0.73	5/51036 (0.0%)	0.73	7/68721 (0.0%)

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	A	0	1
1	E	0	1
1	U	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	92	GLU	CG-CD	6.07	1.61	1.51
1	J	92	GLU	CG-CD	5.89	1.60	1.51
1	S	4	GLU	CG-CD	5.54	1.60	1.51
1	B	81	GLU	CG-CD	5.49	1.60	1.51
1	I	15	ASN	CB-CG	5.38	1.63	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	64	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	B	64	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	D	5	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	P	113	ASP	CB-CG-OD1	5.51	123.26	118.30
1	P	67	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	Y	56	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	G	16	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	78	LYS	Peptide
1	E	78	LYS	Peptide
1	U	1	MET	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1383	0	1352	14	0
1	1	1383	0	1352	12	0
1	2	1383	0	1352	15	0
1	3	1383	0	1352	14	0
1	4	1383	0	1352	14	0
1	5	1383	0	1352	7	0
1	6	1383	0	1352	13	0
1	7	1383	0	1352	18	0
1	8	1383	0	1352	8	0
1	9	1383	0	1352	14	0
1	A	1383	0	1352	8	0
1	B	1383	0	1352	16	0
1	C	1383	0	1352	12	0
1	D	1383	0	1352	9	0
1	E	1383	0	1352	13	0
1	F	1383	0	1352	13	0
1	G	1388	0	1358	9	0
1	H	1383	0	1352	24	0
1	I	1383	0	1352	22	0
1	J	1383	0	1352	5	0
1	K	1383	0	1352	8	0
1	L	1383	0	1352	8	0
1	M	1383	0	1352	20	0
1	N	1383	0	1352	19	0
1	O	1383	0	1352	29	0
1	P	1383	0	1352	22	0
1	Q	1383	0	1352	10	0
1	R	1383	0	1352	10	0
1	S	1383	0	1352	8	0
1	T	1388	0	1358	10	0
1	U	1383	0	1352	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	1383	0	1352	14	0
1	W	1388	0	1358	9	0
1	X	1383	0	1352	9	0
1	Y	1383	0	1352	18	0
1	Z	1383	0	1352	16	0
2	0	3	0	0	0	0
2	1	3	0	0	0	0
2	2	3	0	0	0	0
2	3	3	0	0	0	0
2	4	3	0	0	0	0
2	5	3	0	0	0	0
2	6	3	0	0	0	0
2	7	3	0	0	0	0
2	8	3	0	0	0	0
2	9	3	0	0	0	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	3	0	0	0	0
2	M	3	0	0	0	0
2	N	3	0	0	0	0
2	O	3	0	0	0	0
2	P	3	0	0	0	0
2	Q	3	0	0	0	0
2	R	3	0	0	0	0
2	S	3	0	0	0	0
2	T	3	0	0	0	0
2	U	3	0	0	0	0
2	V	3	0	0	0	0
2	W	3	0	0	0	0
2	X	3	0	0	0	0
2	Y	3	0	0	0	0
2	Z	3	0	0	0	0
3	1	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	5	0	0	0	0
3	3	10	0	0	0	0
3	8	5	0	0	0	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	C	15	0	0	0	0
3	G	10	0	0	0	0
3	H	5	0	0	0	0
3	I	10	0	0	0	0
3	J	5	0	0	0	0
3	O	5	0	0	0	0
3	R	5	0	0	0	0
3	S	5	0	0	0	0
3	T	5	0	0	0	0
3	V	10	0	0	0	0
3	W	5	0	0	0	0
3	Y	10	0	0	1	0
4	0	7	0	0	0	0
4	1	10	0	0	0	0
4	2	7	0	0	1	0
4	3	15	0	0	2	0
4	4	8	0	0	0	0
4	5	5	0	0	0	0
4	6	8	0	0	0	0
4	7	11	0	0	0	0
4	8	9	0	0	0	0
4	9	7	0	0	0	0
4	A	13	0	0	1	0
4	B	17	0	0	2	0
4	C	8	0	0	1	0
4	D	16	0	0	1	0
4	E	18	0	0	2	0
4	F	21	0	0	1	0
4	G	14	0	0	1	0
4	H	2	0	0	2	0
4	I	5	0	0	0	0
4	J	16	0	0	1	0
4	K	4	0	0	1	0
4	L	9	0	0	1	0
4	M	11	0	0	0	0
4	N	3	0	0	0	0
4	O	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	5	0	0	0	0
4	Q	9	0	0	0	0
4	R	5	0	0	0	0
4	S	17	0	0	1	0
4	T	13	0	0	0	0
4	U	18	0	0	1	0
4	V	13	0	0	2	0
4	W	9	0	0	0	0
4	X	14	0	0	1	0
4	Y	11	0	0	0	0
4	Z	5	0	0	0	0
All	All	50409	0	48690	417	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 4.

All (417) 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:S:15:ASN:HB3	4:S:2004:HOH:O	1.48	1.11
1:A:2:LEU:O	1:A:3:SER:HB3	1.50	1.07
1:V:15:ASN:HB3	4:V:2002:HOH:O	1.51	1.06
1:5:69:GLU:HG3	1:N:78:LYS:HD2	1.36	1.05
1:B:15:ASN:HB3	4:B:2001:HOH:O	1.55	1.05
1:H:15:ASN:HB3	4:H:2001:HOH:O	1.66	0.95
1:G:166:PRO:HB2	4:G:2014:HOH:O	1.63	0.95
1:4:69:GLU:HG3	1:M:78:LYS:HD2	1.49	0.95
1:N:149:GLN:HE21	1:N:149:GLN:H	1.16	0.92
1:N:56:ARG:HG2	1:N:56:ARG:HH11	1.34	0.92
1:Z:81:GLU:H	1:Z:85:LYS:HD2	1.34	0.92
1:V:167:GLY:HA3	4:V:2012:HOH:O	1.70	0.92
1:P:116:THR:O	1:P:120:LEU:HD12	1.68	0.91
1:X:15:ASN:HB3	4:X:2003:HOH:O	1.71	0.90
1:H:145:LYS:HB2	4:H:2002:HOH:O	1.73	0.86
1:U:15:ASN:HB2	4:U:2008:HOH:O	1.75	0.85
1:2:5:ARG:HD2	4:2:2003:HOH:O	1.77	0.82
1:O:15:ASN:HB2	4:O:2001:HOH:O	1.82	0.80
1:0:67:ARG:NH2	1:I:30:TYR:HA	1.97	0.80
1:P:13:GLN:OE1	1:P:16:ARG:HD2	1.83	0.78
1:J:15:ASN:HB2	4:J:2002:HOH:O	1.82	0.77
1:K:149:GLN:H	1:K:149:GLN:HE21	1.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:165:LEU:O	1:3:167:GLY:N	2.21	0.74
1:P:116:THR:HG22	1:P:120:LEU:HD11	1.68	0.73
1:8:104:LEU:HD22	1:8:120:LEU:HD11	1.72	0.72
1:4:40:ALA:O	1:4:44:LYS:HG3	1.90	0.72
1:X:91:TYR:CZ	1:X:135:LYS:HD3	2.25	0.71
1:N:138:LEU:HD23	1:N:138:LEU:C	2.10	0.71
1:1:58:TYR:OH	1:J:32:GLU:HG3	1.91	0.71
1:O:11:ASN:OD1	1:O:69:GLU:N	2.22	0.70
1:H:81:GLU:HB2	1:H:85:LYS:HG3	1.73	0.70
1:F:144:ALA:HB2	1:F:150:ILE:HG21	1.73	0.70
1:N:56:ARG:HG2	1:N:56:ARG:NH1	2.07	0.70
1:H:144:ALA:HB2	1:H:150:ILE:CG2	2.21	0.70
1:O:11:ASN:ND2	1:O:61:ILE:HD13	2.08	0.69
1:D:62:TYR:CE2	1:D:68:VAL:HG23	2.28	0.68
1:D:72:GLU:OE1	1:V:72:GLU:OE1	2.11	0.68
1:I:6:MET:HE3	1:I:108:ALA:HA	1.76	0.67
1:9:15:ASN:HD21	1:9:71:ASP:H	1.42	0.67
1:P:113:ASP:OD2	1:P:116:THR:OG1	2.11	0.66
1:7:165:LEU:O	1:7:167:GLY:N	2.28	0.66
1:Q:144:ALA:HB2	1:Q:150:ILE:HG21	1.78	0.65
1:F:48:GLU:OE2	1:F:165:LEU:HB2	1.96	0.65
1:Z:3:SER:OG	1:Z:6:MET:HB2	1.97	0.65
1:M:91:TYR:CZ	1:M:135:LYS:HD3	2.32	0.65
1:F:88:GLU:HG3	1:F:138:LEU:HD11	1.79	0.65
1:6:78:LYS:HD3	1:O:69:GLU:HG3	1.79	0.64
1:O:11:ASN:HD21	1:O:68:VAL:HA	1.62	0.64
1:R:11:ASN:HD21	1:R:68:VAL:HA	1.63	0.64
1:3:136:LYS:HE3	1:K:37:GLU:OE2	1.97	0.64
1:D:112:LYS:HE3	1:Y:99:LYS:HE2	1.77	0.64
1:6:32:GLU:HG2	1:6:40:ALA:HB1	1.80	0.64
1:I:11:ASN:HD21	1:I:68:VAL:HA	1.62	0.64
1:C:72:GLU:OE1	1:U:72:GLU:OE1	2.16	0.63
1:3:149:GLN:H	1:3:149:GLN:NE2	1.96	0.63
1:I:88:GLU:HG3	1:I:138:LEU:HD11	1.81	0.63
1:O:46:GLN:HB2	1:O:161:ARG:HH12	1.64	0.62
1:5:72:GLU:OE2	1:N:72:GLU:OE1	2.18	0.62
1:1:46:GLN:NE2	1:1:130:GLU:OE1	2.32	0.62
1:4:22:TYR:CE1	1:M:73:ILE:HD11	2.34	0.62
1:Y:5:ARG:HD2	1:Y:111:GLU:OE2	2.00	0.62
1:0:135:LYS:HE3	1:0:139:ASP:OD2	2.00	0.61
1:Q:99:LYS:O	1:Q:103:GLU:HG2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:13:GLN:OE1	1:P:13:GLN:HA	2.00	0.61
1:C:78:LYS:O	1:U:67:ARG:NH2	2.34	0.61
1:0:72:GLU:OE1	1:I:72:GLU:OE1	2.19	0.60
1:B:149:GLN:HE21	1:B:149:GLN:H	1.48	0.60
1:O:11:ASN:HD22	1:O:61:ILE:HD13	1.66	0.60
1:Z:81:GLU:N	1:Z:85:LYS:HD2	2.13	0.60
1:9:149:GLN:H	1:9:149:GLN:HE21	1.49	0.60
1:X:138:LEU:HD23	1:X:138:LEU:O	2.02	0.60
1:P:42:TRP:CD1	1:P:158:LEU:HD22	2.37	0.59
1:Y:64:ARG:O	1:Y:65:ASN:HB3	2.01	0.59
1:B:37:GLU:HG3	4:B:2002:HOH:O	2.00	0.59
1:B:14:LEU:HD23	1:B:14:LEU:C	2.23	0.59
1:7:91:TYR:CZ	1:7:135:LYS:HD3	2.37	0.59
1:E:140:LYS:HD3	1:E:154:LEU:HD21	1.85	0.59
1:Y:6:MET:HE3	1:Y:108:ALA:HB2	1.85	0.59
1:M:13:GLN:NE2	1:M:16:ARG:HH11	2.01	0.59
1:5:165:LEU:HB3	1:5:166:PRO:HD3	1.86	0.58
1:4:72:GLU:OE1	1:M:72:GLU:OE1	2.21	0.58
1:1:37:GLU:OE2	1:I:136:LYS:HD3	2.03	0.58
1:T:91:TYR:CZ	1:T:135:LYS:HD3	2.39	0.58
1:J:149:GLN:H	1:J:149:GLN:HE21	1.51	0.58
1:A:2:LEU:O	1:A:3:SER:CB	2.35	0.57
1:I:6:MET:CE	1:I:108:ALA:HA	2.33	0.57
1:F:144:ALA:HB2	1:F:150:ILE:CG2	2.34	0.57
1:W:4:GLU:O	1:W:8:LYS:HG2	2.04	0.57
1:2:144:ALA:HB2	1:2:150:ILE:CG2	2.35	0.57
1:7:117:ARG:HG3	1:7:117:ARG:HH11	1.69	0.57
1:E:149:GLN:HE21	1:X:149:GLN:HG3	1.70	0.57
1:3:149:GLN:H	1:3:149:GLN:HE21	1.52	0.56
1:4:48:GLU:OE2	1:4:165:LEU:HB2	2.06	0.56
1:3:78:LYS:HE3	1:L:69:GLU:HB2	1.87	0.56
1:0:67:ARG:HG2	1:0:67:ARG:HH11	1.70	0.56
1:Y:138:LEU:O	1:Y:138:LEU:HD23	2.05	0.56
1:Z:138:LEU:HD23	1:Z:138:LEU:O	2.06	0.56
1:5:17:GLU:O	1:5:20:SER:HB2	2.06	0.56
1:R:77:PRO:HB2	1:R:80:TRP:CZ2	2.41	0.56
1:V:144:ALA:O	1:V:145:LYS:C	2.44	0.55
1:K:15:ASN:HB2	4:K:2002:HOH:O	2.06	0.55
1:3:6:MET:CE	1:3:116:THR:HG21	2.37	0.55
1:E:81:GLU:HB2	1:E:85:LYS:HG3	1.89	0.55
1:W:13:GLN:HB2	1:W:104:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:144:ALA:HB2	1:L:150:ILE:CG2	2.37	0.55
1:T:144:ALA:HB2	1:T:150:ILE:HG21	1.87	0.55
1:1:107:LEU:O	1:1:111:GLU:HG3	2.07	0.54
1:I:11:ASN:ND2	1:I:69:GLU:H	2.03	0.54
1:Y:48:GLU:OE2	1:Y:165:LEU:HB2	2.08	0.54
1:Z:13:GLN:OE1	1:Z:13:GLN:HA	2.08	0.54
1:6:165:LEU:O	1:6:167:GLY:N	2.41	0.54
1:O:99:LYS:HA	1:O:102:TYR:HD2	1.71	0.54
1:I:48:GLU:OE2	1:I:165:LEU:HB3	2.08	0.54
1:F:69:GLU:HB2	1:X:78:LYS:HD2	1.89	0.54
1:W:5:ARG:HD2	1:W:111:GLU:OE2	2.08	0.54
1:A:91:TYR:CZ	1:A:135:LYS:HG2	2.43	0.53
1:0:67:ARG:HH22	1:I:30:TYR:HA	1.71	0.53
1:1:165:LEU:HD13	1:J:165:LEU:HD12	1.91	0.53
1:O:81:GLU:HB2	1:O:85:LYS:HG2	1.90	0.53
1:F:15:ASN:HD21	1:F:71:ASP:H	1.55	0.53
1:E:91:TYR:CZ	1:E:135:LYS:HD3	2.43	0.53
1:F:92:GLU:HG2	4:F:2012:HOH:O	2.09	0.53
1:O:38:GLY:HA3	1:O:155:ASP:O	2.09	0.53
1:L:144:ALA:HB2	1:L:150:ILE:HG21	1.90	0.53
1:1:42:TRP:CD1	1:1:158:LEU:HD22	2.44	0.53
1:6:72:GLU:OE1	1:O:72:GLU:OE1	2.28	0.52
1:7:65:ASN:HD21	1:Z:135:LYS:HE3	1.74	0.52
1:O:6:MET:HE2	1:O:10:LEU:HG	1.91	0.52
1:G:165:LEU:HD13	1:Y:165:LEU:HD13	1.90	0.52
1:3:15:ASN:HD21	1:3:71:ASP:H	1.58	0.52
1:V:14:LEU:C	1:V:14:LEU:HD23	2.30	0.52
1:B:70:LEU:HD12	1:T:26:ALA:HB2	1.92	0.52
1:H:165:LEU:O	1:H:166:PRO:C	2.48	0.52
1:Q:165:LEU:O	1:Q:167:GLY:N	2.43	0.52
1:9:165:LEU:O	1:9:167:GLY:N	2.43	0.51
1:H:144:ALA:HB2	1:H:150:ILE:HG21	1.92	0.51
1:U:107:LEU:O	1:U:111:GLU:HG3	2.10	0.51
1:R:15:ASN:HD21	1:R:71:ASP:H	1.59	0.51
1:9:40:ALA:O	1:9:44:LYS:HG3	2.11	0.51
1:S:91:TYR:CZ	1:S:135:LYS:HD3	2.46	0.51
1:N:60:TYR:CZ	1:N:64:ARG:HG3	2.46	0.51
1:V:14:LEU:HD23	1:V:14:LEU:O	2.11	0.51
1:0:57:PHE:CE2	1:0:123:PHE:CZ	2.98	0.51
1:3:78:LYS:HD3	4:3:2010:HOH:O	2.10	0.51
1:B:138:LEU:C	1:B:138:LEU:HD23	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:135:LYS:NZ	1:X:139:ASP:OD1	2.42	0.50
1:H:18:LEU:O	1:H:21:ALA:HB3	2.11	0.50
1:H:144:ALA:HB2	1:H:150:ILE:HG22	1.94	0.50
1:Y:91:TYR:CZ	1:Y:135:LYS:HD3	2.47	0.50
1:Y:5:ARG:HG3	3:Y:1669:SO4:O4	2.12	0.50
1:2:149:GLN:O	1:2:153:MET:HG3	2.12	0.50
1:M:15:ASN:ND2	1:M:71:ASP:HB2	2.26	0.50
1:3:97:ILE:HD11	4:3:2004:HOH:O	2.10	0.50
1:R:140:LYS:HB3	1:R:154:LEU:HD11	1.94	0.50
1:7:22:TYR:CE1	1:P:70:LEU:HD13	2.47	0.49
1:H:13:GLN:OE1	1:H:16:ARG:NH1	2.43	0.49
1:4:149:GLN:HA	1:P:150:ILE:HD11	1.94	0.49
1:8:6:MET:CE	1:8:108:ALA:HA	2.42	0.49
1:H:17:GLU:O	1:H:20:SER:HB2	2.12	0.49
1:M:27:MET:HG2	1:M:80:TRP:CH2	2.47	0.49
1:O:149:GLN:O	1:O:152:PHE:HB3	2.13	0.49
1:W:6:MET:HE3	1:W:108:ALA:HA	1.95	0.49
1:7:22:TYR:OH	1:P:70:LEU:HB3	2.13	0.49
1:B:149:GLN:H	1:B:149:GLN:NE2	2.10	0.49
1:E:135:LYS:NZ	1:E:139:ASP:OD1	2.46	0.48
1:L:91:TYR:CZ	1:L:135:LYS:HD3	2.48	0.48
1:P:5:ARG:NH1	1:P:111:GLU:OE2	2.45	0.48
1:Q:144:ALA:HB2	1:Q:150:ILE:CG2	2.43	0.48
1:7:117:ARG:HG3	1:7:117:ARG:NH1	2.28	0.48
1:9:149:GLN:H	1:9:149:GLN:NE2	2.10	0.48
1:6:13:GLN:HB2	1:6:104:LEU:HD11	1.95	0.48
1:8:25:PHE:O	1:8:28:ALA:HB3	2.13	0.48
1:9:15:ASN:ND2	1:9:71:ASP:H	2.10	0.48
1:9:38:GLY:N	1:9:155:ASP:OD1	2.47	0.48
1:C:64:ARG:O	1:C:65:ASN:HB3	2.13	0.48
1:R:60:TYR:CZ	1:R:64:ARG:HG3	2.48	0.48
1:0:6:MET:HE3	1:0:108:ALA:HB2	1.95	0.48
1:7:104:LEU:HD22	1:7:120:LEU:HD11	1.94	0.48
1:M:152:PHE:O	1:M:155:ASP:HB3	2.14	0.48
1:7:72:GLU:OE1	1:P:72:GLU:OE1	2.32	0.48
1:7:84:LEU:HA	1:7:141:LEU:HD13	1.96	0.48
1:A:15:ASN:HB2	4:A:2004:HOH:O	2.14	0.48
1:T:165:LEU:O	1:T:166:PRO:C	2.52	0.47
1:2:144:ALA:HB2	1:2:150:ILE:HG22	1.96	0.47
1:P:130:GLU:O	1:P:134:VAL:HG23	2.13	0.47
1:Q:42:TRP:CD1	1:Q:158:LEU:HD22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:75:LYS:HD2	1:Z:71:ASP:HA	1.97	0.47
1:V:165:LEU:O	1:V:166:PRO:C	2.53	0.47
1:9:13:GLN:OE1	1:9:16:ARG:HD2	2.14	0.47
1:P:116:THR:C	1:P:120:LEU:HD12	2.31	0.47
1:6:72:GLU:HB3	1:O:75:LYS:H	1.79	0.47
1:8:140:LYS:HB3	1:8:154:LEU:HD11	1.95	0.47
1:N:56:ARG:NH1	1:N:56:ARG:CG	2.76	0.47
1:N:138:LEU:HD23	1:N:138:LEU:O	2.14	0.47
1:V:165:LEU:O	1:V:167:GLY:N	2.48	0.47
1:E:138:LEU:C	1:E:138:LEU:HD23	2.34	0.47
1:Z:91:TYR:CZ	1:Z:135:LYS:HD3	2.49	0.47
1:Y:165:LEU:O	1:Y:166:PRO:C	2.53	0.47
1:F:91:TYR:CZ	1:F:135:LYS:HD3	2.49	0.47
1:O:11:ASN:HD22	1:O:61:ILE:CD1	2.27	0.47
1:V:38:GLY:HA3	1:V:155:ASP:O	2.14	0.47
1:9:72:GLU:OE1	1:R:72:GLU:OE1	2.33	0.46
1:Z:38:GLY:HA3	1:Z:155:ASP:O	2.15	0.46
1:6:78:LYS:O	1:O:67:ARG:NH2	2.47	0.46
1:G:165:LEU:O	1:G:166:PRO:C	2.53	0.46
1:P:116:THR:HG22	1:P:120:LEU:CD1	2.43	0.46
1:X:138:LEU:HD23	1:X:138:LEU:C	2.36	0.46
1:4:70:LEU:HD12	1:M:26:ALA:HB2	1.96	0.46
1:C:165:LEU:HB3	1:C:166:PRO:HD3	1.96	0.46
1:E:138:LEU:HD23	1:E:138:LEU:O	2.16	0.46
1:T:144:ALA:O	1:T:145:LYS:C	2.53	0.46
1:2:156:LYS:O	1:2:159:SER:OG	2.28	0.46
1:B:14:LEU:HD23	1:B:14:LEU:O	2.15	0.46
1:C:135:LYS:HE3	1:C:139:ASP:OD2	2.16	0.46
1:P:64:ARG:HD2	1:P:64:ARG:HA	1.62	0.46
1:R:42:TRP:CD1	1:R:158:LEU:HD22	2.50	0.46
1:7:22:TYR:CZ	1:P:70:LEU:HB3	2.50	0.46
1:9:46:GLN:NE2	1:9:130:GLU:OE1	2.48	0.46
1:B:26:ALA:HB2	1:T:70:LEU:HD12	1.98	0.46
1:F:88:GLU:HG3	1:F:138:LEU:CD1	2.46	0.46
1:N:138:LEU:C	1:N:138:LEU:CD2	2.83	0.46
1:D:62:TYR:CE2	1:D:68:VAL:CG2	2.98	0.46
1:I:22:TYR:CD2	1:I:76:PRO:HD3	2.51	0.46
1:N:3:SER:OG	1:N:6:MET:HB2	2.16	0.46
1:S:17:GLU:O	1:S:20:SER:HB2	2.15	0.46
1:T:82:SER:HB2	1:T:83:PRO:HD2	1.98	0.46
1:W:91:TYR:CZ	1:W:135:LYS:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:72:GLU:HB3	1:O:75:LYS:N	2.30	0.46
1:9:107:LEU:O	1:9:111:GLU:HG3	2.16	0.46
1:B:3:SER:CB	1:B:6:MET:H	2.29	0.46
1:C:144:ALA:HB1	1:C:150:ILE:HB	1.97	0.46
1:E:15:ASN:HB2	4:E:2006:HOH:O	2.16	0.46
1:V:27:MET:O	1:V:31:PHE:HD2	1.98	0.46
1:4:26:ALA:HB2	1:M:70:LEU:HD12	1.98	0.45
1:E:151:LEU:HD12	1:E:151:LEU:HA	1.81	0.45
1:4:22:TYR:HE1	1:M:18:LEU:HD13	1.80	0.45
1:I:2:LEU:HG	1:I:64:ARG:HB3	1.98	0.45
1:Y:165:LEU:HD12	1:Y:165:LEU:HA	1.81	0.45
1:5:70:LEU:HD13	1:N:22:TYR:CE1	2.52	0.45
1:7:48:GLU:OE1	1:7:164:LYS:HB2	2.17	0.45
1:9:20:SER:O	1:9:21:ALA:C	2.55	0.45
1:F:17:GLU:O	1:F:20:SER:HB2	2.16	0.45
1:M:116:THR:HG22	1:M:120:LEU:HD12	1.98	0.45
1:P:3:SER:O	1:P:4:GLU:C	2.54	0.45
1:D:140:LYS:HB3	1:D:154:LEU:HD11	1.99	0.45
1:I:64:ARG:HA	1:I:64:ARG:HD2	1.65	0.45
1:M:13:GLN:NE2	1:M:16:ARG:NH1	2.63	0.45
1:N:27:MET:HG2	1:N:80:TRP:CH2	2.52	0.45
1:O:102:TYR:CD1	1:P:114:TYR:HD1	2.34	0.45
1:H:71:ASP:OD1	1:Z:75:LYS:NZ	2.49	0.45
1:I:14:LEU:HD23	1:I:14:LEU:C	2.37	0.45
1:2:46:GLN:NE2	1:2:130:GLU:OE1	2.46	0.45
1:4:81:GLU:HB2	1:4:85:LYS:HG3	1.98	0.45
1:8:95:LYS:O	1:8:99:LYS:HG3	2.16	0.45
1:1:91:TYR:CZ	1:1:95:LYS:HE2	2.52	0.45
1:C:56:ARG:HD3	4:C:2003:HOH:O	2.16	0.45
1:G:56:ARG:HG2	1:G:56:ARG:HH11	1.82	0.45
1:O:6:MET:HE3	1:O:9:ALA:HB3	1.98	0.45
1:3:26:ALA:HA	1:L:70:LEU:HD12	1.98	0.45
1:E:165:LEU:O	1:E:166:PRO:C	2.55	0.45
1:F:149:GLN:HG2	1:S:149:GLN:HG3	1.98	0.45
1:O:154:LEU:O	1:O:155:ASP:C	2.55	0.45
1:R:11:ASN:ND2	1:R:69:GLU:H	2.14	0.45
1:V:140:LYS:HB3	1:V:154:LEU:HD11	1.98	0.45
1:D:2:LEU:HB2	4:D:2007:HOH:O	2.15	0.44
1:G:140:LYS:HD3	1:G:154:LEU:HD21	1.99	0.44
1:O:165:LEU:O	1:O:166:PRO:C	2.56	0.44
1:6:64:ARG:HA	1:6:64:ARG:HD2	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ALA:HB1	1:B:150:ILE:HB	1.98	0.44
1:H:144:ALA:O	1:H:146:ASP:N	2.49	0.44
1:M:138:LEU:C	1:M:138:LEU:HD23	2.38	0.44
1:H:6:MET:HE3	1:H:108:ALA:HB2	2.00	0.44
1:2:149:GLN:HG3	1:H:150:ILE:HD11	2.00	0.44
1:2:149:GLN:HE21	1:G:149:GLN:HG2	1.83	0.44
1:4:6:MET:HE3	1:4:108:ALA:HB2	1.99	0.44
1:9:38:GLY:HA3	1:9:155:ASP:O	2.18	0.44
1:M:13:GLN:HE21	1:M:16:ARG:NH1	2.14	0.44
1:7:144:ALA:O	1:7:145:LYS:C	2.56	0.44
1:8:143:PHE:HZ	1:M:151:LEU:HD23	1.82	0.44
1:F:72:GLU:OE1	1:X:72:GLU:OE1	2.36	0.44
1:H:147:SER:HA	1:H:148:PRO:HD2	1.71	0.44
1:R:140:LYS:HD3	1:R:154:LEU:HD21	2.00	0.44
1:Z:64:ARG:HD2	1:Z:64:ARG:HA	1.81	0.44
1:1:13:GLN:HG2	1:1:57:PHE:CZ	2.53	0.44
1:4:64:ARG:HA	1:4:64:ARG:HD2	1.87	0.44
1:8:67:ARG:NH2	1:Q:78:LYS:O	2.51	0.44
1:D:11:ASN:O	1:D:12:ASP:C	2.54	0.44
1:N:144:ALA:O	1:N:145:LYS:C	2.57	0.44
1:5:69:GLU:OE2	1:N:75:LYS:NZ	2.35	0.43
1:H:102:TYR:CE1	1:K:114:TYR:HB2	2.53	0.43
1:M:165:LEU:C	1:M:167:GLY:H	2.20	0.43
1:O:55:LEU:HD23	1:O:55:LEU:HA	1.82	0.43
1:1:58:TYR:HH	1:J:32:GLU:HG3	1.83	0.43
1:W:150:ILE:O	1:W:154:LEU:HB2	2.17	0.43
1:N:149:GLN:H	1:N:149:GLN:NE2	1.98	0.43
1:W:34:LEU:HD12	1:W:34:LEU:HA	1.82	0.43
1:A:144:ALA:HB2	1:A:150:ILE:CG2	2.48	0.43
1:Y:116:THR:O	1:Y:120:LEU:HG	2.18	0.43
1:I:5:ARG:H	1:I:5:ARG:HD3	1.83	0.43
1:0:67:ARG:HG2	1:0:67:ARG:NH1	2.33	0.43
1:6:46:GLN:NE2	1:6:130:GLU:OE1	2.52	0.43
1:I:40:ALA:O	1:I:44:LYS:HG3	2.19	0.43
1:B:64:ARG:HD2	1:B:64:ARG:HA	1.72	0.43
1:G:149:GLN:H	1:G:149:GLN:NE2	2.17	0.43
1:O:64:ARG:HA	1:O:64:ARG:HD2	1.71	0.43
1:V:62:TYR:CE2	1:V:68:VAL:HG23	2.53	0.43
1:Y:6:MET:HE3	1:Y:108:ALA:CB	2.49	0.43
1:4:57:PHE:CE2	1:4:123:PHE:CZ	3.06	0.43
1:Z:34:LEU:HD12	1:Z:36:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:135:LYS:HE3	1:0:139:ASP:CG	2.39	0.43
1:2:144:ALA:HB2	1:2:150:ILE:HG21	2.00	0.43
1:3:6:MET:HE1	1:3:116:THR:HG21	2.01	0.43
1:I:67:ARG:NH1	1:I:68:VAL:O	2.52	0.43
1:Q:107:LEU:HD12	1:Q:107:LEU:HA	1.83	0.43
1:0:17:GLU:O	1:0:20:SER:HB2	2.19	0.43
1:0:31:PHE:HE1	1:0:83:PRO:HB3	1.83	0.43
1:I:97:ILE:HD13	1:I:97:ILE:HA	1.92	0.43
1:2:15:ASN:HD21	1:2:71:ASP:H	1.66	0.42
1:7:58:TYR:CD1	1:7:58:TYR:C	2.93	0.42
1:C:93:HIS:O	1:C:96:PHE:HB3	2.19	0.42
1:2:138:LEU:C	1:2:138:LEU:HD23	2.40	0.42
1:G:15[B]:ASN:ND2	1:Y:22:TYR:OH	2.51	0.42
1:O:85:LYS:HD2	1:O:85:LYS:HA	1.44	0.42
1:0:70:LEU:HD12	1:I:26:ALA:HA	2.02	0.42
1:A:3:SER:O	1:A:4:GLU:C	2.57	0.42
1:U:57:PHE:CE1	1:U:119:PHE:HE2	2.38	0.42
1:F:165:LEU:O	1:F:167:GLY:N	2.52	0.42
1:M:13:GLN:HE21	1:M:16:ARG:HH11	1.65	0.42
1:S:81:GLU:HB2	1:S:85:LYS:HG3	2.01	0.42
1:B:165:LEU:O	1:B:166:PRO:C	2.55	0.42
1:C:144:ALA:HB2	1:C:150:ILE:HG21	2.02	0.42
1:H:14:LEU:O	1:H:14:LEU:HD23	2.20	0.42
1:Z:55:LEU:HA	1:Z:55:LEU:HD23	1.64	0.42
1:G:149:GLN:H	1:G:149:GLN:HE21	1.66	0.42
1:H:38:GLY:HA3	1:H:155:ASP:O	2.20	0.42
1:2:165:LEU:HB3	1:2:166:PRO:HD3	2.02	0.42
1:8:27:MET:O	1:8:30:TYR:HB3	2.20	0.42
1:H:60:TYR:CZ	1:H:64:ARG:HG3	2.55	0.42
1:Y:138:LEU:HD23	1:Y:138:LEU:C	2.39	0.42
1:A:147:SER:HA	1:A:148:PRO:HD2	1.91	0.42
1:M:23:LEU:O	1:M:27:MET:HG3	2.20	0.42
1:O:55:LEU:O	1:O:58:TYR:HB3	2.20	0.42
1:C:23:LEU:O	1:C:26:ALA:HB3	2.20	0.42
1:H:58:TYR:CD1	1:H:58:TYR:C	2.93	0.42
1:N:135:LYS:HZ3	1:N:139:ASP:CG	2.23	0.42
1:2:91:TYR:CZ	1:2:135:LYS:HD3	2.55	0.41
1:E:107:LEU:O	1:E:111:GLU:HG3	2.20	0.41
1:H:143:PHE:C	1:H:145:LYS:H	2.23	0.41
1:H:144:ALA:O	1:H:145:LYS:C	2.58	0.41
1:K:138:LEU:HD23	1:K:138:LEU:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:97:ILE:HD13	1:N:97:ILE:HA	1.91	0.41
1:O:99:LYS:HA	1:O:102:TYR:CD2	2.54	0.41
1:P:148:PRO:HD2	1:P:149:GLN:OE1	2.20	0.41
1:Q:87:PHE:CE1	1:Q:137:ILE:HG21	2.55	0.41
1:6:20:SER:O	1:6:21:ALA:C	2.57	0.41
1:7:64:ARG:O	1:7:65:ASN:CB	2.68	0.41
1:7:83:PRO:O	1:7:86:ALA:HB3	2.20	0.41
1:D:22:TYR:CD2	1:D:76:PRO:HD3	2.55	0.41
1:Z:20:SER:O	1:Z:24:TYR:CD2	2.73	0.41
1:Z:99:LYS:HA	1:Z:102:TYR:HD2	1.85	0.41
1:0:26:ALA:HA	1:I:70:LEU:HD12	2.01	0.41
1:3:82:SER:O	1:3:83:PRO:C	2.58	0.41
1:B:55:LEU:HD23	1:B:55:LEU:HA	1.93	0.41
1:C:154:LEU:HD23	1:C:154:LEU:HA	1.82	0.41
1:E:72:GLU:CD	1:W:72:GLU:OE1	2.59	0.41
1:O:6:MET:HE2	1:O:6:MET:O	2.20	0.41
1:V:138:LEU:C	1:V:138:LEU:HD23	2.41	0.41
1:0:67:ARG:HD3	1:I:78:LYS:HE2	2.02	0.41
1:O:99:LYS:HB3	1:O:99:LYS:HE2	1.84	0.41
1:A:117:ARG:O	1:A:117:ARG:HG3	2.19	0.41
1:K:144:ALA:O	1:K:145:LYS:C	2.59	0.41
1:P:68:VAL:HG12	1:P:69:GLU:N	2.36	0.41
1:S:13:GLN:HG2	1:S:57:PHE:CZ	2.55	0.41
1:X:64:ARG:HA	1:X:64:ARG:HD2	1.93	0.41
1:R:15:ASN:ND2	1:R:71:ASP:H	2.19	0.41
1:Y:6:MET:HE3	1:Y:108:ALA:CA	2.51	0.41
1:O:18:LEU:HD23	1:O:18:LEU:HA	1.95	0.41
1:T:1:MET:CE	1:U:131:GLU:OE1	2.68	0.41
1:3:6:MET:O	1:3:7:LEU:C	2.59	0.41
1:3:38:GLY:HA3	1:3:155:ASP:O	2.21	0.41
1:6:32:GLU:HG2	1:6:40:ALA:CB	2.48	0.41
1:B:135:LYS:HE3	1:B:139:ASP:OD2	2.21	0.41
1:D:14:LEU:C	1:D:14:LEU:HD23	2.41	0.41
1:K:147:SER:HA	1:K:148:PRO:HD2	1.85	0.41
1:K:154:LEU:HA	1:K:154:LEU:HD23	1.86	0.41
1:M:144:ALA:HB1	1:M:150:ILE:HB	2.03	0.41
1:P:21:ALA:HA	1:P:47:ALA:HA	2.02	0.41
1:S:64:ARG:HD2	1:S:64:ARG:HA	1.74	0.41
1:T:60:TYR:CZ	1:T:64:ARG:HG3	2.55	0.41
1:1:24:TYR:HD1	1:1:43:MET:SD	2.43	0.41
1:1:60:TYR:O	1:1:63:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:48:GLU:OE2	1:2:163:PRO:HB2	2.21	0.41
1:I:60:TYR:HB2	1:I:119:PHE:CE1	2.56	0.41
1:Q:46:GLN:O	1:Q:50:GLU:HG2	2.21	0.41
1:1:77:PRO:HB2	1:1:80:TRP:CZ2	2.55	0.40
1:4:165:LEU:O	1:4:166:PRO:C	2.58	0.40
1:5:64:ARG:HA	1:5:64:ARG:HD2	1.63	0.40
1:9:154:LEU:HD23	1:9:154:LEU:HA	1.94	0.40
1:B:22:TYR:CZ	1:T:70:LEU:HB3	2.56	0.40
1:E:95:LYS:HD3	4:E:2016:HOH:O	2.21	0.40
1:L:10:LEU:HB3	1:L:61:ILE:HD11	2.03	0.40
1:Z:82:SER:O	1:Z:83:PRO:C	2.59	0.40
1:7:135:LYS:NZ	1:7:139:ASP:OD1	2.54	0.40
1:L:15:ASN:HB2	4:L:2002:HOH:O	2.20	0.40
1:L:114:TYR:HB3	1:Q:124:ILE:HD13	2.03	0.40
1:S:57:PHE:O	1:S:61:ILE:HG13	2.21	0.40
1:W:31:PHE:O	1:W:32:GLU:C	2.59	0.40
1:Y:81:GLU:HB2	1:Y:85:LYS:HG3	2.03	0.40
1:7:117:ARG:HD2	1:7:117:ARG:HA	1.65	0.40
1:H:64:ARG:HA	1:H:64:ARG:HD2	1.86	0.40
1:6:13:GLN:OE1	1:6:16:ARG:HD2	2.22	0.40
1:N:46:GLN:NE2	1:N:130:GLU:OE1	2.54	0.40
1:2:60:TYR:CZ	1:2:64:ARG:HG3	2.56	0.40
1:C:64:ARG:HA	1:C:64:ARG:HD2	1.86	0.40
1:P:13:GLN:HA	1:P:16:ARG:HB2	2.03	0.40
1:V:42:TRP:CD1	1:V:158:LEU:HD22	2.57	0.40
1:Y:144:ALA:O	1:Y:146:ASP:N	2.55	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	0	165/174 (95%)	161 (98%)	1 (1%)	3 (2%)	8	28
1	1	165/174 (95%)	159 (96%)	5 (3%)	1 (1%)	25	56
1	2	165/174 (95%)	160 (97%)	2 (1%)	3 (2%)	8	28
1	3	165/174 (95%)	160 (97%)	2 (1%)	3 (2%)	8	28
1	4	165/174 (95%)	157 (95%)	8 (5%)	0	100	100
1	5	165/174 (95%)	161 (98%)	4 (2%)	0	100	100
1	6	165/174 (95%)	157 (95%)	7 (4%)	1 (1%)	25	56
1	7	165/174 (95%)	160 (97%)	3 (2%)	2 (1%)	13	39
1	8	165/174 (95%)	158 (96%)	5 (3%)	2 (1%)	13	39
1	9	165/174 (95%)	160 (97%)	3 (2%)	2 (1%)	13	39
1	A	165/174 (95%)	158 (96%)	2 (1%)	5 (3%)	4	15
1	B	165/174 (95%)	160 (97%)	4 (2%)	1 (1%)	25	56
1	C	165/174 (95%)	157 (95%)	7 (4%)	1 (1%)	25	56
1	D	165/174 (95%)	159 (96%)	3 (2%)	3 (2%)	8	28
1	E	165/174 (95%)	161 (98%)	2 (1%)	2 (1%)	13	39
1	F	165/174 (95%)	158 (96%)	5 (3%)	2 (1%)	13	39
1	G	166/174 (95%)	158 (95%)	7 (4%)	1 (1%)	25	56
1	H	165/174 (95%)	157 (95%)	6 (4%)	2 (1%)	13	39
1	I	165/174 (95%)	159 (96%)	5 (3%)	1 (1%)	25	56
1	J	165/174 (95%)	161 (98%)	2 (1%)	2 (1%)	13	39
1	K	165/174 (95%)	160 (97%)	4 (2%)	1 (1%)	25	56
1	L	165/174 (95%)	156 (94%)	9 (6%)	0	100	100
1	M	165/174 (95%)	153 (93%)	9 (6%)	3 (2%)	8	28
1	N	165/174 (95%)	163 (99%)	1 (1%)	1 (1%)	25	56
1	O	165/174 (95%)	155 (94%)	6 (4%)	4 (2%)	6	20
1	P	165/174 (95%)	158 (96%)	4 (2%)	3 (2%)	8	28
1	Q	165/174 (95%)	160 (97%)	3 (2%)	2 (1%)	13	39
1	R	165/174 (95%)	158 (96%)	5 (3%)	2 (1%)	13	39
1	S	165/174 (95%)	160 (97%)	3 (2%)	2 (1%)	13	39
1	T	166/174 (95%)	160 (96%)	5 (3%)	1 (1%)	25	56
1	U	165/174 (95%)	159 (96%)	4 (2%)	2 (1%)	13	39
1	V	165/174 (95%)	159 (96%)	4 (2%)	2 (1%)	13	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	166/174 (95%)	163 (98%)	2 (1%)	1 (1%)	25	56
1	X	165/174 (95%)	159 (96%)	4 (2%)	2 (1%)	13	39
1	Y	165/174 (95%)	158 (96%)	6 (4%)	1 (1%)	25	56
1	Z	165/174 (95%)	158 (96%)	6 (4%)	1 (1%)	25	56
All	All	5943/6264 (95%)	5720 (96%)	158 (3%)	65 (1%)	14	41

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	145	LYS
1	3	166	PRO
1	7	166	PRO
1	9	145	LYS
1	A	3	SER
1	D	145	LYS
1	P	145	LYS
1	Q	145	LYS
1	S	145	LYS
1	V	145	LYS
1	V	166	PRO
1	0	166	PRO
1	7	145	LYS
1	8	145	LYS
1	F	166	PRO
1	G	145	LYS
1	H	145	LYS
1	I	145	LYS
1	M	115	SER
1	M	145	LYS
1	P	65	ASN
1	U	145	LYS
1	W	145	LYS
1	X	145	LYS
1	Y	145	LYS
1	Z	145	LYS
1	6	166	PRO
1	A	165	LEU
1	A	166	PRO
1	D	166	PRO
1	F	145	LYS
1	J	145	LYS

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Mol	Chain	Res	Type
1	K	145	LYS
1	O	145	LYS
1	O	146	ASP
1	R	165	LEU
1	0	145	LYS
1	9	166	PRO
1	A	146	ASP
1	A	147	SER
1	C	166	PRO
1	D	165	LEU
1	O	147	SER
1	P	166	PRO
1	R	145	LYS
1	2	144	ALA
1	2	145	LYS
1	2	166	PRO
1	3	145	LYS
1	H	146	ASP
1	O	166	PRO
1	T	143	PHE
1	U	166	PRO
1	3	148	PRO
1	J	166	PRO
1	X	166	PRO
1	0	165	LEU
1	E	165	LEU
1	M	166	PRO
1	S	165	LEU
1	B	166	PRO
1	E	166	PRO
1	Q	166	PRO
1	8	166	PRO
1	N	166	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	142/147 (97%)	128 (90%)	14 (10%)	8	23
1	1	142/147 (97%)	133 (94%)	9 (6%)	18	46
1	2	142/147 (97%)	134 (94%)	8 (6%)	21	51
1	3	142/147 (97%)	132 (93%)	10 (7%)	15	40
1	4	142/147 (97%)	135 (95%)	7 (5%)	25	57
1	5	142/147 (97%)	138 (97%)	4 (3%)	43	77
1	6	142/147 (97%)	136 (96%)	6 (4%)	30	63
1	7	142/147 (97%)	128 (90%)	14 (10%)	8	23
1	8	142/147 (97%)	132 (93%)	10 (7%)	15	40
1	9	142/147 (97%)	133 (94%)	9 (6%)	18	46
1	A	142/147 (97%)	135 (95%)	7 (5%)	25	57
1	B	142/147 (97%)	134 (94%)	8 (6%)	21	51
1	C	142/147 (97%)	136 (96%)	6 (4%)	30	63
1	D	142/147 (97%)	134 (94%)	8 (6%)	21	51
1	E	142/147 (97%)	135 (95%)	7 (5%)	25	57
1	F	142/147 (97%)	132 (93%)	10 (7%)	15	40
1	G	143/147 (97%)	137 (96%)	6 (4%)	30	63
1	H	142/147 (97%)	134 (94%)	8 (6%)	21	51
1	I	142/147 (97%)	135 (95%)	7 (5%)	25	57
1	J	142/147 (97%)	136 (96%)	6 (4%)	30	63
1	K	142/147 (97%)	132 (93%)	10 (7%)	15	40
1	L	142/147 (97%)	135 (95%)	7 (5%)	25	57
1	M	142/147 (97%)	132 (93%)	10 (7%)	15	40
1	N	142/147 (97%)	137 (96%)	5 (4%)	36	70
1	O	142/147 (97%)	130 (92%)	12 (8%)	10	31
1	P	142/147 (97%)	135 (95%)	7 (5%)	25	57
1	Q	142/147 (97%)	133 (94%)	9 (6%)	18	46
1	R	142/147 (97%)	134 (94%)	8 (6%)	21	51
1	S	142/147 (97%)	134 (94%)	8 (6%)	21	51
1	T	143/147 (97%)	138 (96%)	5 (4%)	36	70
1	U	142/147 (97%)	137 (96%)	5 (4%)	36	70
1	V	142/147 (97%)	134 (94%)	8 (6%)	21	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	143/147 (97%)	137 (96%)	6 (4%)	30	63
1	X	142/147 (97%)	136 (96%)	6 (4%)	30	63
1	Y	142/147 (97%)	136 (96%)	6 (4%)	30	63
1	Z	142/147 (97%)	136 (96%)	6 (4%)	30	63
All	All	5115/5292 (97%)	4833 (94%)	282 (6%)	21	52

All (282) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	1	MET
1	0	4	GLU
1	0	5	ARG
1	0	6	MET
1	0	8	LYS
1	0	22	TYR
1	0	72	GLU
1	0	79	GLU
1	0	85	LYS
1	0	96	PHE
1	0	100	SER
1	0	110	GLU
1	0	133	SER
1	0	154	LEU
1	1	1	MET
1	1	5	ARG
1	1	6	MET
1	1	22	TYR
1	1	32	GLU
1	1	72	GLU
1	1	100	SER
1	1	149	GLN
1	1	154	LEU
1	2	15	ASN
1	2	22	TYR
1	2	65	ASN
1	2	98	SER
1	2	100	SER
1	2	133	SER
1	2	149	GLN
1	2	156	LYS
1	3	1	MET

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Mol	Chain	Res	Type
1	3	5	ARG
1	3	15	ASN
1	3	22	TYR
1	3	72	GLU
1	3	136	LYS
1	3	143	PHE
1	3	146	ASP
1	3	149	GLN
1	3	165	LEU
1	4	1	MET
1	4	6	MET
1	4	15	ASN
1	4	72	GLU
1	4	96	PHE
1	4	104	LEU
1	4	109	GLU
1	5	22	TYR
1	5	72	GLU
1	5	100	SER
1	5	104	LEU
1	6	6	MET
1	6	22	TYR
1	6	72	GLU
1	6	78	LYS
1	6	88	GLU
1	6	149	GLN
1	7	4	GLU
1	7	22	TYR
1	7	58	TYR
1	7	65	ASN
1	7	98	SER
1	7	100	SER
1	7	104	LEU
1	7	109	GLU
1	7	117	ARG
1	7	119	PHE
1	7	133	SER
1	7	146	ASP
1	7	154	LEU
1	7	164	LYS
1	8	1	MET
1	8	5	ARG

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Mol	Chain	Res	Type
1	8	6	MET
1	8	20	SER
1	8	22	TYR
1	8	85	LYS
1	8	104	LEU
1	8	133	SER
1	8	154	LEU
1	8	165	LEU
1	9	5	ARG
1	9	15	ASN
1	9	22	TYR
1	9	65	ASN
1	9	133	SER
1	9	136	LYS
1	9	143	PHE
1	9	149	GLN
1	9	165	LEU
1	A	1	MET
1	A	3	SER
1	A	22	TYR
1	A	72	GLU
1	A	110	GLU
1	A	135	LYS
1	A	149	GLN
1	B	5	ARG
1	B	20	SER
1	B	22	TYR
1	B	34	LEU
1	B	67	ARG
1	B	72	GLU
1	B	149	GLN
1	B	154	LEU
1	C	1	MET
1	C	5	ARG
1	C	6	MET
1	C	34	LEU
1	C	72	GLU
1	C	149	GLN
1	D	1	MET
1	D	6	MET
1	D	22	TYR
1	D	72	GLU

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Mol	Chain	Res	Type
1	D	92	GLU
1	D	104	LEU
1	D	145	LYS
1	D	149	GLN
1	E	6	MET
1	E	22	TYR
1	E	67	ARG
1	E	92	GLU
1	E	104	LEU
1	E	110	GLU
1	E	149	GLN
1	F	1	MET
1	F	6	MET
1	F	15	ASN
1	F	22	TYR
1	F	72	GLU
1	F	100	SER
1	F	119	PHE
1	F	146	ASP
1	F	152	PHE
1	F	165	LEU
1	G	1	MET
1	G	67	ARG
1	G	78	LYS
1	G	81	GLU
1	G	100	SER
1	G	149	GLN
1	H	1	MET
1	H	6	MET
1	H	22	TYR
1	H	58	TYR
1	H	67	ARG
1	H	110	GLU
1	H	119	PHE
1	H	147	SER
1	I	5	ARG
1	I	72	GLU
1	I	104	LEU
1	I	119	PHE
1	I	136	LYS
1	I	143	PHE
1	I	145	LYS

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Mol	Chain	Res	Type
1	J	22	TYR
1	J	33	ASP
1	J	72	GLU
1	J	112	LYS
1	J	149	GLN
1	J	165	LEU
1	K	1	MET
1	K	6	MET
1	K	22	TYR
1	K	33	ASP
1	K	72	GLU
1	K	81	GLU
1	K	104	LEU
1	K	121	GLU
1	K	149	GLN
1	K	165	LEU
1	L	6	MET
1	L	22	TYR
1	L	69	GLU
1	L	92	GLU
1	L	133	SER
1	L	149	GLN
1	L	165	LEU
1	M	1	MET
1	M	6	MET
1	M	22	TYR
1	M	69	GLU
1	M	72	GLU
1	M	99	LYS
1	M	103	GLU
1	M	149	GLN
1	M	154	LEU
1	M	164	LYS
1	N	4	GLU
1	N	6	MET
1	N	22	TYR
1	N	56	ARG
1	N	149	GLN
1	O	1	MET
1	O	4	GLU
1	O	11	ASN
1	O	22	TYR

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Mol	Chain	Res	Type
1	O	72	GLU
1	O	83	PRO
1	O	85	LYS
1	O	92	GLU
1	O	98	SER
1	O	99	LYS
1	O	100	SER
1	O	133	SER
1	P	22	TYR
1	P	95	LYS
1	P	100	SER
1	P	133	SER
1	P	149	GLN
1	P	153	MET
1	P	164	LYS
1	Q	1	MET
1	Q	6	MET
1	Q	22	TYR
1	Q	75	LYS
1	Q	100	SER
1	Q	103	GLU
1	Q	145	LYS
1	Q	146	ASP
1	Q	156	LYS
1	R	1	MET
1	R	5	ARG
1	R	6	MET
1	R	15	ASN
1	R	22	TYR
1	R	72	GLU
1	R	110	GLU
1	R	165	LEU
1	S	1	MET
1	S	22	TYR
1	S	34	LEU
1	S	67	ARG
1	S	99	LYS
1	S	146	ASP
1	S	149	GLN
1	S	165	LEU
1	T	1	MET
1	T	22	TYR

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Mol	Chain	Res	Type
1	T	34	LEU
1	T	72	GLU
1	T	154	LEU
1	U	1	MET
1	U	34	LEU
1	U	72	GLU
1	U	154	LEU
1	U	165	LEU
1	V	1	MET
1	V	6	MET
1	V	72	GLU
1	V	103	GLU
1	V	145	LYS
1	V	149	GLN
1	V	153	MET
1	V	154	LEU
1	W	34	LEU
1	W	81	GLU
1	W	119	PHE
1	W	135	LYS
1	W	149	GLN
1	W	154	LEU
1	X	5	ARG
1	X	22	TYR
1	X	65	ASN
1	X	104	LEU
1	X	149	GLN
1	X	157	GLU
1	Y	5	ARG
1	Y	67	ARG
1	Y	100	SER
1	Y	104	LEU
1	Y	149	GLN
1	Y	165	LEU
1	Z	6	MET
1	Z	11	ASN
1	Z	22	TYR
1	Z	72	GLU
1	Z	149	GLN
1	Z	165	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	149	GLN
1	2	15	ASN
1	2	149	GLN
1	3	15	ASN
1	3	149	GLN
1	6	149	GLN
1	7	15	ASN
1	7	65	ASN
1	8	149	GLN
1	9	15	ASN
1	9	65	ASN
1	9	149	GLN
1	B	149	GLN
1	F	15	ASN
1	G	149	GLN
1	I	11	ASN
1	I	149	GLN
1	J	149	GLN
1	K	149	GLN
1	M	13	GLN
1	M	15	ASN
1	N	65	ASN
1	N	149	GLN
1	O	149	GLN
1	Q	149	GLN
1	R	11	ASN
1	R	15	ASN
1	R	149	GLN
1	S	149	GLN
1	U	149	GLN
1	W	149	GLN
1	X	149	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 134 ligands modelled in this entry, 108 are monoatomic - leaving 26 for Mogul analysis.

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	$\#\|Z\| > 2$
3	SO4	C	1168	-	4,4,4	0.13	0	6,6,6	0.26	0
3	SO4	I	1168	-	4,4,4	0.38	0	6,6,6	0.51	0
3	SO4	I	1169	-	4,4,4	0.17	0	6,6,6	0.68	0
3	SO4	R	1168	-	4,4,4	0.18	0	6,6,6	0.25	0
3	SO4	V	1668	-	4,4,4	0.17	0	6,6,6	0.44	0
3	SO4	3	1669	-	4,4,4	0.23	0	6,6,6	0.53	0
3	SO4	B	1168	-	4,4,4	0.20	0	6,6,6	0.23	0
3	SO4	H	1168	-	4,4,4	0.17	0	6,6,6	0.43	0
3	SO4	Y	1669	-	4,4,4	0.24	0	6,6,6	0.29	0
3	SO4	G	1168	-	4,4,4	0.23	0	6,6,6	0.38	0
3	SO4	2	1668	-	4,4,4	0.16	0	6,6,6	0.25	0
3	SO4	Y	1668	-	4,4,4	0.19	0	6,6,6	0.30	0
3	SO4	3	1668	-	4,4,4	0.12	0	6,6,6	0.53	0
3	SO4	G	1169	-	4,4,4	0.18	0	6,6,6	0.27	0
3	SO4	O	1168	-	4,4,4	0.12	0	6,6,6	0.48	0
3	SO4	W	1668	-	4,4,4	0.20	0	6,6,6	0.40	0
3	SO4	S	1668	-	4,4,4	0.16	0	6,6,6	0.21	0
3	SO4	V	1669	-	4,4,4	0.14	0	6,6,6	0.44	0
3	SO4	8	1668	-	4,4,4	0.16	0	6,6,6	0.36	0
3	SO4	J	1168	-	4,4,4	0.20	0	6,6,6	0.27	0
3	SO4	C	1169	-	4,4,4	0.29	0	6,6,6	0.51	0
3	SO4	C	1170	-	4,4,4	0.15	0	6,6,6	0.30	0
3	SO4	T	1668	-	4,4,4	0.21	0	6,6,6	0.37	0
3	SO4	1	1668	-	4,4,4	0.18	0	6,6,6	0.18	0
3	SO4	A	1168	-	4,4,4	0.17	0	6,6,6	0.44	0
3	SO4	B	1169	-	4,4,4	0.15	0	6,6,6	0.50	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Y	1669	SO4	1	0

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.