



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 03:16 AM BST

PDB ID : 6KRK  
Title : Peroxiredoxin from *Aeropyrum pernix* K1 (ApPrx) 0Cys mutant  
Authors : Himiyama, T.; Nakamura, T.  
Deposited on : 2019-08-22  
Resolution : 1.80 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](mailto: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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

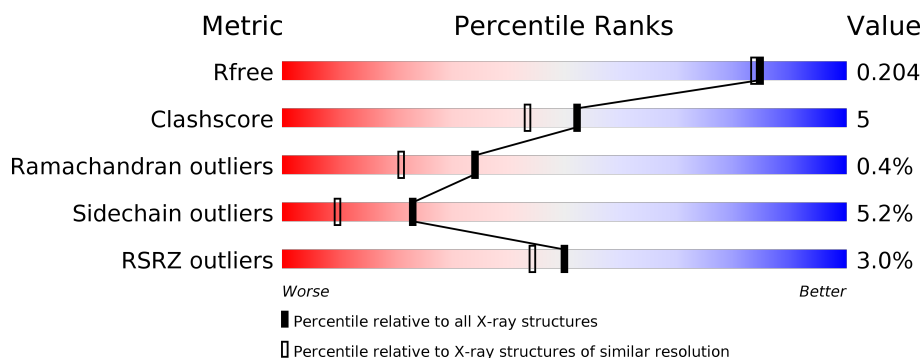
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	250	<div> <div>4%</div> <div>81% 16% .</div> </div>
1	B	250	<div> <div>2%</div> <div>82% 14% ..</div> </div>
1	C	250	<div> <div>3%</div> <div>82% 14% ...</div> </div>
1	D	250	<div> <div>3%</div> <div>82% 15% ..</div> </div>
1	E	250	<div> <div>2%</div> <div>82% 14% ..</div> </div>
1	F	250	<div> <div>2%</div> <div>82% 14% ..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	250	<div><div></div><div>2%</div><div>80%</div><div>15%</div><div>...</div></div>
1	H	250	<div><div></div><div>4%</div><div>81%</div><div>14%</div><div>..</div></div>
1	I	250	<div><div></div><div>3%</div><div>84%</div><div>12%</div><div>..</div></div>
1	J	250	<div><div></div><div>3%</div><div>82%</div><div>13%</div><div>...</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21085 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	244	Total 1973	C 1268	N 347	O 354	S 4	0	0	0
1	B	244	Total 1973	C 1268	N 347	O 354	S 4	0	0	0
1	C	244	Total 1973	C 1268	N 347	O 354	S 4	0	0	0
1	D	244	Total 1973	C 1268	N 347	O 354	S 4	0	0	0
1	E	244	Total 1973	C 1268	N 347	O 354	S 4	0	0	0
1	F	244	Total 1973	C 1268	N 347	O 354	S 4	0	0	0
1	G	244	Total 1973	C 1268	N 347	O 354	S 4	0	0	0
1	H	244	Total 1973	C 1268	N 347	O 354	S 4	0	0	0
1	I	244	Total 1973	C 1268	N 347	O 354	S 4	0	0	0
1	J	244	Total 1973	C 1268	N 347	O 354	S 4	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

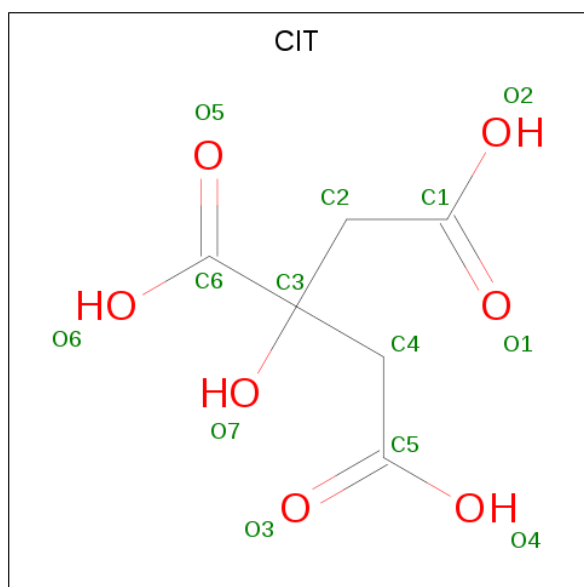
Chain	Residue	Modelled	Actual	Comment	Reference
A	50	SER	CYS	engineered mutation	UNP Q9Y9L0
A	207	SER	CYS	engineered mutation	UNP Q9Y9L0
A	213	SER	CYS	engineered mutation	UNP Q9Y9L0
B	50	SER	CYS	engineered mutation	UNP Q9Y9L0
B	207	SER	CYS	engineered mutation	UNP Q9Y9L0
B	213	SER	CYS	engineered mutation	UNP Q9Y9L0
C	50	SER	CYS	engineered mutation	UNP Q9Y9L0
C	207	SER	CYS	engineered mutation	UNP Q9Y9L0
C	213	SER	CYS	engineered mutation	UNP Q9Y9L0

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	50	SER	CYS	engineered mutation	UNP Q9Y9L0
D	207	SER	CYS	engineered mutation	UNP Q9Y9L0
D	213	SER	CYS	engineered mutation	UNP Q9Y9L0
E	50	SER	CYS	engineered mutation	UNP Q9Y9L0
E	207	SER	CYS	engineered mutation	UNP Q9Y9L0
E	213	SER	CYS	engineered mutation	UNP Q9Y9L0
F	50	SER	CYS	engineered mutation	UNP Q9Y9L0
F	207	SER	CYS	engineered mutation	UNP Q9Y9L0
F	213	SER	CYS	engineered mutation	UNP Q9Y9L0
G	50	SER	CYS	engineered mutation	UNP Q9Y9L0
G	207	SER	CYS	engineered mutation	UNP Q9Y9L0
G	213	SER	CYS	engineered mutation	UNP Q9Y9L0
H	50	SER	CYS	engineered mutation	UNP Q9Y9L0
H	207	SER	CYS	engineered mutation	UNP Q9Y9L0
H	213	SER	CYS	engineered mutation	UNP Q9Y9L0
I	50	SER	CYS	engineered mutation	UNP Q9Y9L0
I	207	SER	CYS	engineered mutation	UNP Q9Y9L0
I	213	SER	CYS	engineered mutation	UNP Q9Y9L0
J	50	SER	CYS	engineered mutation	UNP Q9Y9L0
J	207	SER	CYS	engineered mutation	UNP Q9Y9L0
J	213	SER	CYS	engineered mutation	UNP Q9Y9L0

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		
2	G	1	Total	C	O	0	0
			13	6	7		
2	H	1	Total	C	O	0	0
			13	6	7		
2	I	1	Total	C	O	0	0
			13	6	7		
2	J	1	Total	C	O	0	0
			13	6	7		

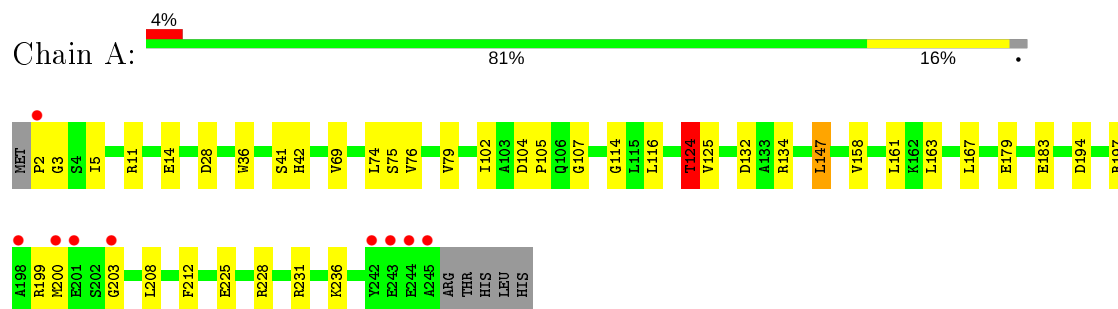
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		
3	B	123	Total	O	0	0
			123	123		
3	C	138	Total	O	0	0
			138	138		
3	D	123	Total	O	0	0
			123	123		
3	E	124	Total	O	0	0
			124	124		
3	F	126	Total	O	0	0
			126	126		
3	G	117	Total	O	0	0
			117	117		
3	H	121	Total	O	0	0
			121	121		
3	I	116	Total	O	0	0
			116	116		
3	J	109	Total	O	0	0
			109	109		

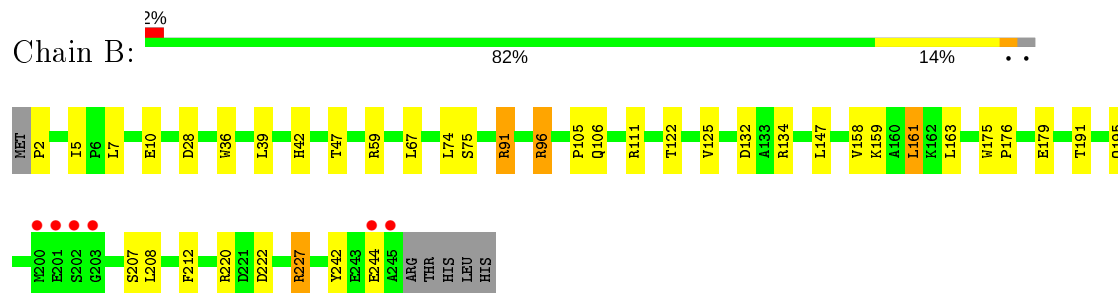
### 3 Residue-property plots [i](#)

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

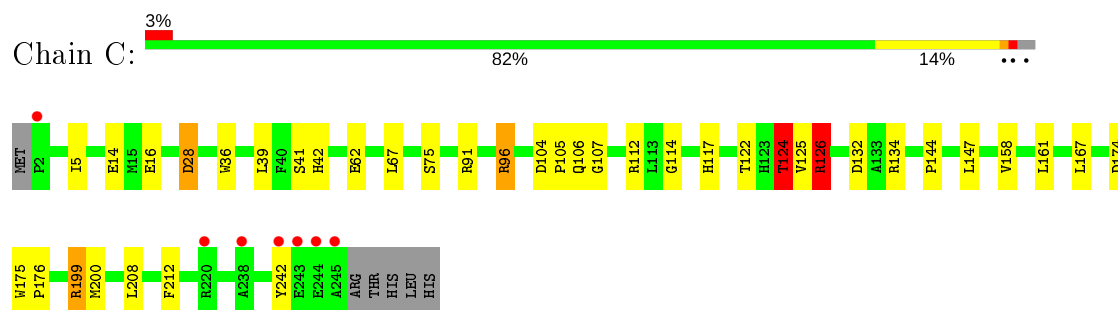
#### • Molecule 1: Peroxiredoxin



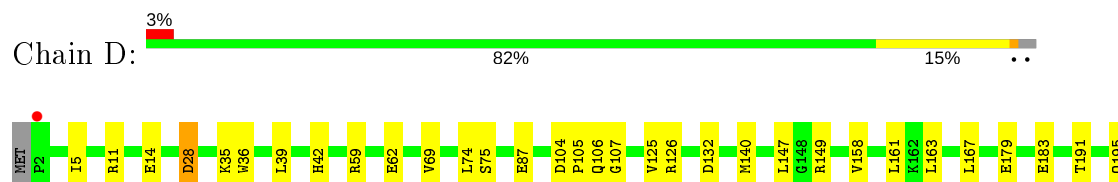
#### • Molecule 1: Peroxiredoxin



#### • Molecule 1: Peroxiredoxin

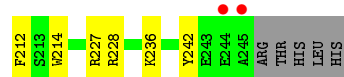
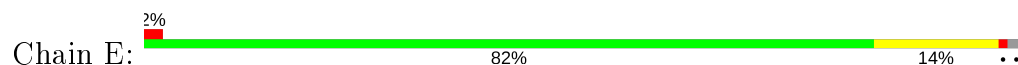


#### • Molecule 1: Peroxiredoxin

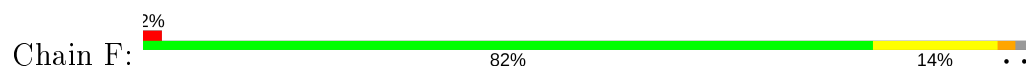




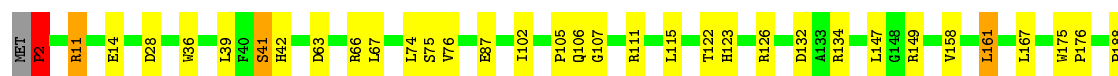
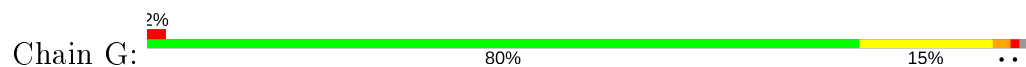
• Molecule 1: Peroxiredoxin



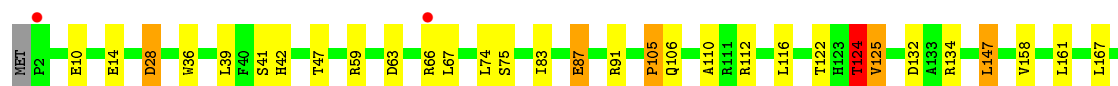
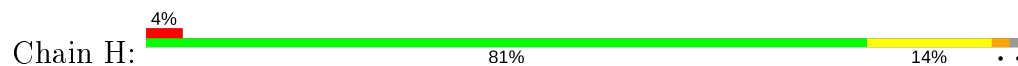
• Molecule 1: Peroxiredoxin



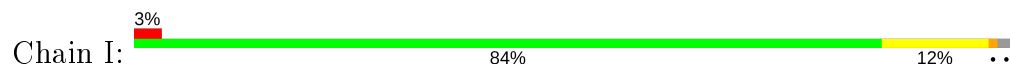
• Molecule 1: Peroxiredoxin



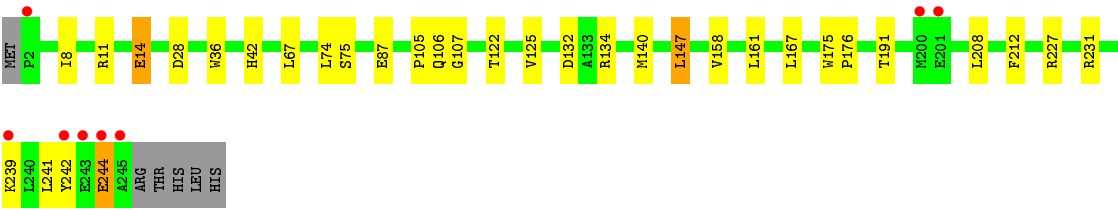
• Molecule 1: Peroxiredoxin



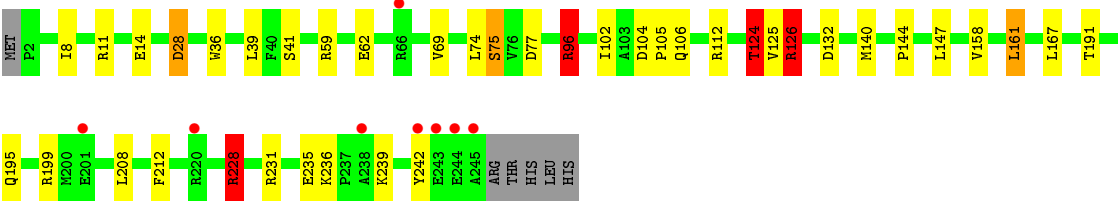
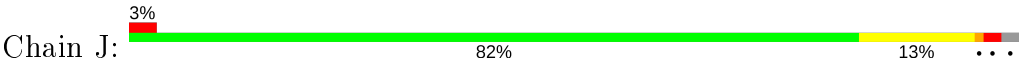
• Molecule 1: Peroxiredoxin







● Molecule 1: Peroxiredoxin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.83Å 102.79Å 104.44Å 105.88° 105.14° 92.46°	Depositor
Resolution (Å)	49.43 – 1.80 49.38 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (49.43-1.80) 97.4 (49.38-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.159 , 0.194 0.171 , 0.204	Depositor DCC
$R_{free}$ test set	13261 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21085	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: CIT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.84	2/2028 (0.1%)	0.98	5/2757 (0.2%)
1	B	0.80	1/2028 (0.0%)	0.96	3/2757 (0.1%)
1	C	0.79	1/2028 (0.0%)	1.37	11/2757 (0.4%)
1	D	0.87	3/2028 (0.1%)	0.97	4/2757 (0.1%)
1	E	0.76	2/2028 (0.1%)	1.17	8/2757 (0.3%)
1	F	0.94	3/2028 (0.1%)	0.97	7/2757 (0.3%)
1	G	0.78	0/2028	0.97	8/2757 (0.3%)
1	H	0.74	1/2028 (0.0%)	0.94	5/2757 (0.2%)
1	I	0.76	1/2028 (0.0%)	0.91	2/2757 (0.1%)
1	J	0.78	2/2028 (0.1%)	1.24	9/2757 (0.3%)
All	All	0.81	16/20280 (0.1%)	1.06	62/27570 (0.2%)

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	C	0	1
1	E	0	1
1	J	0	1
All	All	0	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	179	GLU	CD-OE2	17.60	1.45	1.25
1	F	179	GLU	CD-OE1	14.66	1.41	1.25
1	A	179	GLU	CD-OE2	14.04	1.41	1.25
1	D	179	GLU	CD-OE2	13.96	1.41	1.25
1	B	179	GLU	CD-OE2	10.86	1.37	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	GLU	CD-OE2	6.74	1.33	1.25
1	J	62	GLU	CD-OE2	6.68	1.32	1.25
1	H	87	GLU	CD-OE1	6.58	1.32	1.25
1	F	183	GLU	CD-OE2	6.58	1.32	1.25
1	E	126	ARG	CD-NE	-6.41	1.35	1.46
1	C	126	ARG	CD-NE	-6.16	1.35	1.46
1	D	183	GLU	CD-OE2	5.84	1.32	1.25
1	D	62	GLU	CD-OE2	5.49	1.31	1.25
1	I	87	GLU	CD-OE1	5.34	1.31	1.25
1	E	146	GLU	CD-OE2	5.25	1.31	1.25
1	J	126	ARG	CD-NE	-5.10	1.37	1.46

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	126	ARG	NE-CZ-NH2	-35.78	102.41	120.30
1	J	126	ARG	NE-CZ-NH2	-28.08	106.26	120.30
1	C	126	ARG	NE-CZ-NH1	27.26	133.93	120.30
1	E	126	ARG	NE-CZ-NH2	-27.21	106.69	120.30
1	J	126	ARG	NE-CZ-NH1	23.77	132.19	120.30
1	E	126	ARG	NE-CZ-NH1	22.24	131.42	120.30
1	C	126	ARG	CD-NE-CZ	14.44	143.82	123.60
1	D	231	ARG	NE-CZ-NH2	-13.10	113.75	120.30
1	C	96	ARG	NE-CZ-NH1	12.53	126.56	120.30
1	J	96	ARG	NE-CZ-NH1	12.34	126.47	120.30
1	E	126	ARG	CD-NE-CZ	11.05	139.07	123.60
1	G	231	ARG	NE-CZ-NH2	-10.48	115.06	120.30
1	B	96	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	J	126	ARG	CD-NE-CZ	8.79	135.91	123.60
1	E	2	PRO	CA-N-CD	-8.74	99.26	111.50
1	E	126	ARG	CG-CD-NE	-8.61	93.72	111.80
1	F	231	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	J	126	ARG	CG-CD-NE	-8.58	93.79	111.80
1	C	134	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	D	231	ARG	NE-CZ-NH1	8.49	124.54	120.30
1	G	2	PRO	CA-N-CD	-8.09	100.18	111.50
1	G	231	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	C	124	THR	N-CA-CB	-7.34	96.36	110.30
1	A	231	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	C	134	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	E	134	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	F	124	THR	N-CA-CB	-7.20	96.61	110.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	134	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	A	124	THR	N-CA-CB	-7.01	96.98	110.30
1	A	134	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	G	228	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	H	231	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	H	124	THR	N-CA-CB	-6.44	98.06	110.30
1	J	124	THR	N-CA-CB	-6.41	98.13	110.30
1	J	199	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	G	199	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	F	124	THR	CA-CB-OG1	6.29	122.21	109.00
1	D	199	ARG	CG-CD-NE	-6.24	98.69	111.80
1	A	134	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	J	96	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	134	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	J	228	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	G	199	ARG	CG-CD-NE	-5.89	99.43	111.80
1	C	126	ARG	CG-CD-NE	-5.78	99.65	111.80
1	D	199	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	H	134	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	E	134	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	E	227	ARG	CG-CD-NE	-5.58	100.09	111.80
1	G	134	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	F	199	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	I	231	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	199	ARG	CG-CD-NE	-5.29	100.70	111.80
1	C	199	ARG	CG-CD-NE	-5.25	100.77	111.80
1	I	134	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	C	96	ARG	CD-NE-CZ	5.21	130.89	123.60
1	F	227	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	F	199	ARG	CG-CD-NE	-5.16	100.97	111.80
1	H	124	THR	CA-CB-OG1	5.14	119.78	109.00
1	F	231	ARG	CG-CD-NE	-5.12	101.04	111.80
1	B	227	ARG	CG-CD-NE	-5.11	101.06	111.80
1	C	124	THR	CA-CB-OG1	5.09	119.69	109.00
1	H	199	ARG	CG-CD-NE	-5.09	101.11	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	126	ARG	Sidechain
1	E	126	ARG	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	J	126	ARG	Sidechain

## 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	1973	0	1959	30	0
1	B	1973	0	1959	23	0
1	C	1973	0	1959	25	0
1	D	1973	0	1959	20	0
1	E	1973	0	1959	25	0
1	F	1973	0	1959	21	0
1	G	1973	0	1959	31	0
1	H	1973	0	1959	28	0
1	I	1973	0	1959	18	0
1	J	1973	0	1959	27	0
2	A	13	0	5	0	0
2	B	13	0	5	2	0
2	C	13	0	5	1	0
2	D	13	0	5	0	0
2	E	13	0	5	1	0
2	F	13	0	5	0	0
2	G	13	0	5	0	0
2	H	13	0	5	3	0
2	I	13	0	5	0	0
2	J	13	0	5	0	0
3	A	128	0	0	7	0
3	B	123	0	0	1	0
3	C	138	0	0	2	0
3	D	123	0	0	3	1
3	E	124	0	0	6	0
3	F	126	0	0	3	1
3	G	117	0	0	6	0
3	H	121	0	0	3	0
3	I	116	0	0	0	0
3	J	109	0	0	3	0
All	All	21085	0	19640	217	1

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 5.

All (217) 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:E:76:VAL:HG12	3:E:449:HOH:O	1.26	1.30
1:A:76:VAL:HG12	3:A:475:HOH:O	1.37	1.20
1:G:76:VAL:HB	3:G:488:HOH:O	1.01	1.18
1:E:126:ARG:HD2	1:E:144:PRO:O	1.67	0.92
1:I:11:ARG:NH1	1:I:14:GLU:OE1	2.04	0.90
1:H:222:ASP:OD2	3:H:401:HOH:O	1.90	0.90
1:H:245:ALA:HB1	3:H:407:HOH:O	1.74	0.87
1:D:11:ARG:NH1	1:D:14:GLU:OE2	2.09	0.85
1:C:105:PRO:O	1:H:105:PRO:O	1.96	0.83
1:E:11:ARG:NH1	1:E:14:GLU:OE1	2.10	0.82
1:D:14:GLU:OE1	1:D:28:ASP:OD1	1.99	0.80
1:A:11:ARG:NH1	1:A:14:GLU:OE1	2.13	0.80
1:E:76:VAL:CG1	3:E:449:HOH:O	1.96	0.78
1:A:236:LYS:HE2	3:A:415:HOH:O	1.82	0.78
1:C:126:ARG:HD2	1:C:144:PRO:O	1.84	0.78
1:G:63:ASP:OD2	1:G:228:ARG:NH2	2.19	0.76
1:B:91:ARG:NH1	3:B:401:HOH:O	2.19	0.75
1:J:11:ARG:NH1	1:J:14:GLU:OE2	2.18	0.75
1:C:199:ARG:HG3	1:C:200:MET:HE2	1.70	0.73
1:H:14:GLU:OE1	1:H:28:ASP:OD1	2.06	0.73
1:H:47:THR:HB	2:H:301:CIT:H21	1.70	0.73
1:F:91:ARG:NH2	3:F:401:HOH:O	2.21	0.73
1:F:220:ARG:NH1	3:F:402:HOH:O	2.23	0.72
1:D:87:GLU:OE2	3:D:401:HOH:O	2.09	0.71
1:C:67:LEU:HD13	1:C:158:VAL:HG23	1.72	0.70
1:E:105:PRO:O	1:G:105:PRO:O	2.11	0.69
1:A:107:GLY:HA3	1:J:106:GLN:HE22	1.57	0.69
1:B:106:GLN:HE22	1:D:107:GLY:HA3	1.58	0.68
1:G:2:PRO:HB2	1:H:10:GLU:OE2	1.94	0.67
1:J:126:ARG:HD2	1:J:144:PRO:O	1.94	0.67
1:E:2:PRO:HB2	1:F:10:GLU:OE2	1.95	0.67
1:J:69:VAL:HG21	1:J:158:VAL:HG11	1.75	0.67
1:F:105:PRO:O	1:I:105:PRO:O	2.13	0.66
1:A:200:MET:HG2	3:A:519:HOH:O	1.94	0.66
1:B:105:PRO:O	1:D:105:PRO:O	2.14	0.66
1:A:236:LYS:CE	3:A:415:HOH:O	2.43	0.64
1:G:41:SER:OG	1:G:115:LEU:HD13	1.98	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:LEU:HD13	1:E:158:VAL:HG23	1.80	0.63
1:H:47:THR:HB	2:H:301:CIT:C2	2.29	0.63
1:J:236:LYS:HE3	3:J:416:HOH:O	1.97	0.63
1:A:2:PRO:O	1:B:5:ILE:O	2.16	0.63
1:G:122:THR:HG23	1:G:123:HIS:CD2	2.34	0.62
1:G:106:GLN:O	1:G:111:ARG:NH2	2.34	0.60
1:J:236:LYS:CE	3:J:416:HOH:O	2.50	0.59
1:C:107:GLY:HA3	1:H:106:GLN:HE22	1.67	0.59
1:G:76:VAL:CB	3:G:488:HOH:O	1.84	0.58
1:H:63:ASP:OD1	1:H:66:ARG:NH2	2.36	0.58
1:A:74:LEU:HD23	1:A:102:ILE:CG2	2.34	0.57
1:G:76:VAL:CG1	3:G:488:HOH:O	2.34	0.57
1:A:236:LYS:HD2	1:B:227:ARG:NH2	2.19	0.57
1:G:11:ARG:NH1	1:G:14:GLU:OE2	2.38	0.57
1:G:74:LEU:HD13	1:G:74:LEU:C	2.25	0.57
1:E:107:GLY:HA3	1:G:106:GLN:HE22	1.69	0.57
1:A:105:PRO:O	1:J:105:PRO:O	2.23	0.57
1:J:8:ILE:HG13	1:J:140:MET:HE2	1.86	0.57
1:J:228:ARG:HH11	1:J:228:ARG:HB3	1.69	0.57
1:A:74:LEU:HD23	1:A:102:ILE:HB	1.86	0.56
1:E:105:PRO:HG2	1:G:122:THR:OG1	2.04	0.56
1:G:67:LEU:HD13	1:G:158:VAL:HG23	1.85	0.56
1:A:2:PRO:HB2	1:B:10:GLU:OE2	2.06	0.56
1:H:41:SER:HB2	1:H:124:THR:HG21	1.88	0.56
1:I:67:LEU:HD13	1:I:158:VAL:HG23	1.86	0.56
1:E:174:ASP:HB3	3:F:438:HOH:O	2.05	0.56
1:E:106:GLN:HE22	1:G:107:GLY:HA3	1.71	0.55
1:H:67:LEU:HD13	1:H:158:VAL:HG23	1.89	0.55
1:F:106:GLN:HE22	1:I:107:GLY:HA3	1.72	0.55
1:J:74:LEU:HD23	1:J:102:ILE:HB	1.89	0.55
1:A:200:MET:CG	3:A:519:HOH:O	2.55	0.54
1:H:91:ARG:NH1	3:H:402:HOH:O	2.39	0.54
1:F:69:VAL:HG21	1:F:158:VAL:HG11	1.89	0.54
1:G:63:ASP:CG	1:G:228:ARG:HH22	2.10	0.54
1:J:74:LEU:HD23	1:J:102:ILE:CG2	2.37	0.53
1:B:47:THR:HB	2:B:301:CIT:H42	1.90	0.53
1:I:227:ARG:NH2	1:J:236:LYS:HD2	2.22	0.53
1:F:107:GLY:HA3	1:I:106:GLN:HE22	1.74	0.53
1:J:14:GLU:OE1	1:J:28:ASP:OD1	2.26	0.53
1:A:69:VAL:HG21	1:A:158:VAL:HG11	1.91	0.53
1:J:96:ARG:NH2	3:J:403:HOH:O	2.42	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:231:ARG:O	1:J:235:GLU:HG3	2.08	0.52
1:G:220:ARG:HB3	1:G:220:ARG:NH1	2.25	0.52
3:E:446:HOH:O	1:F:206:ARG:HD3	2.09	0.52
1:E:236:LYS:NZ	3:E:402:HOH:O	2.39	0.52
1:H:59:ARG:NH2	1:H:241:LEU:HD21	2.24	0.52
1:B:106:GLN:O	1:B:111:ARG:NH2	2.43	0.52
1:E:126:ARG:CD	1:E:144:PRO:O	2.50	0.51
1:E:74:LEU:C	1:E:74:LEU:HD13	2.31	0.51
1:A:79:VAL:HG11	1:I:191:THR:O	2.12	0.50
1:I:74:LEU:HD13	1:I:75:SER:N	2.27	0.50
1:E:104:ASP:N	1:E:105:PRO:HD3	2.27	0.50
1:A:41:SER:HB2	1:A:124:THR:HG21	1.94	0.49
1:G:228:ARG:HH21	1:G:232:ARG:NH1	2.11	0.49
1:D:69:VAL:HG21	1:D:158:VAL:HG11	1.94	0.49
1:D:191:THR:H	1:D:195:GLN:NE2	2.11	0.49
1:I:8:ILE:HG13	1:I:140:MET:HE2	1.95	0.49
1:A:2:PRO:CB	1:B:10:GLU:OE2	2.61	0.48
1:H:74:LEU:C	1:H:74:LEU:HD13	2.33	0.48
1:H:83:ILE:O	1:H:87:GLU:HG3	2.14	0.48
1:B:163:LEU:HD21	1:B:222:ASP:OD2	2.13	0.48
1:B:39:LEU:C	1:B:39:LEU:HD23	2.33	0.48
1:B:74:LEU:C	1:B:74:LEU:HD13	2.34	0.48
1:B:36:TRP:CD2	1:B:132:ASP:HA	2.49	0.48
1:I:36:TRP:CD2	1:I:132:ASP:HA	2.48	0.48
1:A:42:HIS:CE1	1:A:75:SER:HB3	2.48	0.48
1:C:117:HIS:HE1	1:D:140:MET:HE3	1.77	0.48
1:B:67:LEU:HD13	1:B:158:VAL:HG23	1.96	0.48
1:H:191:THR:H	1:H:195:GLN:NE2	2.12	0.48
1:B:191:THR:H	1:B:195:GLN:NE2	2.11	0.47
1:D:225:GLU:HG2	3:D:444:HOH:O	2.13	0.47
1:C:5:ILE:HD13	1:D:5:ILE:HD13	1.95	0.47
1:E:200:MET:HG2	1:E:210:TRP:HB3	1.97	0.47
1:I:147:LEU:HG	1:J:161:LEU:HD13	1.96	0.47
1:C:199:ARG:HG3	1:C:200:MET:CE	2.42	0.47
1:F:74:LEU:HD13	1:F:74:LEU:C	2.35	0.47
1:J:75:SER:HB3	1:J:77:ASP:H	1.79	0.47
1:E:228:ARG:HD3	3:E:505:HOH:O	2.14	0.47
2:C:301:CIT:O1	2:C:301:CIT:O5	2.33	0.47
1:D:36:TRP:CD2	1:D:132:ASP:HA	2.50	0.47
1:C:104:ASP:N	1:C:105:PRO:HD3	2.30	0.46
3:E:402:HOH:O	1:F:183:GLU:HG2	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:GLU:OE1	1:F:28:ASP:OD1	2.32	0.46
1:A:74:LEU:HD21	1:A:104:ASP:HB2	1.98	0.46
1:J:104:ASP:N	1:J:105:PRO:HD3	2.31	0.46
1:D:74:LEU:C	1:D:74:LEU:HD13	2.36	0.46
1:A:36:TRP:CD2	1:A:132:ASP:HA	2.50	0.46
1:D:163:LEU:HD11	1:D:222:ASP:HB3	1.98	0.46
1:J:74:LEU:HD21	1:J:104:ASP:HB2	1.98	0.46
1:D:39:LEU:HD23	1:D:39:LEU:C	2.36	0.46
1:A:200:MET:HA	3:A:519:HOH:O	2.15	0.46
1:A:74:LEU:C	1:A:74:LEU:HD13	2.36	0.46
1:C:91:ARG:NH2	3:C:404:HOH:O	2.49	0.46
1:G:161:LEU:HD13	1:H:147:LEU:HG	1.98	0.46
1:B:122:THR:HA	1:D:106:GLN:OE1	2.16	0.46
1:G:36:TRP:CD2	1:G:132:ASP:HA	2.51	0.46
1:E:74:LEU:HD13	1:E:75:SER:N	2.31	0.45
1:E:36:TRP:CD2	1:E:132:ASP:HA	2.52	0.45
1:H:36:TRP:CD2	1:H:132:ASP:HA	2.51	0.45
1:D:42:HIS:CE1	1:D:75:SER:HB3	2.51	0.45
1:G:42:HIS:CE1	1:G:75:SER:HB3	2.51	0.45
1:B:47:THR:HB	2:B:301:CIT:C4	2.46	0.45
1:C:36:TRP:CD2	1:C:132:ASP:HA	2.52	0.45
1:I:227:ARG:NH2	1:J:236:LYS:CD	2.79	0.45
1:A:3:GLY:HA3	1:B:7:LEU:HD21	1.99	0.45
1:D:74:LEU:HD13	1:D:75:SER:N	2.32	0.45
1:G:74:LEU:HD23	1:G:102:ILE:CG2	2.47	0.44
1:A:104:ASP:N	1:A:105:PRO:HD3	2.32	0.44
1:E:208:LEU:HD13	1:E:214:TRP:CZ3	2.52	0.44
1:F:119:GLU:OE2	1:F:146:GLU:OE2	2.35	0.44
1:J:191:THR:H	1:J:195:GLN:NE2	2.15	0.44
1:B:59:ARG:HD3	1:B:59:ARG:HA	1.84	0.44
1:A:194:ASP:OD1	1:A:197:ARG:NH2	2.50	0.44
1:E:67:LEU:CD1	1:E:158:VAL:HG23	2.46	0.44
1:A:5:ILE:HG22	1:A:114:GLY:HA3	2.00	0.44
1:J:41:SER:HB2	1:J:124:THR:HG21	2.00	0.44
1:B:42:HIS:CE1	1:B:75:SER:HB3	2.52	0.44
1:E:67:LEU:O	1:E:162:LYS:HE3	2.18	0.44
1:G:39:LEU:HD23	1:G:39:LEU:C	2.37	0.44
1:H:67:LEU:CD1	1:H:158:VAL:HG23	2.47	0.44
1:A:76:VAL:CG1	3:A:475:HOH:O	2.20	0.43
1:F:106:GLN:O	1:F:111:ARG:NH2	2.51	0.43
1:G:175:TRP:CG	1:G:176:PRO:HA	2.53	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:39:LEU:C	1:H:39:LEU:HD23	2.37	0.43
1:H:42:HIS:CE1	1:H:75:SER:HB3	2.53	0.43
1:H:41:SER:HB2	1:H:124:THR:CG2	2.47	0.43
1:A:69:VAL:CG2	1:A:158:VAL:HG11	2.48	0.43
1:F:179:GLU:CD	1:F:179:GLU:H	2.21	0.43
1:G:87:GLU:OE2	3:G:401:HOH:O	2.21	0.43
3:G:432:HOH:O	1:H:174:ASP:HB3	2.17	0.43
1:A:147:LEU:HG	1:B:161:LEU:HD13	2.00	0.43
2:E:301:CIT:O2	2:E:301:CIT:O3	2.37	0.43
1:G:188:PRO:O	1:G:199:ARG:NH2	2.49	0.43
1:A:74:LEU:HD23	1:A:102:ILE:CB	2.48	0.43
1:F:74:LEU:HD13	1:F:75:SER:N	2.34	0.43
1:I:67:LEU:CD1	1:I:158:VAL:HG23	2.48	0.43
1:C:42:HIS:O	1:C:124:THR:HG22	2.19	0.43
1:D:126:ARG:HB3	1:D:149:ARG:CZ	2.48	0.43
1:E:5:ILE:HG22	1:E:114:GLY:HA3	2.01	0.43
1:C:39:LEU:C	1:C:39:LEU:HD23	2.39	0.42
1:F:20:ASP:HA	1:F:79:VAL:CG2	2.49	0.42
1:G:126:ARG:HB3	1:G:149:ARG:CZ	2.50	0.42
1:G:106:GLN:NE2	3:G:409:HOH:O	2.53	0.42
1:C:124:THR:HG23	1:C:125:VAL:O	2.20	0.42
1:E:11:ARG:HG2	1:E:11:ARG:HH11	1.85	0.42
1:F:105:PRO:HG2	1:I:122:THR:HB	2.02	0.42
1:F:40:PHE:HA	1:F:127:GLY:O	2.20	0.42
1:B:175:TRP:CG	1:B:176:PRO:HA	2.55	0.42
1:C:14:GLU:OE2	1:C:28:ASP:OD1	2.37	0.42
1:I:42:HIS:CE1	1:I:75:SER:HB3	2.55	0.42
1:J:124:THR:HG23	1:J:125:VAL:O	2.20	0.42
1:C:106:GLN:HG3	1:H:122:THR:HA	2.01	0.41
1:C:5:ILE:HG22	1:C:114:GLY:HA3	2.02	0.41
1:C:175:TRP:CG	1:C:176:PRO:HA	2.55	0.41
1:G:63:ASP:OD1	1:G:66:ARG:NH1	2.54	0.41
1:H:110:ALA:HB1	1:H:116:LEU:HD22	2.02	0.41
1:C:67:LEU:CD1	1:C:158:VAL:HG23	2.46	0.41
1:F:104:ASP:N	1:F:105:PRO:CD	2.83	0.41
1:C:41:SER:HB2	1:C:124:THR:HG21	2.03	0.41
1:C:112:ARG:NH1	3:C:406:HOH:O	2.53	0.41
1:D:104:ASP:N	1:D:105:PRO:HD3	2.35	0.41
1:C:122:THR:HB	1:H:105:PRO:HG2	2.02	0.41
1:F:124:THR:HG23	1:F:125:VAL:O	2.21	0.41
1:J:69:VAL:CG2	1:J:158:VAL:HG11	2.47	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LEU:HD21	1:B:159:LYS:HD3	2.03	0.41
1:C:174:ASP:HB3	3:D:425:HOH:O	2.20	0.41
1:J:39:LEU:HD23	1:J:39:LEU:C	2.41	0.41
1:H:124:THR:HG23	1:H:125:VAL:O	2.21	0.41
1:I:241:LEU:HA	1:I:244:GLU:HG2	2.03	0.41
1:I:74:LEU:HD13	1:I:74:LEU:C	2.41	0.41
1:J:74:LEU:HD13	1:J:74:LEU:C	2.41	0.41
1:G:74:LEU:HD23	1:G:102:ILE:HB	2.03	0.40
1:I:175:TRP:CG	1:I:176:PRO:HA	2.56	0.40
1:C:5:ILE:HG21	1:D:5:ILE:HD11	2.03	0.40
1:C:42:HIS:CE1	1:C:75:SER:HB3	2.56	0.40
1:F:200:MET:HG2	1:F:210:TRP:HB3	2.02	0.40
1:J:36:TRP:CD2	1:J:132:ASP:HA	2.56	0.40
1:E:208:LEU:HD13	1:E:214:TRP:HZ3	1.85	0.40
1:G:215:ASP:OD1	1:G:217:PRO:HD3	2.21	0.40
1:H:47:THR:HB	2:H:301:CIT:C1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:444:HOH:O	3:F:492:HOH:O[1_544]	2.16	0.04

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	242/250 (97%)	232 (96%)	8 (3%)	2 (1%)	19	7
1	B	242/250 (97%)	239 (99%)	2 (1%)	1 (0%)	34	21
1	C	242/250 (97%)	238 (98%)	4 (2%)	0	100	100
1	D	242/250 (97%)	237 (98%)	4 (2%)	1 (0%)	34	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	242/250 (97%)	237 (98%)	4 (2%)	1 (0%)	34	21
1	F	242/250 (97%)	237 (98%)	4 (2%)	1 (0%)	34	21
1	G	242/250 (97%)	238 (98%)	4 (2%)	0	100	100
1	H	242/250 (97%)	237 (98%)	3 (1%)	2 (1%)	19	7
1	I	242/250 (97%)	237 (98%)	4 (2%)	1 (0%)	34	21
1	J	242/250 (97%)	238 (98%)	4 (2%)	0	100	100
All	All	2420/2500 (97%)	2370 (98%)	41 (2%)	9 (0%)	34	21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	244	GLU
1	A	203	GLY
1	E	125	VAL
1	F	125	VAL
1	A	125	VAL
1	D	125	VAL
1	I	125	VAL
1	B	125	VAL
1	H	125	VAL

### 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	210/216 (97%)	199 (95%)	11 (5%)	23	10
1	B	210/216 (97%)	198 (94%)	12 (6%)	20	8
1	C	210/216 (97%)	199 (95%)	11 (5%)	23	10
1	D	210/216 (97%)	199 (95%)	11 (5%)	23	10
1	E	210/216 (97%)	200 (95%)	10 (5%)	25	11
1	F	210/216 (97%)	199 (95%)	11 (5%)	23	10

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	210/216 (97%)	199 (95%)	11 (5%)	23	10
1	H	210/216 (97%)	201 (96%)	9 (4%)	29	14
1	I	210/216 (97%)	200 (95%)	10 (5%)	25	11
1	J	210/216 (97%)	196 (93%)	14 (7%)	16	5
All	All	2100/2160 (97%)	1990 (95%)	110 (5%)	23	10

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	116	LEU
1	A	124	THR
1	A	147	LEU
1	A	161	LEU
1	A	163	LEU
1	A	167	LEU
1	A	183	GLU
1	A	208	LEU
1	A	212	PHE
1	A	228	ARG
1	B	2	PRO
1	B	28	ASP
1	B	91	ARG
1	B	96	ARG
1	B	147	LEU
1	B	161	LEU
1	B	207	SER
1	B	208	LEU
1	B	212	PHE
1	B	220	ARG
1	B	242	TYR
1	B	244	GLU
1	C	16	GLU
1	C	28	ASP
1	C	62	GLU
1	C	96	ARG
1	C	124	THR
1	C	147	LEU
1	C	161	LEU
1	C	167	LEU
1	C	208	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	212	PHE
1	C	242	TYR
1	D	28	ASP
1	D	35	LYS
1	D	59	ARG
1	D	147	LEU
1	D	161	LEU
1	D	167	LEU
1	D	199	ARG
1	D	202	SER
1	D	208	LEU
1	D	212	PHE
1	D	242	TYR
1	E	2	PRO
1	E	16	GLU
1	E	28	ASP
1	E	74	LEU
1	E	116	LEU
1	E	147	LEU
1	E	167	LEU
1	E	204	GLN
1	E	212	PHE
1	E	242	TYR
1	F	4	SER
1	F	28	ASP
1	F	124	THR
1	F	147	LEU
1	F	161	LEU
1	F	167	LEU
1	F	207	SER
1	F	208	LEU
1	F	212	PHE
1	F	228	ARG
1	F	244	GLU
1	G	2	PRO
1	G	11	ARG
1	G	28	ASP
1	G	41	SER
1	G	147	LEU
1	G	161	LEU
1	G	167	LEU
1	G	199	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	208	LEU
1	G	212	PHE
1	G	242	TYR
1	H	28	ASP
1	H	105	PRO
1	H	112	ARG
1	H	124	THR
1	H	147	LEU
1	H	161	LEU
1	H	167	LEU
1	H	208	LEU
1	H	212	PHE
1	I	14	GLU
1	I	28	ASP
1	I	147	LEU
1	I	161	LEU
1	I	167	LEU
1	I	208	LEU
1	I	212	PHE
1	I	239	LYS
1	I	242	TYR
1	I	244	GLU
1	J	28	ASP
1	J	59	ARG
1	J	75	SER
1	J	96	ARG
1	J	112	ARG
1	J	124	THR
1	J	147	LEU
1	J	161	LEU
1	J	167	LEU
1	J	208	LEU
1	J	212	PHE
1	J	228	ARG
1	J	239	LYS
1	J	242	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	B	106	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	195	GLN
1	B	204	GLN
1	C	65	GLN
1	D	195	GLN
1	E	106	GLN
1	F	106	GLN
1	F	195	GLN
1	F	204	GLN
1	G	106	GLN
1	H	106	GLN
1	H	195	GLN
1	H	204	GLN
1	I	65	GLN
1	I	106	GLN
1	I	123	HIS
1	J	106	GLN
1	J	195	GLN
1	J	204	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](#)

10 ligands 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	$\# Z  > 2$
2	CIT	J	301	-	3,12,12	0.61	0	3,17,17	0.96	0
2	CIT	C	301	-	3,12,12	1.01	0	3,17,17	0.95	0
2	CIT	A	301	-	3,12,12	1.59	1 (33%)	3,17,17	1.09	0
2	CIT	F	301	-	3,12,12	1.39	1 (33%)	3,17,17	0.49	0
2	CIT	G	301	-	3,12,12	1.20	0	3,17,17	0.99	0
2	CIT	D	301	-	3,12,12	1.47	1 (33%)	3,17,17	0.73	0
2	CIT	E	301	-	3,12,12	1.41	1 (33%)	3,17,17	1.19	0
2	CIT	H	301	-	3,12,12	1.58	1 (33%)	3,17,17	1.55	1 (33%)
2	CIT	I	301	-	3,12,12	1.37	1 (33%)	3,17,17	1.44	0
2	CIT	B	301	-	3,12,12	1.41	1 (33%)	3,17,17	2.14	1 (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
2	CIT	J	301	-	-	0/6/16/16	-
2	CIT	C	301	-	-	1/6/16/16	-
2	CIT	A	301	-	-	4/6/16/16	-
2	CIT	F	301	-	-	3/6/16/16	-
2	CIT	G	301	-	-	3/6/16/16	-
2	CIT	D	301	-	-	3/6/16/16	-
2	CIT	E	301	-	-	6/6/16/16	-
2	CIT	H	301	-	-	1/6/16/16	-
2	CIT	I	301	-	-	3/6/16/16	-
2	CIT	B	301	-	-	3/6/16/16	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CIT	C2-C3	-2.59	1.51	1.54
2	H	301	CIT	C2-C3	-2.56	1.51	1.54
2	D	301	CIT	C4-C3	-2.35	1.51	1.54
2	B	301	CIT	C4-C3	-2.23	1.51	1.54
2	I	301	CIT	C4-C3	-2.17	1.51	1.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	CIT	C4-C3	-2.09	1.51	1.54
2	F	301	CIT	C2-C3	-2.04	1.52	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	CIT	C3-C2-C1	3.08	119.92	114.98
2	H	301	CIT	C3-C4-C5	2.20	118.51	114.98

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	CIT	C2-C3-C4-C5
2	A	301	CIT	O7-C3-C4-C5
2	A	301	CIT	C6-C3-C4-C5
2	F	301	CIT	C2-C3-C4-C5
2	F	301	CIT	O7-C3-C4-C5
2	F	301	CIT	C6-C3-C4-C5
2	G	301	CIT	C1-C2-C3-O7
2	G	301	CIT	C1-C2-C3-C4
2	G	301	CIT	C1-C2-C3-C6
2	D	301	CIT	C1-C2-C3-O7
2	D	301	CIT	C1-C2-C3-C4
2	D	301	CIT	C1-C2-C3-C6
2	E	301	CIT	C1-C2-C3-O7
2	E	301	CIT	C1-C2-C3-C4
2	E	301	CIT	C1-C2-C3-C6
2	I	301	CIT	C1-C2-C3-O7
2	I	301	CIT	C1-C2-C3-C4
2	I	301	CIT	C1-C2-C3-C6
2	B	301	CIT	C1-C2-C3-O7
2	E	301	CIT	C2-C3-C4-C5
2	C	301	CIT	C2-C3-C4-C5
2	B	301	CIT	C1-C2-C3-C4
2	E	301	CIT	O7-C3-C4-C5
2	E	301	CIT	C6-C3-C4-C5
2	B	301	CIT	C1-C2-C3-C6
2	H	301	CIT	O7-C3-C4-C5
2	A	301	CIT	C1-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	CIT	1	0
2	E	301	CIT	1	0
2	H	301	CIT	3	0
2	B	301	CIT	2	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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	244/250 (97%)	-0.18	9 (3%)	41 36	17, 23, 47, 82	0
1	B	244/250 (97%)	-0.31	6 (2%)	57 52	15, 22, 45, 84	0
1	C	244/250 (97%)	-0.44	7 (2%)	51 46	14, 21, 43, 81	0
1	D	244/250 (97%)	-0.30	7 (2%)	51 46	14, 21, 41, 84	0
1	E	244/250 (97%)	-0.37	6 (2%)	57 52	16, 22, 45, 90	0
1	F	244/250 (97%)	-0.30	6 (2%)	57 52	16, 23, 43, 75	0
1	G	244/250 (97%)	-0.21	6 (2%)	57 52	17, 23, 48, 84	0
1	H	244/250 (97%)	-0.31	9 (3%)	41 36	16, 24, 47, 87	0
1	I	244/250 (97%)	-0.33	8 (3%)	46 40	16, 23, 46, 87	0
1	J	244/250 (97%)	-0.22	8 (3%)	46 40	16, 24, 47, 87	0
All	All	2440/2500 (97%)	-0.30	72 (2%)	50 44	14, 23, 46, 90	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	245	ALA	7.3
1	E	245	ALA	6.3
1	I	245	ALA	6.2
1	J	245	ALA	6.2
1	B	245	ALA	5.0
1	G	245	ALA	4.8
1	C	245	ALA	4.7
1	H	245	ALA	4.6
1	F	245	ALA	4.3
1	I	244	GLU	4.2
1	H	244	GLU	4.1
1	I	243	GLU	3.9
1	C	244	GLU	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	201	GLU	3.9
1	A	245	ALA	3.7
1	B	202	SER	3.5
1	B	200	MET	3.5
1	E	200	MET	3.5
1	G	243	GLU	3.3
1	D	200	MET	3.2
1	I	242	TYR	3.2
1	H	220	ARG	3.2
1	F	202	SER	3.1
1	E	203	GLY	3.1
1	E	202	SER	3.0
1	E	201	GLU	3.0
1	A	244	GLU	2.9
1	I	239	LYS	2.9
1	H	242	TYR	2.9
1	C	2	PRO	2.9
1	F	2	PRO	2.9
1	G	242	TYR	2.8
1	J	244	GLU	2.8
1	E	244	GLU	2.7
1	A	200	MET	2.7
1	I	200	MET	2.7
1	G	244	GLU	2.7
1	A	2	PRO	2.7
1	F	201	GLU	2.7
1	H	66	ARG	2.7
1	I	2	PRO	2.6
1	J	243	GLU	2.6
1	A	242	TYR	2.6
1	J	242	TYR	2.6
1	H	238	ALA	2.6
1	B	203	GLY	2.6
1	H	2	PRO	2.5
1	H	201	GLU	2.5
1	A	201	GLU	2.5
1	B	244	GLU	2.5
1	D	2	PRO	2.5
1	C	242	TYR	2.4
1	D	242	TYR	2.4
1	A	243	GLU	2.4
1	A	203	GLY	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	238	ALA	2.3
1	D	201	GLU	2.3
1	F	244	GLU	2.3
1	H	203	GLY	2.3
1	D	202	SER	2.3
1	J	201	GLU	2.2
1	J	238	ALA	2.2
1	I	201	GLU	2.1
1	J	66	ARG	2.1
1	C	243	GLU	2.1
1	D	243	GLU	2.1
1	A	198	ALA	2.1
1	C	220	ARG	2.0
1	F	203	GLY	2.0
1	G	202	SER	2.0
1	J	220	ARG	2.0
1	G	201	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CIT	J	301	13/13	0.89	0.13	20,39,48,49	0
2	CIT	B	301	13/13	0.90	0.16	21,39,56,63	0
2	CIT	I	301	13/13	0.92	0.13	21,33,43,45	0
2	CIT	G	301	13/13	0.93	0.12	21,37,52,58	0
2	CIT	E	301	13/13	0.93	0.10	22,36,48,49	0
2	CIT	H	301	13/13	0.93	0.13	18,36,54,64	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CIT	C	301	13/13	0.93	0.13	18,33,47,54	0
2	CIT	F	301	13/13	0.93	0.12	20,32,46,51	0
2	CIT	A	301	13/13	0.94	0.10	21,33,42,44	0
2	CIT	D	301	13/13	0.94	0.13	18,31,46,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.