Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 04:12 AM JST

PDB ID	:	6KRQ
Title	:	Peroxiredoxin from Aeropyrum pernix K1 (ApPrx) 0Cys F80A mutant
Authors	:	Himiyama, T.; Nakamura, T.
Deposited on	:	2019-08-22
Resolution	:	2.10 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 (1)) were used in the production of this report:

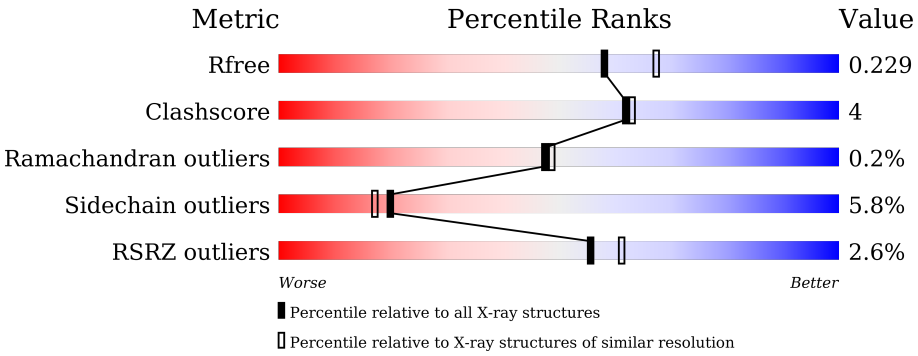
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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% 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	244	2% 85% 13% •
1	B	244	4% 82% 17% •
1	C	244	3% 84% 14% ••
1	D	244	% 86% 13% •
1	E	244	2% 86% 13% •
1	F	244	4% 86% 12% •

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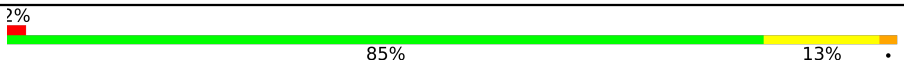
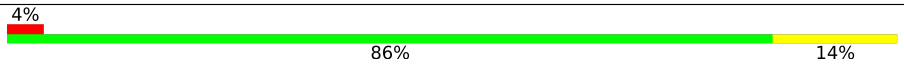
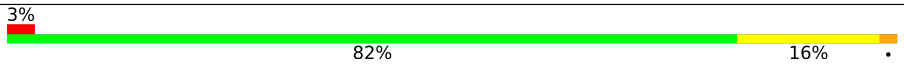
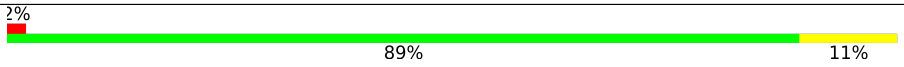
Mol	Chain	Length	Quality of chain
1	G	244	
1	H	244	
1	I	244	
1	J	244	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20741 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	C	N	O	S	0	0	0
			1967	1262	347	354	4			
1	B	244	Total	C	N	O	S	0	0	0
			1967	1262	347	354	4			
1	C	244	Total	C	N	O	S	0	0	0
			1967	1262	347	354	4			
1	D	244	Total	C	N	O	S	0	0	0
			1967	1262	347	354	4			
1	E	244	Total	C	N	O	S	0	0	0
			1967	1262	347	354	4			
1	F	244	Total	C	N	O	S	0	0	0
			1967	1262	347	354	4			
1	G	244	Total	C	N	O	S	0	0	0
			1967	1262	347	354	4			
1	H	244	Total	C	N	O	S	0	0	0
			1967	1262	347	354	4			
1	I	244	Total	C	N	O	S	0	0	0
			1967	1262	347	354	4			
1	J	244	Total	C	N	O	S	0	0	0
			1967	1262	347	354	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	SER	CYS	engineered mutation	UNP Q9Y9L0
A	80	ALA	PHE	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	80	ALA	PHE	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

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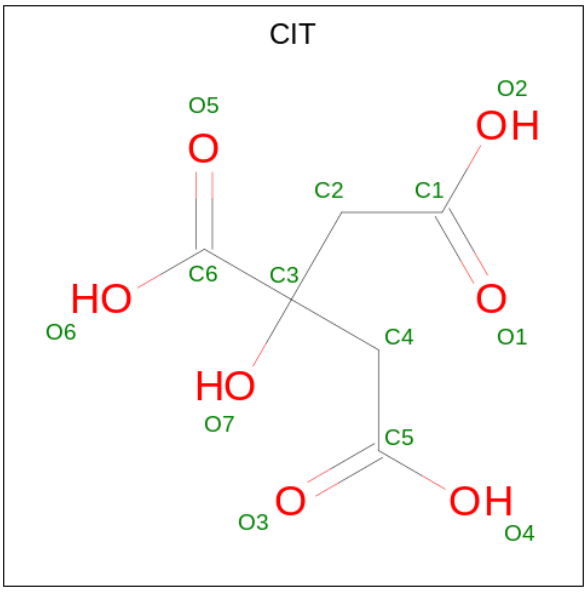
Chain	Residue	Modelled	Actual	Comment	Reference
C	80	ALA	PHE	engineered mutation	UNP Q9Y9L0
C	207	SER	CYS	engineered mutation	UNP Q9Y9L0
C	213	SER	CYS	engineered mutation	UNP Q9Y9L0
D	50	SER	CYS	engineered mutation	UNP Q9Y9L0
D	80	ALA	PHE	engineered mutation	UNP Q9Y9L0
D	207	SER	CYS	engineered mutation	UNP Q9Y9L0
D	213	SER	CYS	engineered mutation	UNP Q9Y9L0
E	50	SER	CYS	engineered mutation	UNP Q9Y9L0
E	80	ALA	PHE	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	80	ALA	PHE	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	80	ALA	PHE	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	80	ALA	PHE	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	80	ALA	PHE	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	80	ALA	PHE	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: $C_6H_8O_7$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	91	Total O 91 91	0	0
3	B	106	Total O 106 106	0	0

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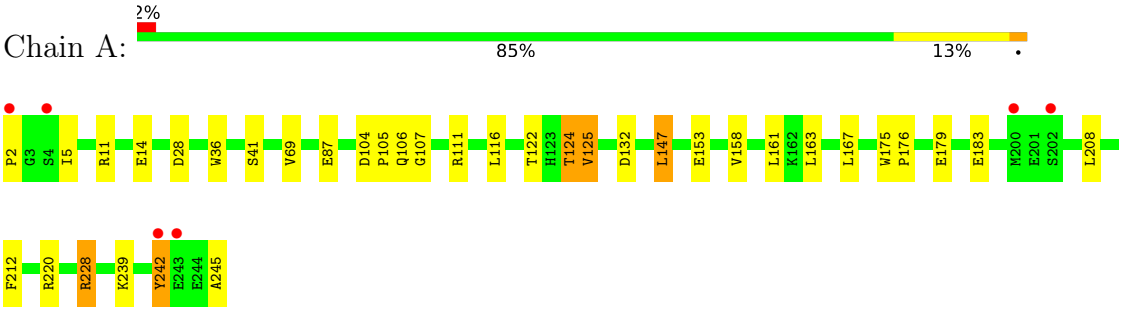
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	135	Total O 135 135	0	0
3	D	91	Total O 91 91	0	0
3	E	81	Total O 81 81	0	0
3	F	92	Total O 92 92	0	0
3	G	89	Total O 89 89	0	0
3	H	77	Total O 77 77	0	0
3	I	99	Total O 99 99	0	0
3	J	80	Total O 80 80	0	0

3 Residue-property plots (i)

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

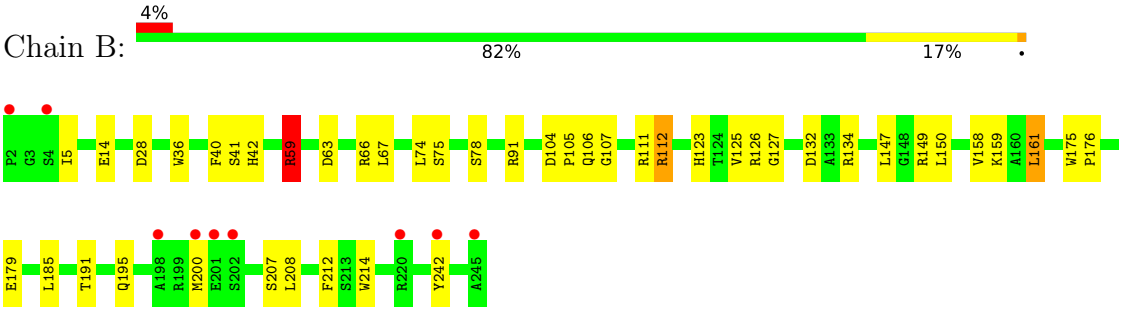
• Molecule 1: Peroxiredoxin

Chain A:



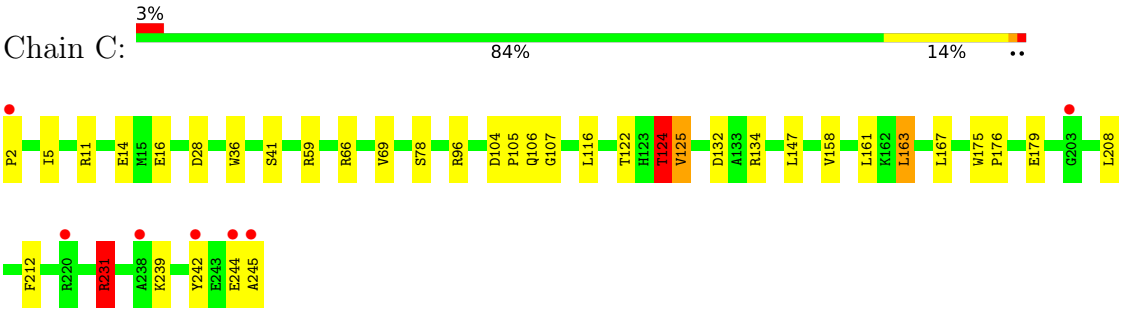
• Molecule 1: Peroxiredoxin

Chain B:



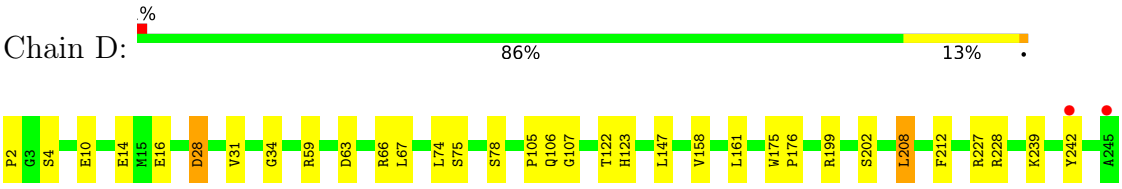
• Molecule 1: Peroxiredoxin

Chain C:



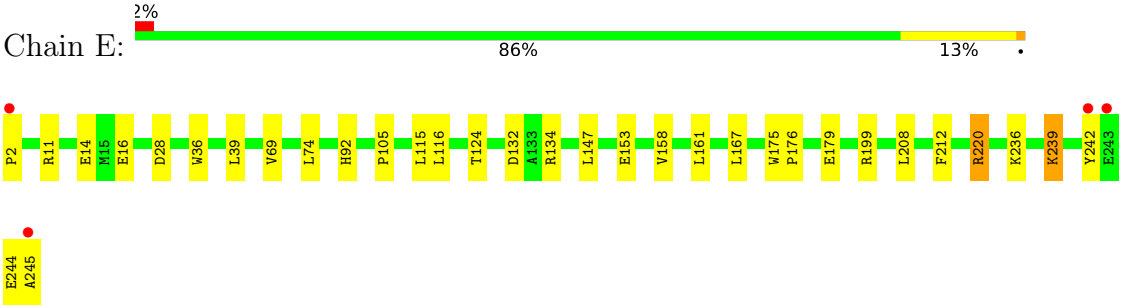
• Molecule 1: Peroxiredoxin

Chain D:



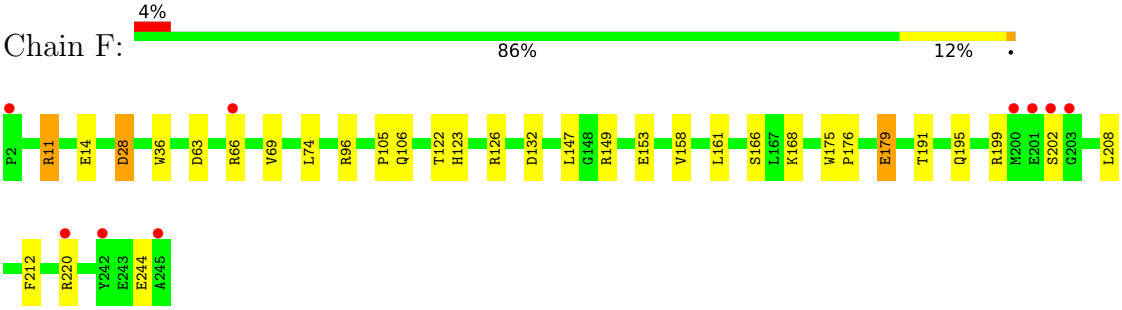
• Molecule 1: Peroxiredoxin

Chain E:



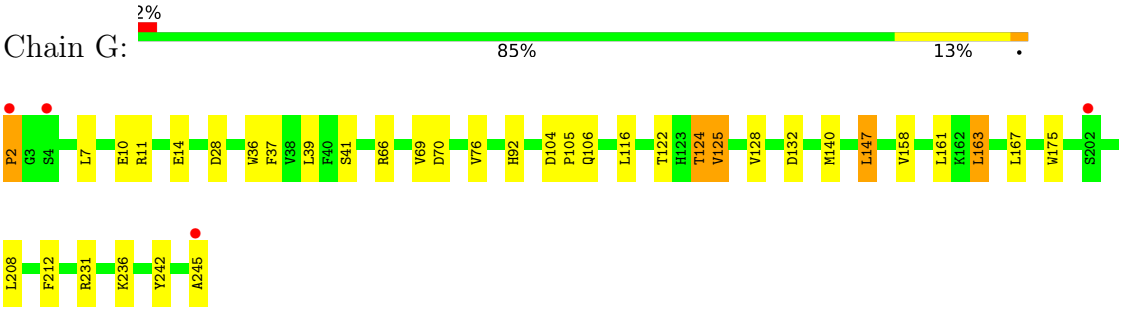
• Molecule 1: Peroxiredoxin

Chain F:



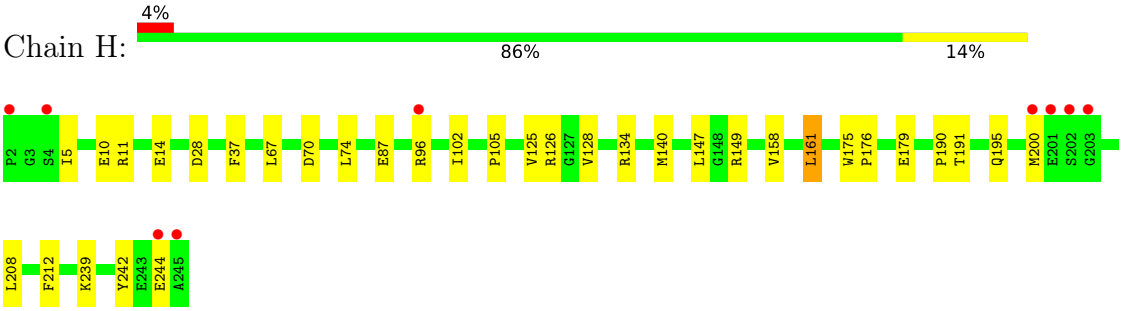
• Molecule 1: Peroxiredoxin

Chain G:



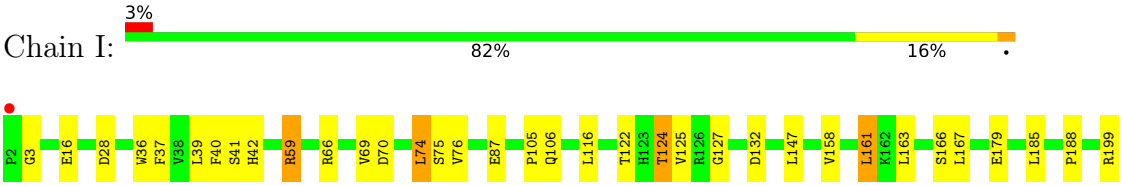
• Molecule 1: Peroxiredoxin

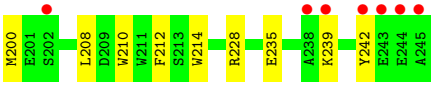
Chain H:



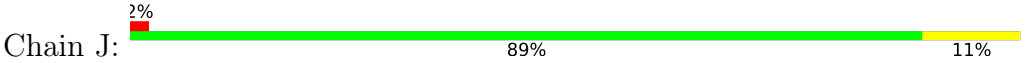
• Molecule 1: Peroxiredoxin

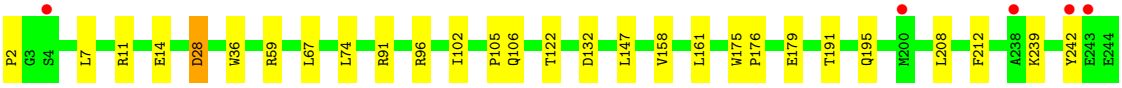
Chain I:





• Molecule 1: Peroxiredoxin





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	76.15Å 103.16Å 105.35Å 106.09° 105.02° 92.40°	Depositor
Resolution (Å)	49.23 – 2.10 49.18 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.23-2.10) 97.7 (49.18-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.169 , 0.221 0.182 , 0.229	Depositor DCC
R_{free} test set	8383 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	24.3	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 36.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20741	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.71	2/2021 (0.1%)	0.88	1/2748 (0.0%)
1	B	0.71	1/2021 (0.0%)	0.87	2/2748 (0.1%)
1	C	0.69	0/2021	0.90	3/2748 (0.1%)
1	D	0.71	0/2021	0.87	3/2748 (0.1%)
1	E	0.72	1/2021 (0.0%)	0.87	2/2748 (0.1%)
1	F	0.68	0/2021	0.85	1/2748 (0.0%)
1	G	0.70	0/2021	0.88	2/2748 (0.1%)
1	H	0.73	2/2021 (0.1%)	0.95	4/2748 (0.1%)
1	I	0.70	1/2021 (0.0%)	0.87	0/2748
1	J	0.70	1/2021 (0.0%)	0.84	1/2748 (0.0%)
All	All	0.70	8/20210 (0.0%)	0.88	19/27480 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	GLU	CD-OE2	7.87	1.34	1.25
1	B	179	GLU	CD-OE2	7.33	1.33	1.25
1	H	179	GLU	CD-OE2	6.92	1.33	1.25
1	E	179	GLU	CD-OE2	6.48	1.32	1.25
1	H	96	ARG	NE-CZ	5.78	1.40	1.33
1	J	179	GLU	CD-OE2	5.47	1.31	1.25
1	I	87	GLU	CD-OE1	5.23	1.31	1.25
1	A	87	GLU	CD-OE1	5.03	1.31	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	96	ARG	NE-CZ-NH1	15.06	127.83	120.30
1	A	228	ARG	CG-CD-NE	6.61	125.67	111.80
1	H	96	ARG	CD-NE-CZ	6.57	132.79	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	96	ARG	CB-CG-CD	6.52	128.54	111.60
1	C	231	ARG	CG-CD-NE	5.88	124.15	111.80
1	H	96	ARG	NH1-CZ-NH2	-5.84	112.98	119.40
1	D	227	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	E	2	PRO	CA-N-CD	-5.63	103.61	111.50
1	D	227	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	C	124	THR	N-CA-CB	-5.44	99.96	110.30
1	D	228	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	134	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	F	199	ARG	CG-CD-NE	-5.23	100.81	111.80
1	B	134	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	G	231	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	59	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	G	2	PRO	CA-N-CD	-5.03	104.45	111.50
1	E	134	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	J	2	PRO	CA-N-CD	-5.01	104.49	111.50

There are no chirality outliers.

There are no planarity outliers.

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	A	1967	0	1955	20	0
1	B	1967	0	1955	31	0
1	C	1967	0	1955	25	0
1	D	1967	0	1955	18	0
1	E	1967	0	1955	17	0
1	F	1967	0	1955	19	0
1	G	1967	0	1955	23	0
1	H	1967	0	1955	15	0
1	I	1967	0	1955	21	0
1	J	1967	0	1955	17	0
2	A	13	0	5	0	0
2	B	13	0	5	0	0
2	C	13	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	13	0	5	0	0
2	E	13	0	5	0	0
2	F	13	0	5	0	0
2	G	13	0	5	0	0
2	H	13	0	5	0	0
2	I	13	0	5	0	0
2	J	13	0	5	0	0
3	A	91	0	0	1	0
3	B	106	0	0	0	0
3	C	135	0	0	3	0
3	D	91	0	0	0	0
3	E	81	0	0	5	0
3	F	92	0	0	0	0
3	G	89	0	0	2	0
3	H	77	0	0	0	0
3	I	99	0	0	1	0
3	J	80	0	0	1	0
All	All	20741	0	19600	173	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 (173) 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:220:ARG:NH2	3:E:401:HOH:O	2.12	0.82
1:I:69:VAL:HG21	1:I:158:VAL:HG11	1.68	0.75
1:C:69:VAL:HG21	1:C:158:VAL:HG11	1.72	0.71
1:A:2:PRO:O	1:B:5:ILE:O	2.08	0.71
1:C:107:GLY:HA3	1:F:106:GLN:HE22	1.55	0.70
1:H:11:ARG:NH1	1:H:14:GLU:OE2	2.26	0.67
1:I:179:GLU:OE2	1:J:59:ARG:HG3	1.97	0.65
1:F:69:VAL:HG21	1:F:158:VAL:HG11	1.77	0.65
1:C:124:THR:HB	3:C:452:HOH:O	1.96	0.64
1:I:228:ARG:HD3	3:I:490:HOH:O	1.96	0.64
1:G:69:VAL:HG21	1:G:158:VAL:HG11	1.78	0.64
1:B:191:THR:H	1:B:195:GLN:NE2	1.97	0.63
1:E:124:THR:HG22	3:E:417:HOH:O	1.98	0.63
1:D:31:VAL:O	1:D:34:GLY:N	2.31	0.62
1:E:69:VAL:HG21	1:E:158:VAL:HG11	1.82	0.62
1:C:41:SER:HB2	1:C:124:THR:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:ARG:CZ	3:E:401:HOH:O	2.45	0.60
1:C:231:ARG:NH1	3:C:401:HOH:O	2.33	0.60
1:E:115:LEU:HB3	1:E:124:THR:OG1	2.03	0.59
1:B:63:ASP:OD1	1:B:66:ARG:NH1	2.36	0.58
1:A:107:GLY:HA3	1:J:106:GLN:HE22	1.68	0.58
1:F:63:ASP:OD1	1:F:66:ARG:NH1	2.36	0.57
1:I:188:PRO:O	1:I:199:ARG:NH2	2.38	0.57
1:J:11:ARG:NH1	1:J:14:GLU:OE2	2.32	0.57
1:I:39:LEU:C	1:I:39:LEU:HD23	2.26	0.56
1:G:2:PRO:HB2	1:H:10:GLU:OE2	2.05	0.56
1:B:123:HIS:HE1	1:D:78:SER:OG	1.89	0.56
1:C:105:PRO:O	1:F:105:PRO:O	2.23	0.56
1:E:236:LYS:HE3	3:E:420:HOH:O	2.04	0.56
1:B:200:MET:HA	1:B:200:MET:CE	2.37	0.55
1:H:74:LEU:HD23	1:H:102:ILE:HB	1.87	0.55
1:E:220:ARG:NH1	3:E:401:HOH:O	2.39	0.54
1:H:67:LEU:HD13	1:H:158:VAL:HG23	1.90	0.54
1:B:78:SER:OG	1:D:123:HIS:HE1	1.89	0.54
1:B:59:ARG:HH11	1:B:59:ARG:HG3	1.73	0.54
1:A:122:THR:HA	1:J:106:GLN:HG2	1.91	0.53
1:A:124:THR:HB	3:A:423:HOH:O	2.09	0.53
1:C:231:ARG:HB2	1:C:231:ARG:HH11	1.74	0.53
1:B:106:GLN:HG2	1:D:122:THR:HA	1.91	0.52
1:I:3:GLY:HA3	1:J:7:LEU:HD21	1.91	0.52
1:C:179:GLU:OE1	1:D:59:ARG:CZ	2.58	0.52
1:A:41:SER:HB2	1:A:124:THR:HG21	1.91	0.52
1:J:14:GLU:OE1	1:J:28:ASP:OD1	2.28	0.52
1:A:69:VAL:HG21	1:A:158:VAL:HG11	1.92	0.51
1:B:106:GLN:HE22	1:D:107:GLY:HA3	1.74	0.51
1:B:67:LEU:HD13	1:B:158:VAL:HG23	1.91	0.51
1:A:104:ASP:N	1:A:105:PRO:HD3	2.26	0.51
1:C:78:SER:OG	1:F:123:HIS:HE1	1.94	0.51
1:J:191:THR:H	1:J:195:GLN:NE2	2.09	0.51
1:G:122:THR:HA	1:I:106:GLN:HG2	1.92	0.50
1:D:67:LEU:HD13	1:D:158:VAL:HG23	1.94	0.50
1:G:105:PRO:O	1:I:105:PRO:O	2.31	0.49
1:A:124:THR:HG23	1:A:125:VAL:O	2.12	0.49
1:C:5:ILE:O	1:D:2:PRO:HB3	2.12	0.49
1:I:74:LEU:HD13	1:I:75:SER:N	2.27	0.49
1:A:242:TYR:O	1:A:245:ALA:HB2	2.12	0.49
1:B:107:GLY:HA3	1:D:106:GLN:HE22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:TRP:CG	1:F:176:PRO:HA	2.48	0.48
1:G:41:SER:HB2	1:G:124:THR:HG21	1.94	0.48
1:F:244:GLU:HG2	1:F:244:GLU:O	2.13	0.48
1:I:41:SER:HB2	1:I:124:THR:HG21	1.95	0.48
1:A:11:ARG:NH1	1:A:14:GLU:OE1	2.38	0.48
1:C:104:ASP:N	1:C:105:PRO:HD3	2.29	0.48
1:B:59:ARG:HH11	1:B:59:ARG:CG	2.27	0.47
1:G:106:GLN:NE2	1:I:76:VAL:HG11	2.28	0.47
1:D:175:TRP:CG	1:D:176:PRO:HA	2.49	0.47
1:G:37:PHE:HA	1:G:70:ASP:O	2.14	0.47
1:I:36:TRP:CD2	1:I:132:ASP:HA	2.49	0.47
1:C:41:SER:HB2	1:C:124:THR:CG2	2.43	0.47
1:J:74:LEU:HD23	1:J:102:ILE:HB	1.97	0.47
1:C:122:THR:HA	1:F:106:GLN:HG2	1.95	0.47
1:E:239:LYS:HE3	1:E:244:GLU:OE2	2.14	0.47
1:F:191:THR:H	1:F:195:GLN:NE2	2.12	0.47
1:A:106:GLN:HG2	1:J:122:THR:HA	1.97	0.47
1:B:42:HIS:CE1	1:B:75:SER:HB3	2.49	0.47
1:E:69:VAL:CG2	1:E:158:VAL:HG11	2.44	0.47
1:E:74:LEU:C	1:E:74:LEU:HD13	2.35	0.47
1:J:28:ASP:OD1	1:J:28:ASP:N	2.48	0.47
1:B:175:TRP:CG	1:B:176:PRO:HA	2.50	0.46
1:A:175:TRP:CG	1:A:176:PRO:HA	2.50	0.46
1:B:36:TRP:CD2	1:B:132:ASP:HA	2.51	0.46
1:F:126:ARG:HB3	1:F:149:ARG:CZ	2.46	0.46
1:B:14:GLU:O	1:B:112:ARG:NH2	2.49	0.46
1:C:124:THR:HG23	1:C:125:VAL:O	2.16	0.46
1:G:92:HIS:O	1:G:245:ALA:HB1	2.15	0.46
1:J:175:TRP:CG	1:J:176:PRO:HA	2.51	0.46
1:A:106:GLN:O	1:A:111:ARG:NH2	2.47	0.46
1:G:11:ARG:NH1	1:G:14:GLU:OE1	2.35	0.46
1:E:36:TRP:CD2	1:E:132:ASP:HA	2.51	0.46
1:G:147:LEU:HG	1:H:161:LEU:HD13	1.97	0.46
1:C:175:TRP:CG	1:C:176:PRO:HA	2.51	0.45
1:E:11:ARG:NH1	1:E:14:GLU:OE1	2.44	0.45
1:G:69:VAL:CG2	1:G:158:VAL:HG11	2.46	0.45
1:A:69:VAL:CG2	1:A:158:VAL:HG11	2.46	0.45
1:D:63:ASP:OD1	1:D:66:ARG:NH1	2.49	0.45
1:E:105:PRO:O	1:H:105:PRO:O	2.35	0.45
1:F:153:GLU:HA	1:F:153:GLU:OE1	2.17	0.45
1:A:5:ILE:HD13	1:B:5:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:74:LEU:HD13	1:I:74:LEU:C	2.38	0.45
1:G:163:LEU:HD23	1:G:175:TRP:CH2	2.51	0.44
1:H:190:PRO:HB3	1:H:195:GLN:HB3	1.98	0.44
1:H:191:THR:H	1:H:195:GLN:NE2	2.14	0.44
1:I:200:MET:HG3	1:I:210:TRP:HB3	2.00	0.44
1:F:11:ARG:NH1	1:F:14:GLU:OE2	2.50	0.44
1:E:39:LEU:C	1:E:39:LEU:HD23	2.37	0.44
1:J:36:TRP:CD2	1:J:132:ASP:HA	2.51	0.44
1:C:2:PRO:HB2	1:D:10:GLU:OE2	2.17	0.44
1:H:11:ARG:HG2	1:H:11:ARG:HH11	1.83	0.44
1:D:74:LEU:HD13	1:D:74:LEU:C	2.38	0.44
1:E:92:HIS:O	1:E:245:ALA:HB1	2.17	0.44
1:F:244:GLU:OE2	1:F:244:GLU:N	2.36	0.44
1:A:36:TRP:CD2	1:A:132:ASP:HA	2.52	0.44
1:J:91:ARG:NH2	3:J:406:HOH:O	2.51	0.44
1:B:105:PRO:O	1:D:105:PRO:O	2.35	0.44
1:G:36:TRP:CD2	1:G:132:ASP:HA	2.53	0.44
1:E:175:TRP:CG	1:E:176:PRO:HA	2.52	0.43
1:H:37:PHE:HA	1:H:70:ASP:O	2.18	0.43
1:H:175:TRP:CG	1:H:176:PRO:HA	2.53	0.43
1:F:28:ASP:OD1	1:F:28:ASP:N	2.50	0.43
1:C:106:GLN:HG3	1:F:122:THR:HA	2.01	0.43
1:D:74:LEU:HD13	1:D:75:SER:N	2.33	0.43
1:F:14:GLU:OE1	1:F:28:ASP:OD1	2.36	0.43
1:D:14:GLU:OE1	1:D:28:ASP:OD1	2.36	0.43
1:B:185:LEU:O	1:B:214:TRP:HB2	2.18	0.43
1:G:39:LEU:C	1:G:39:LEU:HD23	2.39	0.43
1:I:59:ARG:O	1:I:59:ARG:HG3	2.17	0.43
1:J:67:LEU:HD13	1:J:158:VAL:HG23	2.01	0.43
1:F:179:GLU:H	1:F:179:GLU:HG2	1.63	0.43
1:G:236:LYS:HE2	3:G:411:HOH:O	2.19	0.43
1:C:106:GLN:CG	1:F:122:THR:HA	2.49	0.43
1:C:163:LEU:HD12	1:C:163:LEU:HA	1.92	0.42
1:G:124:THR:HG23	1:G:125:VAL:O	2.18	0.42
1:H:200:MET:HA	1:H:200:MET:CE	2.49	0.42
1:C:96:ARG:NH1	3:C:407:HOH:O	2.52	0.42
1:I:161:LEU:HD12	1:I:161:LEU:HA	1.91	0.42
1:A:105:PRO:O	1:J:105:PRO:O	2.37	0.42
1:B:67:LEU:HD21	1:B:159:LYS:HD3	2.00	0.42
1:B:104:ASP:N	1:B:105:PRO:CD	2.82	0.42
1:A:147:LEU:HG	1:B:161:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:SER:HA	1:B:74:LEU:O	2.20	0.42
1:I:42:HIS:O	1:I:124:THR:HG22	2.20	0.42
1:C:231:ARG:HA	1:C:231:ARG:HD3	1.86	0.42
1:G:104:ASP:N	1:G:105:PRO:HD3	2.34	0.42
1:B:106:GLN:O	1:B:111:ARG:NH2	2.53	0.41
1:C:36:TRP:CD2	1:C:132:ASP:HA	2.55	0.41
1:F:36:TRP:CD2	1:F:132:ASP:HA	2.54	0.41
1:J:74:LEU:C	1:J:74:LEU:HD13	2.40	0.41
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.86	0.41
1:C:11:ARG:NH1	1:C:14:GLU:OE1	2.49	0.41
1:I:40:PHE:HA	1:I:127:GLY:O	2.21	0.41
1:A:153:GLU:OE1	1:B:150:LEU:HD22	2.21	0.41
1:B:40:PHE:HA	1:B:127:GLY:O	2.21	0.41
1:B:59:ARG:HG3	1:B:59:ARG:NH1	2.35	0.41
1:C:244:GLU:O	1:C:245:ALA:C	2.58	0.41
1:G:124:THR:HB	3:G:412:HOH:O	2.20	0.41
1:G:76:VAL:O	1:G:105:PRO:HA	2.21	0.41
1:J:74:LEU:HD23	1:J:102:ILE:CG2	2.50	0.41
1:H:128:VAL:O	1:H:140:MET:HA	2.21	0.41
1:B:59:ARG:HA	1:B:59:ARG:HD2	1.77	0.41
1:B:67:LEU:CD1	1:B:158:VAL:HG23	2.51	0.41
1:E:153:GLU:HA	1:E:153:GLU:OE1	2.21	0.41
1:G:106:GLN:HG2	1:I:122:THR:HA	2.03	0.41
1:H:126:ARG:HB3	1:H:149:ARG:CZ	2.50	0.41
1:I:37:PHE:HA	1:I:70:ASP:O	2.20	0.41
1:I:185:LEU:O	1:I:214:TRP:HB2	2.21	0.41
1:G:163:LEU:HD12	1:G:163:LEU:HA	1.99	0.41
1:G:7:LEU:O	1:G:10:GLU:HB2	2.22	0.40
1:G:128:VAL:O	1:G:140:MET:HA	2.21	0.40
1:C:11:ARG:NH1	1:C:11:ARG:HG2	2.36	0.40
1:D:208:LEU:HD12	1:D:208:LEU:HA	1.90	0.40
1:B:126:ARG:HB3	1:B:149:ARG:CZ	2.50	0.40
1:H:74:LEU:HD23	1:H:102:ILE:CG2	2.51	0.40
1:B:105:PRO:HG2	1:D:122:THR:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/244 (99%)	237 (98%)	4 (2%)	1 (0%)	34	32
1	B	242/244 (99%)	237 (98%)	4 (2%)	1 (0%)	34	32
1	C	242/244 (99%)	239 (99%)	2 (1%)	1 (0%)	34	32
1	D	242/244 (99%)	240 (99%)	2 (1%)	0	100	100
1	E	242/244 (99%)	237 (98%)	5 (2%)	0	100	100
1	F	242/244 (99%)	238 (98%)	4 (2%)	0	100	100
1	G	242/244 (99%)	236 (98%)	5 (2%)	1 (0%)	34	32
1	H	242/244 (99%)	238 (98%)	3 (1%)	1 (0%)	34	32
1	I	242/244 (99%)	238 (98%)	3 (1%)	1 (0%)	34	32
1	J	242/244 (99%)	239 (99%)	3 (1%)	0	100	100
All	All	2420/2440 (99%)	2379 (98%)	35 (1%)	6 (0%)	47	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	VAL
1	B	125	VAL
1	C	125	VAL
1	H	125	VAL
1	I	125	VAL
1	G	125	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	209/209 (100%)	196 (94%)	13 (6%)	18 15
1	B	209/209 (100%)	199 (95%)	10 (5%)	25 24
1	C	209/209 (100%)	194 (93%)	15 (7%)	14 11
1	D	209/209 (100%)	198 (95%)	11 (5%)	22 20
1	E	209/209 (100%)	197 (94%)	12 (6%)	20 18
1	F	209/209 (100%)	196 (94%)	13 (6%)	18 15
1	G	209/209 (100%)	198 (95%)	11 (5%)	22 20
1	H	209/209 (100%)	198 (95%)	11 (5%)	22 20
1	I	209/209 (100%)	192 (92%)	17 (8%)	11 8
1	J	209/209 (100%)	201 (96%)	8 (4%)	33 34
All	All	2090/2090 (100%)	1969 (94%)	121 (6%)	20 17

All (121) 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	167	LEU
1	A	183	GLU
1	A	208	LEU
1	A	212	PHE
1	A	220	ARG
1	A	228	ARG
1	A	239	LYS
1	A	242	TYR
1	B	28	ASP
1	B	59	ARG
1	B	91	ARG
1	B	112	ARG
1	B	147	LEU
1	B	161	LEU
1	B	207	SER
1	B	208	LEU
1	B	212	PHE
1	B	242	TYR
1	C	16	GLU

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Mol	Chain	Res	Type
1	C	28	ASP
1	C	59	ARG
1	C	66	ARG
1	C	116	LEU
1	C	124	THR
1	C	147	LEU
1	C	161	LEU
1	C	163	LEU
1	C	167	LEU
1	C	208	LEU
1	C	212	PHE
1	C	231	ARG
1	C	239	LYS
1	C	242	TYR
1	D	4	SER
1	D	16	GLU
1	D	28	ASP
1	D	147	LEU
1	D	161	LEU
1	D	199	ARG
1	D	202	SER
1	D	208	LEU
1	D	212	PHE
1	D	239	LYS
1	D	242	TYR
1	E	16	GLU
1	E	28	ASP
1	E	116	LEU
1	E	147	LEU
1	E	161	LEU
1	E	167	LEU
1	E	199	ARG
1	E	208	LEU
1	E	212	PHE
1	E	220	ARG
1	E	239	LYS
1	E	242	TYR
1	F	11	ARG
1	F	28	ASP
1	F	74	LEU
1	F	96	ARG
1	F	147	LEU

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Mol	Chain	Res	Type
1	F	161	LEU
1	F	166	SER
1	F	168	LYS
1	F	179	GLU
1	F	202	SER
1	F	208	LEU
1	F	212	PHE
1	F	220	ARG
1	G	28	ASP
1	G	66	ARG
1	G	116	LEU
1	G	124	THR
1	G	147	LEU
1	G	161	LEU
1	G	163	LEU
1	G	167	LEU
1	G	208	LEU
1	G	212	PHE
1	G	242	TYR
1	H	5	ILE
1	H	28	ASP
1	H	87	GLU
1	H	134	ARG
1	H	147	LEU
1	H	161	LEU
1	H	208	LEU
1	H	212	PHE
1	H	239	LYS
1	H	242	TYR
1	H	244	GLU
1	I	16	GLU
1	I	28	ASP
1	I	59	ARG
1	I	66	ARG
1	I	74	LEU
1	I	116	LEU
1	I	124	THR
1	I	147	LEU
1	I	161	LEU
1	I	163	LEU
1	I	166	SER
1	I	167	LEU

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Mol	Chain	Res	Type
1	I	208	LEU
1	I	212	PHE
1	I	235	GLU
1	I	239	LYS
1	I	242	TYR
1	J	28	ASP
1	J	96	ARG
1	J	147	LEU
1	J	161	LEU
1	J	208	LEU
1	J	212	PHE
1	J	239	LYS
1	J	242	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

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

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Mol	Chain	Res	Type
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	I	301	-	12,12,12	1.24	1 (8%)	17,17,17	1.45	3 (17%)
2	CIT	F	301	-	12,12,12	1.16	1 (8%)	17,17,17	1.54	2 (11%)
2	CIT	G	301	-	12,12,12	1.31	1 (8%)	17,17,17	1.68	3 (17%)
2	CIT	E	301	-	12,12,12	1.30	1 (8%)	17,17,17	1.26	3 (17%)
2	CIT	D	301	-	12,12,12	1.03	1 (8%)	17,17,17	1.91	5 (29%)
2	CIT	H	301	-	12,12,12	1.22	1 (8%)	17,17,17	1.31	2 (11%)
2	CIT	J	301	-	12,12,12	1.39	1 (8%)	17,17,17	1.42	3 (17%)
2	CIT	B	301	-	12,12,12	1.26	2 (16%)	17,17,17	1.34	2 (11%)
2	CIT	A	301	-	12,12,12	1.06	0	17,17,17	1.54	3 (17%)
2	CIT	C	301	-	12,12,12	1.25	1 (8%)	17,17,17	1.42	4 (23%)

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	I	301	-	-	12/16/16/16	-
2	CIT	F	301	-	-	4/16/16/16	-
2	CIT	G	301	-	-	7/16/16/16	-
2	CIT	E	301	-	-	9/16/16/16	-
2	CIT	D	301	-	-	5/16/16/16	-
2	CIT	H	301	-	-	7/16/16/16	-
2	CIT	J	301	-	-	7/16/16/16	-
2	CIT	B	301	-	-	7/16/16/16	-
2	CIT	A	301	-	-	13/16/16/16	-
2	CIT	C	301	-	-	11/16/16/16	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	CIT	C3-C6	3.43	1.57	1.53
2	E	301	CIT	C3-C6	3.36	1.56	1.53
2	J	301	CIT	C3-C6	3.07	1.56	1.53
2	H	301	CIT	C3-C6	2.90	1.56	1.53
2	I	301	CIT	C3-C6	2.87	1.56	1.53
2	C	301	CIT	C3-C6	2.67	1.56	1.53
2	F	301	CIT	O2-C1	-2.30	1.23	1.30
2	B	301	CIT	C3-C6	2.27	1.55	1.53
2	D	301	CIT	C3-C6	2.21	1.55	1.53
2	B	301	CIT	O4-C5	-2.06	1.23	1.30

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	CIT	O5-C6-C3	-4.94	115.26	122.25
2	F	301	CIT	O5-C6-C3	-4.65	115.67	122.25
2	A	301	CIT	O5-C6-C3	-4.42	115.99	122.25
2	G	301	CIT	O5-C6-C3	-4.13	116.41	122.25
2	G	301	CIT	O6-C6-C3	3.84	119.72	113.05
2	D	301	CIT	O6-C6-C3	3.81	119.66	113.05
2	B	301	CIT	O5-C6-C3	-3.80	116.87	122.25
2	J	301	CIT	O5-C6-C3	-3.48	117.33	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	301	CIT	O5-C6-C3	-3.44	117.38	122.25
2	H	301	CIT	O5-C6-C3	-3.21	117.71	122.25
2	F	301	CIT	O6-C6-C3	3.06	118.36	113.05
2	J	301	CIT	O6-C6-C3	3.06	118.36	113.05
2	A	301	CIT	O6-C6-C3	2.84	117.97	113.05
2	I	301	CIT	O6-C6-C3	2.82	117.95	113.05
2	B	301	CIT	O6-C6-C3	2.80	117.91	113.05
2	C	301	CIT	O5-C6-C3	-2.77	118.34	122.25
2	C	301	CIT	O3-C5-C4	-2.75	114.92	122.94
2	I	301	CIT	C3-C4-C5	2.55	119.98	113.81
2	J	301	CIT	C3-C4-C5	2.52	119.91	113.81
2	E	301	CIT	O3-C5-C4	-2.52	115.59	122.94
2	D	301	CIT	O1-C1-C2	-2.47	115.74	122.94
2	D	301	CIT	O3-C5-C4	-2.39	115.95	122.94
2	H	301	CIT	O6-C6-C3	2.34	117.11	113.05
2	C	301	CIT	O6-C6-C3	2.28	117.01	113.05
2	C	301	CIT	O1-C1-C2	-2.17	116.61	122.94
2	A	301	CIT	C3-C4-C5	2.10	118.91	113.81
2	E	301	CIT	O4-C5-C4	2.09	121.05	114.35
2	G	301	CIT	O3-C5-C4	-2.07	116.89	122.94
2	D	301	CIT	O4-C5-C4	2.07	120.98	114.35
2	E	301	CIT	O5-C6-C3	-2.00	119.42	122.25

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	CIT	C1-C2-C3-O7
2	A	301	CIT	C1-C2-C3-C4
2	A	301	CIT	C1-C2-C3-C6
2	A	301	CIT	C2-C3-C4-C5
2	A	301	CIT	C2-C3-C6-O5
2	A	301	CIT	C2-C3-C6-O6
2	A	301	CIT	O7-C3-C6-O5
2	A	301	CIT	O7-C3-C6-O6
2	B	301	CIT	C1-C2-C3-O7
2	B	301	CIT	C1-C2-C3-C4
2	B	301	CIT	C1-C2-C3-C6
2	B	301	CIT	C2-C3-C6-O5
2	B	301	CIT	C2-C3-C6-O6
2	B	301	CIT	O7-C3-C6-O5
2	B	301	CIT	O7-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	301	CIT	C1-C2-C3-O7
2	C	301	CIT	C1-C2-C3-C4
2	C	301	CIT	C1-C2-C3-C6
2	C	301	CIT	C2-C3-C6-O6
2	C	301	CIT	O7-C3-C6-O5
2	C	301	CIT	O7-C3-C6-O6
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	E	301	CIT	O7-C3-C6-O5
2	E	301	CIT	O7-C3-C6-O6
2	E	301	CIT	C4-C3-C6-O5
2	E	301	CIT	C4-C3-C6-O6
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	O7-C3-C6-O6
2	G	301	CIT	C4-C3-C6-O6
2	H	301	CIT	C2-C3-C4-C5
2	H	301	CIT	O7-C3-C4-C5
2	H	301	CIT	C6-C3-C4-C5
2	H	301	CIT	O7-C3-C6-O5
2	H	301	CIT	O7-C3-C6-O6
2	H	301	CIT	C4-C3-C6-O5
2	H	301	CIT	C4-C3-C6-O6
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	I	301	CIT	C2-C3-C6-O5
2	I	301	CIT	C2-C3-C6-O6
2	I	301	CIT	O7-C3-C6-O5
2	I	301	CIT	O7-C3-C6-O6
2	J	301	CIT	C1-C2-C3-O7
2	J	301	CIT	C1-C2-C3-C4
2	J	301	CIT	C1-C2-C3-C6
2	J	301	CIT	C2-C3-C6-O5
2	J	301	CIT	C2-C3-C6-O6
2	J	301	CIT	O7-C3-C6-O5
2	J	301	CIT	O7-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	301	CIT	C6-C3-C4-C5
2	I	301	CIT	C2-C3-C4-C5
2	C	301	CIT	C2-C3-C6-O5
2	I	301	CIT	C6-C3-C4-C5
2	E	301	CIT	C3-C4-C5-O3
2	E	301	CIT	C3-C4-C5-O4
2	A	301	CIT	C4-C3-C6-O5
2	A	301	CIT	C4-C3-C6-O6
2	C	301	CIT	C4-C3-C6-O5
2	C	301	CIT	C4-C3-C6-O6
2	D	301	CIT	C3-C4-C5-O3
2	A	301	CIT	O7-C3-C4-C5
2	D	301	CIT	C3-C4-C5-O4
2	C	301	CIT	C3-C4-C5-O3
2	C	301	CIT	C3-C4-C5-O4
2	G	301	CIT	C2-C3-C6-O6
2	G	301	CIT	C4-C3-C6-O5
2	I	301	CIT	C4-C3-C6-O6
2	G	301	CIT	C3-C4-C5-O4
2	I	301	CIT	O7-C3-C4-C5
2	G	301	CIT	C3-C4-C5-O3
2	G	301	CIT	C2-C3-C6-O5
2	I	301	CIT	C4-C3-C6-O5
2	F	301	CIT	C1-C2-C3-C4
2	A	301	CIT	O2-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	244/244 (100%)	-0.21	6 (2%)	57	62	22, 31, 52, 91	0
1	B	244/244 (100%)	-0.34	9 (3%)	41	48	21, 29, 53, 77	0
1	C	244/244 (100%)	-0.36	7 (2%)	51	57	19, 27, 55, 97	0
1	D	244/244 (100%)	-0.23	2 (0%)	86	88	20, 28, 51, 96	0
1	E	244/244 (100%)	-0.21	4 (1%)	72	75	23, 31, 55, 84	0
1	F	244/244 (100%)	-0.22	9 (3%)	41	48	21, 30, 56, 91	0
1	G	244/244 (100%)	-0.27	4 (1%)	72	75	22, 30, 53, 80	0
1	H	244/244 (100%)	-0.24	9 (3%)	41	48	22, 30, 55, 86	0
1	I	244/244 (100%)	-0.32	8 (3%)	46	53	22, 30, 55, 91	0
1	J	244/244 (100%)	-0.22	6 (2%)	57	62	23, 32, 57, 94	0
All	All	2440/2440 (100%)	-0.26	64 (2%)	56	61	19, 30, 55, 97	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	245	ALA	5.6
1	F	245	ALA	5.4
1	D	245	ALA	4.4
1	C	245	ALA	4.3
1	J	238	ALA	4.3
1	H	4	SER	4.3
1	H	202	SER	4.3
1	H	200	MET	4.0
1	I	2	PRO	4.0
1	B	200	MET	3.8
1	B	201	GLU	3.7
1	C	2	PRO	3.7
1	G	245	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	245	ALA	3.6
1	C	244	GLU	3.6
1	B	202	SER	3.5
1	I	238	ALA	3.4
1	A	4	SER	3.4
1	A	2	PRO	3.3
1	E	245	ALA	3.2
1	I	243	GLU	3.2
1	B	245	ALA	3.1
1	A	200	MET	3.1
1	H	203	GLY	3.0
1	G	2	PRO	3.0
1	B	220	ARG	2.9
1	I	242	TYR	2.8
1	A	242	TYR	2.7
1	F	242	TYR	2.7
1	J	242	TYR	2.7
1	H	201	GLU	2.6
1	F	200	MET	2.6
1	C	203	GLY	2.6
1	F	203	GLY	2.6
1	H	244	GLU	2.6
1	I	245	ALA	2.6
1	I	202	SER	2.5
1	H	2	PRO	2.5
1	C	242	TYR	2.5
1	G	4	SER	2.4
1	F	201	GLU	2.4
1	E	242	TYR	2.4
1	H	96	ARG	2.3
1	I	244	GLU	2.3
1	J	4	SER	2.3
1	F	2	PRO	2.3
1	F	202	SER	2.3
1	F	220	ARG	2.3
1	B	198	ALA	2.3
1	E	2	PRO	2.3
1	C	238	ALA	2.2
1	C	220	ARG	2.2
1	G	202	SER	2.2
1	E	243	GLU	2.2
1	F	66	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	243	GLU	2.2
1	A	202	SER	2.1
1	B	4	SER	2.1
1	I	239	LYS	2.1
1	A	243	GLU	2.1
1	J	200	MET	2.1
1	D	242	TYR	2.1
1	B	242	TYR	2.1
1	B	2	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CIT	C	301	13/13	0.90	0.14	28,41,58,65	0
2	CIT	H	301	13/13	0.90	0.17	30,45,56,60	0
2	CIT	E	301	13/13	0.92	0.12	27,50,57,61	0
2	CIT	G	301	13/13	0.92	0.14	31,50,62,69	0
2	CIT	D	301	13/13	0.92	0.12	29,48,58,67	0
2	CIT	I	301	13/13	0.92	0.14	33,52,58,64	0
2	CIT	A	301	13/13	0.93	0.14	26,49,59,62	0
2	CIT	B	301	13/13	0.93	0.12	28,48,59,64	0
2	CIT	F	301	13/13	0.95	0.12	28,46,59,63	0
2	CIT	J	301	13/13	0.95	0.11	30,48,57,64	0

6.5 Other polymers (i)

There are no such residues in this entry.