



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:42 AM UTC

PDB ID : 3A2X / pdb_00003a2x
Title : Peroxiredoxin (C50S) from *Aeropyrum pernix* K1 (acetate-bound form)
Authors : Nakamura, T.; Kado, Y.; Yamaguchi, F.; Matsumura, H.; Ishikawa, K.; Inoue, T.
Deposited on : 2009-06-04
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

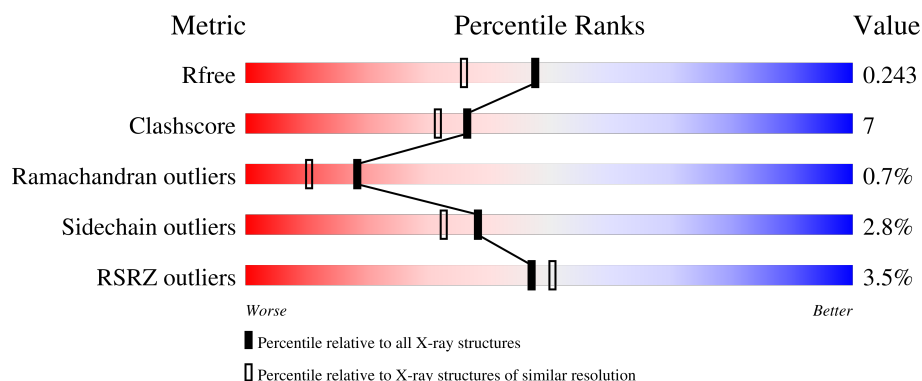
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	249	4% 80% 14% ...
1	B	249	5% 79% 18% ..
1	C	249	4% 81% 16% ..
1	D	249	4% 80% 15% ..
1	E	249	5% 79% 17% ..

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Mol	Chain	Length	Quality of chain
1	F	249	3% 80% 16%
1	G	249	2% 81% 14%
1	H	249	2% 81% 15%
1	I	249	2% 83% 13%
1	J	249	4% 83% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21180 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 Probable peroxiredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1968	1265	346	351	6			
1	B	242	Total	C	N	O	S	0	0	0
			1959	1260	345	348	6			
1	C	244	Total	C	N	O	S	0	0	0
			1973	1268	347	352	6			
1	D	243	Total	C	N	O	S	0	0	0
			1968	1265	346	351	6			
1	E	243	Total	C	N	O	S	0	0	0
			1968	1265	346	351	6			
1	F	244	Total	C	N	O	S	0	0	0
			1973	1268	347	352	6			
1	G	243	Total	C	N	O	S	0	0	0
			1968	1265	346	351	6			
1	H	243	Total	C	N	O	S	0	0	0
			1968	1265	346	351	6			
1	I	243	Total	C	N	O	S	0	0	0
			1968	1265	346	351	6			
1	J	243	Total	C	N	O	S	0	0	0
			1968	1265	346	351	6			

There are 10 discrepancies between the modelled and reference sequences:

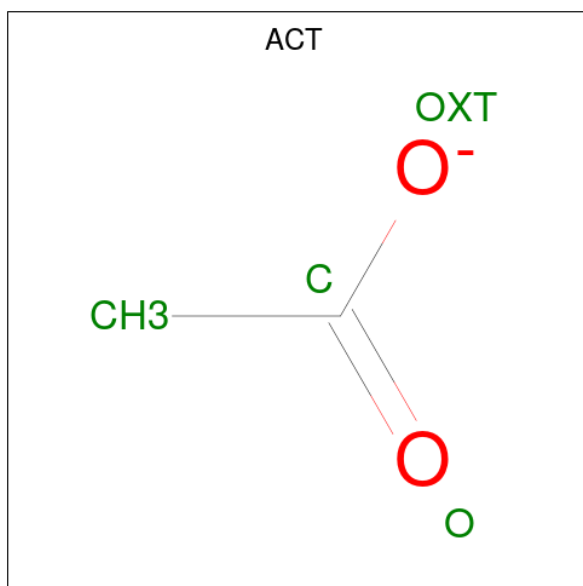
Chain	Residue	Modelled	Actual	Comment	Reference
A	50	SER	CYS	engineered mutation	UNP Q9Y9L0
B	50	SER	CYS	engineered mutation	UNP Q9Y9L0
C	50	SER	CYS	engineered mutation	UNP Q9Y9L0
D	50	SER	CYS	engineered mutation	UNP Q9Y9L0
E	50	SER	CYS	engineered mutation	UNP Q9Y9L0
F	50	SER	CYS	engineered mutation	UNP Q9Y9L0
G	50	SER	CYS	engineered mutation	UNP Q9Y9L0
H	50	SER	CYS	engineered mutation	UNP Q9Y9L0
I	50	SER	CYS	engineered mutation	UNP Q9Y9L0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	50	SER	CYS	engineered mutation	UNP Q9Y9L0

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		

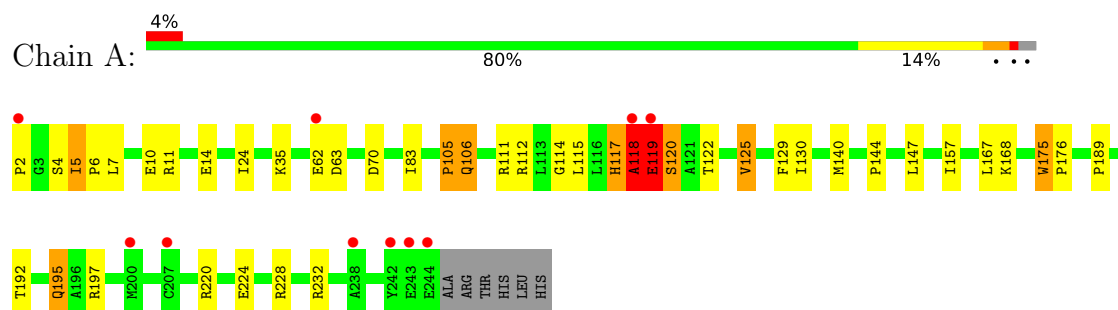
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total 145	O 145	0	0
3	B	148	Total 148	O 148	0	0
3	C	129	Total 129	O 129	0	0
3	D	147	Total 147	O 147	0	0
3	E	142	Total 142	O 142	0	0
3	F	153	Total 153	O 153	0	0
3	G	141	Total 141	O 141	0	0
3	H	147	Total 147	O 147	0	0
3	I	150	Total 150	O 150	0	0
3	J	157	Total 157	O 157	0	0

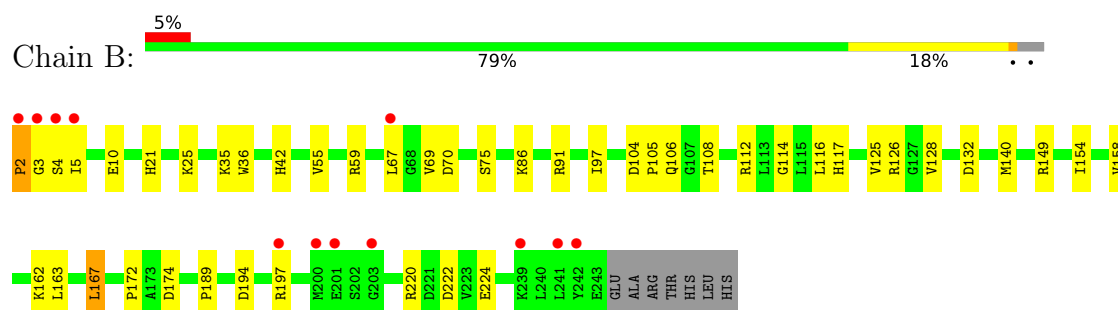
3 Residue-property plots [i](#)

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.

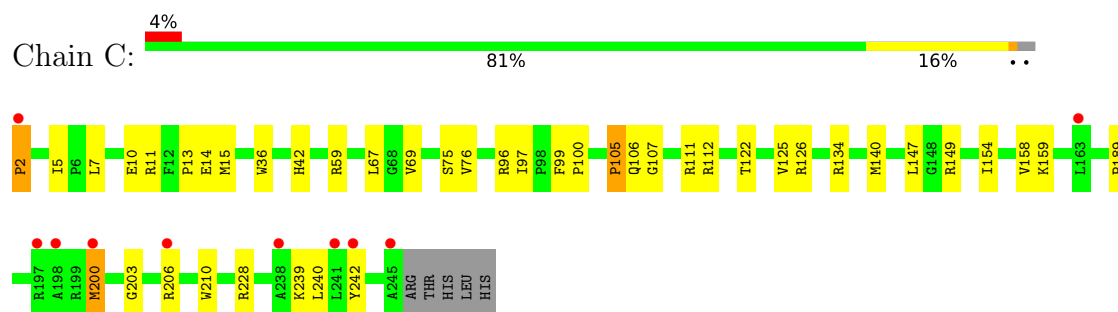
- Molecule 1: Probable peroxiredoxin



- Molecule 1: Probable peroxiredoxin

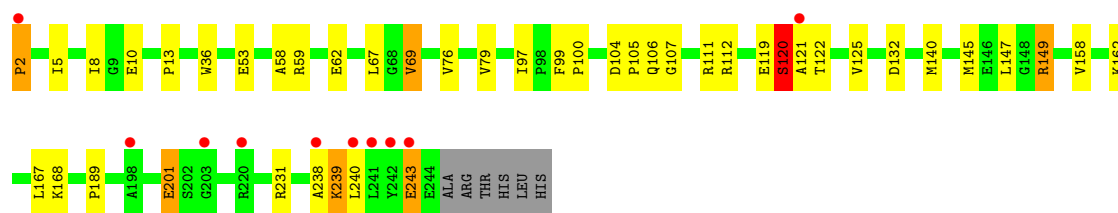


- Molecule 1: Probable peroxiredoxin

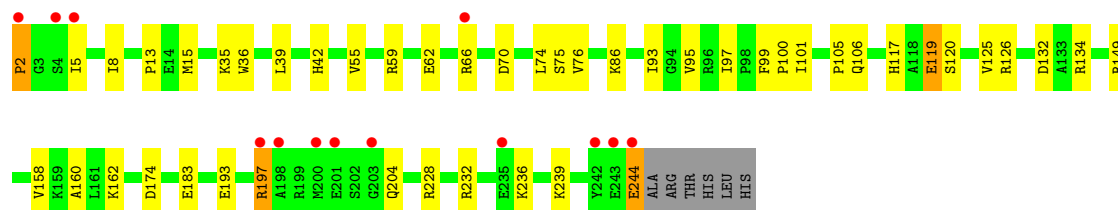
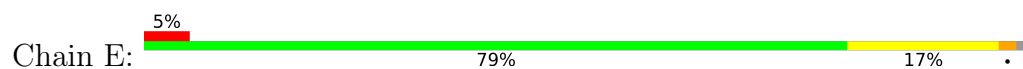


- Molecule 1: Probable peroxiredoxin

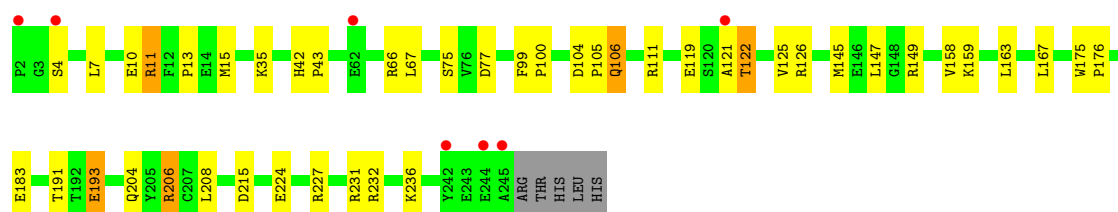
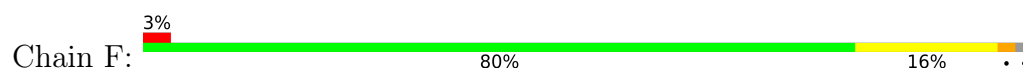




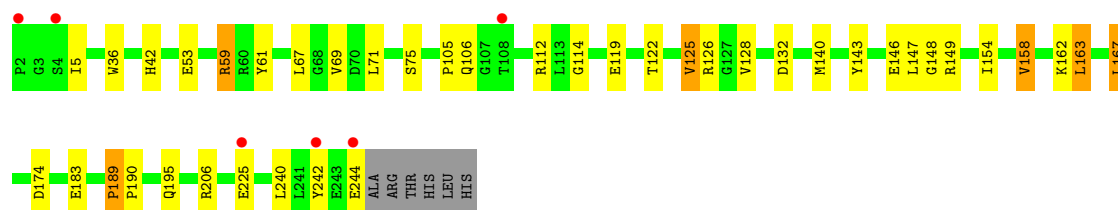
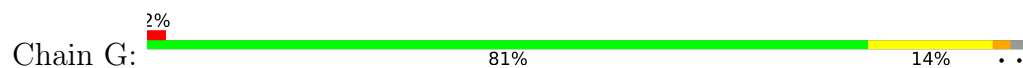
● Molecule 1: Probable peroxiredoxin



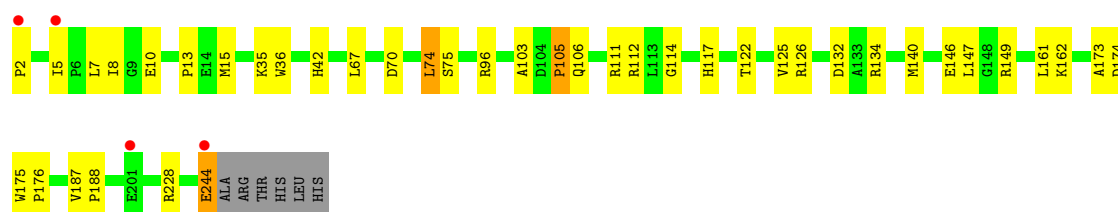
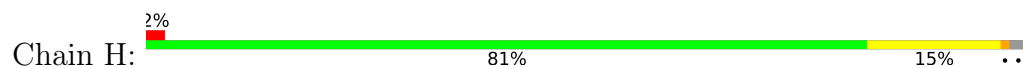
● Molecule 1: Probable peroxiredoxin



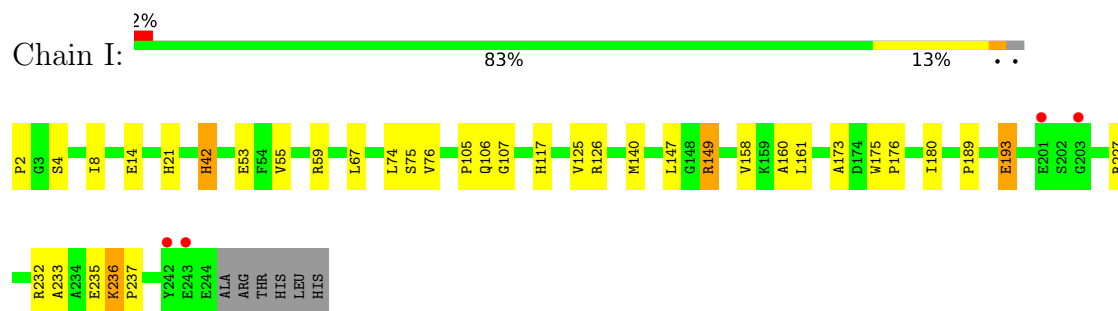
● Molecule 1: Probable peroxiredoxin



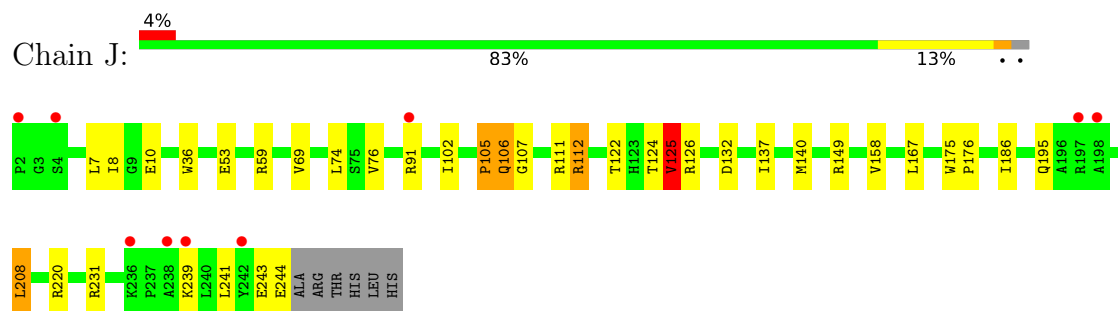
● Molecule 1: Probable peroxiredoxin



- Molecule 1: Probable peroxiredoxin



- Molecule 1: Probable peroxiredoxin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.83Å 102.92Å 104.14Å 105.99° 105.12° 92.80°	Depositor
Resolution (Å)	95.78 – 1.90 95.78 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.8 (95.78-1.90) 93.8 (95.78-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.243 0.196 , 0.243	Depositor DCC
R_{free} test set	10674 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21180	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.11	4/2023 (0.2%)	1.09	6/2750 (0.2%)
1	B	1.12	2/2014 (0.1%)	1.09	4/2738 (0.1%)
1	C	1.02	1/2028 (0.0%)	1.07	4/2757 (0.1%)
1	D	1.07	2/2023 (0.1%)	1.13	8/2750 (0.3%)
1	E	1.11	2/2023 (0.1%)	1.14	7/2750 (0.3%)
1	F	1.10	1/2028 (0.0%)	1.10	6/2757 (0.2%)
1	G	1.07	0/2023	1.09	4/2750 (0.1%)
1	H	1.05	0/2023	1.08	5/2750 (0.2%)
1	I	1.13	4/2023 (0.2%)	1.12	3/2750 (0.1%)
1	J	1.21	2/2023 (0.1%)	1.12	2/2750 (0.1%)
All	All	1.10	18/20231 (0.1%)	1.10	49/27502 (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	A	0	2
1	D	0	1
1	E	0	1
1	F	0	1
1	J	0	1
All	All	0	6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	189	PRO	CA-C	6.80	1.55	1.51
1	I	233	ALA	CA-CB	6.67	1.63	1.53
1	E	160	ALA	CA-CB	6.62	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	PRO	CA-C	6.29	1.55	1.51
1	J	186	ILE	CA-CB	-5.71	1.47	1.54
1	E	95	VAL	CA-CB	5.62	1.61	1.54
1	J	137	ILE	CA-CB	-5.46	1.47	1.54
1	D	189	PRO	CA-C	5.42	1.54	1.51
1	I	42	HIS	C-O	-5.38	1.19	1.24
1	F	193	GLU	N-CA	-5.36	1.40	1.46
1	A	175	TRP	CA-C	5.35	1.58	1.53
1	A	118	ALA	CA-C	-5.29	1.44	1.52
1	I	21	HIS	N-CA	5.17	1.52	1.46
1	A	120	SER	C-O	-5.14	1.17	1.24
1	B	172	PRO	C-O	5.13	1.29	1.23
1	D	69	VAL	CA-CB	5.09	1.60	1.54
1	I	160	ALA	CA-CB	5.08	1.61	1.53
1	A	125	VAL	CB-CG1	5.04	1.69	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	120	SER	N-CA-C	9.91	125.17	109.50
1	F	122	THR	N-CA-C	-9.59	103.69	114.62
1	I	149	ARG	NE-CZ-NH1	-8.21	113.29	121.50
1	D	149	ARG	NE-CZ-NH2	8.19	126.57	119.20
1	D	149	ARG	NE-CZ-NH1	-7.91	113.59	121.50
1	J	125	VAL	N-CA-C	7.86	125.69	109.34
1	I	149	ARG	NE-CZ-NH2	7.29	125.77	119.20
1	F	104	ASP	CA-C-N	-6.56	113.20	119.76
1	F	104	ASP	C-N-CA	-6.56	113.20	119.76
1	I	189	PRO	O-C-N	6.40	124.16	121.15
1	D	104	ASP	CA-C-N	-6.16	113.61	119.76
1	D	104	ASP	C-N-CA	-6.16	113.61	119.76
1	A	120	SER	N-CA-C	6.09	123.76	110.80
1	A	189	PRO	N-CA-C	5.95	116.95	110.58
1	E	119	GLU	N-CA-C	5.86	118.90	111.69
1	E	228	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	D	120	SER	CA-C-N	5.75	132.53	121.54
1	D	120	SER	C-N-CA	5.75	132.53	121.54
1	A	117	HIS	N-CA-C	-5.72	98.61	110.80
1	E	120	SER	N-CA-CB	-5.65	101.08	111.37
1	H	187	VAL	CA-C-N	-5.65	114.56	120.38
1	H	187	VAL	C-N-CA	-5.65	114.56	120.38
1	A	119	GLU	O-C-N	-5.47	115.31	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ALA	CA-C-O	-5.47	114.83	121.89
1	J	105	PRO	N-CA-C	-5.37	102.84	111.38
1	E	5	ILE	CA-C-N	-5.37	115.24	120.98
1	E	5	ILE	C-N-CA	-5.37	115.24	120.98
1	G	189	PRO	O-C-N	5.30	123.64	121.15
1	A	105	PRO	N-CA-C	-5.29	102.89	111.19
1	G	183	GLU	CA-C-N	5.25	125.09	120.10
1	G	183	GLU	C-N-CA	5.25	125.09	120.10
1	B	189	PRO	N-CA-C	5.23	115.49	110.47
1	B	104	ASP	CA-C-N	-5.23	114.53	119.76
1	B	104	ASP	C-N-CA	-5.23	114.53	119.76
1	F	122	THR	N-CA-CB	5.19	119.38	111.18
1	D	5	ILE	CA-C-N	-5.18	115.24	120.21
1	D	5	ILE	C-N-CA	-5.18	115.24	120.21
1	F	215	ASP	CA-C-N	-5.15	116.91	123.15
1	F	215	ASP	C-N-CA	-5.15	116.91	123.15
1	C	105	PRO	N-CA-C	-5.15	103.11	111.19
1	C	97	ILE	N-CA-C	-5.10	102.61	107.76
1	C	5	ILE	CA-C-N	-5.09	113.47	119.84
1	C	5	ILE	C-N-CA	-5.09	113.47	119.84
1	B	189	PRO	O-C-N	5.06	123.64	121.31
1	G	225	GLU	N-CA-C	-5.04	105.69	111.14
1	H	105	PRO	N-CA-C	-5.03	103.38	111.38
1	H	96	ARG	CA-C-N	-5.02	119.19	122.60
1	H	96	ARG	C-N-CA	-5.02	119.19	122.60
1	E	97	ILE	CB-CA-C	-5.02	105.13	110.95

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	HIS	Peptide
1	A	118	ALA	Peptide
1	D	120	SER	Peptide
1	E	119	GLU	Peptide
1	F	121	ALA	Peptide
1	J	124	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1968	0	1954	40	0
1	B	1959	0	1948	32	0
1	C	1973	0	1959	29	0
1	D	1968	0	1954	29	0
1	E	1968	0	1954	36	0
1	F	1973	0	1959	35	0
1	G	1968	0	1954	34	0
1	H	1968	0	1954	27	0
1	I	1968	0	1954	25	0
1	J	1968	0	1954	36	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
2	E	4	0	3	0	0
2	F	4	0	3	0	0
2	G	4	0	3	0	0
2	H	4	0	3	0	0
2	I	4	0	3	0	0
2	J	4	0	3	0	0
3	A	145	0	0	7	1
3	B	148	0	0	3	0
3	C	129	0	0	9	0
3	D	147	0	0	7	0
3	E	142	0	0	5	0
3	F	153	0	0	8	0
3	G	141	0	0	6	0
3	H	147	0	0	6	0
3	I	150	0	0	4	0
3	J	157	0	0	6	1
All	All	21180	0	19574	281	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 7.

All (281) 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:G:206:ARG:HD3	3:G:1217:HOH:O	1.39	1.21
1:E:76:VAL:HG12	3:E:1314:HOH:O	1.50	1.10
1:F:35:LYS:NZ	3:F:1142:HOH:O	1.84	1.09
1:D:53:GLU:OE2	1:D:149:ARG:HD2	1.54	1.08
1:G:125:VAL:HG12	3:G:1123:HOH:O	1.54	1.07
1:G:59:ARG:HH11	1:G:59:ARG:HG2	1.03	1.06
1:G:69:VAL:HG21	1:G:158:VAL:HG21	1.47	0.96
1:J:112:ARG:HH21	1:J:112:ARG:HG3	1.28	0.95
1:I:53:GLU:OE2	1:I:149:ARG:HD2	1.67	0.95
1:G:59:ARG:HG2	1:G:59:ARG:NH1	1.75	0.95
1:G:105:PRO:O	1:G:106:GLN:HB2	1.65	0.94
1:D:111:ARG:HD2	3:D:1153:HOH:O	1.65	0.94
1:B:222:ASP:OD2	3:B:1134:HOH:O	1.85	0.93
1:F:11:ARG:HH11	1:F:11:ARG:HG2	1.35	0.90
1:E:8:ILE:HG22	1:F:119:GLU:HG3	1.56	0.87
1:G:119:GLU:OE1	3:G:1123:HOH:O	1.92	0.87
1:G:163:LEU:HD22	1:G:167:LEU:HD22	1.57	0.87
1:J:112:ARG:HH21	1:J:112:ARG:CG	1.87	0.86
1:E:134:ARG:NH1	3:E:482:HOH:O	2.08	0.85
1:J:112:ARG:CD	3:J:1023:HOH:O	2.23	0.85
1:C:59:ARG:HD3	3:C:1172:HOH:O	1.76	0.85
1:G:59:ARG:HH11	1:G:59:ARG:CG	1.88	0.84
1:F:43:PRO:HB3	1:F:145:MET:HE1	1.58	0.84
1:J:105:PRO:O	1:J:106:GLN:HB2	1.77	0.84
1:D:105:PRO:O	1:D:106:GLN:HB2	1.80	0.80
1:F:224:GLU:OE2	1:F:231:ARG:NH2	2.15	0.80
1:F:206:ARG:HD2	3:F:939:HOH:O	1.79	0.80
1:D:53:GLU:OE2	1:D:149:ARG:CD	2.30	0.80
1:J:69:VAL:HG21	1:J:158:VAL:HG11	1.63	0.79
1:D:240:LEU:O	1:D:243:GLU:HG3	1.86	0.76
1:A:118:ALA:H	1:A:119:GLU:HB3	1.50	0.76
1:B:106:GLN:HE22	1:C:107:GLY:HA3	1.49	0.76
1:J:105:PRO:O	1:J:106:GLN:CB	2.34	0.76
1:G:105:PRO:O	1:G:106:GLN:CB	2.28	0.75
1:I:55:VAL:O	1:I:59:ARG:HG2	1.87	0.75
1:I:53:GLU:OE2	1:I:149:ARG:CD	2.33	0.74
1:F:204:GLN:NE2	3:F:737:HOH:O	2.20	0.73
1:C:10:GLU:OE2	1:D:2:PRO:HB2	1.90	0.71
1:E:2:PRO:HB2	1:F:10:GLU:OE2	1.89	0.71
1:H:122:THR:HB	1:I:105:PRO:HG2	1.72	0.71
1:D:168:LYS:NZ	3:D:268:HOH:O	2.23	0.71
1:E:35:LYS:HD3	1:E:70:ASP:OD2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:MET:HE2	1:C:210:TRP:HB3	1.72	0.70
1:F:67:LEU:HD13	1:F:158:VAL:HG23	1.73	0.70
1:F:111:ARG:HD3	3:F:1165:HOH:O	1.92	0.69
1:H:112:ARG:NE	3:H:830:HOH:O	2.24	0.69
1:C:112:ARG:NE	3:C:1214:HOH:O	2.18	0.69
1:C:2:PRO:HB2	1:D:10:GLU:OE1	1.92	0.69
1:D:105:PRO:O	1:D:106:GLN:CB	2.42	0.68
1:B:5:ILE:HG22	1:B:114:GLY:HA3	1.76	0.68
1:H:244:GLU:OE1	3:H:1413:HOH:O	2.11	0.68
1:F:11:ARG:HG2	1:F:11:ARG:NH1	2.04	0.68
1:H:35:LYS:HD3	1:H:70:ASP:OD2	1.93	0.68
1:H:188:PRO:O	3:H:659:HOH:O	2.12	0.68
1:A:105:PRO:O	1:A:106:GLN:HB2	1.94	0.67
1:C:96:ARG:HD3	3:C:794:HOH:O	1.92	0.67
1:J:126:ARG:HB3	1:J:149:ARG:CZ	2.25	0.67
1:B:69:VAL:HG21	1:B:158:VAL:HG11	1.76	0.66
1:I:105:PRO:O	3:I:1144:HOH:O	2.14	0.66
1:G:143:TYR:HD2	1:G:147:LEU:HD12	1.61	0.66
1:C:105:PRO:O	1:C:106:GLN:HB2	1.96	0.65
1:F:204:GLN:O	3:F:826:HOH:O	2.14	0.65
1:A:118:ALA:N	1:A:119:GLU:HB3	2.10	0.65
1:E:105:PRO:O	1:E:106:GLN:HB2	1.95	0.65
1:A:10:GLU:OE2	1:B:2:PRO:HB2	1.95	0.65
1:C:126:ARG:HB3	1:C:149:ARG:CZ	2.26	0.65
1:E:239:LYS:HE3	1:E:244:GLU:HG2	1.79	0.65
1:D:62:GLU:OE2	3:D:578:HOH:O	2.14	0.64
1:A:232:ARG:O	3:A:263:HOH:O	2.15	0.64
1:E:183:GLU:OE1	1:F:236:LYS:NZ	2.29	0.63
1:H:126:ARG:HB3	1:H:149:ARG:CZ	2.27	0.63
1:E:126:ARG:HB3	1:E:149:ARG:CZ	2.28	0.63
1:A:111:ARG:HD2	3:A:1051:HOH:O	2.00	0.62
1:H:105:PRO:O	1:H:106:GLN:HB2	1.98	0.62
1:I:235:GLU:OE2	3:I:881:HOH:O	2.16	0.62
1:J:112:ARG:NE	3:J:1023:HOH:O	2.31	0.61
1:A:105:PRO:O	1:A:106:GLN:CB	2.48	0.61
1:A:224:GLU:HG2	3:A:977:HOH:O	2.00	0.60
1:E:193:GLU:O	1:E:197:ARG:CD	2.49	0.60
1:B:105:PRO:O	1:B:106:GLN:HB2	2.01	0.60
1:B:42:HIS:CE1	1:B:75:SER:HB3	2.37	0.59
1:F:105:PRO:O	1:F:106:GLN:HB2	2.02	0.59
1:D:238:ALA:O	1:D:239:LYS:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:ARG:HB3	1:G:149:ARG:CZ	2.33	0.59
1:E:55:VAL:O	1:E:59:ARG:HG2	2.03	0.59
1:H:8:ILE:HG13	1:H:140:MET:HE2	1.84	0.58
1:E:62:GLU:OE1	1:E:66:ARG:NH1	2.37	0.58
1:F:105:PRO:O	1:F:106:GLN:CB	2.49	0.58
1:E:99:PHE:HB2	1:E:100:PRO:HD2	1.85	0.58
1:C:67:LEU:HD21	1:C:159:LYS:HD3	1.86	0.57
1:D:13:PRO:HB3	1:D:112:ARG:CZ	2.33	0.57
1:B:194:ASP:OD2	1:B:197:ARG:NH2	2.37	0.57
1:E:193:GLU:O	1:E:197:ARG:HD2	2.04	0.57
1:B:91:ARG:HD2	3:B:682:HOH:O	2.04	0.56
1:F:43:PRO:HB3	1:F:145:MET:CE	2.33	0.56
1:C:154:ILE:O	1:C:158:VAL:HG22	2.04	0.56
1:D:8:ILE:HG13	1:D:140:MET:HE2	1.88	0.56
1:J:112:ARG:CG	1:J:112:ARG:NH2	2.56	0.56
1:A:118:ALA:H	1:A:119:GLU:CB	2.15	0.56
1:G:36:TRP:HB2	1:G:69:VAL:HG22	1.88	0.56
1:B:106:GLN:OE1	1:C:76:VAL:HG11	2.05	0.56
1:D:79:VAL:HG11	1:F:191:THR:O	2.06	0.55
1:A:2:PRO:HB3	1:B:10:GLU:OE2	2.07	0.55
1:D:107:GLY:HA3	1:E:106:GLN:OE1	2.06	0.55
1:G:143:TYR:CD2	1:G:147:LEU:HD12	2.40	0.55
1:C:105:PRO:O	1:C:106:GLN:CB	2.54	0.55
1:C:134:ARG:NH1	3:C:548:HOH:O	2.39	0.55
1:D:120:SER:O	3:D:1085:HOH:O	2.17	0.54
1:F:119:GLU:OE1	1:F:145:MET:HG2	2.07	0.54
1:A:4:SER:HA	1:B:4:SER:HA	1.90	0.54
1:D:231:ARG:NH2	3:D:1119:HOH:O	2.40	0.54
1:J:74:LEU:HD13	1:J:102:ILE:CG2	2.37	0.53
1:E:197:ARG:HD2	1:E:197:ARG:N	2.23	0.53
1:G:67:LEU:O	1:G:162:LYS:HE3	2.08	0.53
1:B:55:VAL:O	1:B:59:ARG:HG3	2.08	0.53
1:B:106:GLN:HE21	1:C:111:ARG:HH22	1.57	0.53
1:I:236:LYS:HD3	1:I:237:PRO:HD2	1.90	0.53
1:G:154:ILE:O	1:G:158:VAL:HG12	2.09	0.52
1:A:11:ARG:NE	3:A:751:HOH:O	2.13	0.52
1:C:42:HIS:CE1	1:C:75:SER:HB3	2.45	0.52
1:J:69:VAL:CG2	1:J:158:VAL:HG11	2.36	0.52
1:F:67:LEU:HD13	1:F:158:VAL:CG2	2.40	0.52
1:E:174:ASP:HB3	3:F:721:HOH:O	2.08	0.52
1:E:66:ARG:CD	3:E:965:HOH:O	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:MET:CE	1:H:117:HIS:HE1	2.23	0.51
1:J:112:ARG:HG3	1:J:112:ARG:NH2	2.10	0.51
1:A:111:ARG:NE	3:A:1208:HOH:O	2.36	0.51
1:A:192:THR:OG1	1:A:195:GLN:HB2	2.10	0.51
1:D:99:PHE:HB2	1:D:100:PRO:HD2	1.92	0.51
1:H:106:GLN:OE1	1:I:107:GLY:HA3	2.09	0.51
1:E:193:GLU:O	1:E:197:ARG:HD3	2.11	0.51
1:D:36:TRP:CD2	1:D:132:ASP:HA	2.46	0.51
1:J:112:ARG:HD2	3:J:1023:HOH:O	2.02	0.51
1:I:126:ARG:HB3	1:I:149:ARG:CZ	2.41	0.51
1:H:74:LEU:C	1:H:74:LEU:HD13	2.36	0.50
1:D:122:THR:HB	1:E:105:PRO:HG2	1.92	0.50
1:F:122:THR:HB	1:G:105:PRO:HG2	1.94	0.50
1:E:93:ILE:HD11	1:F:208:LEU:HD23	1.94	0.50
1:A:106:GLN:NE2	1:J:76:VAL:HG11	2.27	0.49
1:A:118:ALA:N	1:A:119:GLU:CB	2.74	0.49
1:I:8:ILE:HG13	1:I:140:MET:HE2	1.94	0.49
1:H:106:GLN:NE2	1:I:76:VAL:HG11	2.27	0.49
1:I:232:ARG:O	3:I:281:HOH:O	2.19	0.49
1:A:130:ILE:HD13	1:A:157:ILE:HG21	1.94	0.49
1:B:35:LYS:HD3	1:B:70:ASP:OD2	2.13	0.49
1:F:176:PRO:HG2	1:F:227:ARG:HG2	1.94	0.49
1:A:83:ILE:HG12	1:I:193:GLU:HG2	1.95	0.49
1:A:5:ILE:HG12	1:B:5:ILE:HG12	1.95	0.49
1:I:175:TRP:CG	1:I:176:PRO:HA	2.48	0.48
1:J:74:LEU:HD13	1:J:102:ILE:HG21	1.95	0.48
1:D:112:ARG:NE	3:D:920:HOH:O	2.28	0.48
1:E:232:ARG:O	3:E:525:HOH:O	2.20	0.48
1:A:106:GLN:HE21	1:J:76:VAL:HG11	1.77	0.48
1:B:105:PRO:O	1:B:106:GLN:CB	2.61	0.48
1:C:228:ARG:HG3	3:C:628:HOH:O	2.14	0.48
1:A:119:GLU:HA	1:A:119:GLU:OE2	2.12	0.48
1:A:14:GLU:HG2	3:A:751:HOH:O	2.13	0.48
1:J:36:TRP:CD2	1:J:132:ASP:HA	2.49	0.48
1:H:42:HIS:CE1	1:H:75:SER:HB3	2.48	0.48
1:I:173:ALA:HB2	1:J:53:GLU:HG2	1.96	0.48
1:C:59:ARG:CD	3:C:1172:HOH:O	2.50	0.47
1:F:105:PRO:HG2	1:G:122:THR:HB	1.95	0.47
1:H:105:PRO:O	1:H:106:GLN:CB	2.62	0.47
1:H:2:PRO:N	3:H:1373:HOH:O	2.47	0.47
1:A:5:ILE:HG22	1:A:114:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:TRP:CD2	1:E:132:ASP:HA	2.50	0.47
1:B:21:HIS:HB3	3:B:601:HOH:O	2.15	0.47
1:B:67:LEU:O	1:B:162:LYS:HE3	2.14	0.47
1:I:117:HIS:HA	1:J:7:LEU:HD13	1.97	0.47
1:D:36:TRP:HB2	1:D:69:VAL:HG22	1.97	0.47
1:G:174:ASP:HB3	3:G:783:HOH:O	2.14	0.47
1:B:220:ARG:O	1:B:224:GLU:HG3	2.15	0.46
1:C:99:PHE:HB2	1:C:100:PRO:HD2	1.96	0.46
1:H:175:TRP:CG	1:H:176:PRO:HA	2.50	0.46
1:J:195:GLN:OE1	3:J:1427:HOH:O	2.21	0.46
1:H:103:ALA:C	1:H:105:PRO:HD3	2.40	0.46
1:I:2:PRO:N	1:J:10:GLU:OE2	2.49	0.46
1:J:107:GLY:O	1:J:111:ARG:HG3	2.15	0.46
1:C:59:ARG:NH1	3:C:1172:HOH:O	2.46	0.46
1:D:76:VAL:HG11	1:E:106:GLN:NE2	2.31	0.46
1:E:105:PRO:O	1:E:106:GLN:CB	2.62	0.46
1:F:42:HIS:CE1	1:F:75:SER:HB3	2.51	0.46
1:G:42:HIS:CE1	1:G:75:SER:HB3	2.51	0.46
1:H:7:LEU:O	1:H:10:GLU:HB2	2.15	0.46
1:J:8:ILE:HG13	1:J:140:MET:HE2	1.97	0.46
1:A:63:ASP:OD2	1:A:228:ARG:NH2	2.49	0.46
1:F:126:ARG:HB3	1:F:149:ARG:CZ	2.46	0.46
1:J:91:ARG:NH2	3:J:280:HOH:O	2.48	0.46
1:G:240:LEU:HD12	1:G:242:TYR:HE2	1.81	0.46
1:I:105:PRO:O	1:I:106:GLN:HB2	2.16	0.46
1:C:203:GLY:HA2	3:C:1076:HOH:O	2.16	0.45
1:E:66:ARG:HD3	3:E:965:HOH:O	2.17	0.45
1:A:175:TRP:CG	1:A:176:PRO:HA	2.51	0.45
1:F:232:ARG:O	3:F:272:HOH:O	2.21	0.45
1:G:5:ILE:HG22	1:G:114:GLY:HA3	1.98	0.45
1:I:74:LEU:C	1:I:74:LEU:HD23	2.42	0.45
1:I:42:HIS:CE1	1:I:75:SER:HB3	2.52	0.45
1:J:239:LYS:HE2	1:J:243:GLU:HB2	1.98	0.45
1:G:163:LEU:HD22	1:G:167:LEU:CD2	2.39	0.45
1:G:146:GLU:HG3	3:H:1008:HOH:O	2.16	0.45
1:H:134:ARG:NH1	3:H:1181:HOH:O	2.49	0.45
1:J:243:GLU:O	1:J:244:GLU:HB2	2.17	0.45
1:H:67:LEU:O	1:H:162:LYS:HE3	2.17	0.44
1:H:106:GLN:O	1:H:111:ARG:NH2	2.50	0.44
1:A:140:MET:HE1	1:B:117:HIS:HE1	1.82	0.44
1:H:5:ILE:HG22	1:H:114:GLY:HA3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:227:ARG:HD2	3:I:378:HOH:O	2.18	0.44
1:F:13:PRO:HB2	1:F:15:MET:HE3	1.99	0.44
1:D:201:GLU:HG2	3:D:1368:HOH:O	2.17	0.44
1:G:143:TYR:HD2	1:G:147:LEU:CD1	2.30	0.44
1:H:36:TRP:CD2	1:H:132:ASP:HA	2.53	0.44
1:C:13:PRO:HB2	1:C:15:MET:HE3	1.99	0.44
1:C:36:TRP:HB2	1:C:69:VAL:HG22	2.00	0.44
1:J:175:TRP:CG	1:J:176:PRO:HA	2.53	0.44
1:A:144:PRO:HD2	1:A:147:LEU:HB3	2.00	0.44
1:A:220:ARG:NH1	1:A:224:GLU:OE2	2.51	0.44
1:A:105:PRO:HG2	1:J:122:THR:HB	2.00	0.43
1:B:128:VAL:O	1:B:140:MET:HA	2.18	0.43
1:A:7:LEU:HD21	1:B:3:GLY:HA3	2.00	0.43
3:A:707:HOH:O	1:B:174:ASP:HB3	2.17	0.43
1:E:2:PRO:CB	1:F:10:GLU:OE2	2.64	0.43
1:J:231:ARG:HH11	1:J:231:ARG:HD2	1.67	0.43
1:D:162:LYS:HB3	1:D:162:LYS:HE3	1.80	0.43
3:G:821:HOH:O	1:H:174:ASP:HB3	2.18	0.43
1:B:154:ILE:O	1:B:158:VAL:HG23	2.18	0.43
1:E:86:LYS:HE3	1:E:101:ILE:CD1	2.48	0.43
1:F:67:LEU:HD21	1:F:159:LYS:HD3	2.00	0.43
1:G:36:TRP:CD2	1:G:132:ASP:HA	2.53	0.43
1:A:5:ILE:HD12	1:A:6:PRO:O	2.18	0.43
1:J:59:ARG:HG2	1:J:59:ARG:NH2	2.33	0.43
1:B:163:LEU:HD22	1:B:167:LEU:HD22	2.00	0.43
1:E:42:HIS:CE1	1:E:75:SER:HB3	2.53	0.43
1:G:128:VAL:O	1:G:140:MET:HA	2.19	0.43
1:J:7:LEU:O	1:J:10:GLU:HB2	2.19	0.43
1:E:117:HIS:HA	1:F:7:LEU:HD13	2.00	0.42
1:A:122:THR:HA	1:J:106:GLN:HG3	1.99	0.42
1:A:140:MET:HE3	1:A:140:MET:HB2	1.86	0.42
1:C:7:LEU:HA	1:C:140:MET:HE1	2.00	0.42
1:A:4:SER:HB2	1:B:3:GLY:O	2.20	0.42
1:F:175:TRP:CG	1:F:176:PRO:HA	2.55	0.42
1:B:105:PRO:HG2	1:C:122:THR:HB	2.01	0.42
1:D:119:GLU:OE1	1:D:145:MET:HG2	2.20	0.42
1:B:126:ARG:HB3	1:B:149:ARG:CZ	2.50	0.42
1:G:147:LEU:HD13	1:G:147:LEU:C	2.45	0.42
1:H:13:PRO:HB2	1:H:15:MET:HE3	2.01	0.42
1:C:240:LEU:HD12	1:C:242:TYR:HE2	1.84	0.42
1:G:61:TYR:HD1	1:G:71:LEU:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:220:ARG:NE	3:J:1132:HOH:O	2.36	0.41
1:A:115:LEU:HD21	1:A:129:PHE:HE1	1.85	0.41
1:D:58:ALA:HB2	1:D:97:ILE:HD12	2.02	0.41
1:A:197:ARG:HH12	1:C:96:ARG:HH21	1.67	0.41
1:I:175:TRP:CD1	1:I:176:PRO:HA	2.56	0.41
1:A:35:LYS:HG3	1:A:70:ASP:OD2	2.21	0.41
1:G:53:GLU:HG2	1:H:173:ALA:HB2	2.03	0.41
1:D:132:ASP:OD1	1:D:132:ASP:C	2.64	0.41
1:F:183:GLU:H	1:F:183:GLU:HG2	1.67	0.41
1:I:180:ILE:HA	1:J:241:LEU:HB2	2.03	0.41
1:J:59:ARG:HG2	1:J:59:ARG:HH21	1.86	0.41
1:B:86:LYS:HG2	1:B:97:ILE:HB	2.03	0.41
1:E:197:ARG:HD2	1:E:197:ARG:H	1.85	0.41
1:F:77:ASP:OD2	3:F:1328:HOH:O	2.22	0.41
1:G:147:LEU:HD13	1:G:148:GLY:O	2.20	0.41
1:I:105:PRO:O	1:I:106:GLN:CB	2.68	0.41
1:D:67:LEU:HD13	1:D:158:VAL:HG23	2.02	0.41
1:E:13:PRO:HB2	1:E:15:MET:HE3	2.03	0.41
1:E:39:LEU:HD23	1:E:39:LEU:C	2.46	0.40
1:E:74:LEU:HD23	1:E:74:LEU:C	2.46	0.40
1:F:99:PHE:HB2	1:F:100:PRO:HD2	2.03	0.40
1:G:189:PRO:HA	1:G:190:PRO:HD3	1.89	0.40
3:G:447:HOH:O	1:H:146:GLU:HG3	2.21	0.40
1:I:67:LEU:HD13	1:I:158:VAL:HG23	2.03	0.40
1:C:11:ARG:NH1	1:C:14:GLU:OE1	2.55	0.40
1:C:203:GLY:N	3:C:1076:HOH:O	2.50	0.40
1:E:93:ILE:HD11	1:F:208:LEU:CD2	2.51	0.40
1:E:158:VAL:O	1:E:162:LYS:HG3	2.20	0.40
1:B:36:TRP:CD2	1:B:132:ASP:HA	2.56	0.40
1:J:208:LEU:CD2	1:J:208:LEU:N	2.85	0.40
1:A:63:ASP:CG	1:A:228:ARG:HH22	2.29	0.40
1:A:112:ARG:HA	1:A:112:ARG:HD2	1.89	0.40
1:G:190:PRO:HB3	1:G:195:GLN:HG2	2.03	0.40
1:A:140:MET:CE	1:B:117:HIS:HE1	2.34	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:A:1031:HOH:O	3:J:1020:HOH:O[1_455]	2.15	0.05

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	241/249 (97%)	232 (96%)	5 (2%)	4 (2%)	7	2
1	B	240/249 (96%)	236 (98%)	3 (1%)	1 (0%)	30	22
1	C	242/249 (97%)	235 (97%)	6 (2%)	1 (0%)	30	22
1	D	241/249 (97%)	229 (95%)	9 (4%)	3 (1%)	10	4
1	E	241/249 (97%)	235 (98%)	5 (2%)	1 (0%)	30	22
1	F	242/249 (97%)	234 (97%)	6 (2%)	2 (1%)	16	8
1	G	241/249 (97%)	235 (98%)	5 (2%)	1 (0%)	30	22
1	H	241/249 (97%)	233 (97%)	7 (3%)	1 (0%)	30	22
1	I	241/249 (97%)	234 (97%)	6 (2%)	1 (0%)	30	22
1	J	241/249 (97%)	233 (97%)	6 (2%)	2 (1%)	16	8
All	All	2411/2490 (97%)	2336 (97%)	58 (2%)	17 (1%)	18	10

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	GLU
1	D	121	ALA
1	J	125	VAL
1	D	239	LYS
1	A	120	SER
1	D	125	VAL
1	F	106	GLN
1	F	125	VAL
1	J	106	GLN
1	A	106	GLN
1	A	125	VAL
1	E	125	VAL
1	G	125	VAL
1	I	125	VAL

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Mol	Chain	Res	Type
1	C	125	VAL
1	H	125	VAL
1	B	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	210/215 (98%)	203 (97%)	7 (3%)	33	26
1	B	209/215 (97%)	203 (97%)	6 (3%)	37	31
1	C	210/215 (98%)	205 (98%)	5 (2%)	43	38
1	D	210/215 (98%)	204 (97%)	6 (3%)	37	31
1	E	210/215 (98%)	205 (98%)	5 (2%)	43	38
1	F	210/215 (98%)	202 (96%)	8 (4%)	29	21
1	G	210/215 (98%)	204 (97%)	6 (3%)	37	31
1	H	210/215 (98%)	205 (98%)	5 (2%)	43	38
1	I	210/215 (98%)	204 (97%)	6 (3%)	37	31
1	J	210/215 (98%)	206 (98%)	4 (2%)	50	47
All	All	2099/2150 (98%)	2041 (97%)	58 (3%)	38	32

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	24	ILE
1	A	62	GLU
1	A	119	GLU
1	A	167	LEU
1	A	168	LYS
1	A	195	GLN
1	B	2	PRO
1	B	25	LYS
1	B	108	THR

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Mol	Chain	Res	Type
1	B	112	ARG
1	B	116	LEU
1	B	167	LEU
1	C	2	PRO
1	C	147	LEU
1	C	200	MET
1	C	206	ARG
1	C	239	LYS
1	D	2	PRO
1	D	59	ARG
1	D	147	LEU
1	D	167	LEU
1	D	201	GLU
1	D	243	GLU
1	E	2	PRO
1	E	197	ARG
1	E	204	GLN
1	E	236	LYS
1	E	244	GLU
1	F	4	SER
1	F	11	ARG
1	F	66	ARG
1	F	147	LEU
1	F	163	LEU
1	F	167	LEU
1	F	193	GLU
1	F	206	ARG
1	G	59	ARG
1	G	112	ARG
1	G	158	VAL
1	G	163	LEU
1	G	167	LEU
1	G	244	GLU
1	H	74	LEU
1	H	147	LEU
1	H	161	LEU
1	H	228	ARG
1	H	244	GLU
1	I	4	SER
1	I	14	GLU
1	I	147	LEU
1	I	161	LEU

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Mol	Chain	Res	Type
1	I	193	GLU
1	I	236	LYS
1	J	112	ARG
1	J	125	VAL
1	J	167	LEU
1	J	208	LEU

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

Mol	Chain	Res	Type
1	A	204	GLN
1	B	33	GLN
1	B	106	GLN
1	B	123	HIS
1	B	204	GLN
1	C	123	HIS
1	D	123	HIS
1	D	204	GLN
1	F	204	GLN
1	G	106	GLN
1	G	204	GLN
1	H	33	GLN
1	H	204	GLN
1	J	204	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	ACT	I	251	-	3,3,3	0.44	0	3,3,3	1.41	0
2	ACT	H	251	-	3,3,3	1.25	0	3,3,3	0.97	0
2	ACT	F	251	-	3,3,3	1.17	0	3,3,3	0.93	0
2	ACT	D	251	-	3,3,3	0.54	0	3,3,3	1.23	0
2	ACT	J	251	-	3,3,3	1.03	0	3,3,3	1.30	0
2	ACT	G	251	-	3,3,3	0.98	0	3,3,3	0.48	0
2	ACT	A	1	-	3,3,3	0.66	0	3,3,3	0.89	0
2	ACT	B	251	-	3,3,3	1.17	0	3,3,3	0.59	0
2	ACT	E	251	-	3,3,3	0.43	0	3,3,3	1.17	0
2	ACT	C	251	-	3,3,3	0.32	0	3,3,3	1.45	1 (33%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	251	ACT	OXT-C-CH3	2.02	123.53	115.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	243/249 (97%)	0.29	10 (4%) 41 44	16, 23, 38, 57	0
1	B	242/249 (97%)	0.39	12 (4%) 34 36	16, 25, 37, 50	0
1	C	244/249 (97%)	0.42	10 (4%) 41 44	18, 27, 43, 61	0
1	D	243/249 (97%)	0.33	10 (4%) 41 44	17, 26, 42, 58	0
1	E	243/249 (97%)	0.36	13 (5%) 32 34	15, 24, 38, 53	0
1	F	244/249 (97%)	0.34	7 (2%) 53 57	16, 24, 37, 53	0
1	G	243/249 (97%)	0.29	6 (2%) 58 62	17, 24, 40, 51	0
1	H	243/249 (97%)	0.20	4 (1%) 70 74	17, 25, 39, 51	0
1	I	243/249 (97%)	0.12	4 (1%) 70 74	14, 22, 38, 54	0
1	J	243/249 (97%)	0.31	9 (3%) 45 48	14, 23, 37, 49	0
All	All	2431/2490 (97%)	0.30	85 (3%) 47 50	14, 24, 40, 61	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	245	ALA	4.7
1	C	242	TYR	4.4
1	A	119	GLU	4.4
1	F	245	ALA	4.4
1	B	242	TYR	4.2
1	D	238	ALA	4.1
1	G	242	TYR	3.9
1	A	2	PRO	3.7
1	E	2	PRO	3.7
1	C	200	MET	3.6
1	C	2	PRO	3.6
1	A	244	GLU	3.5
1	E	198	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	242	TYR	3.4
1	B	4	SER	3.4
1	A	118	ALA	3.4
1	I	242	TYR	3.4
1	J	242	TYR	3.3
1	E	200	MET	3.2
1	E	242	TYR	3.2
1	J	91	ARG	3.2
1	F	244	GLU	3.1
1	D	243	GLU	3.1
1	F	242	TYR	3.0
1	E	203	GLY	2.9
1	D	220	ARG	2.9
1	B	200	MET	2.9
1	H	5	ILE	2.9
1	B	241	LEU	2.8
1	A	242	TYR	2.8
1	B	197	ARG	2.8
1	B	201	GLU	2.7
1	D	241	LEU	2.7
1	B	2	PRO	2.7
1	J	2	PRO	2.7
1	E	197	ARG	2.7
1	H	2	PRO	2.7
1	J	238	ALA	2.7
1	B	67	LEU	2.7
1	D	198	ALA	2.6
1	E	244	GLU	2.6
1	H	201	GLU	2.6
1	D	203	GLY	2.6
1	C	241	LEU	2.6
1	E	201	GLU	2.6
1	G	4	SER	2.6
1	C	197	ARG	2.5
1	E	235	GLU	2.5
1	A	62	GLU	2.5
1	G	244	GLU	2.5
1	J	197	ARG	2.4
1	C	163	LEU	2.4
1	G	225	GLU	2.4
1	J	198	ALA	2.3
1	B	239	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	238	ALA	2.3
1	F	4	SER	2.3
1	H	244	GLU	2.3
1	F	121	ALA	2.2
1	I	203	GLY	2.2
1	B	5	ILE	2.2
1	G	2	PRO	2.2
1	A	238	ALA	2.2
1	J	236	LYS	2.2
1	G	108	THR	2.2
1	A	207	CYS	2.2
1	B	3	GLY	2.2
1	J	4	SER	2.2
1	D	2	PRO	2.2
1	C	198	ALA	2.2
1	F	2	PRO	2.1
1	E	5	ILE	2.1
1	B	203	GLY	2.1
1	E	66	ARG	2.1
1	A	243	GLU	2.1
1	E	243	GLU	2.1
1	I	243	GLU	2.1
1	A	200	MET	2.1
1	F	62	GLU	2.1
1	D	240	LEU	2.1
1	D	121	ALA	2.1
1	C	206	ARG	2.1
1	I	201	GLU	2.0
1	J	239	LYS	2.0
1	E	4	SER	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	A	1	4/4	0.93	0.11	25,27,27,27	0
2	ACT	I	251	4/4	0.93	0.11	22,23,24,24	0
2	ACT	F	251	4/4	0.94	0.09	22,24,24,25	0
2	ACT	E	251	4/4	0.95	0.08	23,23,24,25	0
2	ACT	C	251	4/4	0.95	0.07	22,23,24,24	0
2	ACT	D	251	4/4	0.95	0.07	23,23,24,24	0
2	ACT	J	251	4/4	0.95	0.08	20,21,22,22	0
2	ACT	H	251	4/4	0.96	0.09	20,22,22,23	0
2	ACT	G	251	4/4	0.97	0.05	20,21,21,22	0
2	ACT	B	251	4/4	0.98	0.05	21,22,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.