



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 1, 2021 – 12:43 PM EDT

PDB ID : 3A2X
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
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) : 2.23.2

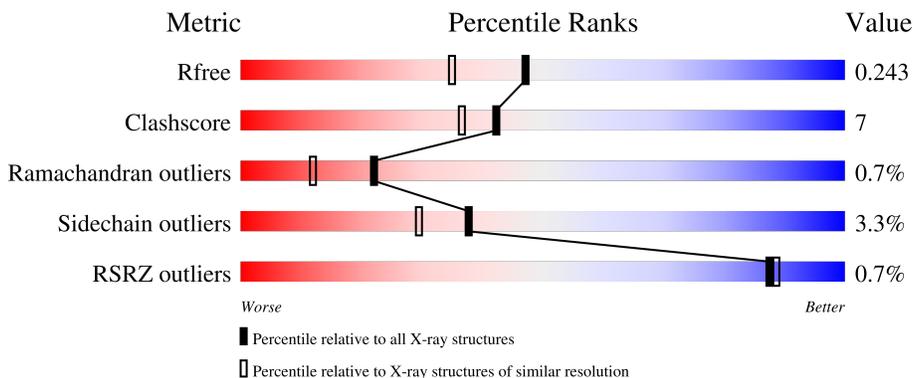
1 Overall quality at a glance

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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	 2% 80% 16% ..
1	B	249	 79% 17% ..
1	C	249	 82% 15% .
1	D	249	 80% 16% ..
1	E	249	 80% 16% ..

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Mol	Chain	Length	Quality of chain
1	F	249	 80% 16% ..
1	G	249	%  80% 16% ..
1	H	249	%  82% 14% ..
1	I	249	 83% 14% ..
1	J	249	 82% 14% ..

2 Entry composition [i](#)

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

There are 10 discrepancies between the modelled and reference sequences:

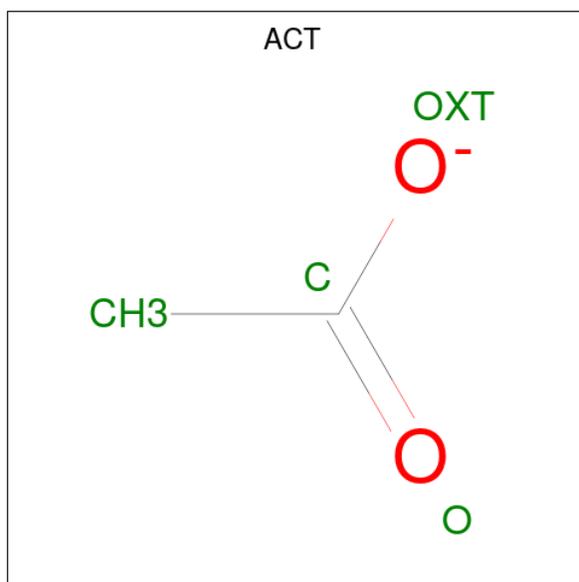
Chain	Residue	Modelled	Actual	Comment	Reference
A	50	SER	CYS	engineered mutation	UNP Q9Y9L0
B	50	SER	CYS	engineered mutation	UNP Q9Y9L0
C	50	SER	CYS	engineered mutation	UNP Q9Y9L0
D	50	SER	CYS	engineered mutation	UNP Q9Y9L0
E	50	SER	CYS	engineered mutation	UNP Q9Y9L0
F	50	SER	CYS	engineered mutation	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 (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

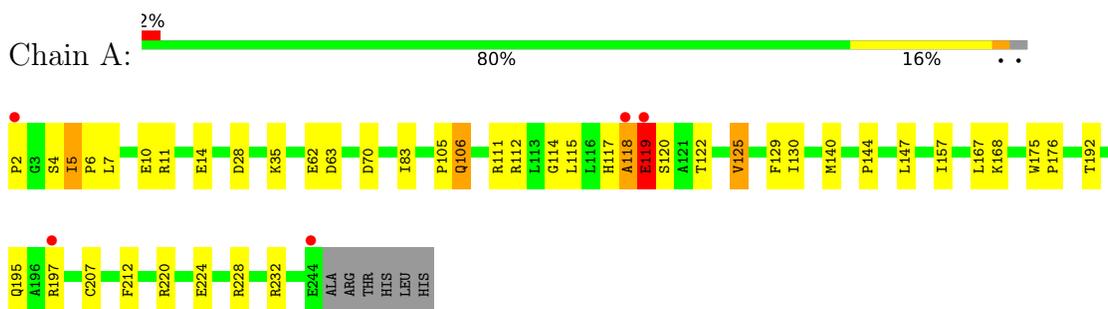
- Molecule 3 is water.

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

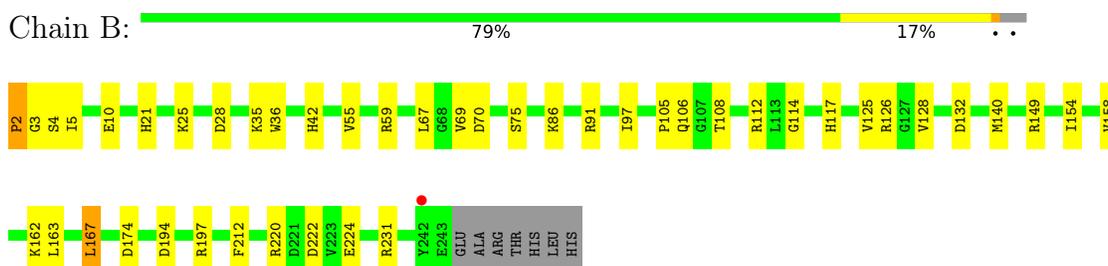
3 Residue-property plots

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.

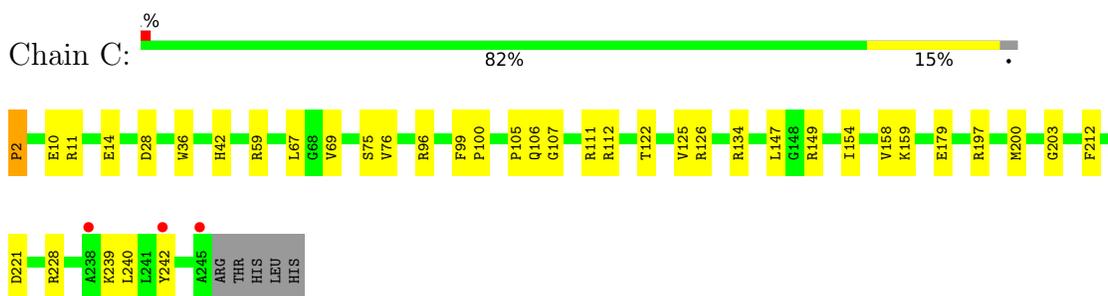
- Molecule 1: Probable peroxiredoxin



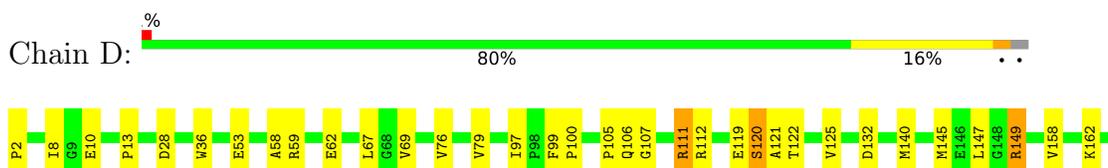
- Molecule 1: Probable peroxiredoxin

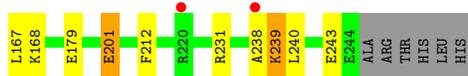


- Molecule 1: Probable peroxiredoxin

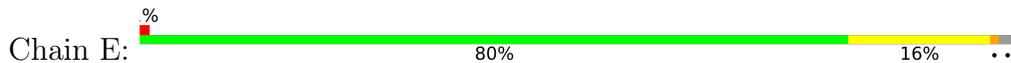


- Molecule 1: Probable peroxiredoxin





- Molecule 1: Probable peroxiredoxin



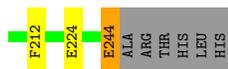
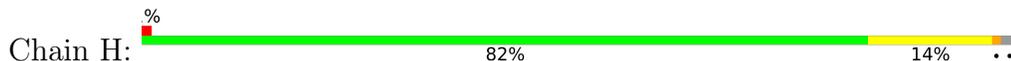
- Molecule 1: Probable peroxiredoxin



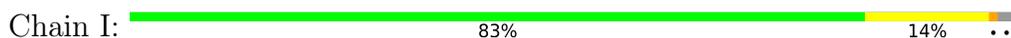
- Molecule 1: Probable peroxiredoxin

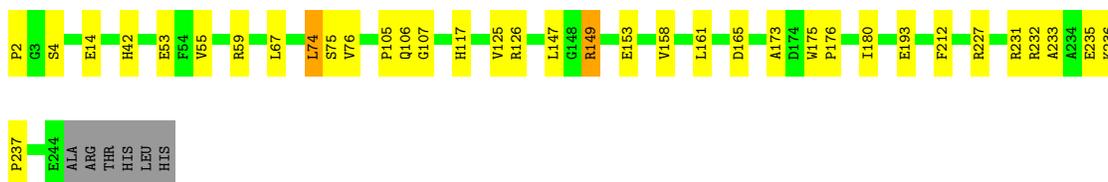


- Molecule 1: Probable peroxiredoxin



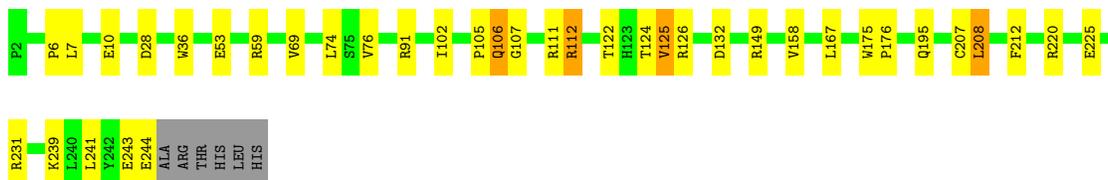
- Molecule 1: Probable peroxiredoxin





- Molecule 1: Probable peroxiredoxin

Chain J: 82% 14% ..



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 72.58 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.8 (95.78-1.90) 93.8 (72.58-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.90Å)	Xtrriage
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	Xtrriage
Anisotropy	0.008	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 i

5.1 Standard geometry i

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	0.94	1/2023 (0.0%)	0.87	0/2750
1	B	0.91	0/2014	0.84	1/2738 (0.0%)
1	C	0.86	2/2028 (0.1%)	0.83	1/2757 (0.0%)
1	D	0.88	1/2023 (0.0%)	0.94	2/2750 (0.1%)
1	E	0.91	1/2023 (0.0%)	0.93	5/2750 (0.2%)
1	F	0.91	1/2028 (0.0%)	0.89	2/2757 (0.1%)
1	G	0.89	1/2023 (0.0%)	0.85	0/2750
1	H	0.87	1/2023 (0.0%)	0.81	1/2750 (0.0%)
1	I	0.93	2/2023 (0.1%)	0.93	4/2750 (0.1%)
1	J	1.01	2/2023 (0.1%)	0.89	1/2750 (0.0%)
All	All	0.91	12/20231 (0.1%)	0.88	17/27502 (0.1%)

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

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	VAL	CB-CG1	7.78	1.69	1.52
1	C	179	GLU	CB-CG	6.51	1.64	1.52
1	C	179	GLU	CG-CD	6.44	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	224	GLU	CG-CD	5.48	1.60	1.51
1	J	225	GLU	CG-CD	5.39	1.60	1.51

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	149	ARG	NE-CZ-NH1	-14.01	113.29	120.30
1	D	149	ARG	NE-CZ-NH1	-13.42	113.59	120.30
1	D	149	ARG	NE-CZ-NH2	12.54	126.57	120.30
1	I	149	ARG	NE-CZ-NH2	10.93	125.77	120.30
1	E	228	ARG	NE-CZ-NH2	8.30	124.45	120.30

There are no chirality outliers.

5 of 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

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	1968	0	1954	39	0
1	B	1959	0	1948	33	0
1	C	1973	0	1959	26	0
1	D	1968	0	1954	28	0
1	E	1968	0	1954	33	0
1	F	1973	0	1959	34	0
1	G	1968	0	1954	35	0
1	H	1968	0	1954	28	0
1	I	1968	0	1954	24	0
1	J	1968	0	1954	35	0
2	A	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	270	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.

The worst 5 of 270 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

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 [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	241/249 (97%)	232 (96%)	5 (2%)	4 (2%)	9	2
1	B	240/249 (96%)	236 (98%)	3 (1%)	1 (0%)	34	24
1	C	242/249 (97%)	235 (97%)	6 (2%)	1 (0%)	34	24
1	D	241/249 (97%)	229 (95%)	9 (4%)	3 (1%)	13	4
1	E	241/249 (97%)	235 (98%)	5 (2%)	1 (0%)	34	24
1	F	242/249 (97%)	234 (97%)	6 (2%)	2 (1%)	19	9
1	G	241/249 (97%)	235 (98%)	5 (2%)	1 (0%)	34	24
1	H	241/249 (97%)	233 (97%)	7 (3%)	1 (0%)	34	24
1	I	241/249 (97%)	234 (97%)	6 (2%)	1 (0%)	34	24
1	J	241/249 (97%)	233 (97%)	6 (2%)	2 (1%)	19	9
All	All	2411/2490 (97%)	2336 (97%)	58 (2%)	17 (1%)	22	12

5 of 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

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%)	202 (96%)	8 (4%)	33	24
1	B	209/215 (97%)	202 (97%)	7 (3%)	38	29
1	C	210/215 (98%)	203 (97%)	7 (3%)	38	29
1	D	210/215 (98%)	203 (97%)	7 (3%)	38	29
1	E	210/215 (98%)	203 (97%)	7 (3%)	38	29
1	F	210/215 (98%)	202 (96%)	8 (4%)	33	24
1	G	210/215 (98%)	202 (96%)	8 (4%)	33	24
1	H	210/215 (98%)	204 (97%)	6 (3%)	42	35
1	I	210/215 (98%)	204 (97%)	6 (3%)	42	35
1	J	210/215 (98%)	204 (97%)	6 (3%)	42	35
All	All	2099/2150 (98%)	2029 (97%)	70 (3%)	38	29

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	244	GLU
1	I	14	GLU
1	J	28	ASP
1	D	111	ARG
1	D	59	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	123	HIS
1	F	204	GLN
1	J	204	GLN
1	H	204	GLN
1	I	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	ACT	G	251	-	1,3,3	0.86	0	0,3,3	-	-
2	ACT	I	251	-	1,3,3	2.19	1 (100%)	0,3,3	-	-
2	ACT	D	251	-	1,3,3	2.06	1 (100%)	0,3,3	-	-
2	ACT	F	251	-	1,3,3	1.93	0	0,3,3	-	-
2	ACT	B	251	-	1,3,3	1.84	0	0,3,3	-	-
2	ACT	C	251	-	1,3,3	0.28	0	0,3,3	-	-
2	ACT	A	1	-	1,3,3	1.24	0	0,3,3	-	-
2	ACT	E	251	-	1,3,3	0.51	0	0,3,3	-	-
2	ACT	H	251	-	1,3,3	0.70	0	0,3,3	-	-
2	ACT	J	251	-	1,3,3	1.99	0	0,3,3	-	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	251	ACT	CH3-C	2.19	1.51	1.48
2	D	251	ACT	CH3-C	2.06	1.51	1.48

There are no bond angle outliers.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.10	5 (2%) 63 66	16, 23, 38, 57	0
1	B	242/249 (97%)	-0.13	1 (0%) 92 93	16, 25, 37, 50	0
1	C	244/249 (97%)	-0.06	3 (1%) 79 81	18, 27, 43, 61	0
1	D	243/249 (97%)	-0.19	2 (0%) 86 87	17, 26, 42, 58	0
1	E	243/249 (97%)	-0.04	2 (0%) 86 87	15, 24, 38, 53	0
1	F	244/249 (97%)	-0.07	0 100 100	16, 24, 37, 53	0
1	G	243/249 (97%)	-0.17	3 (1%) 79 81	17, 24, 40, 51	0
1	H	243/249 (97%)	-0.21	2 (0%) 86 87	17, 25, 39, 51	0
1	I	243/249 (97%)	-0.24	0 100 100	14, 22, 38, 54	0
1	J	243/249 (97%)	-0.04	0 100 100	14, 23, 37, 49	0
All	All	2431/2490 (97%)	-0.13	18 (0%) 87 88	14, 24, 40, 61	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	245	ALA	4.2
1	D	238	ALA	3.9
1	A	119	GLU	3.2
1	H	5	ILE	3.0
1	C	242	TYR	2.7

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACT	D	251	4/4	0.95	0.08	23,23,24,24	0
2	ACT	F	251	4/4	0.95	0.10	22,24,24,25	0
2	ACT	I	251	4/4	0.95	0.11	22,23,24,24	0
2	ACT	A	1	4/4	0.96	0.12	25,27,27,27	0
2	ACT	E	251	4/4	0.96	0.10	23,23,24,25	0
2	ACT	J	251	4/4	0.96	0.09	20,21,22,22	0
2	ACT	C	251	4/4	0.97	0.08	22,23,24,24	0
2	ACT	H	251	4/4	0.97	0.10	20,22,22,23	0
2	ACT	G	251	4/4	0.98	0.09	20,21,21,22	0
2	ACT	B	251	4/4	0.98	0.09	21,22,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.