

Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2021 – 12:13 AM EDT

PDB ID	:	3A2V
Title	:	Peroxiredoxin (C207S) from Aeropyrum pernix K1 complexed with hydrogen
		peroxide
Authors	:	Nakamura, T.; Kado, Y.; Yamaguchi, F.; Ishikawa, K.; Matsumura, H.; Inoue,
		Т.
Deposited on	:	2009-06-04
Resolution	:	1.65 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 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	:	2.23.2
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 (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 1.65 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	Similar resolution		
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R_{free}	130704	1827 (1.66-1.66)		
Clashscore	141614	$1931 \ (1.66-1.66)$		
Ramachandran outliers	138981	$1891 \ (1.66-1.66)$		
Sidechain outliers	138945	1891 (1.66-1.66)		
RSRZ outliers	127900	1791 (1.66-1.66)		

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	А	249	% • 80%	17%	•••
1	В	249	3%	9%	
1	C	249	5%	16%	
1	D	249	3% 85%	10%	
1	Е	249	2% 87%	10%	••



Contr	nued from	n previous	page			
Mol	Chain	Length	Quality of chain			
1	F	249	3% 	12%		
1	G	249	86%	10%		
1		240	4%			
1		243	87% 2%	9%	· ·	,
1	1	249	88%	9%	•	
1	J	249	80%	16%	•••	

 α Jf n tin



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20999 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.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
1	Δ	243	Total	С	Ν	0	S	0	15	0
1	Л	240	2050	1334	350	359	7	0	10	0
1	В	949	Total	С	Ν	Ο	\mathbf{S}	0	6	0
1	D		1993	1287	348	352	6	0	0	0
1	C	2/3	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	11	0
1	U	240	2038	1318	358	354	8	0	11	0
1	а	240	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	7	0
1	D	240	1978	1276	349	346	7		1	0
1	E	949	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	5	0
		242	1990	1281	352	351	6		0	
1	F	944	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	7	0
1	T,	244	2014	1302	348	357	7	0	1	0
1	G	2/3	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	5	0
1	u	240	1998	1288	350	353	7	0	0	0
1	н	949	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	5	0
1	11		1996	1292	349	349	6	0	0	0
1	т	949	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	5	0
	1		1993	1286	352	349	6	0	0	
1	T	2/3	Total	C	Ν	0	S	0	6	0
	J	240	2019	1300	353	358	8	0	0	0

• Molecule 1 is a protein called Probable peroxiredoxin.

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	207	SER	CYS	engineered mutation	UNP Q9Y9L0
В	207	SER	CYS	engineered mutation	UNP Q9Y9L0
С	207	SER	CYS	engineered mutation	UNP Q9Y9L0
D	207	SER	CYS	engineered mutation	UNP Q9Y9L0
Е	207	SER	CYS	engineered mutation	UNP Q9Y9L0
F	207	SER	CYS	engineered mutation	UNP Q9Y9L0
G	207	SER	CYS	engineered mutation	UNP Q9Y9L0
Н	207	SER	CYS	engineered mutation	UNP Q9Y9L0
Ι	207	SER	CYS	engineered mutation	UNP Q9Y9L0



Chain	Residue	Modelled	Actual Comment		Reference
J	207	SER	CYS	engineered mutation	UNP Q9Y9L0

• Molecule 2 is PEROXIDE ION (three-letter code: PER) (formula: O_2).

PER	
01 0 - 0 - 02	

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total O 2 2	0	0
2	В	1	Total O 2 2	0	0
2	С	1	Total O 2 2	0	0
2	D	1	Total O 2 2	0	0
2	Ε	1	Total O 2 2	0	0
2	\mathbf{F}	1	Total O 2 2	0	0
2	G	1	Total O 2 2	0	0
2	Н	1	Total O 2 2	0	0
2	Ι	1	Total O 2 2	0	0
2	J	1	Total O 2 2	0	0

• Molecule 3 is water.



9	٨	0	17
О.	Η	-2	v

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	106	Total O 106 106	0	0
3	В	79	Total O 79 79	0	0
3	С	77	Total O 77 77	0	0
3	D	88	Total O 88 88	0	0
3	Е	79	Total O 79 79	0	0
3	F	76	Total O 76 76	0	0
3	G	93	Total O 93 93	0	0
3	Н	85	Total O 85 85	0	0
3	Ι	124	Total O 124 124	0	0
3	J	103	Total O 103 103	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

GLU ALA ARG HIS HIS LEU HIS





• Molecule 1: Probable peroxired oxin





 \bullet Molecule 1: Probable peroxired oxin









• Molecule 1: Probable peroxired oxin





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	76.21Å 103.11Å 104.40Å	Depositor
a, b, c, α , β , γ	106.02° 104.91° 92.97°	Depositor
Bosolution(A)	39.25 - 1.65	Depositor
Resolution (A)	39.24 - 1.65	EDS
% Data completeness	94.0 (39.25-1.65)	Depositor
(in resolution range)	94.0 (39.24-1.65)	EDS
R_{merge}	0.05	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.79 (at 1.65 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
B B.	0.194 , 0.223	Depositor
II, II free	0.193 , 0.222	DCC
R_{free} test set	16633 reflections (5.05%)	wwPDB-VP
Wilson B-factor $(Å^2)$	23.1	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.44 , 51.2	EDS
L-test for $twinning^2$	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20999	wwPDB-VP
Average B, all atoms $(Å^2)$	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: PER

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	
WIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.66	0/2153	0.71	0/2927
1	В	0.63	0/2066	0.69	1/2808~(0.0%)
1	С	0.58	0/2128	0.67	0/2889
1	D	0.63	0/2053	0.72	1/2788~(0.0%)
1	Е	0.64	0/2060	0.70	1/2797~(0.0%)
1	F	0.63	0/2093	0.68	0/2846
1	G	0.66	0/2070	0.69	0/2813
1	Н	0.63	0/2069	0.71	0/2814
1	Ι	0.71	0/2065	0.73	0/2807
1	J	0.73	0/2076	0.76	2/2822~(0.1%)
All	All	0.65	0/20833	0.71	5/28311~(0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	В	231	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	D	199	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	J	147	LEU	CB-CG-CD2	5.25	119.93	111.00
1	Е	215	ASP	CB-CG-OD1	5.05	122.85	118.30
1	J	169	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2050	0	2084	38	0
1	В	1993	0	2004	24	0
1	С	2038	0	2064	34	0
1	D	1978	0	2001	20	0
1	Е	1990	0	1998	24	0
1	F	2014	0	2012	31	0
1	G	1998	0	1996	23	0
1	Н	1996	0	2000	28	0
1	Ι	1993	0	1998	24	0
1	J	2019	0	2001	34	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
2	D	2	0	0	0	0
2	Е	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	Н	2	0	0	0	0
2	Ι	2	0	0	0	0
2	J	2	0	0	0	0
3	А	106	0	0	1	0
3	В	79	0	0	0	0
3	С	77	0	0	1	0
3	D	88	0	0	1	0
3	Ε	79	0	0	1	0
3	F	76	0	0	1	0
3	G	93	0	0	0	0
3	Н	85	0	0	1	0
3	Ι	124	0	0	1	0
3	J	103	0	0	1	0
All	All	20999	0	20158	221	0

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.

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (221) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-1 Atom-2		Clash overlap (Å)
1:I:242:TYR:CD1 1:J:214[B]:TRP:HH2		1.55	1.23



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:59:ARG:HD3	1:F:179[B]:GLU:OE1	1.41	1.20	
1:E:59:ARG:CD	1:F:179[B]:GLU:OE1	1.91	1.16	
1:E:59:ARG:HD2	1:F:179[B]:GLU:OE2	1.49	1.12	
1:E:59:ARG:HD2	1:F:179[B]:GLU:CD	1.71	1.10	
1:I:242:TYR:CD1	1:J:214[B]:TRP:CH2	2.40	1.09	
1:A:214[A]:TRP:HH2	1:B:242:TYR:CD1	1.73	1.05	
1:I:242:TYR:CE1	1:J:214[B]:TRP:HH2	1.78	0.99	
1:G:105:PRO:O	1:G:106:GLN:HB2	1.66	0.94	
1:I:242:TYR:CE1	1:J:214[B]:TRP:CH2	2.54	0.94	
1:A:214[A]:TRP:CH2	1:B:242:TYR:CD1	2.56	0.93	
1:F:105:PRO:O	1:F:106:GLN:HB2	1.69	0.92	
1:C:59:ARG:HD2	1:D:179:GLU:OE2	1.74	0.88	
1:B:11[A]:ARG:NH1	1:B:14[A]:GLU:OE2	2.06	0.87	
1:B:69:VAL:HG21	1:B:158[A]:VAL:HG11	1.56	0.87	
1:C:208[A]:LEU:CD1	1:C:214[A]:TRP:HZ3	1.88	0.85	
1:B:194:ASP:OD2	1:B:197:ARG:NH2	2.10	0.85	
1:E:105:PRO:O	1:E:106:GLN:HB2	1.73	0.85	
1:E:241:LEU:HD11	1:F:179[B]:GLU:OE2	1.78	0.83	
1:I:69:VAL:HG21	1:I:158[A]:VAL:HG11	1.61	0.83	
1:C:69:VAL:HG21	1:C:158:VAL:HG11	1.59	0.81	
1:J:69:VAL:HG21	1:J:158[A]:VAL:HG21	1.64	0.80	
1:J:105:PRO:O	1:J:106:GLN:HB2	1.82	0.79	
1:D:45:ASP:OD2	1:D:82:HIS:HD2	1.68	0.77	
1:A:125[A]:VAL:HG22	1:A:143:TYR:O	1.84	0.76	
1:E:8:ILE:HG22	1:F:119:GLU:HG3	1.67	0.76	
1:I:179:GLU:OE1	1:J:241:LEU:HD11	1.86	0.75	
1:C:208[A]:LEU:CD1	1:C:214[A]:TRP:CZ3	2.70	0.74	
1:G:106:GLN:O	1:G:111:ARG:NH2	2.20	0.74	
1:F:129:PHE:HE2	1:F:140:MET:HE3	1.53	0.74	
1:H:106:GLN:O	1:H:111:ARG:NH2	2.20	0.73	
1:B:105:PRO:O	1:B:106:GLN:HB2	1.88	0.72	
1:H:134:ARG:NH1	3:H:1139:HOH:O	2.22	0.72	
1:D:105:PRO:O	1:D:106:GLN:HB2	1.88	0.71	
1:C:179:GLU:OE1	1:D:241:LEU:HD11	1.90	0.71	
1:I:200:MET:HA	1:I:200:MET:HE2	1.72	0.70	
1:C:119:GLU:HB3	3:C:445:HOH:O	1.92	0.69	
1:G:163:LEU:HD22	1:G:167:LEU:HD22	1.74	0.68	
1:A:105:PRO:O	1:A:106:GLN:HB2	1.93	0.68	
1:C:43:PRO:HG3	1:C:145[A]:MET:HG3	1.74	0.68	
1:H:69:VAL:HG21	1:H:158[B]:VAL:HG11	1.76	0.68	
1:F:200:MET:HE2	1:F:200:MET:HA	1.76	0.67	



Atom-1	Atom-2	Interatomic	Clash	
	2100HT 2	distance (Å)	overlap (Å)	
1:A:214[A]:TRP:HH2	1:B:242:TYR:CE1	2.12	0.67	
1:J:105:PRO:O	1:J:106:GLN:CB	2.43	0.67	
1:H:122:THR:HG23	1:H:123:HIS:CD2	2.29	0.66	
1:C:208[A]:LEU:HD12	1:C:214[A]:TRP:HZ3	1.59	0.66	
1:H:35:LYS:HD3	1:H:70:ASP:OD2	1.96	0.66	
1:E:11:ARG:HD3	3:E:392:HOH:O	1.95	0.66	
1:C:224:GLU:OE2	1:C:231:ARG:NH1	2.29	0.65	
1:H:122:THR:HG21	3:I:627:HOH:O	1.97	0.65	
1:A:214[A]:TRP:CH2	1:B:242:TYR:CE1	2.85	0.64	
1:A:224[B]:GLU:OE2	1:A:231:ARG:NH2	2.30	0.64	
1:F:122:THR:HB	1:G:105:PRO:HG2	1.78	0.63	
1:H:122:THR:CG2	1:H:123:HIS:CD2	2.81	0.63	
1:J:110:ALA:HB1	1:J:116:LEU:CD2	2.28	0.63	
1:C:105:PRO:O	1:C:106[A]:GLN:HB2	1.99	0.63	
1:F:129:PHE:CE2	1:F:140:MET:HE3	2.34	0.62	
1:F:140:MET:CE	1:F:142:TYR:OH	2.47	0.61	
1:F:140:MET:HE1	1:F:142:TYR:OH	2.01	0.61	
1:E:59:ARG:CD	1:F:179[B]:GLU:CD	2.45	0.61	
1:D:105:PRO:O	1:D:106:GLN:CB	2.48	0.61	
1:F:129:PHE:CE2	1:F:140:MET:CE	2.84	0.61	
1:J:225:GLU:CD	1:J:228:ARG:HH21	2.05	0.60	
1:A:105:PRO:HG2	1:J:122:THR:HB	1.84	0.60	
1:I:105:PRO:O	1:I:106:GLN:HB2	2.02	0.59	
1:I:176:PRO:HG2	1:I:227:ARG:HG2	1.85	0.59	
1:H:105:PRO:O	1:H:106:GLN:HB2	2.03	0.59	
1:A:106:GLN:O	1:A:111:ARG:NH2	2.36	0.58	
1:A:69:VAL:HG21	1:A:158[A]:VAL:HG11	1.84	0.58	
1:B:106:GLN:NE2	1:C:116:LEU:HD22	2.18	0.57	
1:B:42:HIS:CE1	1:B:75:SER:HB3	2.38	0.57	
1:E:35[B]:LYS:HD2	1:E:70:ASP:OD2	2.03	0.57	
1:D:106:GLN:O	1:D:111:ARG:NH2	2.37	0.57	
1:D:176:PRO:HG2	1:D:227:ARG:HG2	1.85	0.57	
1:A:185:LEU:O	1:A:214[A]:TRP:HB2	2.05	0.57	
1:A:106:GLN:HG2	1:J:122:THR:HA	1.87	0.56	
1:C:10:GLU:OE2	1:D:2:PRO:HB2	2.05	0.56	
1:B:74:LEU:HD23	1:B:102:ILE:HB	1.87	0.56	
1:E:119:GLU:OE2	1:E:145:MET:HG2	2.05	0.56	
1:G:124:THR:HG23	1:G:125:VAL:O	2.07	0.55	
1:I:105:PRO:O	1:I:106:GLN:CB	2.54	0.55	
1:C:200[A]:MET:CE	1:C:200[A]:MET:HA	2.37	0.54	
1:I:200:MET:HE2	1:I:200:MET:CA	2.36	0.54	

1 0 \sim , ·



Continued from previou	is page			
Atom-1	Atom-2	Interatomic	Clash	
		distance (A)	overlap (A)	
1:A:105:PRO:O	1:A:106:GLN:CB	2.55	0.54	
1:B:122:THR:HG23	1:B:123:HIS:CD2	2.42	0.54	
1:H:105:PRO:HG2	1:I:122:THR:HB	1.90	0.54	
1:B:130:ILE:HD13	1:B:157:ILE:HG21	1.89	0.54	
1:A:125[A]:VAL:HG21	1:B:8:ILE:HD12	1.89	0.53	
1:A:119:GLU:HG3	1:B:8:ILE:HG22	1.91	0.53	
1:I:200:MET:HA	1:I:200:MET:CE	2.39	0.53	
1:H:106:GLN:HE22	1:I:107:GLY:HA3	1.73	0.52	
1:C:105:PRO:O	1:C:106[B]:GLN:CB	2.57	0.52	
1:G:59:ARG:HG3	1:H:179:GLU:OE1	2.08	0.52	
1:H:130:ILE:HD13	1:H:157:ILE:HG21	1.91	0.52	
1:D:105:PRO:HG2	1:E:122:THR:HB	1.92	0.52	
1:J:90:GLU:OE2	1:J:96:ARG:HD3	2.09	0.52	
1:A:11:ARG:NH1	1:A:14[A]:GLU:OE2	2.32	0.52	
1:J:14:GLU:O	1:J:112:ARG:NH2	2.40	0.52	
1:A:74[A]:LEU:HD23	1:A:102:ILE:HB	1.92	0.51	
1:I:179:GLU:OE1	1:J:241:LEU:CD1	2.56	0.51	
1:I:194:ASP:OD1	1:I:197:ARG:NH1	2.43	0.51	
1:F:106:GLN:HE22	1:G:111:ARG:HE	1.59	0.51	
1:F:105:PRO:HG2	1:G:122:THR:HB	1.93	0.51	
1:F:200:MET:HE2	1:F:200:MET:CA	2.40	0.51	
1:J:42:HIS:CE1	1:J:75:SER:HB3	2.46	0.51	
1:C:208[A]:LEU:HD13	1:C:214[A]:TRP:CZ3	2.46	0.50	
1:C:200[A]:MET:HG2	1:C:210:TRP:HB3	1.92	0.50	
1:J:185:LEU:O	1:J:214[B]:TRP:HB2	2.11	0.50	
1:A:36:TRP:HB2	1:A:69:VAL:HG22	1.94	0.50	
1:B:74:LEU:HD23	1:B:102:ILE:CG2	2.42	0.50	
1:J:74:LEU:C	1:J:74:LEU:HD13	2.32	0.50	
1:C:241:LEU:HD11	1:D:179:GLU:OE1	2.12	0.50	
1:A:119:GLU:OE2	1:A:145[B]:MET:HG2	2.11	0.49	
1:A:220:ARG:O	1:A:224[A]:GLU:HG3	2.12	0.49	
1:E:119:GLU:HG3	1:F:8:ILE:HG22	1.94	0.49	
1:C:59:ARG:CD	1:D:179:GLU:OE2	2.55	0.49	
1:B:5:ILE:HG22	1:B:114:GLY:HA3	1.93	0.49	
1:D:42:HIS:CE1	1:D:75:SER:HB3	2.48	0.49	
1:E:175:TRP:CG	1:E:176:PRO:HA	2.48	0.49	
1:I:242:TYR:CD1	1:J:214[B]:TRP:CZ2	2.98	0.49	
1:B:69:VAL:CG2	1:B:158[A]:VAL:HG11	2.36	0.48	
1:C:130:ILE:HD13	1:C:157:ILE:HG21	1.95	0.48	
1:B:105:PRO:O	1:B:106:GLN:CB	2.57	0.48	
1:E:93:ILE:HD11	1:F:208:LEU:HD13	1.96	0.48	
			-	

C



Atom 1	Atom 2	Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance (Å)		
1:H:105:PRO:O	1:H:106:GLN:CB	2.62	0.48	
1:D:82:HIS:HE1	1:D:102:ILE:O	1.97	0.48	
1:D:199:ARG:HD3	3:D:472:HOH:O	2.14	0.47	
1:J:119:GLU:OE2	1:J:145[B]:MET:HG2	2.14	0.47	
1:F:185:LEU:O	1:F:214[A]:TRP:HB2	2.14	0.47	
1:J:175:TRP:CG	1:J:176:PRO:HA	2.50	0.47	
1:B:106:GLN:HE22	1:C:116:LEU:HD22	1.78	0.47	
1:I:179:GLU:OE2	1:J:59:ARG:HG3	2.14	0.47	
1:A:125[A]:VAL:HG22	1:A:126:ARG:H	1.79	0.47	
1:J:106:GLN:O	1:J:111:ARG:NH2	2.48	0.47	
1:C:42:HIS:CE1	1:C:75:SER:HB3	2.50	0.47	
1:C:122:THR:HG23	1:C:123:HIS:CD2	2.51	0.47	
1:I:119:GLU:HG3	1:J:8:ILE:HG22	1.96	0.46	
1:G:208:LEU:CD1	1:H:242[B]:TYR:CD1	2.99	0.46	
1:F:42:HIS:CE1	1:F:75:SER:HB3	2.51	0.46	
1:F:140:MET:HE2	1:F:142:TYR:OH	2.15	0.46	
1:J:6:PRO:HG2	1:J:129:PHE:HE2	1.81	0.46	
1:E:5:ILE:HG12	1:F:5:ILE:HG12	1.97	0.46	
1:G:119:GLU:HG3	1:H:8:ILE:HG22	1.97	0.46	
1:G:179:GLU:OE2	1:H:59:ARG:HG3	2.16	0.46	
1:G:193:GLU:O	1:G:197:ARG:HG2	2.15	0.46	
1:H:14:GLU:O	1:H:112[B]:ARG:NH2	2.49	0.46	
1:G:3:GLY:HA3	1:H:7:LEU:HD21	1.97	0.46	
1:A:67:LEU:HD21	1:A:159:LYS:HD3	1.98	0.46	
1:E:146:GLU:HG3	3:F:558:HOH:O	2.16	0.46	
1:J:204:GLN:NE2	3:J:283:HOH:O	2.48	0.46	
1:A:125[A]:VAL:CG2	1:A:143:TYR:O	2.60	0.45	
1:G:208:LEU:CD1	1:H:242[B]:TYR:HD1	2.29	0.45	
1:H:74:LEU:C	1:H:74:LEU:HD13	2.36	0.45	
1:E:42:HIS:CE1	1:E:75:SER:HB3	2.52	0.45	
1:G:186:ILE:HG21	1:H:48:PRO:HG2	1.99	0.45	
1:C:200[B]:MET:HG3	1:C:210:TRP:HB3	1.98	0.45	
1:A:99:PHE:HB2	1:A:100:PRO:HD2	1.97	0.44	
1:F:129:PHE:CE2	1:F:140:MET:HE2	2.51	0.44	
1:E:99:PHE:HB2	1:E:100:PRO:HD2	1.99	0.44	
1:F:47:THR:HB	1:F:48:PRO:HD2	1.97	0.44	
1:D:200:MET:CE	1:D:210:TRP:HA	2.48	0.44	
1:A:176:PRO:HG2	1:A:227:ARG:HG2	2.00	0.44	
1:C:175:TRP:CG	1:C:176:PRO:HA	2.53	0.44	
1:D:36:TRP:CD2	1:D:132:ASP:HA	2.52	0.44	
1:J:200[A]:MET:HA	1:J:200[A]:MET:CE	2.48	0.44	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:C:67:LEU:HD21	1:C:159:LYS:HD3	1.99	0.44	
1:D:194:ASP:OD1	1:D:197:ARG:NH2	2.49	0.44	
1:D:200:MET:HE3	1:D:210:TRP:HA	1.99	0.44	
1:J:154:ILE:O	1:J:158[B]:VAL:HG23	2.17	0.44	
1:F:188:PRO:O	1:F:199:ARG:NH2	2.47	0.43	
1:C:36:TRP:CD2	1:C:132:ASP:HA	2.53	0.43	
1:C:14:GLU:O	1:C:112:ARG:NH2	2.52	0.43	
1:A:175:TRP:CG	1:A:176:PRO:HA	2.54	0.43	
1:A:214[A]:TRP:CZ2	1:B:242:TYR:CD1	3.06	0.43	
1:F:79[B]:VAL:HG11	1:H:191:THR:O	2.19	0.43	
1:G:122:THR:OG1	1:G:123:HIS:HD2	2.01	0.43	
1:C:47:THR:HB	1:C:48:PRO:HD2	2.01	0.43	
1:G:41:SER:HB2	1:G:124:THR:HG21	2.00	0.43	
1:D:5:ILE:HG22	1:D:114:GLY:HA3	2.01	0.43	
1:E:104:ASP:N	1:E:105:PRO:HD3	2.34	0.43	
1:H:106:GLN:HG2	1:I:122:THR:HA	2.01	0.43	
1:A:125[A]:VAL:HG22	1:A:126:ARG:N	2.34	0.43	
1:E:200:MET:CE	1:E:200:MET:HA	2.49	0.43	
1:J:36:TRP:CD2	1:J:132:ASP:HA	2.54	0.42	
1:A:59[A]:ARG:HH21	1:A:241:LEU:HD21	1.85	0.42	
1:G:208:LEU:HD11	1:H:242[B]:TYR:CD1	2.54	0.42	
1:C:28:ASP:OD1	1:C:28:ASP:N	2.51	0.42	
1:A:74[A]:LEU:HD23	1:A:102:ILE:CG2	2.50	0.42	
1:A:154:ILE:O	1:A:158[A]:VAL:HG23	2.20	0.42	
1:F:228:ARG:HG3	1:F:231:ARG:NH1	2.35	0.42	
1:B:106:GLN:NE2	1:C:116:LEU:CD2	2.83	0.42	
1:F:119:GLU:OE2	1:F:145[B]:MET:HG2	2.20	0.41	
1:A:42:HIS:CE1	1:A:75:SER:HB3	2.54	0.41	
1:A:189:PRO:HA	1:A:190:PRO:HD3	1.97	0.41	
1:A:228:ARG:HD3	3:A:387:HOH:O	2.20	0.41	
1:C:126:ARG:HB3	1:C:149:ARG:CZ	2.50	0.41	
1:G:2:PRO:HB2	1:H:10:GLU:OE2	2.20	0.41	
1:B:106:GLN:NE2	1:C:121:ALA:O	2.53	0.41	
1:C:62:GLU:HG2	1:C:66:ARG:NH1	2.35	0.41	
1:A:228:ARG:CZ	1:A:228:ARG:HB3	2.51	0.41	
1:D:107:GLY:HA3	1:E:106:GLN:NE2	2.36	0.41	
1:G:67:LEU:O	1:G:162:LYS:HE3	2.20	0.41	
1:I:59:ARG:HH11	1:I:59:ARG:HD3	1.74	0.41	
1:E:175:TRP:CD1	1:E:176:PRO:HA	2.56	0.41	
1:G:42:HIS:CE1	1:G:75:SER:HB3	2.56	0.41	
1:G:183:GLU:OE2	1:G:220[B]:ARG:NH2	2.42	0.41	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:I:10:GLU:OE2	1:J:2:PRO:HB2	2.21	0.41	
1:J:69:VAL:CG2	1:J:158[A]:VAL:HG21	2.42	0.41	
1:J:130:ILE:HD13	1:J:157:ILE:HG21	2.02	0.41	
1:A:208:LEU:HD13	1:B:93[A]:ILE:CD1	2.51	0.40	
1:H:106:GLN:OE1	1:I:76:VAL:HG11	2.22	0.40	
1:G:117:HIS:HA	1:H:7:LEU:HD13	2.02	0.40	
1:J:110:ALA:CB	1:J:116:LEU:CD2	2.97	0.40	
1:F:36:TRP:CD2	1:F:132:ASP:HA	2.57	0.40	
1:A:43:PRO:HB3	1:A:145[B]:MET:CE	2.51	0.40	
1:C:225:GLU:O	1:C:228[B]:ARG:HB3	2.22	0.40	
1:H:25:LYS:NZ	1:H:28:ASP:OD2	2.54	0.40	
1:A:36:TRP:CD2	1:A:132:ASP:HA	2.56	0.40	
1:I:47:THR:HB	1:I:48:PRO:HD2	2.04	0.40	
1:J:6:PRO:HG2	1:J:129:PHE:CE2	2.57	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	Perce	ntiles
1	А	256/249~(103%)	251~(98%)	4 (2%)	1 (0%)	34	16
1	В	246/249~(99%)	243 (99%)	3 (1%)	0	100	100
1	С	252/249~(101%)	244 (97%)	6 (2%)	2(1%)	19	5
1	D	245/249~(98%)	239~(98%)	4 (2%)	2 (1%)	19	5
1	Ε	245/249~(98%)	238~(97%)	7 (3%)	0	100	100
1	F	249/249~(100%)	245~(98%)	4 (2%)	0	100	100
1	G	246/249~(99%)	241 (98%)	5 (2%)	0	100	100
1	Н	245/249~(98%)	240 (98%)	5 (2%)	0	100	100
1	Ι	245/249~(98%)	241 (98%)	4 (2%)	0	100	100



• • • • • •	j = j	Proceeding Program				
Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	247/249~(99%)	238~(96%)	7 (3%)	2(1%)	19 5
All	All	2476/2490 (99%)	2420 (98%)	49 (2%)	7(0%)	47 22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	106[A]	GLN
1	С	106[B]	GLN
1	D	106	GLN
1	А	106	GLN
1	D	239	LYS
1	J	239	LYS
1	J	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	225/215~(105%)	215~(96%)	10 (4%)	28 7
1	В	215/215~(100%)	212~(99%)	3~(1%)	67 46
1	\mathbf{C}	221/215~(103%)	212~(96%)	9~(4%)	30 8
1	D	214/215~(100%)	209~(98%)	5(2%)	50 25
1	Ε	214/215~(100%)	210~(98%)	4 (2%)	57 34
1	\mathbf{F}	217/215~(101%)	212~(98%)	5(2%)	50 25
1	G	215/215~(100%)	208~(97%)	7 (3%)	38 12
1	Η	214/215~(100%)	208~(97%)	6 (3%)	43 18
1	Ι	214/215~(100%)	211~(99%)	3~(1%)	67 46
1	J	216/215~(100%)	207 (96%)	9 (4%)	30 8
All	All	2165/2150~(101%)	2104 (97%)	61 (3%)	46 18

All (61) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	28	ASP
1	А	147[A]	LEU
1	А	147[B]	LEU
1	А	161[A]	LEU
1	А	161[B]	LEU
1	А	212	PHE
1	А	228	ARG
1	А	239	LYS
1	А	242[A]	TYR
1	А	242[B]	TYR
1	В	28	ASP
1	В	122	THR
1	В	212	PHE
1	С	4	SER
1	С	28	ASP
1	С	59	ARG
1	С	106[A]	GLN
1	С	106[B]	GLN
1	С	145[A]	MET
1	С	145[B]	MET
1	С	197	ARG
1	С	212	PHE
1	D	28	ASP
1	D	159	LYS
1	D	199	ARG
1	D	201	GLU
1	D	212	PHE
1	Е	11	ARG
1	Е	106	GLN
1	Е	111	ARG
1	Е	212	PHE
1	F	28	ASP
1	F	199	ARG
1	F	206	ARG
1	F	212	PHE
1	F	220	ARG
1	G	28	ASP
1	G	112	ARG
1	G	124	THR
1	G	163	LEU
1	G	167	LEU
1	G	208	LEU
1	G	212	PHE



Mol	Chain	Res	
1		14	Type
1	H	14	GLU
1	Н	28	ASP
1	Н	112[A]	ARG
1	Н	112[B]	ARG
1	Н	122	THR
1	Н	212	PHE
1	Ι	7	LEU
1	Ι	28	ASP
1	Ι	212	PHE
1	J	2	PRO
1	J	28	ASP
1	J	62	GLU
1	J	112	ARG
1	J	145[A]	MET
1	J	145[B]	MET
1	J	147	LEU
1	J	212	PHE
1	J	220	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	65	GLN
1	А	106	GLN
1	А	123	HIS
1	А	204	GLN
1	В	106	GLN
1	В	123	HIS
1	В	204	GLN
1	С	123	HIS
1	С	204	GLN
1	D	82	HIS
1	Е	123	HIS
1	F	106	GLN
1	F	123	HIS
1	F	204	GLN
1	G	123	HIS
1	G	204	GLN
1	Н	106	GLN
1	Н	123	HIS
1	Н	204	GLN
1	Ι	204	GLN



Continued from previous page...

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).

Mal	Turne	Chain	Dec		Bond lengths			B	ond angles
	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ # Z > 2
2	PER	А	1	-	0,1,1	-	-	-	
2	PER	Е	251	-	0,1,1	-	-	-	
2	PER	F	251	-	0,1,1	-	-	-	
2	PER	Н	251	-	0,1,1	-	-	-	
2	PER	G	251	-	0,1,1	-	-	-	
2	PER	В	251	-	$0,\!1,\!1$	-	-	-	
2	PER	J	251	-	0,1,1	-	-	-	
2	PER	D	251	-	0,1,1	-	-	-	
2	PER	Ι	251	-	0,1,1	-	-	-	
2	PER	C	251	-	0,1,1	-	-	-	

There are no bond length outliers.



There are no bond angle outliers. There are no chirality outliers. There are no torsion outliers. There are no ring outliers. 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, 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 $>$	#RSR2	Z>2	$OWAB(Å^2)$	Q<0.9
1	А	243/249~(97%)	-0.22	3 (1%) 79	81	16, 22, 36, 48	0
1	В	242/249~(97%)	0.03	8 (3%) 46	5 47	16, 25, 40, 48	0
1	С	243/249~(97%)	0.24	12 (4%) 2	9 28	18, 27, 44, 62	0
1	D	240/249~(96%)	-0.06	7 (2%) 51	52	16, 24, 42, 50	0
1	Ε	242/249~(97%)	-0.13	4 (1%) 70) 73	15, 24, 39, 44	0
1	F	244/249~(97%)	-0.12	7 (2%) 51	52	16, 25, 41, 54	0
1	G	243/249~(97%)	0.03	10 (4%) 3	7 37	17, 24, 40, 59	0
1	Н	242/249~(97%)	0.07	9 (3%) 41	41	16, 24, 36, 47	0
1	Ι	242/249~(97%)	-0.15	6 (2%) 57	7 58	13, 20, 35, 45	0
1	J	243/249~(97%)	-0.16	8 (3%) 46	5 47	14, 21, 37, 56	0
All	All	2424/2490 (97%)	-0.05	74 (3%) 4	9 49	13, 24, 40, 62	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	245	ALA	7.7
1	D	238	ALA	6.3
1	J	238	ALA	6.1
1	Н	242[A]	TYR	4.9
1	G	242	TYR	4.6
1	D	239	LYS	4.4
1	С	238	ALA	4.2
1	С	244	GLU	4.0
1	F	201	GLU	3.9
1	Н	200	MET	3.8
1	F	244	GLU	3.6
1	J	242	TYR	3.4
1	С	220	ARG	3.4



Mol	Chain	Res	Type	RSRZ
1	С	239	LYS	3.3
1	В	242	TYR	3.2
1	Ι	242	TYR	3.2
1	D	200	MET	3.1
1	Е	242	TYR	3.0
1	F	200	MET	3.0
1	G	244	GLU	3.0
1	А	201	GLU	2.9
1	С	243	GLU	2.9
1	Н	243	GLU	2.9
1	J	200[A]	MET	2.9
1	В	238	ALA	2.8
1	F	242[A]	TYR	2.8
1	J	244	GLU	2.7
1	С	242	TYR	2.7
1	С	32	SER	2.7
1	G	32	SER	2.6
1	Н	141	LEU	2.6
1	С	141	LEU	2.6
1	G	238	ALA	2.5
1	В	4	SER	2.5
1	G	118	ALA	2.5
1	G	243	GLU	2.5
1	С	106[A]	GLN	2.5
1	Ι	238	ALA	2.4
1	G	119	GLU	2.4
1	Ι	220	ARG	2.4
1	Ι	243	GLU	2.4
1	Е	32	SER	2.4
1	А	220	ARG	2.4
1	D	2	PRO	2.4
1	В	121	ALA	2.4
1	С	122	THR	2.4
1	Н	154	ILE	2.4
1	G	141	LEU	2.3
1	А	197	ARG	2.3
1	D	141	LEU	2.3
1	F	197	ARG	2.2
1	Н	201	GLU	2.2
1	Н	220	ARG	2.2
1	G	2	PRO	2.2
1	С	200[A]	MET	2.2



3	А	2	V	
U.	11	-	v	

Mol	Chain	Res	Type	RSRZ	
1	В	14[A]	GLU	2.2	
1	В	243	GLU	2.2	
1	J	34	GLY	2.2	
1	F	121	ALA	2.2	
1	J	202	SER	2.1	
1	В	141	LEU	2.1	
1	Ι	203	GLY	2.1	
1	D	220	ARG	2.1	
1	J	32	SER	2.1	
1	Е	4	SER	2.1	
1	D	118	ALA	2.1	
1	Н	2	PRO	2.1	
1	Н	239	LYS	2.1	
1	J	2	PRO	2.1	
1	С	121	ALA	2.0	
1	В	32	SER	2.0	
1	Ι	141	LEU	2.0	
1	Е	238	ALA	2.0	
1	G	201	GLU	2.0	

Continued from previous page...

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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	PER	F	251	2/2	0.90	0.14	$28,\!28,\!28,\!37$	0
2	PER	В	251	2/2	0.91	0.11	$28,\!28,\!28,\!35$	0
2	PER	А	1	2/2	0.91	0.09	25,25,25,31	0
2	PER	J	251	2/2	0.91	0.15	22,22,22,29	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	PER	С	251	2/2	0.93	0.09	$27,\!27,\!27,\!33$	0
2	PER	D	251	2/2	0.93	0.07	30,30,30,35	0
2	PER	Н	251	2/2	0.94	0.06	29,29,29,32	0
2	PER	G	251	2/2	0.94	0.11	29,29,29,33	0
2	PER	Е	251	2/2	0.96	0.08	32,32,32,34	0
2	PER	Ι	251	2/2	0.97	0.08	22,22,22,27	0

Continued from previous page...

6.5 Other polymers (i)

There are no such residues in this entry.

