



Full wwPDB X-ray Structure Validation Report

Jun 26, 2014 – 09:05 PM EDT

PDB ID : 4PIB
Title : Crystal Structure of Uncharacterized Conserved Protein PixA from *Burkholderia thailandensis*
Authors : Kim, Y.; Li, H.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2014-05-08
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

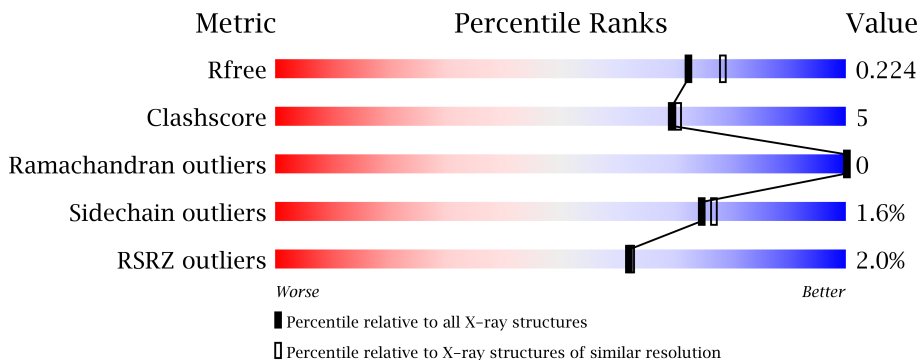
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	FAILED
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23161
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23161

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	193	
1	B	193	
1	C	193	
1	D	193	
1	E	193	
1	F	193	
1	G	193	
1	H	193	
1	I	193	
1	J	193	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	A	206	-	X
4	GOL	B	206	-	X
4	GOL	D	205	-	X
4	GOL	I	204	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14478 atoms, of which 0 are hydrogen and 0 are deuterium.

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 inclusion body protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	Se	0	5	0
			1369	868	225	271	3	2			
1	B	176	Total	C	N	O	S	Se	0	3	0
			1366	866	226	270	2	2			
1	C	176	Total	C	N	O	S	Se	0	5	0
			1383	876	229	274	2	2			
1	D	176	Total	C	N	O	S	Se	0	4	0
			1374	870	227	273	2	2			
1	E	176	Total	C	N	O	S	Se	0	0	0
			1338	847	221	266	2	2			
1	F	174	Total	C	N	O	S	Se	0	1	0
			1335	846	220	265	2	2			
1	G	176	Total	C	N	O	S	Se	0	2	0
			1353	855	223	271	2	2			
1	H	174	Total	C	N	O	S	Se	0	0	0
			1326	841	218	263	2	2			
1	I	176	Total	C	N	O	S	Se	0	2	0
			1355	856	225	270	2	2			
1	J	171	Total	C	N	O	S	Se	0	3	0
			1328	841	218	265	2	2			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	3	Total	Ca	0	0
			3	3		
2	J	2	Total	Ca	0	0
			2	2		
2	D	3	Total	Ca	0	0
			3	3		
2	E	5	Total	Ca	0	0
			5	5		

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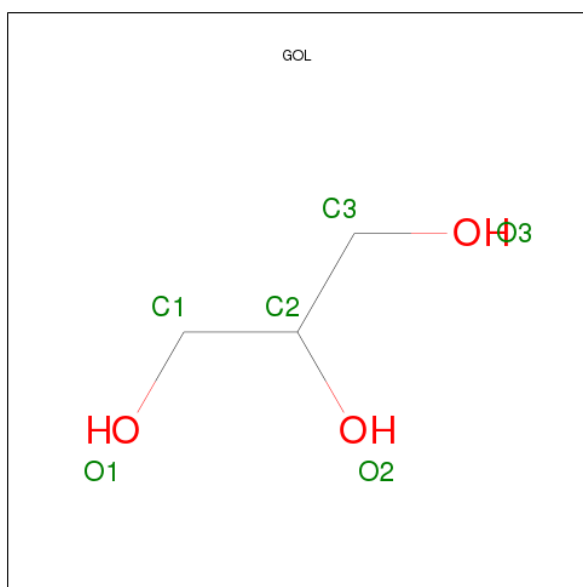
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	3	Total 3	Ca 3	0	0
2	B	3	Total 3	Ca 3	0	0
2	I	3	Total 3	Ca 3	0	0
2	C	4	Total 4	Ca 4	0	0
2	A	3	Total 3	Ca 3	0	0
2	F	2	Total 2	Ca 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

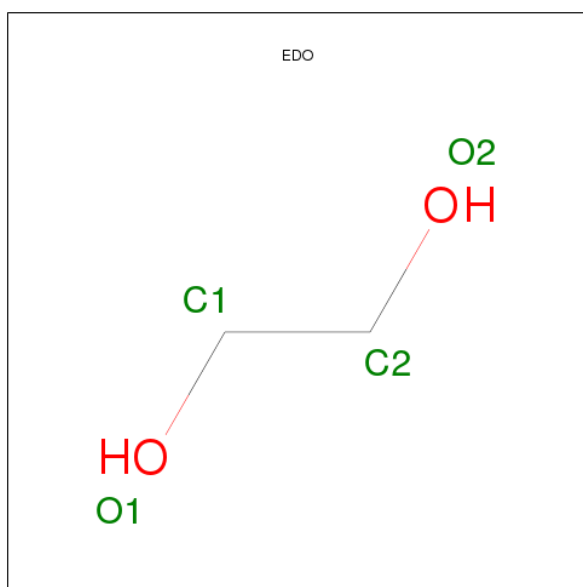
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	1	Total 1	Cl 1	0	0
3	D	1	Total 1	Cl 1	0	0
3	E	1	Total 1	Cl 1	0	0
3	H	1	Total 1	Cl 1	0	0
3	B	1	Total 1	Cl 1	0	0
3	A	1	Total 1	Cl 1	0	0
3	F	1	Total 1	Cl 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	56	Total	O	0	0
			56	56		
6	B	66	Total	O	0	0
			66	66		
6	C	99	Total	O	0	0
			99	99		
6	D	97	Total	O	0	0
			97	97		
6	E	95	Total	O	0	0
			95	95		
6	F	97	Total	O	0	0
			97	97		
6	G	120	Total	O	0	0
			120	120		
6	H	100	Total	O	0	0
			100	100		
6	I	71	Total	O	0	0
			71	71		
6	J	50	Total	O	0	0
			50	50		

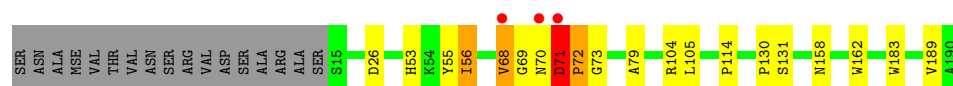
- Molecule 1: inclusion body protein

Chain F:



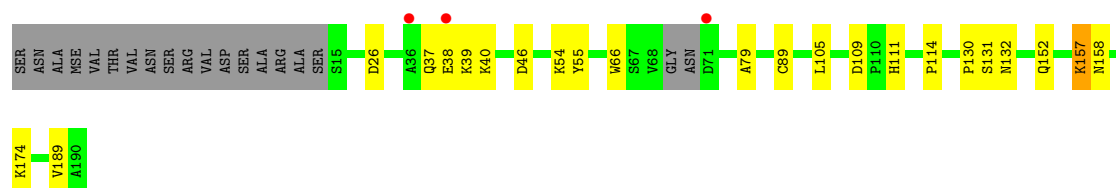
- Molecule 1: inclusion body protein

Chain G:



- Molecule 1: inclusion body protein

Chain H:



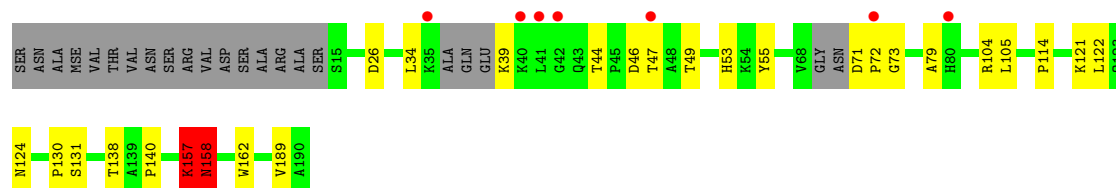
- Molecule 1: inclusion body protein

Chain I:



- Molecule 1: inclusion body protein

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	79.81Å 84.87Å 249.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.11 – 2.00 42.54 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.9 (36.11-2.00) 90.9 (42.54-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.07 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1621)	Depositor
R, R_{free}	0.181 , 0.224 0.181 , 0.224	Depositor DCC
R_{free} test set	5266 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 104291 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14478	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, EDO, CL

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	0.36	1/1401 (0.1%)	0.57	2/1909 (0.1%)
1	B	0.43	1/1399 (0.1%)	0.62	3/1908 (0.2%)
1	C	0.42	2/1416 (0.1%)	0.58	1/1931 (0.1%)
1	D	0.40	1/1407 (0.1%)	0.54	1/1920 (0.1%)
1	E	0.43	1/1370 (0.1%)	0.54	0/1870
1	F	0.39	0/1366	0.53	0/1863
1	G	0.40	1/1385 (0.1%)	0.54	1/1890 (0.1%)
1	H	0.35	0/1357	0.51	0/1851
1	I	0.37	1/1387 (0.1%)	0.52	1/1893 (0.1%)
1	J	0.39	1/1358 (0.1%)	0.62	4/1852 (0.2%)
All	All	0.40	9/13846 (0.1%)	0.56	13/18887 (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	J	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	110	PRO	N-CD	5.48	1.55	1.47
1	D	72	PRO	N-CD	5.44	1.55	1.47
1	C	89	CYS	CB-SG	-5.29	1.73	1.81
1	B	72	PRO	N-CD	5.16	1.55	1.47
1	I	72	PRO	N-CD	5.09	1.54	1.47
1	G	72	PRO	N-CD	5.09	1.54	1.47
1	A	72	PRO	N-CD	5.07	1.54	1.47
1	J	72	PRO	N-CD	5.07	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	72	PRO	N-CD	5.02	1.54	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	ALA	O-C-N	-9.63	107.29	122.70
1	B	156	ALA	CA-C-N	8.19	135.22	117.20
1	J	157	LYS	O-C-N	-7.84	110.15	122.70
1	J	157	LYS	CA-C-N	7.70	134.14	117.20
1	G	71	ASP	C-N-CD	5.96	140.93	128.40
1	C	108	GLY	CA-C-N	5.74	129.84	117.20
1	I	71	ASP	C-N-CD	5.71	140.38	128.40
1	A	71	ASP	C-N-CD	5.67	140.31	128.40
1	J	71[A]	ASP	C-N-CD	5.60	140.16	128.40
1	J	71[B]	ASP	C-N-CD	5.60	140.16	128.40
1	B	71	ASP	C-N-CD	5.51	139.96	128.40
1	D	71	ASP	C-N-CD	5.42	139.79	128.40
1	A	71	ASP	CB-CG-OD2	5.25	123.02	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	158[B]	ASN	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1369	0	1306	15	0
1	B	1366	0	1307	14	0
1	C	1383	0	1323	12	0
1	D	1374	0	1311	9	0
1	E	1338	0	1280	12	0
1	F	1335	0	1277	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1353	0	1289	17	0
1	H	1326	0	1270	15	0
1	I	1355	0	1292	12	0
1	J	1328	0	1263	18	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
2	E	5	0	0	0	0
2	F	2	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
4	A	12	0	16	1	0
4	B	12	0	16	5	0
4	D	12	0	16	3	0
4	G	6	0	8	4	0
4	H	6	0	8	1	0
4	I	6	0	8	0	0
5	B	4	0	6	0	0
5	C	4	0	6	0	0
6	A	56	0	0	0	0
6	B	66	0	0	1	0
6	C	99	0	0	0	0
6	D	97	0	0	0	0
6	E	95	0	0	0	0
6	F	97	0	0	1	0
6	G	120	0	0	0	0
6	H	100	0	0	3	0
6	I	71	0	0	2	0
6	J	50	0	0	1	0
All	All	14478	0	13002	124	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (124) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:68:VAL:HG12	4:D:204:GOL:H32	1.49	0.95
1:G:70:ASN:OD1	1:G:71:ASP:HB2	1.85	0.76
1:E:37:GLN:OE1	1:E:39:LYS:HB2	1.90	0.72
1:A:15:SER:OG	1:A:16:HIS:N	2.18	0.72
1:B:71:ASP:OD2	1:B:71:ASP:N	2.21	0.72
1:B:32:ASP:HA	1:B:35:LYS:HE2	1.75	0.69
1:C:71:ASP:OD2	1:C:72:PRO:HD2	1.94	0.67
1:J:158[B]:ASN:OD1	1:J:158[B]:ASN:N	2.29	0.65
1:B:37:GLN:O	1:B:38:GLU:HB3	1.97	0.64
1:A:40:LYS:HG3	1:A:41:LEU:N	2.13	0.62
1:G:68:VAL:H	4:G:204:GOL:H2	1.64	0.62
1:C:79:ALA:HB3	1:C:189:VAL:HG13	1.81	0.62
1:C:56:ILE:HD11	1:C:73:GLY:HA2	1.82	0.61
1:J:44:THR:HG22	1:J:46:ASP:H	1.65	0.61
1:C:66:TRP:HZ3	1:C:68:VAL:CG2	2.14	0.60
1:I:79:ALA:HB3	1:I:189:VAL:HG13	1.82	0.60
1:B:147:ASP:OD2	4:B:206:GOL:H32	2.00	0.60
1:G:68:VAL:CG2	4:G:204:GOL:H2	2.31	0.60
1:G:68:VAL:HG22	4:G:204:GOL:H2	1.84	0.60
1:E:39:LYS:HE3	1:E:49:THR:HG23	1.84	0.59
1:E:110:PRO:HG3	1:H:132:ASN:ND2	2.17	0.59
1:J:79:ALA:HB3	1:J:189:VAL:HG13	1.84	0.59
1:D:72:PRO:O	1:D:74:ASN:ND2	2.36	0.59
1:A:67:SER:HA	4:A:205:GOL:H31	1.86	0.57
1:C:37:GLN:OE1	1:C:39:LYS:HE2	2.05	0.56
1:C:71:ASP:OD2	1:C:72:PRO:CD	2.54	0.56
1:H:109:ASP:OD2	1:J:104:ARG:NH2	2.39	0.55
4:B:206:GOL:H2	6:B:309:HOH:O	2.05	0.55
1:H:157:LYS:HD3	1:H:157:LYS:H	1.71	0.55
1:D:70:ASN:OD1	1:D:70:ASN:N	2.38	0.54
1:F:15:SER:N	6:F:301:HOH:O	2.40	0.54
1:B:66:TRP:HZ3	1:B:68:VAL:HB	1.73	0.54
1:A:33:GLU:HG3	1:A:55:TYR:HE2	1.73	0.54
1:H:46:ASP:OD2	1:J:157:LYS:HD3	2.09	0.53
1:D:68:VAL:HG12	4:D:204:GOL:C3	2.32	0.53
1:E:56:ILE:HD11	1:E:73:GLY:HA2	1.88	0.53
1:H:174:LYS:NZ	6:H:377:HOH:O	2.40	0.53
1:A:89[A]:CYS:SG	1:A:102:ILE:HG13	2.49	0.53
1:E:79:ALA:HB3	1:E:189:VAL:HG13	1.91	0.53
1:G:56:ILE:O	1:G:56:ILE:HG13	2.09	0.53
1:I:130:PRO:HD3	1:J:121:LYS:HZ3	1.73	0.52
1:I:123[B]:GLN:NE2	6:I:328:HOH:O	2.31	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:69:GLY:O	1:G:70:ASN:HB3	2.10	0.51
1:H:26:ASP:HB3	1:H:55:TYR:HB3	1.92	0.51
1:A:80:HIS:N	1:A:83:ASP:OD2	2.41	0.51
1:D:105:LEU:HB2	1:D:114:PRO:HB3	1.91	0.50
1:D:66:TRP:O	4:D:205:GOL:H2	2.11	0.50
1:B:118:GLU:OE1	4:B:206:GOL:O2	2.23	0.49
1:G:79:ALA:HB3	1:G:189:VAL:HG13	1.94	0.49
1:H:66:TRP:O	4:H:204:GOL:H2	2.13	0.49
1:F:41:LEU:HG	1:F:179:GLY:HA3	1.95	0.49
1:H:37:GLN:HG3	6:H:301:HOH:O	2.13	0.48
1:I:130:PRO:HD3	1:J:121:LYS:NZ	2.27	0.48
1:J:104:ARG:HB3	1:J:162:TRP:HB2	1.95	0.48
1:I:104:ARG:HB3	1:I:162:TRP:HB2	1.95	0.48
1:B:105:LEU:HB2	1:B:114:PRO:HB3	1.96	0.48
1:C:174[A]:LYS:HG3	1:D:124:ASN:HB3	1.95	0.48
1:H:79:ALA:HB3	1:H:189:VAL:HG13	1.94	0.48
1:E:105:LEU:HB2	1:E:114:PRO:HB3	1.97	0.47
1:I:158:ASN:N	6:I:301:HOH:O	2.21	0.47
1:I:56:ILE:HD11	1:I:73:GLY:HA2	1.95	0.47
1:G:158:ASN:OD1	1:G:158:ASN:N	2.47	0.47
1:J:130:PRO:HA	1:J:131:SER:HA	1.67	0.47
1:G:71:ASP:OD2	1:G:72:PRO:HD2	2.14	0.46
1:B:79:ALA:HB3	1:B:189:VAL:HG13	1.96	0.46
1:J:105:LEU:HB2	1:J:114:PRO:HB3	1.98	0.46
1:E:130:PRO:HA	1:E:131:SER:HA	1.68	0.46
1:J:122:LEU:O	1:J:140:PRO:HA	2.16	0.46
1:A:104:ARG:HB3	1:A:162:TRP:HB2	1.97	0.46
1:C:108:GLY:HA2	1:C:158[B]:ASN:OD1	2.16	0.46
1:D:157[B]:LYS:HE3	1:D:157[B]:LYS:HB3	1.79	0.46
1:I:44:THR:HB	1:I:47:THR:OG1	2.16	0.46
1:H:37:GLN:CG	6:H:301:HOH:O	2.64	0.46
1:A:153:GLN:HG2	1:A:189:VAL:HG12	1.99	0.45
1:B:130:PRO:HA	1:B:131:SER:HA	1.73	0.45
1:B:66:TRP:O	4:B:205:GOL:H2	2.17	0.45
1:G:104:ARG:HB3	1:G:162:TRP:HB2	1.97	0.45
1:H:54:LYS:HG3	1:H:55:TYR:CD2	2.52	0.45
1:F:53:HIS:HB2	1:F:73:GLY:HA3	2.00	0.44
1:G:26:ASP:HB3	1:G:55:TYR:HB3	1.99	0.44
1:I:130:PRO:HA	1:I:131:SER:HA	1.67	0.44
1:C:26:ASP:HB3	1:C:55:TYR:HB3	1.99	0.44
1:E:130:PRO:HG2	1:F:121:LYS:HE3	1.99	0.44
1:G:130:PRO:HA	1:G:131:SER:HA	1.71	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:105:LEU:HB2	1:H:114:PRO:HB3	1.99	0.44
1:J:47:THR:HG22	1:J:47:THR:O	2.17	0.44
1:E:173:GLU:OE2	1:F:123[B]:GLN:HG2	2.17	0.44
1:A:98:TYR:CD1	1:A:167:THR:HG22	2.53	0.44
1:E:53:HIS:HB2	1:E:73:GLY:HA3	1.99	0.44
1:F:26:ASP:HB3	1:F:55:TYR:HB3	1.98	0.44
1:B:118:GLU:OE2	4:B:206:GOL:O3	2.31	0.44
1:H:130:PRO:HA	1:H:131:SER:HA	1.60	0.44
1:A:130:PRO:HA	1:A:131:SER:HA	1.69	0.43
1:C:41:LEU:HG	1:C:179:GLY:HA3	2.01	0.43
1:C:88:PHE:CE2	1:C:145:SER:HB3	2.53	0.43
1:G:105:LEU:HB2	1:G:114:PRO:HB3	2.01	0.43
1:J:26:ASP:HB3	1:J:55:TYR:HB3	2.00	0.43
1:A:158[B]:ASN:N	1:A:158[B]:ASN:OD1	2.51	0.43
1:G:56:ILE:HD11	1:G:73:GLY:HA2	2.00	0.43
1:H:39:LYS:HG2	1:H:40:LYS:N	2.34	0.43
1:I:105:LEU:HB2	1:I:114:PRO:HB3	2.00	0.43
1:A:54:LYS:HD2	1:A:55:TYR:CZ	2.55	0.42
1:A:122:LEU:HB2	1:A:125:ALA:HB2	2.02	0.42
1:A:26:ASP:HB3	1:A:55:TYR:HB3	2.01	0.42
1:F:105:LEU:HB2	1:F:114:PRO:HB3	2.02	0.42
1:G:56:ILE:HD13	1:G:183:TRP:NE1	2.33	0.42
1:G:68:VAL:HG23	4:G:204:GOL:H2	2.01	0.42
1:B:39:LYS:HB2	1:B:39:LYS:HE2	1.88	0.42
1:I:44:THR:HG22	1:I:46:ASP:H	1.84	0.42
1:E:124:ASN:ND2	1:E:138:THR:OG1	2.51	0.42
1:B:44:THR:HG22	1:B:46:ASP:H	1.84	0.41
1:D:158[B]:ASN:N	1:D:158[B]:ASN:OD1	2.46	0.41
1:J:53:HIS:ND1	1:J:73:GLY:HA3	2.35	0.41
1:G:53:HIS:HB2	1:G:73:GLY:HA3	2.03	0.41
1:J:121:LYS:NZ	6:J:302:HOH:O	2.46	0.41
1:A:53:HIS:HB2	1:A:73:GLY:HA3	2.01	0.41
1:C:66:TRP:CZ3	1:C:68:VAL:CG2	3.00	0.41
1:J:124:ASN:HB3	1:J:138:THR:HB	2.03	0.41
1:E:39:LYS:HE3	1:E:49:THR:CG2	2.50	0.41
1:J:39:LYS:NZ	1:J:49:THR:HG23	2.36	0.41
1:I:35:LYS:HB2	1:I:35:LYS:HE3	1.75	0.40
1:H:111:HIS:HA	1:H:152:GLN:HB3	2.04	0.40
1:J:34:LEU:O	1:J:39:LYS:N	2.55	0.40
1:B:168:LEU:HD12	1:B:174:LYS:O	2.22	0.40

There are no symmetry-related clashes.

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	175/193 (91%)	170 (97%)	5 (3%)	0	100	100
1	B	177/193 (92%)	172 (97%)	5 (3%)	0	100	100
1	C	179/193 (93%)	175 (98%)	4 (2%)	0	100	100
1	D	178/193 (92%)	174 (98%)	4 (2%)	0	100	100
1	E	174/193 (90%)	169 (97%)	5 (3%)	0	100	100
1	F	171/193 (89%)	167 (98%)	4 (2%)	0	100	100
1	G	176/193 (91%)	171 (97%)	5 (3%)	0	100	100
1	H	170/193 (88%)	164 (96%)	6 (4%)	0	100	100
1	I	176/193 (91%)	170 (97%)	6 (3%)	0	100	100
1	J	167/193 (86%)	157 (94%)	10 (6%)	0	100	100
All	All	1743/1930 (90%)	1689 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	149/156 (96%)	149 (100%)	0	100	100
1	B	148/156 (95%)	143 (97%)	5 (3%)	49	45
1	C	150/156 (96%)	147 (98%)	3 (2%)	68	69
1	D	149/156 (96%)	144 (97%)	5 (3%)	49	45
1	E	145/156 (93%)	143 (99%)	2 (1%)	78	81
1	F	145/156 (93%)	144 (99%)	1 (1%)	91	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	147/156 (94%)	144 (98%)	3 (2%)	68	69
1	H	144/156 (92%)	140 (97%)	4 (3%)	56	54
1	I	147/156 (94%)	146 (99%)	1 (1%)	91	93
1	J	145/156 (93%)	142 (98%)	3 (2%)	66	67
All	All	1469/1560 (94%)	1442 (98%)	27 (2%)	75	73

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	44	THR
1	B	70	ASN
1	B	71	ASP
1	B	157[A]	LYS
1	B	157[B]	LYS
1	C	89	CYS
1	C	109[A]	ASP
1	C	109[B]	ASP
1	D	68	VAL
1	D	70	ASN
1	D	71	ASP
1	D	157[A]	LYS
1	D	157[B]	LYS
1	E	40	LYS
1	E	89	CYS
1	F	71	ASP
1	G	56	ILE
1	G	68	VAL
1	G	71	ASP
1	H	38	GLU
1	H	89	CYS
1	H	157	LYS
1	H	158	ASN
1	I	33	GLU
1	J	157	LYS
1	J	158[A]	ASN
1	J	158[B]	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	B	152	GLN
1	B	155	GLN
1	E	124	ASN
1	G	124	ASN
1	I	124	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

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(Å²)	Q<0.9
1	A	174/193 (90%)	-0.02	6 (3%)	43	43	18, 37, 73, 96	0
1	B	176/193 (91%)	-0.17	2 (1%)	77	78	19, 33, 71, 105	0
1	C	176/193 (91%)	-0.08	6 (3%)	43	43	14, 31, 68, 104	0
1	D	176/193 (91%)	-0.19	2 (1%)	77	78	13, 25, 71, 94	0
1	E	176/193 (91%)	-0.31	2 (1%)	77	78	15, 27, 57, 88	1 (0%)
1	F	174/193 (90%)	-0.35	3 (1%)	67	67	15, 27, 54, 85	0
1	G	176/193 (91%)	-0.18	3 (1%)	67	67	15, 25, 45, 99	0
1	H	174/193 (90%)	-0.26	3 (1%)	67	67	13, 28, 58, 95	0
1	I	176/193 (91%)	-0.08	2 (1%)	77	78	16, 34, 64, 87	0
1	J	171/193 (88%)	0.19	7 (4%)	35	35	19, 45, 82, 96	0
All	All	1749/1930 (90%)	-0.15	36 (2%)	62	61	13, 30, 67, 105	1 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157[A]	LYS	4.2
1	D	36	ALA	4.1
1	B	131	SER	3.5
1	J	41	LEU	3.5
1	C	68	VAL	3.1
1	C	69	GLY	3.0
1	E	70	ASN	3.0
1	J	42	GLY	2.9
1	G	68	VAL	2.9
1	J	72	PRO	2.9
1	C	70	ASN	2.8
1	J	47	THR	2.8
1	G	70	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	36	ALA	2.7
1	A	38	GLU	2.7
1	B	69	GLY	2.6
1	D	40	LYS	2.6
1	F	72	PRO	2.6
1	A	16	HIS	2.5
1	A	36	ALA	2.4
1	F	71	ASP	2.4
1	H	38	GLU	2.4
1	A	37	GLN	2.4
1	I	151	ALA	2.2
1	H	71	ASP	2.2
1	F	15	SER	2.2
1	A	190	ALA	2.2
1	J	40	LYS	2.1
1	C	71	ASP	2.1
1	C	157[A]	LYS	2.1
1	J	35	LYS	2.1
1	J	80	HIS	2.1
1	I	36	ALA	2.1
1	H	36	ALA	2.0
1	G	71	ASP	2.0
1	E	69	GLY	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 carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	A	206	6/6	0.37	10.17	47,52,54,55	0
4	GOL	D	205	6/6	0.19	8.42	56,59,59,61	0
4	GOL	I	204	6/6	0.22	3.42	42,46,47,48	0
4	GOL	B	206	6/6	0.37	3.15	78,81,82,82	0
4	GOL	B	205	6/6	0.20	1.77	51,53,54,54	0
4	GOL	H	204	6/6	0.18	1.34	52,52,53,53	0
5	EDO	B	204	4/4	0.20	0.95	57,57,58,59	0
2	CA	D	200	1/1	0.10	0.93	18,18,18,18	0
4	GOL	G	204	6/6	0.24	0.80	71,72,73,73	0
5	EDO	C	205	4/4	0.18	0.52	55,55,56,56	0
4	GOL	A	205	6/6	0.16	0.00	55,59,60,62	0
2	CA	A	204	1/1	0.11	-0.42	73,73,73,73	0
4	GOL	D	204	6/6	0.16	-0.42	66,67,67,67	0
2	CA	A	203	1/1	0.09	-0.74	46,46,46,46	0
2	CA	B	202	1/1	0.08	-0.81	42,42,42,42	0
3	CL	H	201	1/1	0.09	-0.90	40,40,40,40	0
2	CA	I	202	1/1	0.07	-0.93	28,28,28,28	1
2	CA	E	205	1/1	0.08	-1.00	65,65,65,65	0
2	CA	I	203	1/1	0.08	-1.09	59,59,59,59	0
2	CA	E	203	1/1	0.07	-1.09	54,54,54,54	0
2	CA	J	202	1/1	0.07	-1.22	70,70,70,70	0
2	CA	H	202	1/1	0.07	-1.31	53,53,53,53	0
2	CA	D	202	1/1	0.06	-1.47	58,58,58,58	0
3	CL	J	203	1/1	0.05	-1.48	33,33,33,33	0
2	CA	G	203	1/1	0.07	-1.61	28,28,28,28	0
3	CL	E	202	1/1	0.06	-1.75	26,26,26,26	0
3	CL	F	203	1/1	0.06	-1.83	24,24,24,24	0
2	CA	C	201	1/1	0.06	-1.87	28,28,28,28	0
2	CA	E	201	1/1	0.06	-1.87	22,22,22,22	0
2	CA	E	204	1/1	0.05	-1.88	50,50,50,50	0
2	CA	C	204	1/1	0.05	-1.94	38,38,38,38	0
3	CL	B	201	1/1	0.06	-2.06	27,27,27,27	0
3	CL	A	202	1/1	0.07	-2.08	29,29,29,29	0
2	CA	F	201	1/1	0.05	-2.11	49,49,49,49	0
2	CA	D	203	1/1	0.09	-2.31	68,68,68,68	0
2	CA	B	203	1/1	0.05	-2.40	71,71,71,71	0
2	CA	F	202	1/1	0.04	-2.41	38,38,38,38	0
3	CL	D	201	1/1	0.06	-2.64	20,20,20,20	0
2	CA	B	200	1/1	0.06	-2.74	24,24,24,24	0
2	CA	I	201	1/1	0.03	-2.80	34,34,34,34	0
2	CA	J	201	1/1	0.04	-2.90	32,32,32,32	0
2	CA	G	201	1/1	0.05	-2.92	32,32,32,32	0
2	CA	G	202	1/1	0.05	-2.98	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	C	202	1/1	0.04	-3.58	28,28,28,28	0
2	CA	E	200	1/1	0.05	-3.98	33,33,33,33	0
2	CA	H	200	1/1	0.05	-4.15	26,26,26,26	0
2	CA	C	203	1/1	0.03	-4.43	31,31,31,31	0
2	CA	H	203	1/1	0.04	-5.08	57,57,57,57	0
2	CA	A	201	1/1	0.04	-6.81	38,38,38,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.