



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2017 – 07:47 PM EST

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 : unknown  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

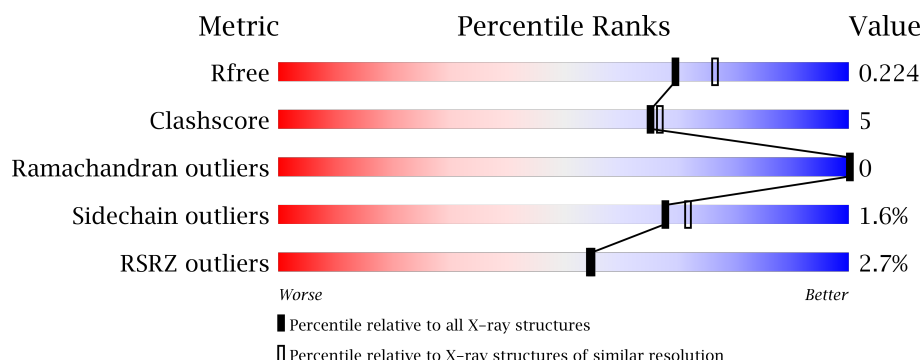
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	193	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>10%</div> </div> </div>
1	B	193	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>••</div> <div>9%</div> </div> </div>
1	C	193	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	193	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>•</div> <div>•</div> <div>9%</div> </div> </div>
1	E	193	<div> <div>•%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>•</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	193	
1	G	193	
1	H	193	
1	I	193	
1	J	193	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	206	-	-	-	X
4	GOL	B	206	-	-	X	X
4	GOL	G	204	-	-	X	-
4	GOL	H	204	-	-	-	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 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 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			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q2SVW5
A	-1	ASN	-	expression tag	UNP Q2SVW5
A	0	ALA	-	expression tag	UNP Q2SVW5
B	-2	SER	-	expression tag	UNP Q2SVW5
B	-1	ASN	-	expression tag	UNP Q2SVW5
B	0	ALA	-	expression tag	UNP Q2SVW5
C	-2	SER	-	expression tag	UNP Q2SVW5
C	-1	ASN	-	expression tag	UNP Q2SVW5
C	0	ALA	-	expression tag	UNP Q2SVW5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP Q2SVW5
D	-1	ASN	-	expression tag	UNP Q2SVW5
D	0	ALA	-	expression tag	UNP Q2SVW5
E	-2	SER	-	expression tag	UNP Q2SVW5
E	-1	ASN	-	expression tag	UNP Q2SVW5
E	0	ALA	-	expression tag	UNP Q2SVW5
F	-2	SER	-	expression tag	UNP Q2SVW5
F	-1	ASN	-	expression tag	UNP Q2SVW5
F	0	ALA	-	expression tag	UNP Q2SVW5
G	-2	SER	-	expression tag	UNP Q2SVW5
G	-1	ASN	-	expression tag	UNP Q2SVW5
G	0	ALA	-	expression tag	UNP Q2SVW5
H	-2	SER	-	expression tag	UNP Q2SVW5
H	-1	ASN	-	expression tag	UNP Q2SVW5
H	0	ALA	-	expression tag	UNP Q2SVW5
I	-2	SER	-	expression tag	UNP Q2SVW5
I	-1	ASN	-	expression tag	UNP Q2SVW5
I	0	ALA	-	expression tag	UNP Q2SVW5
J	-2	SER	-	expression tag	UNP Q2SVW5
J	-1	ASN	-	expression tag	UNP Q2SVW5
J	0	ALA	-	expression tag	UNP Q2SVW5

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	3	Total Ca 3 3	0	0
2	J	2	Total Ca 2 2	0	0
2	D	3	Total Ca 3 3	0	0
2	E	5	Total Ca 5 5	0	0
2	H	3	Total Ca 3 3	0	0
2	B	3	Total Ca 3 3	0	0
2	I	3	Total Ca 3 3	0	0
2	C	4	Total Ca 4 4	0	0
2	A	3	Total Ca 3 3	0	0

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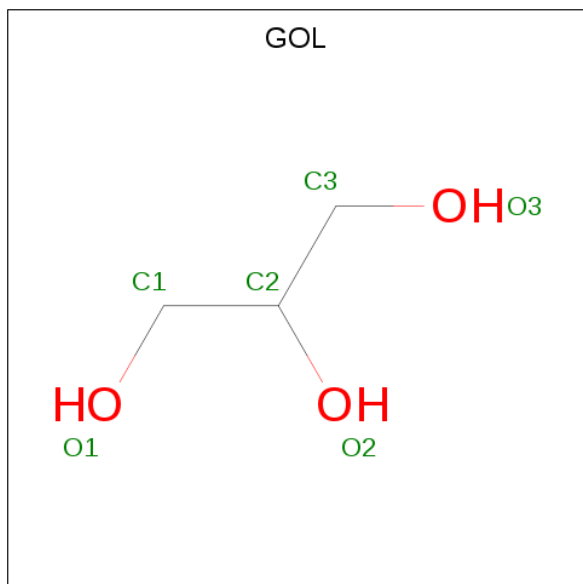
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	2	Total	Ca	0	0
			2	2		

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

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



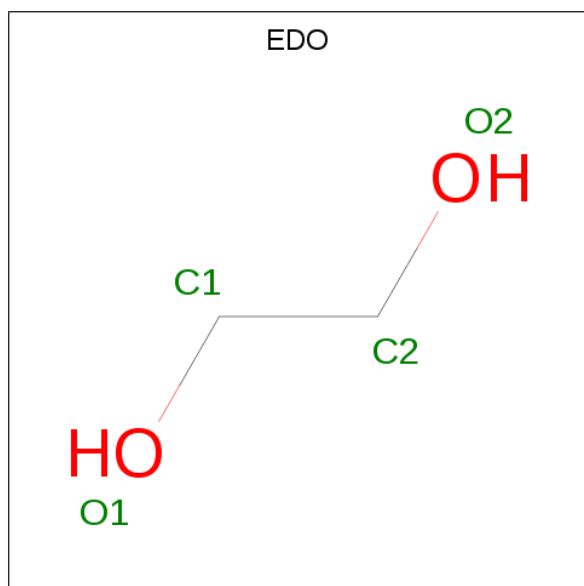
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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.

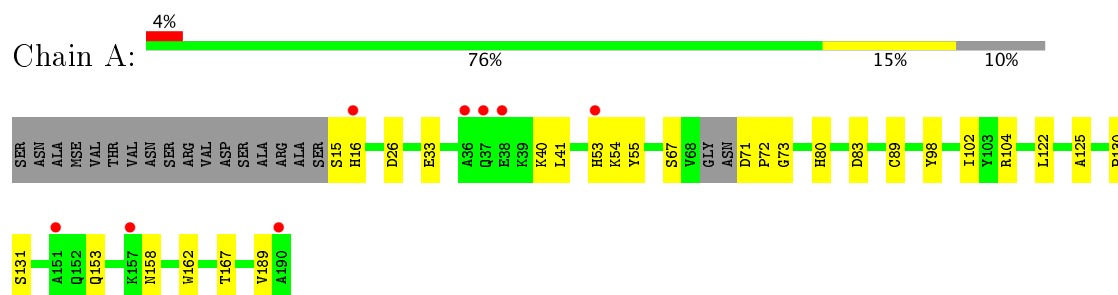
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	56	Total 56	O 56	0	0
6	B	66	Total 66	O 66	0	0
6	C	99	Total 99	O 99	0	0
6	D	97	Total 97	O 97	0	0
6	E	95	Total 95	O 95	0	0
6	F	97	Total 97	O 97	0	0
6	G	120	Total 120	O 120	0	0
6	H	100	Total 100	O 100	0	0
6	I	71	Total 71	O 71	0	0
6	J	50	Total 50	O 50	0	0



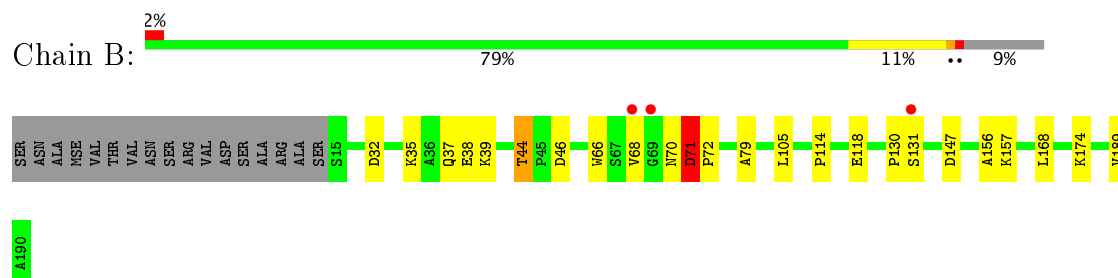
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

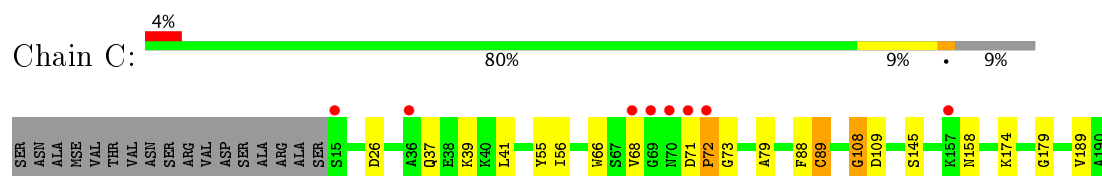
- Molecule 1: inclusion body protein



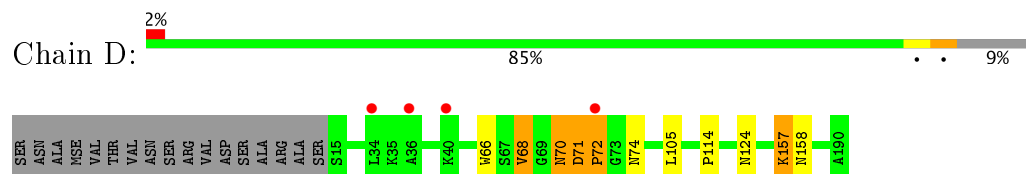
- Molecule 1: inclusion body protein



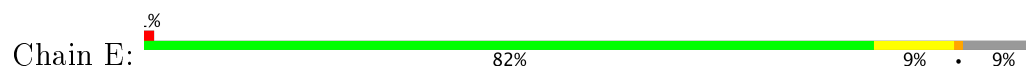
- Molecule 1: inclusion body protein



- Molecule 1: inclusion body protein

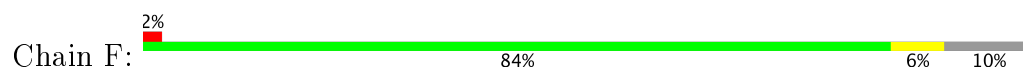


- Molecule 1: inclusion body protein

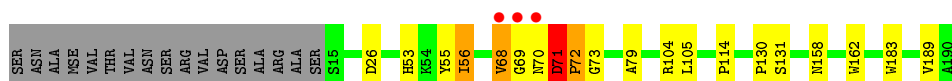
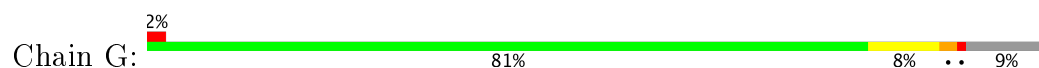




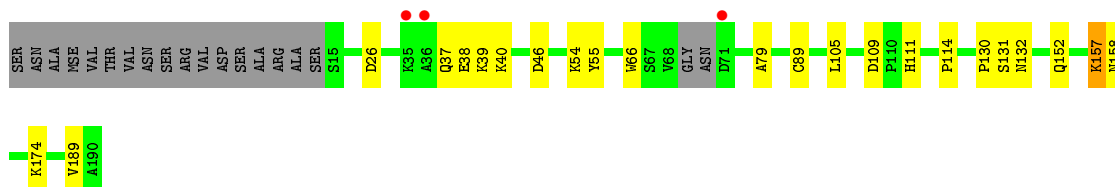
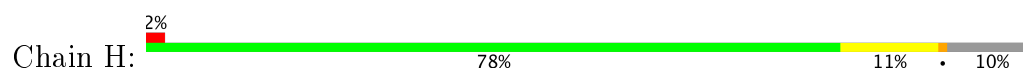
- Molecule 1: inclusion body protein



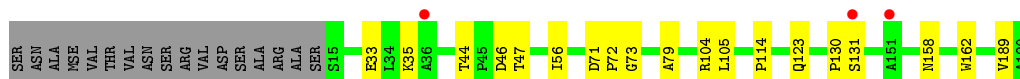
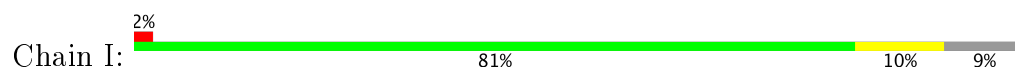
- Molecule 1: inclusion body protein



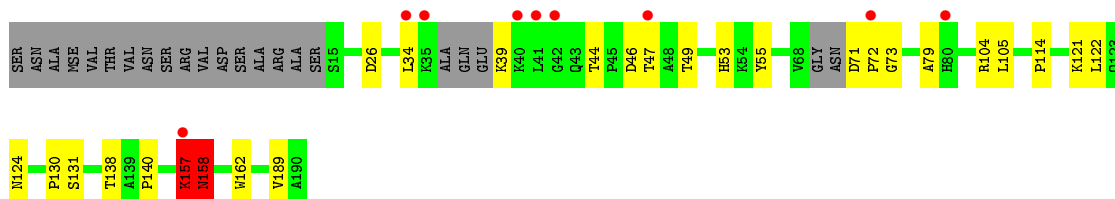
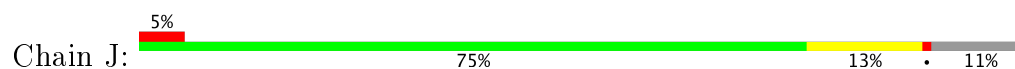
- Molecule 1: inclusion body protein



- Molecule 1: inclusion body protein



- Molecule 1: inclusion body protein



- Molecule 1: inclusion body protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14478	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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 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	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
1	G	1353	0	1289	17	0
1	H	1326	0	1270	15	0

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

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 (124) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:PRO:HA	1:G:131:SER:HA	1.71	0.44
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%)	42	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	150/156 (96%)	147 (98%)	3 (2%)	60	64
1	D	149/156 (96%)	144 (97%)	5 (3%)	42	40
1	E	145/156 (93%)	143 (99%)	2 (1%)	71	76
1	F	145/156 (93%)	144 (99%)	1 (1%)	87	90
1	G	147/156 (94%)	144 (98%)	3 (2%)	60	64
1	H	144/156 (92%)	140 (97%)	4 (3%)	49	49
1	I	147/156 (94%)	146 (99%)	1 (1%)	87	90
1	J	145/156 (93%)	142 (98%)	3 (2%)	59	62
All	All	1469/1560 (94%)	1442 (98%)	27 (2%)	68	68

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

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Mol	Chain	Res	Type
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 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 49 ligands modelled in this entry, 38 are monoatomic - leaving 11 for Mogul analysis.

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	$\# Z  > 2$
4	GOL	A	205	-	5,5,5	0.36	0	5,5,5	0.19	0
4	GOL	A	206	-	5,5,5	0.28	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	B	204	-	3,3,3	0.51	0	2,2,2	0.21	0
4	GOL	B	205	-	5,5,5	0.28	0	5,5,5	0.38	0
4	GOL	B	206	-	5,5,5	0.31	0	5,5,5	0.07	0
5	EDO	C	205	-	3,3,3	0.50	0	2,2,2	0.29	0
4	GOL	D	204	-	5,5,5	0.31	0	5,5,5	0.33	0
4	GOL	D	205	-	5,5,5	0.31	0	5,5,5	0.41	0
4	GOL	G	204	-	5,5,5	0.34	0	5,5,5	0.25	0
4	GOL	H	204	-	5,5,5	0.36	0	5,5,5	0.30	0
4	GOL	I	204	-	5,5,5	0.23	0	5,5,5	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	205	-	-	0/4/4/4	0/0/0/0
4	GOL	A	206	-	-	0/4/4/4	0/0/0/0
5	EDO	B	204	-	-	0/1/1/1	0/0/0/0
4	GOL	B	205	-	-	0/4/4/4	0/0/0/0
4	GOL	B	206	-	-	0/4/4/4	0/0/0/0
5	EDO	C	205	-	-	0/1/1/1	0/0/0/0
4	GOL	D	204	-	-	0/4/4/4	0/0/0/0
4	GOL	D	205	-	-	0/4/4/4	0/0/0/0
4	GOL	G	204	-	-	0/4/4/4	0/0/0/0
4	GOL	H	204	-	-	0/4/4/4	0/0/0/0
4	GOL	I	204	-	-	0/4/4/4	0/0/0/0

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.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	205	GOL	1	0
4	B	205	GOL	1	0
4	B	206	GOL	4	0
4	D	204	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	205	GOL	1	0
4	G	204	GOL	4	0
4	H	204	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	172/193 (89%)	0.01	8 (4%) 32 32	18, 37, 73, 96	0
1	B	174/193 (90%)	-0.17	3 (1%) 70 69	19, 33, 71, 105	0
1	C	174/193 (90%)	-0.03	8 (4%) 33 33	14, 31, 68, 104	0
1	D	174/193 (90%)	-0.13	4 (2%) 61 60	13, 25, 71, 94	0
1	E	174/193 (90%)	-0.31	2 (1%) 80 80	15, 28, 57, 88	1 (0%)
1	F	172/193 (89%)	-0.35	3 (1%) 70 69	15, 27, 54, 85	0
1	G	174/193 (90%)	-0.23	3 (1%) 70 69	15, 25, 45, 99	0
1	H	172/193 (89%)	-0.29	3 (1%) 70 69	13, 28, 58, 95	0
1	I	174/193 (90%)	-0.11	3 (1%) 70 69	16, 35, 64, 87	0
1	J	169/193 (87%)	0.22	9 (5%) 27 27	19, 45, 82, 96	0
All	All	1729/1930 (89%)	-0.14	46 (2%) 55 54	13, 31, 68, 105	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	36	ALA	4.7
1	B	131	SER	3.7
1	A	157[A]	LYS	3.6
1	B	69	GLY	3.6
1	C	36	ALA	3.5
1	J	42	GLY	3.2
1	J	41	LEU	3.2
1	A	16	HIS	3.0
1	E	70	ASN	3.0
1	C	68	VAL	2.9
1	J	47	THR	2.9
1	C	69	GLY	2.8
1	A	190	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	72	PRO	2.7
1	F	72	PRO	2.7
1	G	68	VAL	2.7
1	A	36	ALA	2.7
1	J	35	LYS	2.7
1	J	72	PRO	2.7
1	C	70	ASN	2.6
1	I	36	ALA	2.5
1	E	69	GLY	2.5
1	F	71	ASP	2.5
1	I	151	ALA	2.4
1	I	131	SER	2.4
1	G	70	ASN	2.4
1	F	15	SER	2.4
1	A	38	GLU	2.3
1	C	71	ASP	2.3
1	A	53	HIS	2.2
1	G	69	GLY	2.2
1	J	157	LYS	2.2
1	H	35	LYS	2.2
1	A	151	ALA	2.2
1	D	40	LYS	2.1
1	C	15	SER	2.1
1	J	80	HIS	2.1
1	D	34	LEU	2.1
1	J	34	LEU	2.1
1	H	36	ALA	2.1
1	C	157[A]	LYS	2.0
1	A	37	GLN	2.0
1	H	71	ASP	2.0
1	C	72	PRO	2.0
1	B	68	VAL	2.0
1	J	40	LYS	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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	A	206	6/6	0.75	0.32	7.28	47,52,54,55	0
4	GOL	B	206	6/6	0.70	0.34	2.70	78,81,82,82	0
4	GOL	I	204	6/6	0.82	0.21	2.69	42,46,47,48	0
4	GOL	H	204	6/6	0.76	0.20	2.09	52,52,53,53	0
2	CA	D	200	1/1	1.00	0.10	0.63	18,18,18,18	0
4	GOL	G	204	6/6	0.75	0.20	0.39	71,72,73,73	0
4	GOL	A	205	6/6	0.83	0.16	-0.09	55,59,60,62	0
4	GOL	D	204	6/6	0.80	0.16	-0.47	66,67,67,67	0
2	CA	B	202	1/1	0.92	0.07	-0.91	42,42,42,42	0
2	CA	I	202	1/1	0.97	0.07	-0.96	28,28,28,28	1
3	CL	H	201	1/1	0.97	0.09	-0.98	40,40,40,40	0
2	CA	E	203	1/1	0.94	0.08	-1.14	54,54,54,54	0
2	CA	A	203	1/1	0.98	0.07	-1.23	46,46,46,46	0
2	CA	H	202	1/1	0.93	0.08	-1.31	53,53,53,53	0
2	CA	D	202	1/1	0.94	0.07	-1.36	58,58,58,58	0
2	CA	C	201	1/1	0.99	0.07	-1.40	28,28,28,28	0
3	CL	J	203	1/1	0.99	0.06	-1.53	33,33,33,33	0
2	CA	E	201	1/1	0.99	0.07	-1.54	22,22,22,22	0
3	CL	F	203	1/1	0.99	0.07	-1.65	24,24,24,24	0
2	CA	F	201	1/1	0.97	0.06	-1.83	49,49,49,49	0
3	CL	B	201	1/1	0.99	0.07	-1.84	27,27,27,27	0
3	CL	E	202	1/1	0.99	0.06	-1.94	26,26,26,26	0
3	CL	D	201	1/1	0.99	0.07	-2.16	20,20,20,20	0
2	CA	G	202	1/1	0.97	0.07	-2.17	42,42,42,42	0
3	CL	A	202	1/1	0.98	0.07	-2.18	29,29,29,29	0
2	CA	C	204	1/1	0.98	0.07	-2.55	38,38,38,38	0
2	CA	J	201	1/1	0.98	0.04	-2.69	32,32,32,32	0
2	CA	B	200	1/1	0.99	0.06	-2.86	24,24,24,24	0
2	CA	C	203	1/1	0.99	0.04	-2.87	31,31,31,31	0
2	CA	H	200	1/1	0.99	0.05	-3.57	26,26,26,26	0
2	CA	A	204	1/1	0.85	0.10	-	73,73,73,73	0
2	CA	C	202	1/1	0.98	0.05	-	28,28,28,28	0
5	EDO	C	205	4/4	0.65	0.23	-	55,55,56,56	0
2	CA	I	201	1/1	0.99	0.04	-	34,34,34,34	0
2	CA	D	203	1/1	0.72	0.09	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	G	203	1/1	0.98	0.08	-	28,28,28,28	0
2	CA	E	200	1/1	0.97	0.06	-	33,33,33,33	0
2	CA	E	204	1/1	0.97	0.05	-	50,50,50,50	0
2	CA	H	203	1/1	0.98	0.03	-	57,57,57,57	0
2	CA	F	202	1/1	0.98	0.05	-	38,38,38,38	0
2	CA	I	203	1/1	0.91	0.08	-	59,59,59,59	0
2	CA	G	201	1/1	0.99	0.05	-	32,32,32,32	0
4	GOL	B	205	6/6	0.81	0.18	-	51,53,54,54	0
2	CA	B	203	1/1	0.94	0.06	-	71,71,71,71	0
2	CA	A	201	1/1	0.97	0.03	-	38,38,38,38	0
5	EDO	B	204	4/4	0.61	0.21	-	57,57,58,59	0
2	CA	E	205	1/1	0.89	0.08	-	65,65,65,65	0
2	CA	J	202	1/1	0.84	0.09	-	70,70,70,70	0
4	GOL	D	205	6/6	0.70	0.19	-	56,59,59,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.