



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:02 am BST

PDB ID : 5OHG  
Title : enolase in complex with RNase E  
Authors : Du, D.; Luisi, B.F.  
Deposited on : 2017-07-16  
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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

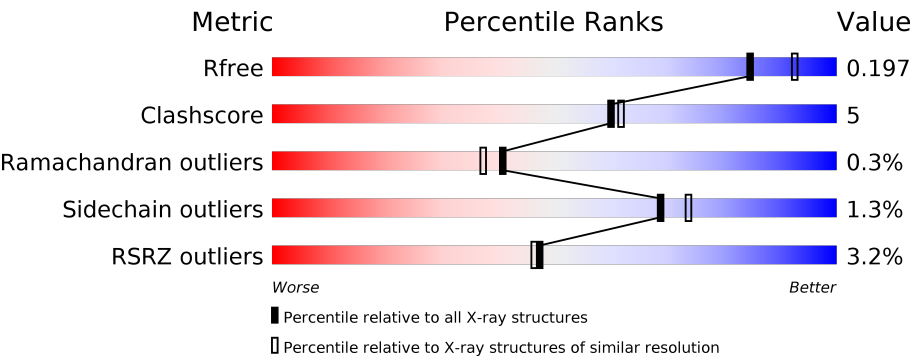
# 1 Overall quality at a glance i

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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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	432	<div><div>%</div><div>93%7%</div></div>
1	B	432	<div><div>%</div><div>92%8%</div></div>
1	H	432	<div><div>%</div><div>92%6%</div></div>
1	I	432	<div><div>%</div><div>92%8%</div></div>
2	C	36	<div><div>39%</div><div>67%22%8%</div></div>
3	J	35	<div><div>74%</div><div>54%43%</div></div>

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
6	PO4	B	503	-	X	-	-
6	PO4	H	503	-	X	-	-
6	PO4	I	504	-	X	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15053 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 Enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3198	2005	546	633	14			
1	B	432	Total	C	N	O	S	0	0	0
			3203	2008	547	634	14			
1	H	431	Total	C	N	O	S	0	0	0
			3198	2005	546	633	14			
1	I	431	Total	C	N	O	S	0	0	0
			3198	2005	546	633	14			

- Molecule 2 is a protein called Ribonuclease E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	36	Total	C	N	O	S	0	1	0
			284	181	53	48	2			

- Molecule 3 is a protein called Ribonuclease E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	35	Total	C	N	O	S	2	1	0
			267	168	47	50	2			

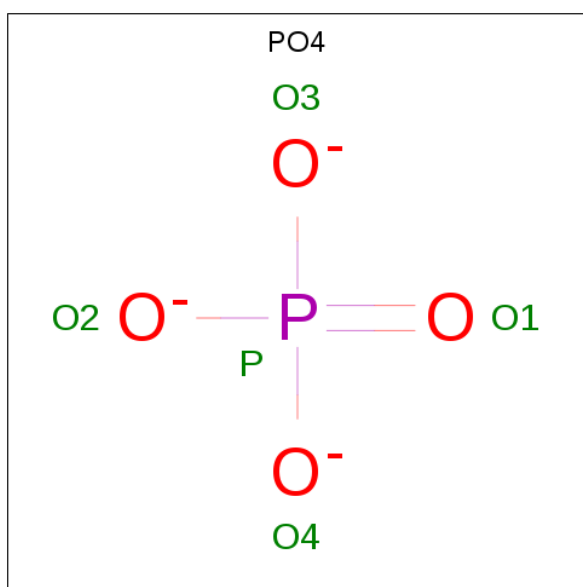
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Na	0	0
			1	1		
5	B	1	Total	Na	0	0
			1	1		
5	A	1	Total	Na	0	0
			1	1		
5	I	2	Total	Na	0	0
			2	2		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	H	1	Total	O	P	0	0
			5	4	1		
6	I	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	421	Total	O	0	0
			421	421		

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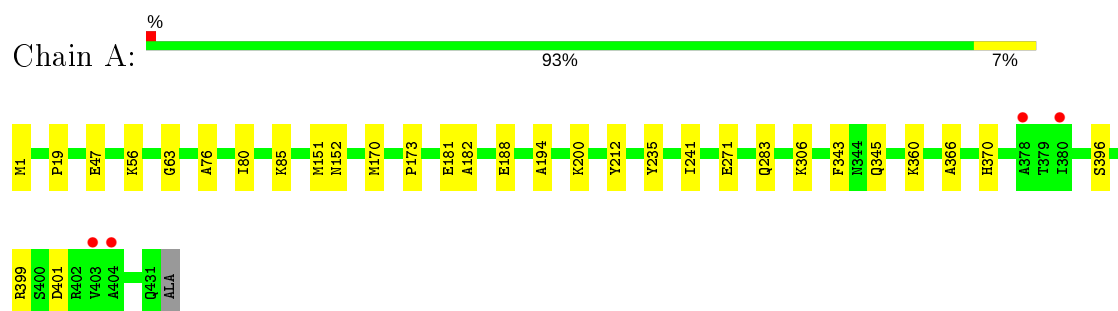
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	359	Total 359	O 359	0	0
7	C	32	Total 32	O 32	0	0
7	H	443	Total 443	O 443	0	0
7	I	387	Total 387	O 387	0	0
7	J	34	Total 34	O 34	0	0

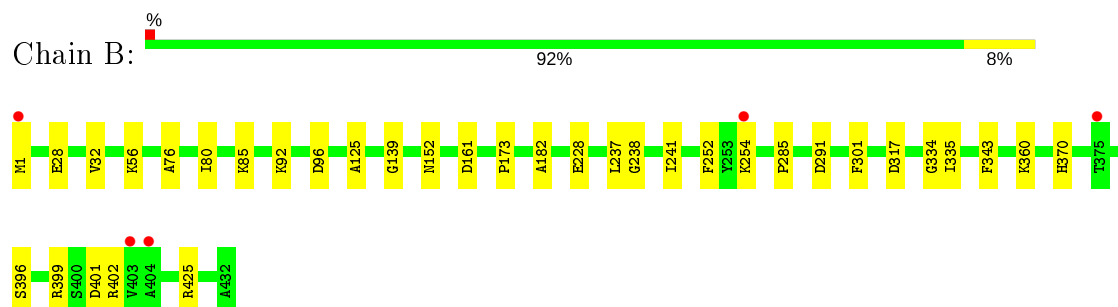
### 3 Residue-property plots [i](#)

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.

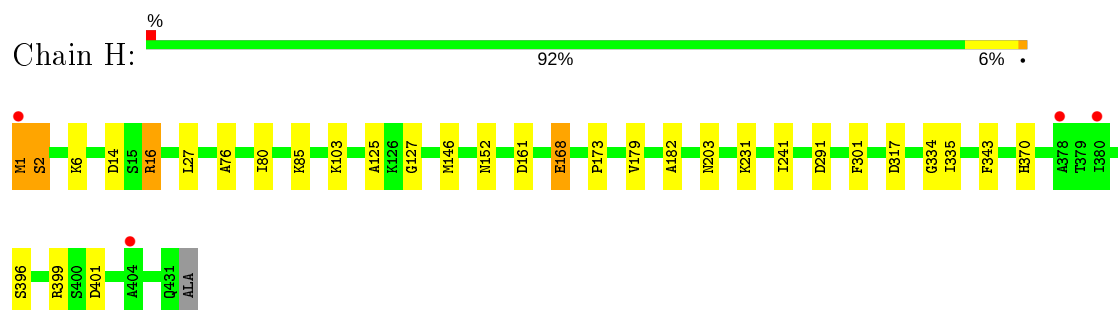
#### • Molecule 1: Enolase



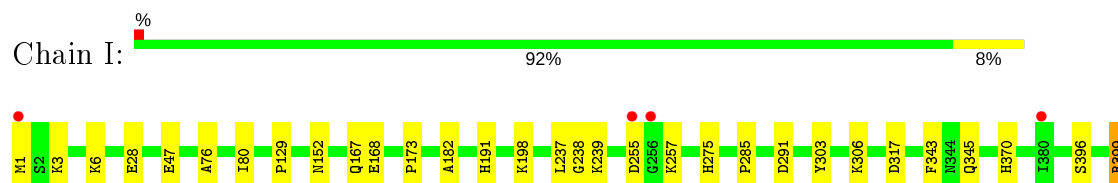
#### • Molecule 1: Enolase



#### • Molecule 1: Enolase

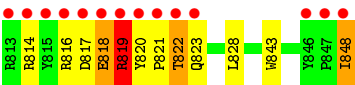


#### • Molecule 1: Enolase

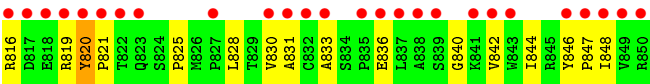




• Molecule 2: Ribonuclease E



• Molecule 3: Ribonuclease E





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.68Å 116.92Å 107.78Å 90.00° 105.43° 90.00°	Depositor
Resolution (Å)	39.24 – 2.00 44.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.24-2.00) 98.6 (44.97-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.161 , 0.197 0.164 , 0.197	Depositor DCC
$R_{free}$ test set	5979 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.8	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	0.96	EDS
Total number of atoms	15053	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: NA, PO4, MG

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	0.49	0/3240	0.60	1/4362 (0.0%)
1	B	0.46	0/3245	0.57	0/4369
1	H	0.52	1/3240 (0.0%)	0.61	3/4362 (0.1%)
1	I	0.52	0/3240	0.63	3/4362 (0.1%)
2	C	0.64	0/292	0.86	0/399
3	J	0.56	0/277	0.74	0/379
All	All	0.50	1/13534 (0.0%)	0.61	7/18233 (0.0%)

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
2	C	0	3
3	J	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	168	GLU	CD-OE2	-5.21	1.20	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	16	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	I	257	LYS	CD-CE-NZ	-6.84	95.97	111.70
1	I	239	LYS	CD-CE-NZ	-6.63	96.46	111.70
1	A	56	LYS	CD-CE-NZ	-5.77	98.42	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	399	ARG	N-CA-CB	5.75	120.94	110.60
1	H	16	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	H	14	ASP	CB-CG-OD1	5.12	122.91	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	817	ASP	Peptide
2	C	818	GLU	Peptide
2	C	819	ARG	Peptide
3	J	848	ILE	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3198	0	3225	17	0
1	B	3203	0	3230	22	0
1	H	3198	0	3225	29	0
1	I	3198	0	3225	21	2
2	C	284	0	279	18	2
3	J	267	0	255	31	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	H	1	0	0	0	0
5	I	2	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	H	5	0	0	0	0
6	I	5	0	0	0	0
7	A	421	0	0	10	1
7	B	359	0	0	3	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	32	0	0	1	0
7	H	443	0	0	6	1
7	I	387	0	0	6	0
7	J	34	0	0	9	0
All	All	15053	0	13439	123	4

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 (123) 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:H:1:MET:HG2	3:J:819:ARG:HE	1.31	0.95
1:H:1:MET:O	1:H:85:LYS:NZ	2.01	0.93
3:J:825:PRO:HG2	3:J:844:ILE:HD11	1.50	0.93
1:I:6:LYS:HE3	7:I:759:HOH:O	1.70	0.91
3:J:844:ILE:HD12	7:J:933:HOH:O	1.76	0.84
1:B:139:GLY:HA2	2:C:814:ARG:HG3	1.62	0.81
1:H:1:MET:HG2	3:J:819:ARG:NE	1.94	0.81
1:H:1:MET:HG3	3:J:819:ARG:HH21	1.46	0.81
1:I:1:MET:N	1:I:28:GLU:OE1	2.12	0.79
7:A:892:HOH:O	2:C:848:ILE:CD1	2.32	0.78
7:A:892:HOH:O	2:C:848:ILE:HG13	1.84	0.76
1:I:418:GLU:HG3	7:I:734:HOH:O	1.87	0.75
1:A:271:GLU:OE2	7:A:601:HOH:O	2.06	0.73
1:H:203:ASN:OD1	7:H:601:HOH:O	2.07	0.72
1:H:334:GLY:HA2	7:H:619:HOH:O	1.90	0.71
3:J:820:TYR:OH	7:J:902:HOH:O	2.09	0.71
1:I:1:MET:HB3	7:I:897:HOH:O	1.90	0.71
3:J:816:ARG:NH1	3:J:821:PRO:HD3	2.05	0.71
2:C:822:THR:HG23	2:C:823[A]:GLN:HG2	1.73	0.69
1:B:228:GLU:OE2	7:B:601:HOH:O	2.11	0.68
1:A:173:PRO:HG2	1:A:182:ALA:HB1	1.77	0.66
1:A:1:MET:HB2	1:A:85:LYS:HZ1	1.61	0.65
3:J:836[A]:GLU:OE1	7:J:903:HOH:O	2.14	0.64
2:C:822:THR:HG23	2:C:823[A]:GLN:OE1	1.98	0.64
1:B:238:GLY:O	1:B:425:ARG:NH2	2.32	0.62
2:C:816:ARG:HA	2:C:819:ARG:NH1	2.14	0.62
1:B:32:VAL:HG11	2:C:828:LEU:HD12	1.81	0.62
1:B:125:ALA:O	2:C:821:PRO:HD2	2.01	0.61
1:H:127:GLY:HA3	3:J:816:ARG:NH1	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:825:PRO:HG2	3:J:844:ILE:CD1	2.29	0.59
1:H:173:PRO:HG2	1:H:182:ALA:HB1	1.85	0.59
1:H:1:MET:SD	1:H:1:MET:N	2.63	0.59
1:H:1:MET:HG3	3:J:819:ARG:NH2	2.17	0.58
1:H:1:MET:CG	3:J:819:ARG:HH21	2.15	0.58
1:H:76:ALA:O	1:H:80:ILE:HG12	2.03	0.57
3:J:840:GLY:HA3	7:J:932:HOH:O	2.04	0.57
1:B:139:GLY:HA2	2:C:814:ARG:CG	2.33	0.57
1:I:6:LYS:CE	7:I:759:HOH:O	2.39	0.56
1:I:173:PRO:HG2	1:I:182:ALA:HB1	1.87	0.56
1:H:1:MET:CG	3:J:819:ARG:NH2	2.68	0.56
1:A:283:GLN:OE1	7:A:602:HOH:O	2.18	0.55
2:C:814:ARG:HB3	2:C:814:ARG:CZ	2.34	0.55
1:A:200:LYS:NZ	7:A:608:HOH:O	2.28	0.55
1:H:152:ASN:ND2	1:H:168:GLU:HG2	2.21	0.55
3:J:825:PRO:CG	3:J:844:ILE:HD11	2.29	0.55
1:H:1:MET:HB2	3:J:819:ARG:CZ	2.38	0.54
1:A:76:ALA:O	1:A:80:ILE:HG12	2.07	0.54
7:A:892:HOH:O	2:C:848:ILE:CG1	2.44	0.54
1:I:275:HIS:NE2	1:I:303:TYR:OH	2.32	0.54
3:J:846:TYR:N	3:J:847:PRO:CD	2.72	0.53
1:B:237:LEU:HG	1:B:285:PRO:HG3	1.91	0.53
1:A:181:GLU:OE2	7:A:603:HOH:O	2.19	0.53
3:J:816:ARG:HD3	3:J:820:TYR:HB2	1.91	0.53
3:J:840:GLY:N	7:J:901:HOH:O	2.42	0.52
1:I:425:ARG:NH1	1:I:431:GLN:OE1	2.35	0.52
1:H:231:LYS:HE3	7:H:959:HOH:O	2.10	0.51
1:B:401:ASP:OD2	1:B:402:ARG:NE	2.37	0.51
3:J:819:ARG:HD2	7:J:904:HOH:O	2.11	0.50
2:C:822:THR:HG23	2:C:823[A]:GLN:CG	2.42	0.50
1:I:238:GLY:O	1:I:425:ARG:NH2	2.45	0.49
1:A:152:ASN:O	1:A:396:SER:HB2	2.11	0.49
1:B:301:PHE:HB3	1:B:335:ILE:HG23	1.94	0.49
3:J:844:ILE:N	7:J:910:HOH:O	2.44	0.49
1:H:152:ASN:O	1:H:396:SER:HB2	2.13	0.49
1:A:360:LYS:HG3	7:A:837:HOH:O	2.13	0.48
1:B:173:PRO:HA	1:B:241:ILE:HD13	1.95	0.48
1:H:1:MET:HA	1:H:2:SER:HA	1.50	0.48
1:H:2:SER:HB3	1:H:27:LEU:HB3	1.94	0.48
1:B:252:PHE:HA	1:B:254:LYS:HE2	1.96	0.48
2:C:822:THR:CG2	2:C:823[A]:GLN:HG2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:816:ARG:HH11	3:J:821:PRO:HD3	1.79	0.48
1:B:173:PRO:HG2	1:B:182:ALA:HB1	1.95	0.47
1:H:1:MET:CG	3:J:819:ARG:NE	2.72	0.47
1:A:306:LYS:HE2	7:A:935:HOH:O	2.14	0.47
1:B:1:MET:HA	1:B:28:GLU:HG3	1.96	0.47
3:J:828:LEU:CD2	3:J:833:ALA:HB3	2.44	0.47
1:B:291:ASP:OD2	1:B:317:ASP:HB3	2.15	0.47
1:I:76:ALA:O	1:I:80:ILE:HG12	2.15	0.47
1:B:85:LYS:NZ	7:B:602:HOH:O	2.25	0.46
1:H:291:ASP:OD2	1:H:317:ASP:HB3	2.15	0.46
1:I:291:ASP:OD2	1:I:317:ASP:HB3	2.15	0.46
1:H:301:PHE:HB3	1:H:335:ILE:HG23	1.98	0.46
1:I:198:LYS:HB2	1:I:198:LYS:HE2	1.51	0.46
7:A:892:HOH:O	2:C:848:ILE:HD12	2.09	0.46
1:A:173:PRO:HA	1:A:241:ILE:HD13	1.98	0.45
1:I:152:ASN:O	1:I:396:SER:HB2	2.16	0.45
1:H:125:ALA:O	3:J:821:PRO:HD2	2.16	0.45
1:H:161:ASP:OD2	1:I:198:LYS:HD3	2.17	0.45
1:A:151:MET:O	1:A:170:MET:HA	2.17	0.45
1:B:152:ASN:O	1:B:396:SER:HB2	2.17	0.44
1:B:161:ASP:OD1	1:B:161:ASP:O	2.34	0.44
1:A:194:ALA:HB2	1:A:212:TYR:OH	2.18	0.44
1:B:334:GLY:HA2	7:B:754:HOH:O	2.18	0.44
3:J:828:LEU:HD21	3:J:830:VAL:O	2.18	0.43
1:A:19:PRO:HG2	1:A:63:GLY:HA2	2.01	0.43
1:H:6:LYS:HD2	7:H:840:HOH:O	2.17	0.43
1:B:76:ALA:O	1:B:80:ILE:HG12	2.18	0.43
2:C:843:TRP:HA	7:C:924:HOH:O	2.19	0.43
1:I:237:LEU:HG	1:I:285:PRO:HG3	2.01	0.43
2:C:819:ARG:HB3	2:C:820:TYR:CG	2.54	0.43
1:B:1:MET:N	1:B:28:GLU:OE2	2.35	0.43
1:B:56:LYS:HD2	1:B:56:LYS:HA	1.74	0.43
1:H:173:PRO:HA	1:H:241:ILE:HD13	2.00	0.43
1:H:103:LYS:NZ	7:H:607:HOH:O	2.41	0.42
1:I:3:LYS:HD3	7:I:672:HOH:O	2.19	0.42
1:A:47:GLU:CD	1:A:345:GLN:HG2	2.40	0.42
1:B:92:LYS:NZ	1:B:96:ASP:OD2	2.41	0.42
3:J:836[B]:GLU:HB2	3:J:842:VAL:HG12	2.02	0.42
1:I:167:GLN:HG2	1:I:168:GLU:HG3	2.01	0.41
3:J:828:LEU:HD11	3:J:831:ALA:N	2.34	0.41
1:I:47:GLU:CD	1:I:345:GLN:HG2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:MET:HE2	1:H:179:VAL:HG11	2.03	0.41
1:A:188:GLU:OE1	1:A:235:TYR:OH	2.30	0.41
1:H:16:ARG:HD2	7:H:675:HOH:O	2.20	0.41
2:C:819:ARG:HD3	2:C:820:TYR:CE2	2.56	0.41
1:I:191:HIS:HD2	7:I:919:HOH:O	2.03	0.41
3:J:836[A]:GLU:HB3	3:J:842:VAL:HG12	2.03	0.41
1:I:306:LYS:HE2	1:I:306:LYS:HB3	1.74	0.41
1:I:129:PRO:HB3	3:J:833:ALA:HA	2.03	0.41
1:A:360:LYS:NZ	1:A:366:ALA:H	2.19	0.40
3:J:840:GLY:HA3	7:J:912:HOH:O	2.21	0.40
2:C:819:ARG:HB3	2:C:820:TYR:CD1	2.56	0.40

All (4) 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)
2:C:818:GLU:CB	1:I:255:ASP:OD1[2_646]	1.27	0.93
2:C:818:GLU:CB	1:I:255:ASP:CG[2_646]	1.93	0.27
7:B:767:HOH:O	7:H:959:HOH:O[2_546]	1.96	0.24
7:A:757:HOH:O	7:B:772:HOH:O[1_655]	2.06	0.14

## 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	429/432 (99%)	417 (97%)	11 (3%)	1 (0%)	47	44
1	B	430/432 (100%)	418 (97%)	11 (3%)	1 (0%)	47	44
1	H	429/432 (99%)	418 (97%)	10 (2%)	1 (0%)	47	44
1	I	429/432 (99%)	415 (97%)	13 (3%)	1 (0%)	47	44
2	C	35/36 (97%)	34 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	34/35 (97%)	27 (79%)	6 (18%)	1 (3%)	4	1
All	All	1786/1799 (99%)	1729 (97%)	52 (3%)	5 (0%)	41	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	820	TYR
1	A	399	ARG
1	B	399	ARG
1	H	399	ARG
1	I	399	ARG

### 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	326/326 (100%)	323 (99%)	3 (1%)	78	83
1	B	326/326 (100%)	323 (99%)	3 (1%)	78	83
1	H	326/326 (100%)	321 (98%)	5 (2%)	65	69
1	I	326/326 (100%)	323 (99%)	3 (1%)	78	83
2	C	29/32 (91%)	26 (90%)	3 (10%)	7	4
3	J	28/31 (90%)	28 (100%)	0	100	100
All	All	1361/1367 (100%)	1344 (99%)	17 (1%)	69	76

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	PHE
1	A	370	HIS
1	A	401	ASP
1	B	343	PHE
1	B	360	LYS
1	B	370	HIS

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Mol	Chain	Res	Type
2	C	819	ARG
2	C	822	THR
2	C	848	ILE
1	H	1	MET
1	H	2	SER
1	H	343	PHE
1	H	370	HIS
1	H	401	ASP
1	I	343	PHE
1	I	370	HIS
1	I	401	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	191	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 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
6	PO4	B	503	-	4,4,4	3.28	4 (100%)	6,6,6	0.95	0
6	PO4	A	503	-	4,4,4	3.39	3 (75%)	6,6,6	0.90	0
6	PO4	I	504	-	4,4,4	4.12	4 (100%)	6,6,6	0.67	0
6	PO4	H	503	-	4,4,4	4.08	4 (100%)	6,6,6	0.67	0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	504	PO4	P-O2	-5.06	1.39	1.54
6	H	503	PO4	P-O4	-4.82	1.40	1.54
6	I	504	PO4	P-O3	-4.13	1.42	1.54
6	I	504	PO4	P-O4	-4.05	1.42	1.54
6	H	503	PO4	P-O3	-4.04	1.42	1.54
6	A	503	PO4	P-O2	-4.03	1.42	1.54
6	A	503	PO4	P-O3	-3.83	1.43	1.54
6	H	503	PO4	P-O2	-3.77	1.43	1.54
6	H	503	PO4	P-O1	-3.60	1.42	1.50
6	B	503	PO4	P-O3	-3.56	1.43	1.54
6	B	503	PO4	P-O2	-3.44	1.44	1.54
6	A	503	PO4	P-O4	-3.44	1.44	1.54
6	B	503	PO4	P-O1	-3.25	1.43	1.50
6	I	504	PO4	P-O1	-2.97	1.43	1.50
6	B	503	PO4	P-O4	-2.81	1.46	1.54

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	431/432 (99%)	-0.30	4 (0%) 84 83	20, 26, 38, 53	0
1	B	432/432 (100%)	-0.31	5 (1%) 79 78	18, 27, 41, 53	0
1	H	431/432 (99%)	-0.36	4 (0%) 84 83	17, 24, 36, 58	0
1	I	431/432 (99%)	-0.24	4 (0%) 84 83	18, 25, 41, 61	0
2	C	36/36 (100%)	2.92	14 (38%) 0 0	29, 41, 83, 101	0
3	J	35/35 (100%)	4.25	26 (74%) 0 0	29, 37, 65, 73	31 (88%)
All	All	1796/1799 (99%)	-0.15	57 (3%) 47 46	17, 26, 41, 101	31 (1%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	815	TYR	19.5
3	J	818	GLU	11.8
3	J	820	TYR	10.8
2	C	818	GLU	10.7
3	J	816	ARG	9.7
3	J	850	ARG	9.0
3	J	849	VAL	8.5
3	J	819	ARG	7.7
2	C	814	ARG	7.7
2	C	817	ASP	6.8
3	J	846	TYR	6.8
2	C	813	ARG	6.6
3	J	817	ASP	6.4
2	C	820	TYR	6.4
3	J	848	ILE	6.1
1	B	1	MET	6.0
2	C	821	PRO	5.7
2	C	816	ARG	5.7
2	C	819	ARG	5.6

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Mol	Chain	Res	Type	RSRZ
3	J	835	PRO	5.5
2	C	822	THR	5.1
3	J	827	PRO	4.9
3	J	822	THR	4.7
3	J	823	GLN	4.4
2	C	823[A]	GLN	4.3
3	J	842	VAL	4.3
3	J	836[A]	GLU	4.0
1	H	1	MET	3.9
3	J	837	LEU	3.7
3	J	841	LYS	3.6
1	I	1	MET	3.6
1	A	404	ALA	3.4
3	J	832	CYS	3.4
1	B	404	ALA	3.3
2	C	846	TYR	3.2
1	H	404	ALA	3.1
1	I	256	GLY	3.1
2	C	847	PRO	3.1
3	J	839	SER	3.1
3	J	843	TRP	3.0
3	J	833	ALA	2.8
3	J	838	ALA	2.7
1	I	255	ASP	2.7
1	I	380	ILE	2.7
1	A	403	VAL	2.7
3	J	821	PRO	2.7
1	H	380	ILE	2.6
1	A	378	ALA	2.6
1	B	375	THR	2.5
1	A	380	ILE	2.5
3	J	831	ALA	2.4
1	B	403	VAL	2.4
2	C	848	ILE	2.2
3	J	830	VAL	2.2
1	H	378	ALA	2.2
3	J	847	PRO	2.1
1	B	254	LYS	2.1

## 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 [i](#)

There are no carbohydrates 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<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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	501	1/1	0.87	0.15	22,22,22,22	0
4	MG	B	501	1/1	0.91	0.13	25,25,25,25	0
4	MG	I	501	1/1	0.94	0.10	20,20,20,20	0
6	PO4	A	503	5/5	0.95	0.18	30,30,30,30	0
4	MG	H	501	1/1	0.96	0.13	18,18,18,18	0
6	PO4	B	503	5/5	0.98	0.16	30,30,30,30	0
6	PO4	H	503	5/5	0.98	0.16	30,30,30,30	0
6	PO4	I	504	5/5	0.98	0.14	30,30,30,30	0
5	NA	B	502	1/1	0.99	0.13	18,18,18,18	0
5	NA	I	502	1/1	0.99	0.09	27,27,27,27	0
5	NA	I	503	1/1	1.00	0.19	17,17,17,17	0
5	NA	A	502	1/1	1.00	0.15	16,16,16,16	0
5	NA	H	502	1/1	1.00	0.15	14,14,14,14	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.