



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 06:03 AM EDT

PDB ID : 2DW7 / pdb\_00002dw7  
Title : Crystal structure of D-tartrate dehydratase from Bradyrhizobium japonicum complexed with Mg<sup>++</sup> and meso-tartrate  
Authors : Fedorov, A.A.; Fedorov, E.V.; Yew, W.S.; Wood, B.M.; Gerlt, J.A.; Almo, S.C.  
Deposited on : 2006-08-07  
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

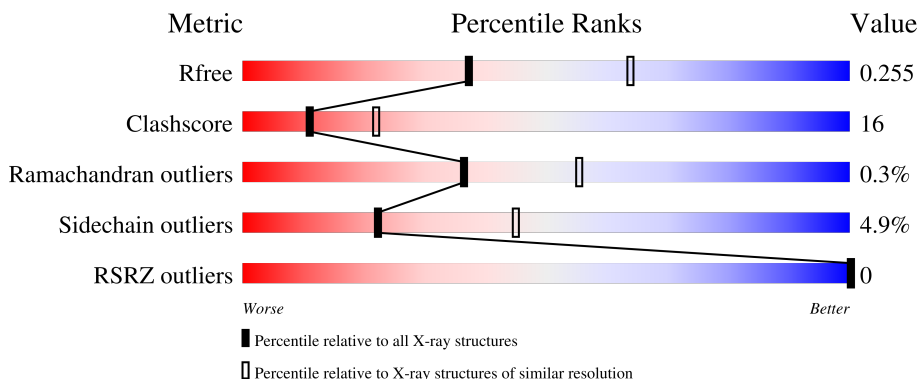
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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  $\geq 3$ , 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	389	
1	B	389	
1	C	389	
1	D	389	
1	E	389	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	389	 68% 29% .
1	G	389	 64% 32% .
1	H	389	 68% 28% .
1	I	389	 70% 26% .
1	J	389	 65% 32% .
1	K	389	 67% 30% .
1	L	389	 66% 31% .
1	M	389	 66% 30% .
1	N	389	 67% 29% .
1	O	389	 66% 30% .
1	P	389	 63% 32% . .

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
3	SRT	A	1001	-	X	-	-
3	SRT	G	1007	-	-	X	-
3	SRT	I	1009	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 48977 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.

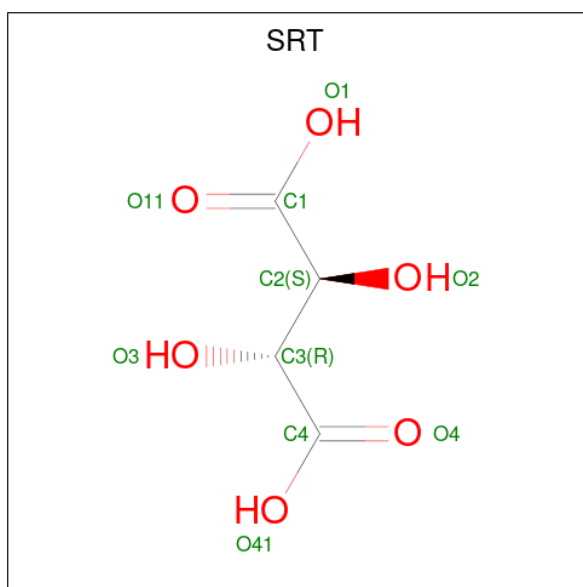
- Molecule 1 is a protein called Bll6730 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3022	1917	530	558	17	0	0	0
1	B	388	3022	1917	530	558	17	0	0	0
1	C	388	3022	1917	530	558	17	0	0	0
1	D	388	3022	1917	530	558	17	0	0	0
1	E	388	3022	1917	530	558	17	0	0	0
1	F	388	3022	1917	530	558	17	0	0	0
1	G	388	3022	1917	530	558	17	0	0	0
1	H	388	3022	1917	530	558	17	0	0	0
1	I	388	3022	1917	530	558	17	0	0	0
1	J	388	3022	1917	530	558	17	0	0	0
1	K	388	3022	1917	530	558	17	0	0	0
1	L	388	3022	1917	530	558	17	0	0	0
1	M	388	3022	1917	530	558	17	0	0	0
1	N	388	3022	1917	530	558	17	0	0	0
1	O	388	3022	1917	530	558	17	0	0	0
1	P	388	3022	1917	530	558	17	0	0	0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0
2	L	1	Total Mg 1 1	0	0
2	M	1	Total Mg 1 1	0	0
2	N	1	Total Mg 1 1	0	0
2	O	1	Total Mg 1 1	0	0
2	P	1	Total Mg 1 1	0	0

- Molecule 3 is S,R MESO-TARTARIC ACID (CCD ID: SRT) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 4 6	0	0
3	B	1	Total C O 10 4 6	0	0
3	C	1	Total C O 10 4 6	0	0
3	D	1	Total C O 10 4 6	0	0
3	E	1	Total C O 10 4 6	0	0
3	F	1	Total C O 10 4 6	0	0
3	G	1	Total C O 10 4 6	0	0
3	H	1	Total C O 10 4 6	0	0
3	I	1	Total C O 10 4 6	0	0
3	J	1	Total C O 10 4 6	0	0
3	K	1	Total C O 10 4 6	0	0
3	L	1	Total C O 10 4 6	0	0
3	M	1	Total C O 10 4 6	0	0
3	N	1	Total C O 10 4 6	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	C	O	0	0
			10	4	6		
3	P	1	Total	C	O	0	0
			10	4	6		

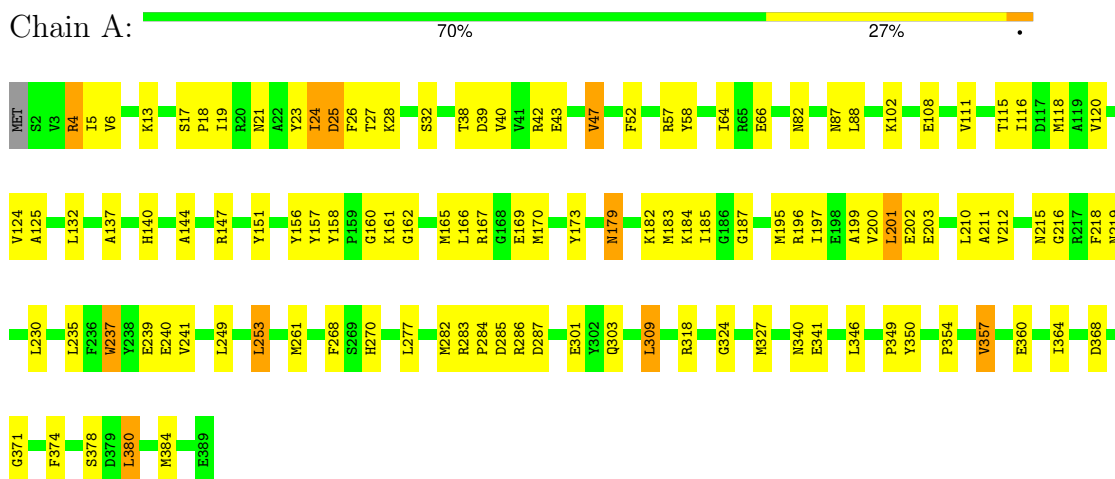
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	21	Total	O	0	0
			21	21		
4	C	61	Total	O	0	0
			61	61		
4	D	49	Total	O	0	0
			49	49		
4	E	29	Total	O	0	0
			29	29		
4	F	53	Total	O	0	0
			53	53		
4	G	41	Total	O	0	0
			41	41		
4	H	22	Total	O	0	0
			22	22		
4	I	20	Total	O	0	0
			20	20		
4	J	12	Total	O	0	0
			12	12		
4	K	29	Total	O	0	0
			29	29		
4	L	20	Total	O	0	0
			20	20		
4	M	12	Total	O	0	0
			12	12		
4	N	20	Total	O	0	0
			20	20		
4	O	5	Total	O	0	0
			5	5		
4	P	12	Total	O	0	0
			12	12		

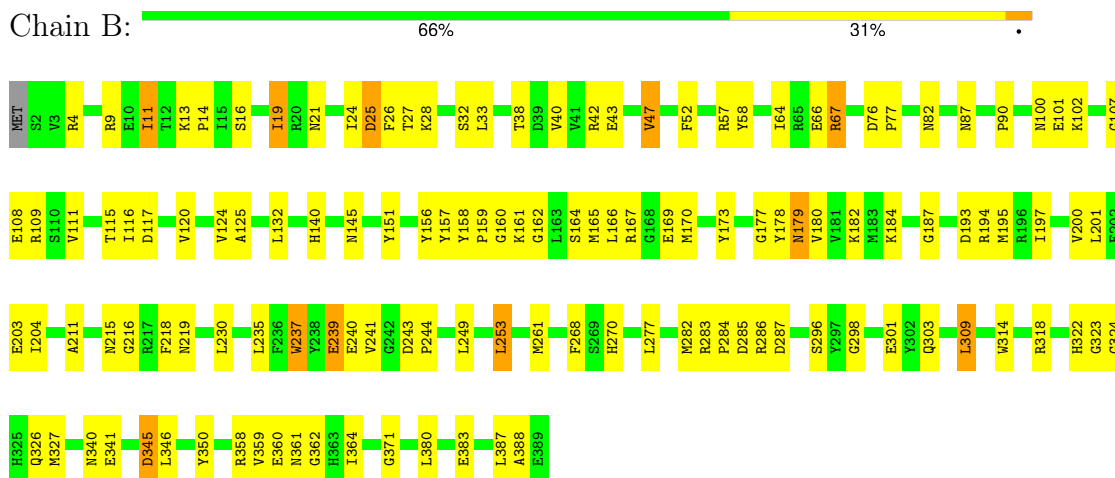
### 3 Residue-property plots [i](#)

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: Bll6730 protein



- Molecule 1: Bll6730 protein

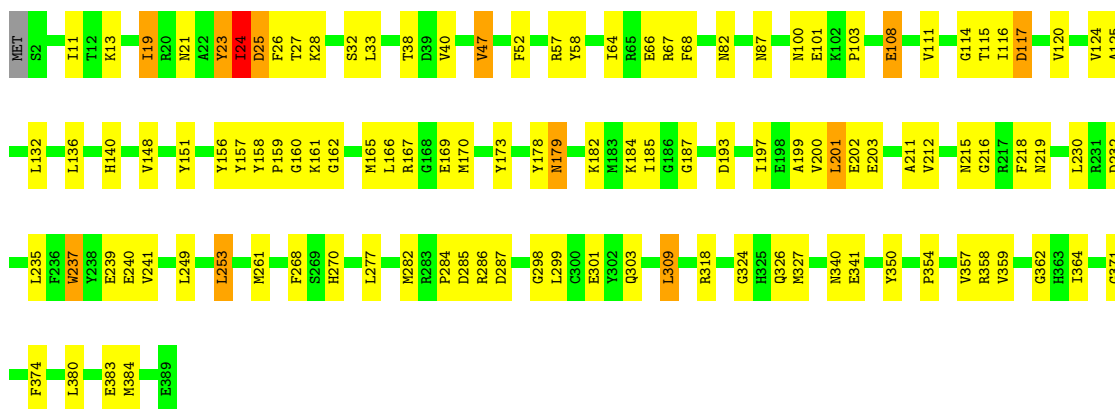


- Molecule 1: Bll6730 protein

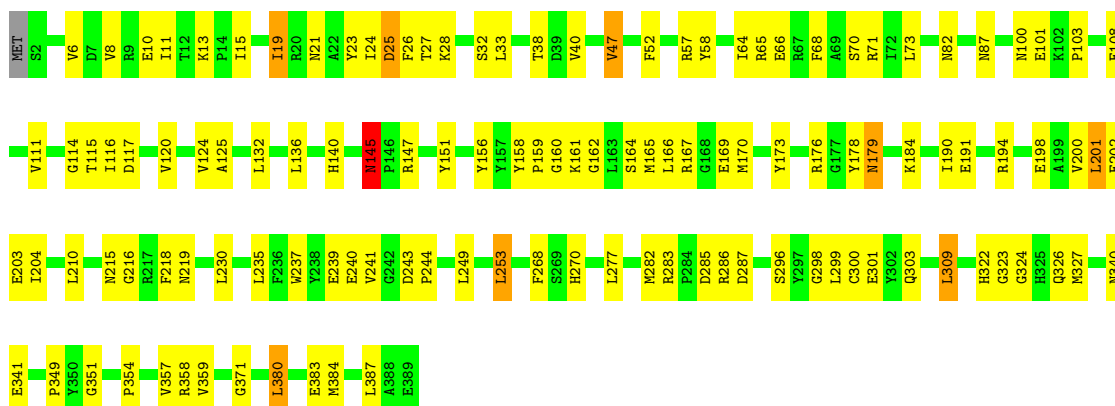




• Molecule 1: Bll6730 protein



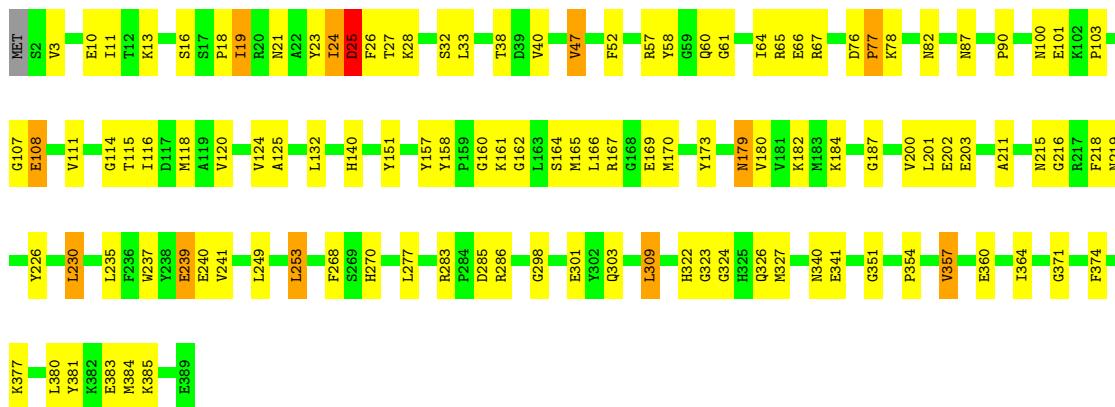
• Molecule 1: Bll6730 protein



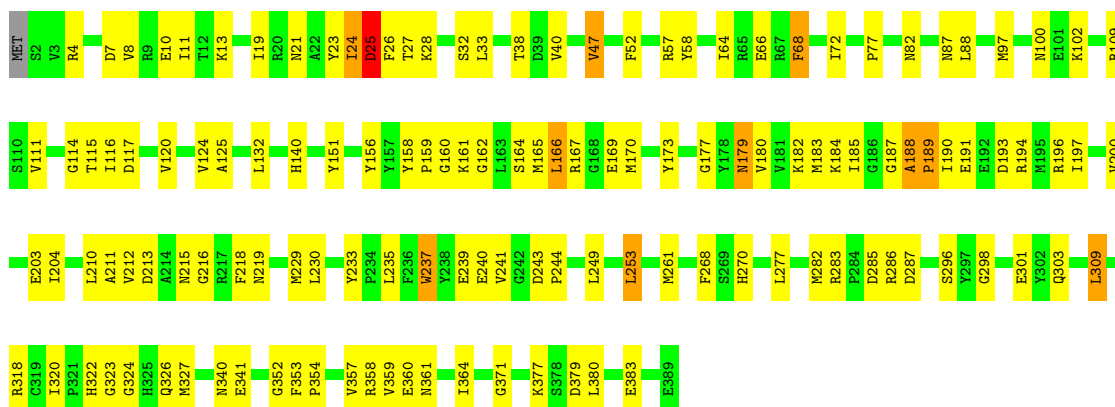
• Molecule 1: Bll6730 protein



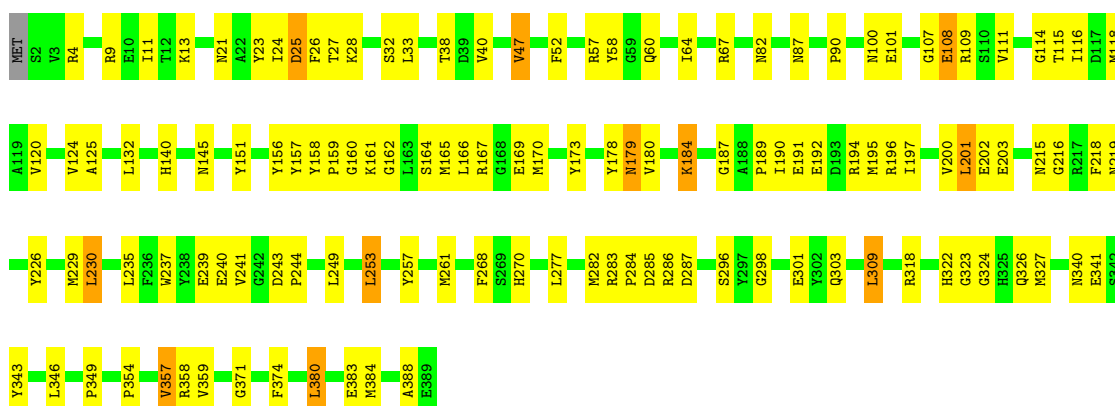




• Molecule 1: Bll6730 protein

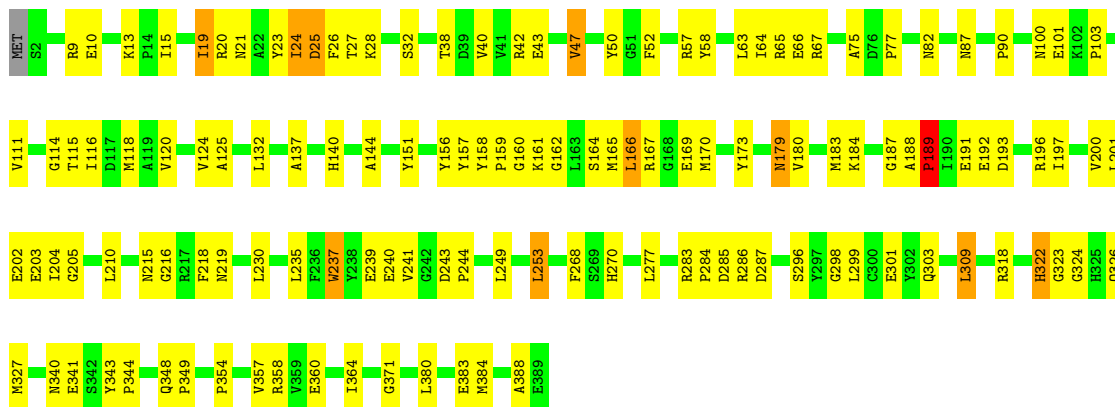


• Molecule 1: Bll6730 protein

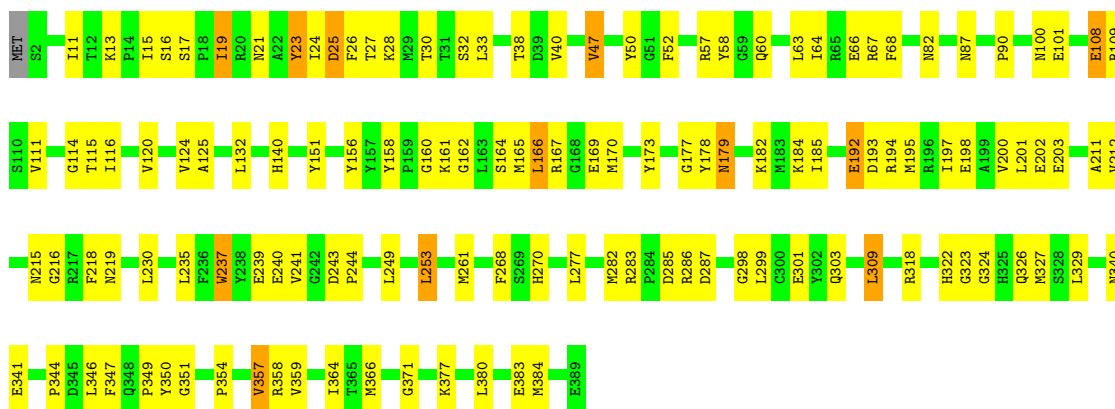


• Molecule 1: Bll6730 protein

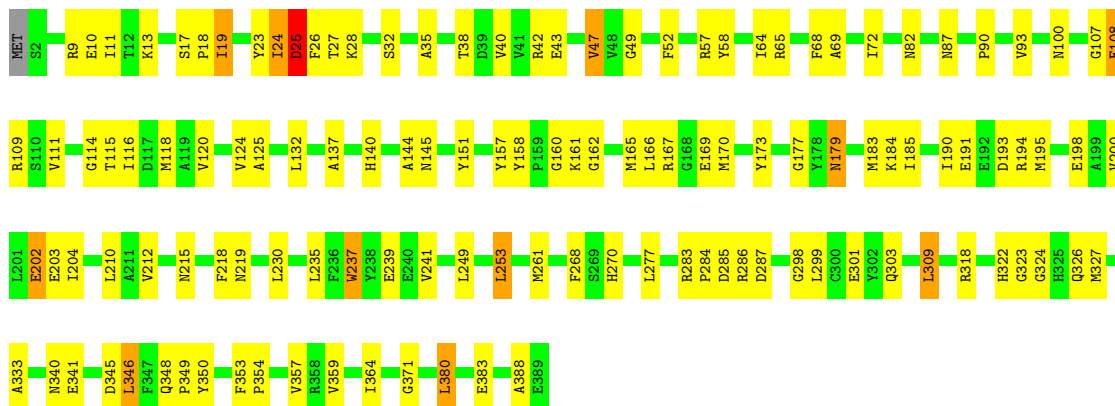




• Molecule 1: Bll6730 protein



• Molecule 1: Bll6730 protein



• Molecule 1: Bll6730 protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.84Å 162.54Å 168.18Å 117.76° 90.03° 90.67°	Depositor
Resolution (Å)	25.00 – 2.50 25.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.50) 92.3 (25.00-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.241 , 0.265 0.232 , 0.255	Depositor DCC
$R_{free}$ test set	11937 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 18.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.064 for h,-k,-l 0.016 for -h,k,-k-l 0.014 for -h,-k,k+l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	48977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: SRT, 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	0.46	0/3092	0.94	7/4177 (0.2%)
1	B	0.43	0/3092	0.94	9/4177 (0.2%)
1	C	0.51	0/3092	0.93	7/4177 (0.2%)
1	D	0.50	0/3092	0.95	8/4177 (0.2%)
1	E	0.44	0/3092	0.93	9/4177 (0.2%)
1	F	0.48	0/3092	0.96	13/4177 (0.3%)
1	G	0.49	0/3092	0.95	10/4177 (0.2%)
1	H	0.43	0/3092	0.94	8/4177 (0.2%)
1	I	0.44	0/3092	0.92	6/4177 (0.1%)
1	J	0.42	0/3092	0.93	10/4177 (0.2%)
1	K	0.46	0/3092	0.95	11/4177 (0.3%)
1	L	0.43	0/3092	0.93	8/4177 (0.2%)
1	M	0.43	0/3092	0.92	6/4177 (0.1%)
1	N	0.40	0/3092	0.93	6/4177 (0.1%)
1	O	0.41	0/3092	0.92	5/4177 (0.1%)
1	P	0.41	0/3092	0.92	6/4177 (0.1%)
All	All	0.45	0/49472	0.94	129/66832 (0.2%)

There are no bond length outliers.

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	66	GLU	N-CA-C	8.69	120.75	111.28
1	H	145	ASN	CA-C-N	8.65	128.30	119.56
1	H	145	ASN	C-N-CA	8.65	128.30	119.56
1	M	66	GLU	N-CA-C	8.51	121.69	111.82
1	N	69	ALA	N-CA-C	-8.13	103.34	113.18

There are no chirality outliers.

There are no planarity outliers.

## 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	3022	0	2975	92	0
1	B	3022	0	2975	108	0
1	C	3022	0	2975	89	0
1	D	3022	0	2975	95	0
1	E	3022	0	2975	99	0
1	F	3022	0	2975	94	0
1	G	3022	0	2975	124	0
1	H	3022	0	2975	110	0
1	I	3022	0	2975	92	0
1	J	3022	0	2975	112	0
1	K	3022	0	2975	101	0
1	L	3022	0	2975	102	0
1	M	3022	0	2975	112	0
1	N	3022	0	2975	113	0
1	O	3022	0	2975	109	0
1	P	3022	0	2975	119	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	10	0	3	3	0
3	B	10	0	3	2	0
3	C	10	0	3	2	0
3	D	10	0	3	3	0
3	E	10	0	3	2	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	10	0	3	1	0
3	G	10	0	4	4	0
3	H	10	0	3	2	0
3	I	10	0	3	4	0
3	J	10	0	3	1	0
3	K	10	0	3	2	0
3	L	10	0	3	3	0
3	M	10	0	3	0	0
3	N	10	0	3	3	0
3	O	10	0	3	0	0
3	P	10	0	4	3	0
4	A	43	0	0	1	0
4	B	21	0	0	0	0
4	C	61	0	0	3	0
4	D	49	0	0	0	0
4	E	29	0	0	1	0
4	F	53	0	0	0	0
4	G	41	0	0	2	0
4	H	22	0	0	0	0
4	I	20	0	0	0	0
4	J	12	0	0	0	0
4	K	29	0	0	0	0
4	L	20	0	0	0	0
4	M	12	0	0	0	0
4	N	20	0	0	0	0
4	O	5	0	0	1	0
4	P	12	0	0	1	0
All	All	48977	0	47650	1577	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 16.

The worst 5 of 1577 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:P:353:PHE:HB2	1:P:357:VAL:HG11	1.37	1.07
1:L:184:LYS:HE3	1:L:215:ASN:HD21	1.19	1.04
1:J:167:ARG:HD3	1:J:203:GLU:HB2	1.35	1.03
1:C:100:ASN:HA	1:D:24:ILE:HG13	1.37	1.03
1:C:24:ILE:HG13	1:D:100:ASN:HA	1.39	1.02

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	Percentiles	
1	A	386/389 (99%)	370 (96%)	16 (4%)	0	100	100
1	B	386/389 (99%)	366 (95%)	20 (5%)	0	100	100
1	C	386/389 (99%)	373 (97%)	11 (3%)	2 (0%)	24	43
1	D	386/389 (99%)	374 (97%)	12 (3%)	0	100	100
1	E	386/389 (99%)	367 (95%)	18 (5%)	1 (0%)	36	55
1	F	386/389 (99%)	367 (95%)	18 (5%)	1 (0%)	36	55
1	G	386/389 (99%)	371 (96%)	14 (4%)	1 (0%)	36	55
1	H	386/389 (99%)	369 (96%)	17 (4%)	0	100	100
1	I	386/389 (99%)	367 (95%)	18 (5%)	1 (0%)	36	55
1	J	386/389 (99%)	367 (95%)	18 (5%)	1 (0%)	36	55
1	K	386/389 (99%)	371 (96%)	15 (4%)	0	100	100
1	L	386/389 (99%)	358 (93%)	26 (7%)	2 (0%)	24	43
1	M	386/389 (99%)	365 (95%)	20 (5%)	1 (0%)	36	55
1	N	386/389 (99%)	365 (95%)	21 (5%)	0	100	100
1	O	386/389 (99%)	367 (95%)	17 (4%)	2 (0%)	24	43
1	P	386/389 (99%)	363 (94%)	15 (4%)	8 (2%)	5	9
All	All	6176/6224 (99%)	5880 (95%)	276 (4%)	20 (0%)	36	55

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	108	GLU
1	J	188	ALA
1	M	350	TYR
1	P	66	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	P	352	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/309 (100%)	293 (95%)	15 (5%)	22	45
1	B	308/309 (100%)	293 (95%)	15 (5%)	22	45
1	C	308/309 (100%)	294 (96%)	14 (4%)	24	49
1	D	308/309 (100%)	292 (95%)	16 (5%)	21	42
1	E	308/309 (100%)	294 (96%)	14 (4%)	24	49
1	F	308/309 (100%)	294 (96%)	14 (4%)	24	49
1	G	308/309 (100%)	292 (95%)	16 (5%)	21	42
1	H	308/309 (100%)	291 (94%)	17 (6%)	19	40
1	I	308/309 (100%)	292 (95%)	16 (5%)	21	42
1	J	308/309 (100%)	296 (96%)	12 (4%)	28	55
1	K	308/309 (100%)	296 (96%)	12 (4%)	28	55
1	L	308/309 (100%)	293 (95%)	15 (5%)	22	45
1	M	308/309 (100%)	294 (96%)	14 (4%)	24	49
1	N	308/309 (100%)	292 (95%)	16 (5%)	21	42
1	O	308/309 (100%)	294 (96%)	14 (4%)	24	49
1	P	308/309 (100%)	287 (93%)	21 (7%)	14	31
All	All	4928/4944 (100%)	4687 (95%)	241 (5%)	22	45

5 of 241 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	237	TRP
1	P	9	ARG
1	J	230	LEU
1	O	380	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	P	253	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 119 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	303	GLN
1	O	303	GLN
1	J	303	GLN
1	O	270	HIS
1	P	340	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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
3	SRT	K	1011	2	9,9,9	1.01	0	12,12,12	1.67	4 (33%)
3	SRT	E	1005	2	9,9,9	1.25	1 (11%)	12,12,12	1.71	3 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SRT	B	1002	2	9,9,9	0.89	1 (11%)	12,12,12	1.73	3 (25%)
3	SRT	F	1006	2	9,9,9	1.01	0	12,12,12	1.67	4 (33%)
3	SRT	H	1008	2	9,9,9	0.98	1 (11%)	12,12,12	1.75	3 (25%)
3	SRT	I	1009	2	9,9,9	1.03	1 (11%)	12,12,12	1.64	3 (25%)
3	SRT	C	1003	2	9,9,9	1.42	1 (11%)	12,12,12	1.66	3 (25%)
3	SRT	N	1014	2	9,9,9	1.01	1 (11%)	12,12,12	1.74	3 (25%)
3	SRT	O	1015	2	9,9,9	0.92	1 (11%)	12,12,12	1.76	3 (25%)
3	SRT	G	1007	2	9,9,9	1.28	1 (11%)	12,12,12	1.71	4 (33%)
3	SRT	M	1013	2	9,9,9	0.91	0	12,12,12	1.71	3 (25%)
3	SRT	D	1004	2	9,9,9	1.09	1 (11%)	12,12,12	1.77	4 (33%)
3	SRT	J	1010	2	9,9,9	1.09	1 (11%)	12,12,12	1.78	3 (25%)
3	SRT	P	1016	2	9,9,9	1.04	1 (11%)	12,12,12	1.72	3 (25%)
3	SRT	A	1001	2	9,9,9	1.06	1 (11%)	12,12,12	1.68	4 (33%)
3	SRT	L	1012	2	9,9,9	1.04	1 (11%)	12,12,12	1.72	3 (25%)

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
3	SRT	K	1011	2	-	8/12/12/12	-
3	SRT	E	1005	2	-	8/12/12/12	-
3	SRT	B	1002	2	-	8/12/12/12	-
3	SRT	F	1006	2	-	8/12/12/12	-
3	SRT	H	1008	2	-	8/12/12/12	-
3	SRT	I	1009	2	-	8/12/12/12	-
3	SRT	C	1003	2	-	8/12/12/12	-
3	SRT	N	1014	2	-	8/12/12/12	-
3	SRT	O	1015	2	-	8/12/12/12	-
3	SRT	G	1007	2	-	8/12/12/12	-
3	SRT	M	1013	2	-	8/12/12/12	-
3	SRT	D	1004	2	-	8/12/12/12	-
3	SRT	J	1010	2	-	8/12/12/12	-
3	SRT	P	1016	2	-	8/12/12/12	-
3	SRT	A	1001	2	-	10/12/12/12	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SRT	L	1012	2	-	8/12/12/12	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1003	SRT	C3-C4	-3.57	1.47	1.52
3	E	1005	SRT	C3-C4	-3.28	1.48	1.52
3	G	1007	SRT	C3-C4	-3.22	1.48	1.52
3	D	1004	SRT	C3-C4	-2.70	1.48	1.52
3	J	1010	SRT	C3-C4	-2.65	1.48	1.52

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1004	SRT	O41-C4-C3	3.32	122.53	113.31
3	J	1010	SRT	O41-C4-C3	3.30	122.49	113.31
3	P	1016	SRT	O41-C4-C3	3.30	122.48	113.31
3	N	1014	SRT	O41-C4-C3	3.29	122.46	113.31
3	O	1015	SRT	O41-C4-C3	3.28	122.43	113.31

There are no chirality outliers.

5 of 130 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	SRT	O3-C3-C4-O4
3	A	1001	SRT	O3-C3-C4-O41
3	B	1002	SRT	O3-C3-C4-O4
3	B	1002	SRT	O3-C3-C4-O41
3	C	1003	SRT	O3-C3-C4-O4

There are no ring outliers.

14 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1011	SRT	2	0
3	E	1005	SRT	2	0
3	B	1002	SRT	2	0
3	F	1006	SRT	1	0
3	H	1008	SRT	2	0
3	I	1009	SRT	4	0
3	C	1003	SRT	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	1014	SRT	3	0
3	G	1007	SRT	4	0
3	D	1004	SRT	3	0
3	J	1010	SRT	1	0
3	P	1016	SRT	3	0
3	A	1001	SRT	3	0
3	L	1012	SRT	3	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 [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<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	388/389 (99%)	-1.68	0 100 100	14, 34, 57, 76	0
1	B	388/389 (99%)	-1.52	0 100 100	21, 49, 68, 84	0
1	C	388/389 (99%)	-1.70	0 100 100	13, 30, 48, 77	0
1	D	388/389 (99%)	-1.69	0 100 100	13, 32, 50, 73	0
1	E	388/389 (99%)	-1.61	0 100 100	16, 43, 66, 89	0
1	F	388/389 (99%)	-1.65	0 100 100	11, 34, 64, 77	0
1	G	388/389 (99%)	-1.61	0 100 100	14, 41, 69, 81	0
1	H	388/389 (99%)	-1.55	0 100 100	18, 49, 67, 82	0
1	I	388/389 (99%)	-1.60	0 100 100	22, 43, 71, 90	0
1	J	388/389 (99%)	-1.55	0 100 100	19, 49, 70, 78	0
1	K	388/389 (99%)	-1.64	0 100 100	14, 38, 63, 84	0
1	L	388/389 (99%)	-1.50	0 100 100	20, 53, 72, 83	0
1	M	388/389 (99%)	-1.53	0 100 100	24, 53, 69, 89	0
1	N	388/389 (99%)	-1.51	0 100 100	26, 58, 77, 87	0
1	O	388/389 (99%)	-1.45	0 100 100	34, 56, 72, 83	0
1	P	388/389 (99%)	-1.43	0 100 100	30, 62, 80, 94	0
All	All	6208/6224 (99%)	-1.58	0 100 100	11, 45, 71, 94	0

There are no RSRZ outliers to report.

### 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 oligosaccharides 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
2	MG	B	2002	1/1	0.99	0.03	62,62,62,62	0
2	MG	D	2004	1/1	0.99	0.02	27,27,27,27	0
2	MG	G	2007	1/1	0.99	0.03	31,31,31,31	0
2	MG	J	2010	1/1	0.99	0.02	41,41,41,41	0
2	MG	N	2014	1/1	0.99	0.02	27,27,27,27	0
3	SRT	A	1001	10/10	0.99	0.03	26,30,32,36	0
3	SRT	B	1002	10/10	0.99	0.03	44,49,53,54	0
3	SRT	C	1003	10/10	0.99	0.03	18,28,38,45	0
3	SRT	E	1005	10/10	0.99	0.03	45,47,50,51	0
3	SRT	F	1006	10/10	0.99	0.02	25,33,37,38	0
3	SRT	G	1007	10/10	0.99	0.03	32,36,40,41	0
3	SRT	H	1008	10/10	0.99	0.02	50,54,56,57	0
3	SRT	I	1009	10/10	0.99	0.03	20,33,36,36	0
3	SRT	J	1010	10/10	0.99	0.03	45,47,52,53	0
3	SRT	K	1011	10/10	0.99	0.03	24,28,35,36	0
3	SRT	L	1012	10/10	0.99	0.02	43,46,48,49	0
3	SRT	M	1013	10/10	0.99	0.03	47,51,52,54	0
3	SRT	N	1014	10/10	0.99	0.03	49,51,52,53	0
3	SRT	O	1015	10/10	0.99	0.03	50,52,56,58	0
3	SRT	P	1016	10/10	0.99	0.03	51,54,55,57	0
2	MG	I	2009	1/1	1.00	0.02	25,25,25,25	0
2	MG	A	2001	1/1	1.00	0.01	20,20,20,20	0
2	MG	K	2011	1/1	1.00	0.01	15,15,15,15	0
2	MG	L	2012	1/1	1.00	0.01	42,42,42,42	0
2	MG	M	2013	1/1	1.00	0.01	36,36,36,36	0
2	MG	E	2005	1/1	1.00	0.03	39,39,39,39	0
2	MG	O	2015	1/1	1.00	0.01	43,43,43,43	0
2	MG	P	2016	1/1	1.00	0.01	45,45,45,45	0
2	MG	F	2006	1/1	1.00	0.01	19,19,19,19	0
2	MG	C	2003	1/1	1.00	0.01	26,26,26,26	0
2	MG	H	2008	1/1	1.00	0.01	42,42,42,42	0
3	SRT	D	1004	10/10	1.00	0.03	21,34,38,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.