



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 10:45 pm GMT

PDB ID : 3O7M  
Title : 1.98 Angstrom resolution crystal structure of a hypoxanthine-guanine phosphoribosyltransferase (hpt-2) from Bacillus anthracis str. 'Ames Ancestor'  
Authors : Halavaty, A.S.; Minasov, G.; Shuvalova, L.; Dubrovskaya, I.; Winsor, J.; Papazisi, L.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2010-07-30  
Resolution : 1.98 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	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

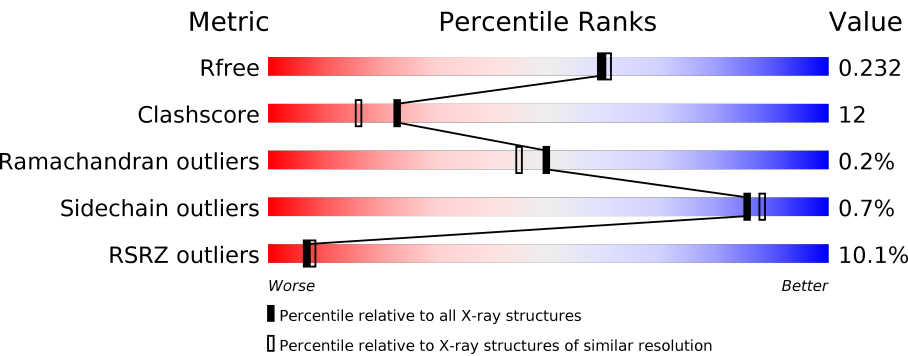
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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))
$R_{free}$	111664	10189 (2.00-1.96)
Clashscore	122126	11405 (2.00-1.96)
Ramachandran outliers	120053	11281 (2.00-1.96)
Sidechain outliers	120020	11280 (2.00-1.96)
RSRZ outliers	108989	9953 (2.00-1.96)

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	186	<div><div>4%</div><div><div></div><div>73%</div><div>16%</div><div>•</div><div>11%</div></div></div>
1	B	186	<div><div>17%</div><div><div></div><div>76%</div><div>16%</div><div>•</div><div>8%</div></div></div>
1	C	186	<div><div>9%</div><div><div></div><div>68%</div><div>20%</div><div>•</div><div>12%</div></div></div>
1	D	186	<div><div>5%</div><div><div></div><div>70%</div><div>17%</div><div>•</div><div>12%</div></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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BME	B	186[B]	-	-	X	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6154 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 Hypoxanthine phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	6	0
			1377	890	222	261	4			
1	B	171	Total	C	N	O	S	0	4	0
			1398	901	226	267	4			
1	C	164	Total	C	N	O	S	0	5	0
			1354	881	216	253	4			
1	D	164	Total	C	N	O	S	0	7	0
			1380	897	222	258	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q81KC7
A	-1	ASN	-	EXPRESSION TAG	UNP Q81KC7
A	0	ALA	-	EXPRESSION TAG	UNP Q81KC7
B	-2	SER	-	EXPRESSION TAG	UNP Q81KC7
B	-1	ASN	-	EXPRESSION TAG	UNP Q81KC7
B	0	ALA	-	EXPRESSION TAG	UNP Q81KC7
C	-2	SER	-	EXPRESSION TAG	UNP Q81KC7
C	-1	ASN	-	EXPRESSION TAG	UNP Q81KC7
C	0	ALA	-	EXPRESSION TAG	UNP Q81KC7
D	-2	SER	-	EXPRESSION TAG	UNP Q81KC7
D	-1	ASN	-	EXPRESSION TAG	UNP Q81KC7
D	0	ALA	-	EXPRESSION TAG	UNP Q81KC7

- Molecule 2 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
2	A	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	1
			12	6	6		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



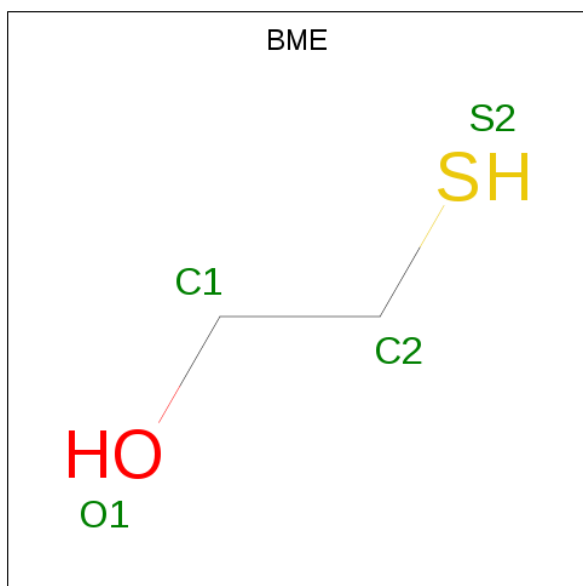
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	1
			4	2	1	1		
4	B	1	Total	C	O	S	0	1
			4	2	1	1		
4	C	1	Total	C	O	S	0	1
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		

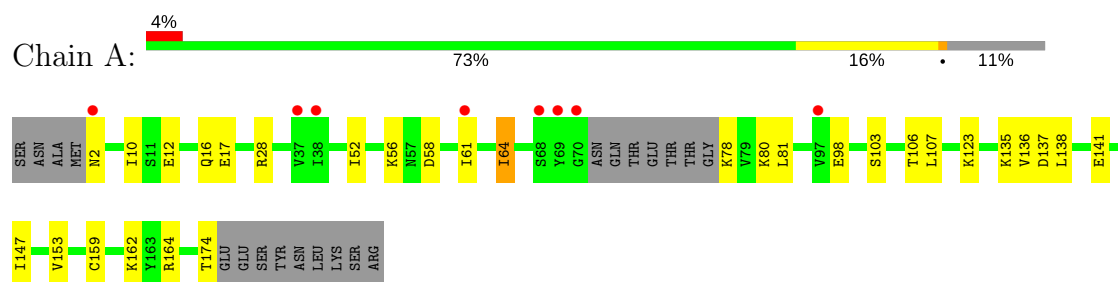
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	192	Total 195	O 195	0	8
5	B	105	Total 107	O 107	0	2
5	C	115	Total 115	O 115	0	0
5	D	146	Total 149	O 149	0	7

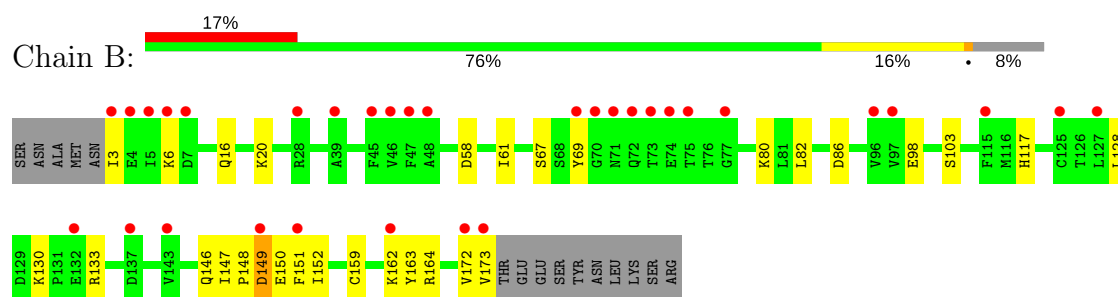
### 3 Residue-property plots [i](#)

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.

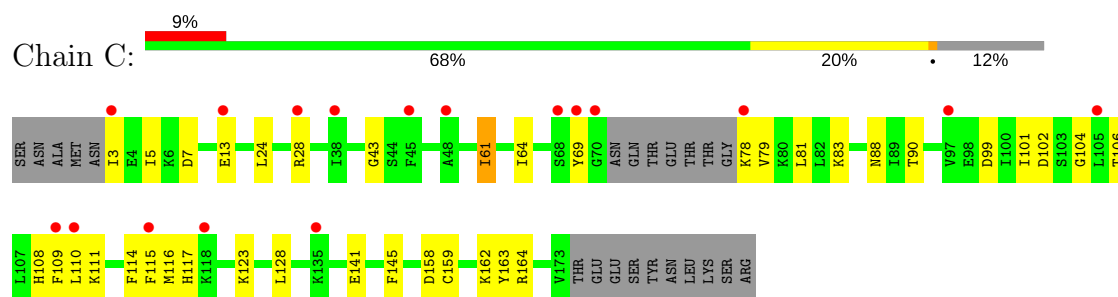
- Molecule 1: Hypoxanthine phosphoribosyltransferase



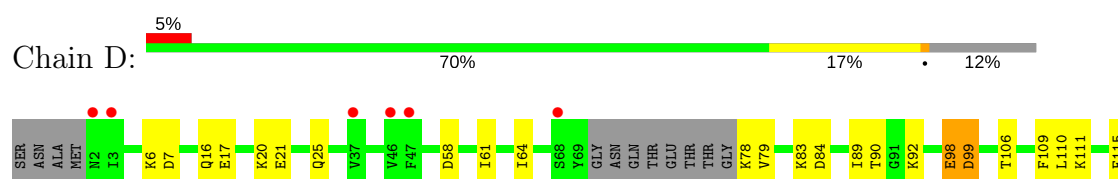
- Molecule 1: Hypoxanthine phosphoribosyltransferase



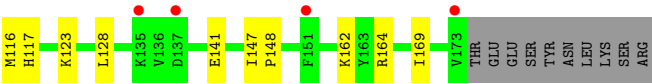
- Molecule 1: Hypoxanthine phosphoribosyltransferase



- Molecule 1: Hypoxanthine phosphoribosyltransferase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.50Å 122.50Å 119.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 1.98 29.71 – 1.98	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.92-1.98) 100.0 (29.71-1.98)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.03 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.167 , 0.206 0.200 , 0.232	Depositor DCC
$R_{free}$ test set	3231 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,-l,-k 0.013 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6154	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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, SO4, BME

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	0.71	0/1398	0.80	1/1883 (0.1%)
1	B	0.61	0/1420	0.78	0/1916
1	C	0.61	0/1376	0.76	0/1854
1	D	0.67	0/1402	0.82	3/1888 (0.2%)
All	All	0.65	0/5596	0.79	4/7541 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	164	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	58	ASP	CB-CG-OD1	6.01	123.71	118.30
1	D	99	ASP	CB-CG-OD1	5.63	123.37	118.30
1	D	84	ASP	CB-CG-OD1	5.07	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen 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	1377	0	1399	36	0
1	B	1398	0	1417	43	0
1	C	1354	0	1380	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1380	0	1407	28	0
2	A	6	0	8	3	0
2	C	12	0	16	6	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	20	0	0	0	0
4	A	4	0	5	0	0
4	B	4	0	5	6	0
4	C	4	0	5	0	0
4	D	4	0	5	0	0
5	A	195	0	0	8	0
5	B	107	0	0	3	0
5	C	115	0	0	6	0
5	D	149	0	0	5	0
All	All	6154	0	5647	139	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 12.

All (139) 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:C:90:THR:HG22	1:C:117:HIS:O	1.47	1.13
1:A:10:ILE:HD11	1:A:147:ILE:CD1	1.89	1.02
1:A:52:ILE:CD1	1:A:61:ILE:HD11	1.88	1.01
1:A:106:THR:H	2:A:184:GOL:H11	1.20	1.00
1:A:10:ILE:HD11	1:A:147:ILE:HD11	1.44	0.98
5:A:410:HOH:O	1:D:162[B]:LYS:HG2	1.66	0.94
1:A:52:ILE:HD12	1:A:61:ILE:HD11	1.52	0.92
1:C:79:VAL:HG21	1:C:106:THR:HA	1.49	0.92
1:C:78:LYS:HZ1	1:D:89:ILE:H	1.18	0.90
1:A:52:ILE:HD13	1:A:61:ILE:CD1	2.09	0.83
1:B:128:LEU:CD1	1:B:152:ILE:HD11	2.09	0.83
1:B:3:ILE:HD13	1:B:159[A]:CYS:SG	2.19	0.82
1:A:52:ILE:HD13	1:A:61:ILE:HD11	1.63	0.81
1:A:52:ILE:CD1	1:A:61:ILE:CD1	2.59	0.81
1:B:16[B]:GLN:OE1	1:B:16[B]:GLN:O	1.98	0.80
1:B:147:ILE:HD13	1:B:152:ILE:HD13	1.63	0.80
1:C:3:ILE:HD13	1:C:159[A]:CYS:SG	2.22	0.79
1:D:16[B]:GLN:OE1	1:D:20:LYS:HE3	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LEU:HD13	1:B:152:ILE:CD1	2.17	0.75
1:B:128:LEU:HD13	1:B:152:ILE:HD11	1.70	0.74
1:C:43:GLY:C	1:C:99[B]:ASP:OD2	2.27	0.73
1:C:61:ILE:HD12	1:C:61:ILE:C	2.09	0.73
1:D:17:GLU:HG2	5:D:342:HOH:O	1.89	0.73
1:C:115[B]:PHE:CD2	1:C:115[B]:PHE:C	2.60	0.72
1:C:7:ASP:HB2	5:C:389:HOH:O	1.89	0.72
1:B:128:LEU:CD1	1:B:152:ILE:CD1	2.67	0.72
1:A:10:ILE:HD11	1:A:147:ILE:HD12	1.73	0.71
1:A:106:THR:N	2:A:184:GOL:H11	2.01	0.71
1:B:69:TYR:CZ	1:B:80:LYS:HB3	2.27	0.69
1:D:123:LYS:HD2	1:D:141:GLU:HG2	1.74	0.69
1:B:151:PHE:CG	4:B:186[B]:BME:H12	2.29	0.68
1:B:146[B]:GLN:HG2	5:B:233:HOH:O	1.94	0.67
1:C:88:ASN:OD1	1:D:78:LYS:NZ	2.25	0.67
1:C:116:MET:HE3	1:D:116:MET:SD	2.35	0.66
1:A:10:ILE:CD1	1:A:147:ILE:HD11	2.23	0.66
1:A:16[A]:GLN:NE2	5:A:292:HOH:O	2.27	0.66
1:B:3:ILE:HG23	1:B:172:VAL:HG11	1.79	0.64
1:A:28:ARG:HG3	5:A:244:HOH:O	1.96	0.64
1:D:92:LYS:NZ	5:D:213[A]:HOH:O	2.29	0.64
1:B:162:LYS:HE3	1:B:163:TYR:CZ	2.32	0.64
1:C:78:LYS:HZ1	1:D:89:ILE:N	1.94	0.63
1:C:64:ILE:HD11	1:C:81:LEU:HD11	1.81	0.63
1:C:79:VAL:CG2	1:C:106:THR:HA	2.27	0.62
1:A:52:ILE:HD13	1:A:61:ILE:HD13	1.81	0.61
1:C:64:ILE:HD13	1:C:110[B]:LEU:HD11	1.81	0.61
1:C:106:THR:HB	2:C:184[B]:GOL:H12	1.80	0.61
1:D:98:GLU:HB2	5:D:470:HOH:O	1.99	0.61
1:C:115[B]:PHE:O	1:C:115[B]:PHE:CD2	2.54	0.60
1:B:151:PHE:CD2	4:B:186[B]:BME:H12	2.37	0.59
1:B:151:PHE:CD1	4:B:186[B]:BME:H12	2.37	0.59
1:C:78:LYS:HE2	1:D:117:HIS:ND1	2.18	0.58
1:B:16[B]:GLN:OE1	1:B:16[B]:GLN:C	2.43	0.57
1:A:80[B]:LYS:NZ	1:B:86:ASP:OD2	2.36	0.57
1:A:56:LYS:HG2	5:A:492:HOH:O	2.04	0.56
5:C:317:HOH:O	1:D:116:MET:HE3	2.05	0.56
1:A:123:LYS:HD2	1:A:141:GLU:HG2	1.88	0.56
1:C:88:ASN:OD1	1:C:90:THR:OG1	2.21	0.55
1:D:79:VAL:HG21	1:D:106:THR:HA	1.88	0.55
1:D:111:LYS:HE3	1:D:115:PHE:HE2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:PRO:O	1:B:150:GLU:HG3	2.07	0.54
1:C:110[B]:LEU:HD11	1:C:114:PHE:CE2	2.43	0.54
1:C:116:MET:CE	1:D:116:MET:SD	2.96	0.54
1:C:69:TYR:CD2	1:C:78:LYS:HB3	2.43	0.53
1:C:43:GLY:O	1:C:99[B]:ASP:OD2	2.27	0.53
1:D:109[B]:PHE:CE2	1:D:110:LEU:HD23	2.43	0.52
1:D:79:VAL:HB	1:D:109[A]:PHE:CD2	2.45	0.51
1:C:79:VAL:HB	1:C:109:PHE:CG	2.46	0.51
1:C:115[B]:PHE:HD2	1:C:115[B]:PHE:C	2.15	0.50
1:C:162:LYS:HD3	5:C:222:HOH:O	2.12	0.50
1:A:103:SER:HB2	1:A:135:LYS:HD2	1.94	0.50
1:B:130:LYS:HE3	1:B:147:ILE:HD11	1.93	0.49
1:C:102:ASP:OD1	2:C:184[B]:GOL:H32	2.12	0.49
1:B:6:LYS:HG3	1:B:173:VAL:HG22	1.95	0.49
1:B:6:LYS:HG3	1:B:173:VAL:CG2	2.43	0.49
1:A:78:LYS:HG3	1:B:117:HIS:HA	1.95	0.48
1:C:101:ILE:HG23	2:C:184[A]:GOL:H32	1.94	0.48
1:B:16[B]:GLN:NE2	1:B:20:LYS:HE3	2.28	0.48
1:C:123:LYS:HD2	1:C:141:GLU:HG2	1.94	0.48
1:A:10:ILE:CD1	1:A:147:ILE:CD1	2.78	0.48
1:C:64:ILE:HG13	1:C:83:LYS:O	2.14	0.47
1:C:64:ILE:HD11	1:C:81:LEU:CD1	2.44	0.47
1:D:16[B]:GLN:NE2	5:D:333[B]:HOH:O	2.47	0.47
1:A:28:ARG:NH2	5:A:569:HOH:O	2.38	0.47
1:C:5:ILE:HD11	1:C:163:TYR:CE2	2.50	0.46
1:A:64:ILE:HD11	1:A:81:LEU:HD11	1.98	0.46
1:B:67:SER:HB3	1:B:82:LEU:HD11	1.96	0.46
1:A:153:VAL:CG1	1:A:159[B]:CYS:HB2	2.45	0.46
1:B:151:PHE:HB3	4:B:186[B]:BME:H21	1.97	0.46
1:D:21[A]:GLU:O	1:D:25[A]:GLN:HG3	2.15	0.46
2:C:184[B]:GOL:H31	5:C:487:HOH:O	2.15	0.46
1:B:164:ARG:HD2	1:C:61:ILE:HG13	1.98	0.45
1:A:103:SER:OG	2:A:184:GOL:H12	2.16	0.45
1:A:80[B]:LYS:CE	1:B:86:ASP:OD2	2.64	0.45
1:B:6:LYS:CG	1:B:173:VAL:HG22	2.47	0.45
1:A:17:GLU:CD	5:A:349:HOH:O	2.55	0.45
1:A:2:ASN:HD22	1:A:2:ASN:N	2.13	0.45
1:B:16[A]:GLN:OE1	5:B:401:HOH:O	2.21	0.45
1:A:107:LEU:HB3	1:A:138:LEU:HD13	1.98	0.45
1:B:6:LYS:HE3	1:B:173:VAL:HG22	1.99	0.45
1:A:174:THR:OG1	5:A:522:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ILE:HD11	1:C:163:TYR:CD2	2.51	0.45
1:B:103:SER:HA	1:B:133:ARG:O	2.17	0.44
1:B:133:ARG:HD2	1:B:149:ASP:OD2	2.17	0.44
1:A:80[B]:LYS:HE3	1:B:86:ASP:OD2	2.16	0.44
1:D:6:LYS:NZ	1:D:7:ASP:OD2	2.43	0.44
1:B:3:ILE:HG23	1:B:172:VAL:CG1	2.45	0.44
1:D:98:GLU:OE2	1:D:99:ASP:OD1	2.35	0.44
1:B:147:ILE:HD13	1:B:152:ILE:CD1	2.41	0.43
1:D:64:ILE:HG13	1:D:83:LYS:O	2.18	0.43
1:C:64:ILE:HD13	1:C:110[B]:LEU:CD1	2.48	0.43
1:D:128:LEU:HD11	1:D:169:ILE:HD13	2.00	0.43
1:B:6:LYS:CE	1:B:173:VAL:HG22	2.48	0.43
1:B:16[B]:GLN:HE22	1:B:20:LYS:HE3	1.82	0.43
1:C:24:LEU:O	1:C:28:ARG:HG2	2.17	0.43
1:C:102:ASP:OD1	2:C:184[A]:GOL:O3	2.33	0.43
1:B:61:ILE:HG22	1:C:164:ARG:HD2	2.01	0.43
1:C:110[B]:LEU:HD11	1:C:114:PHE:CZ	2.54	0.43
1:C:78:LYS:N	5:D:384:HOH:O	2.51	0.42
1:A:164:ARG:HD2	1:D:61:ILE:CG2	2.50	0.42
1:C:104:GLY:H	2:C:184[A]:GOL:C3	2.31	0.42
1:D:109[B]:PHE:CD2	1:D:110:LEU:HD23	2.54	0.42
1:C:110[B]:LEU:HG	1:C:114:PHE:CE2	2.54	0.42
1:A:162:LYS:NZ	1:D:58:ASP:CG	2.73	0.42
1:C:158:ASP:OD2	5:C:500:HOH:O	2.21	0.42
1:B:58[A]:ASP:OD2	1:C:162:LYS:HE3	2.19	0.42
1:C:78:LYS:HE3	1:D:90:THR:OG1	2.20	0.42
1:A:10:ILE:CG1	1:A:147:ILE:HD11	2.50	0.41
1:A:174:THR:N	5:A:522:HOH:O	2.53	0.41
1:B:69:TYR:OH	1:B:80:LYS:HB3	2.20	0.41
1:C:13:GLU:HG3	5:C:307:HOH:O	2.19	0.41
1:C:128:LEU:HD23	1:C:145:PHE:HB2	2.01	0.41
1:B:151:PHE:CD1	4:B:186[B]:BME:C1	3.04	0.41
1:C:108:HIS:O	1:C:111:LYS:HB3	2.21	0.41
1:B:98:GLU:OE2	5:B:419:HOH:O	2.20	0.40
1:A:12:GLU:O	1:A:16[A]:GLN:HG2	2.21	0.40
1:A:136:VAL:HG22	1:A:137[B]:ASP:N	2.36	0.40
1:B:151:PHE:CE2	4:B:186[B]:BME:H12	2.56	0.40
1:B:6:LYS:CG	1:B:173:VAL:CG2	2.99	0.40
1:D:147:ILE:HB	1:D:148:PRO:HD2	2.04	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	168/186 (90%)	164 (98%)	4 (2%)	0	100	100
1	B	173/186 (93%)	168 (97%)	4 (2%)	1 (1%)	27	19
1	C	165/186 (89%)	161 (98%)	4 (2%)	0	100	100
1	D	167/186 (90%)	164 (98%)	3 (2%)	0	100	100
All	All	673/744 (90%)	657 (98%)	15 (2%)	1 (0%)	49	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	ASP

### 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	155/167 (93%)	153 (99%)	2 (1%)	71	74
1	B	157/167 (94%)	157 (100%)	0	100	100
1	C	152/167 (91%)	151 (99%)	1 (1%)	85	88
1	D	155/167 (93%)	154 (99%)	1 (1%)	87	90
All	All	619/668 (93%)	615 (99%)	4 (1%)	85	90

All (4) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	64	ILE
1	A	98	GLU
1	C	61	ILE
1	D	98	GLU

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

Mol	Chain	Res	Type
1	B	25	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GOL	A	184	-	5,5,5	0.49	0	5,5,5	0.84	0
3	SO4	A	185	-	4,4,4	0.20	0	6,6,6	0.65	0
3	SO4	A	186	-	4,4,4	0.29	0	6,6,6	0.33	0
4	BME	A	187[A]	1	3,3,3	0.37	0	1,2,2	0.67	0
3	SO4	B	184	-	4,4,4	0.29	0	6,6,6	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	B	185	-	4,4,4	0.37	0	6,6,6	0.32	0
4	BME	B	186[B]	1	3,3,3	0.34	0	1,2,2	0.41	0
2	GOL	C	184[A]	-	5,5,5	0.25	0	5,5,5	1.12	1 (20%)
2	GOL	C	184[B]	-	5,5,5	0.31	0	5,5,5	0.41	0
3	SO4	C	185	-	4,4,4	0.17	0	6,6,6	0.41	0
4	BME	C	186[B]	1	3,3,3	0.47	0	1,2,2	0.18	0
3	SO4	D	184	-	4,4,4	0.16	0	6,6,6	0.52	0
3	SO4	D	185	-	4,4,4	0.25	0	6,6,6	0.29	0
3	SO4	D	186	-	4,4,4	0.27	0	6,6,6	0.22	0
3	SO4	D	187	-	4,4,4	0.18	0	6,6,6	0.19	0
4	BME	D	188	1	3,3,3	0.40	0	1,2,2	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
2	GOL	A	184	-	-	0/4/4/4	0/0/0/0
3	SO4	A	185	-	-	0/0/0/0	0/0/0/0
3	SO4	A	186	-	-	0/0/0/0	0/0/0/0
4	BME	A	187[A]	1	-	0/1/1/1	0/0/0/0
3	SO4	B	184	-	-	0/0/0/0	0/0/0/0
3	SO4	B	185	-	-	0/0/0/0	0/0/0/0
4	BME	B	186[B]	1	-	0/1/1/1	0/0/0/0
2	GOL	C	184[A]	-	-	0/4/4/4	0/0/0/0
2	GOL	C	184[B]	-	-	0/4/4/4	0/0/0/0
3	SO4	C	185	-	-	0/0/0/0	0/0/0/0
4	BME	C	186[B]	1	-	0/1/1/1	0/0/0/0
3	SO4	D	184	-	-	0/0/0/0	0/0/0/0
3	SO4	D	185	-	-	0/0/0/0	0/0/0/0
3	SO4	D	186	-	-	0/0/0/0	0/0/0/0
3	SO4	D	187	-	-	0/0/0/0	0/0/0/0
4	BME	D	188	1	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	184[A]	GOL	C3-C2-C1	-2.06	103.69	111.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	184	GOL	3	0
4	B	186[B]	BME	6	0
2	C	184[A]	GOL	3	0
2	C	184[B]	GOL	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

### 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	166/186 (89%)	0.24	8 (4%) 30 33	17, 26, 40, 67	0
1	B	171/186 (91%)	1.00	32 (18%) 1 1	22, 35, 61, 81	0
1	C	164/186 (88%)	0.56	17 (10%) 6 7	22, 36, 55, 66	0
1	D	164/186 (88%)	0.40	10 (6%) 21 23	17, 28, 49, 61	0
All	All	665/744 (89%)	0.55	67 (10%) 7 8	17, 32, 54, 81	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	173	VAL	6.9
1	B	149	ASP	6.0
1	B	5	ILE	4.7
1	A	70	GLY	4.6
1	D	68	SER	4.4
1	B	132	GLU	4.3
1	B	172	VAL	4.2
1	B	4	GLU	4.2
1	D	3	ILE	4.0
1	B	6	LYS	4.0
1	C	70	GLY	3.8
1	C	115[A]	PHE	3.8
1	A	68	SER	3.7
1	A	2	ASN	3.6
1	A	69	TYR	3.6
1	C	69	TYR	3.4
1	B	151	PHE	3.4
1	B	137	ASP	3.4
1	D	2	ASN	3.4
1	B	74	GLU	3.3
1	B	73	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	97	VAL	3.3
1	C	3	ILE	3.3
1	B	7	ASP	3.2
1	C	28	ARG	3.2
1	B	72	GLN	3.2
1	B	71	ASN	3.1
1	B	70	GLY	3.1
1	D	135	LYS	3.1
1	B	3	ILE	3.1
1	B	127	LEU	3.0
1	C	68	SER	3.0
1	B	45	PHE	2.9
1	C	135	LYS	2.9
1	B	77	GLY	2.9
1	B	96	VAL	2.9
1	B	75	THR	2.7
1	D	46	VAL	2.6
1	C	45	PHE	2.6
1	B	47	PHE	2.6
1	C	13	GLU	2.5
1	B	39	ALA	2.5
1	D	151	PHE	2.5
1	B	46	VAL	2.4
1	B	115	PHE	2.4
1	C	110[A]	LEU	2.4
1	C	78	LYS	2.4
1	D	47	PHE	2.4
1	C	48	ALA	2.4
1	D	173	VAL	2.4
1	A	38	ILE	2.3
1	B	143	VAL	2.3
1	A	97	VAL	2.3
1	C	97	VAL	2.3
1	C	105	LEU	2.3
1	B	48	ALA	2.2
1	A	37	VAL	2.2
1	A	61	ILE	2.2
1	B	69	TYR	2.2
1	D	137	ASP	2.2
1	C	118	LYS	2.2
1	C	109	PHE	2.1
1	D	37	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	38	ILE	2.1
1	B	162	LYS	2.1
1	B	28	ARG	2.1
1	B	125	CYS	2.1

## 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 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(Å <sup>2</sup> )	Q<0.9
4	BME	B	186[B]	4/4	0.75	0.53	61,61,61,62	4
3	SO4	D	186	5/5	0.83	0.16	46,46,52,54	5
2	GOL	C	184[B]	6/6	0.89	0.17	38,40,41,42	6
2	GOL	C	184[A]	6/6	0.89	0.17	30,33,34,35	6
3	SO4	B	185	5/5	0.89	0.17	47,48,51,52	5
2	GOL	A	184	6/6	0.91	0.12	38,42,45,47	0
3	SO4	D	187	5/5	0.92	0.19	73,73,73,74	5
3	SO4	A	186	5/5	0.94	0.13	51,54,55,56	5
4	BME	C	186[B]	4/4	0.94	0.24	53,53,53,54	4
3	SO4	D	185	5/5	0.94	0.21	59,61,61,63	0
4	BME	D	188	4/4	0.94	0.26	57,57,57,57	0
4	BME	A	187[A]	4/4	0.95	0.16	42,42,43,44	0
3	SO4	B	184	5/5	0.97	0.07	42,45,48,48	0
3	SO4	A	185	5/5	0.99	0.08	31,33,36,37	0
3	SO4	C	185	5/5	0.99	0.07	40,44,47,49	0
3	SO4	D	184	5/5	0.99	0.06	33,37,39,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.