



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:37 AM GMT

PDB ID : 3FEF  
Title : Crystal structure of putative glucosidase lplD from bacillus subtilis  
Authors : Ramagopal, U.A.; Rajashankar, K.R.; Toro, R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2008-11-28  
Resolution : 2.20 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

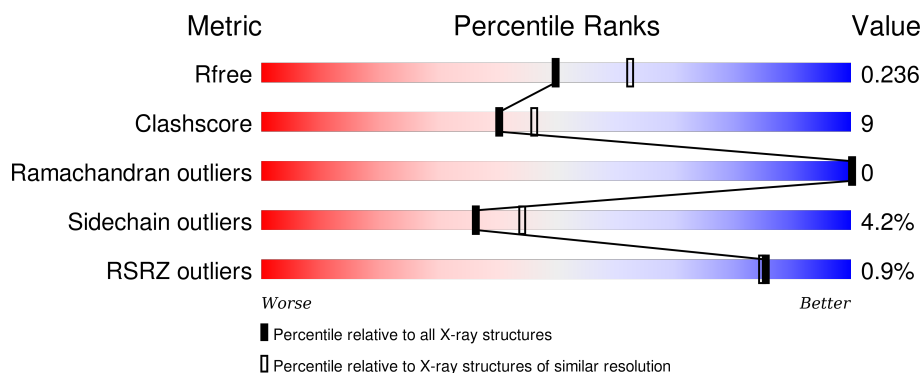
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	450	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>• •</div> </div> </div>
1	B	450	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>
1	C	450	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
1	D	450	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14117 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 Putative glucosidase lplD, ALPHA-GALACTURONIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	Se	0	1	0
			3388	2149	594	631	6	8			
1	B	434	Total	C	N	O	S	Se	0	0	0
			3383	2146	594	629	6	8			
1	C	434	Total	C	N	O	S	Se	0	0	0
			3386	2147	594	631	6	8			
1	D	434	Total	C	N	O	S	Se	0	0	0
			3386	2147	594	631	6	8			

There are 40 discrepancies between the modelled and reference sequences:

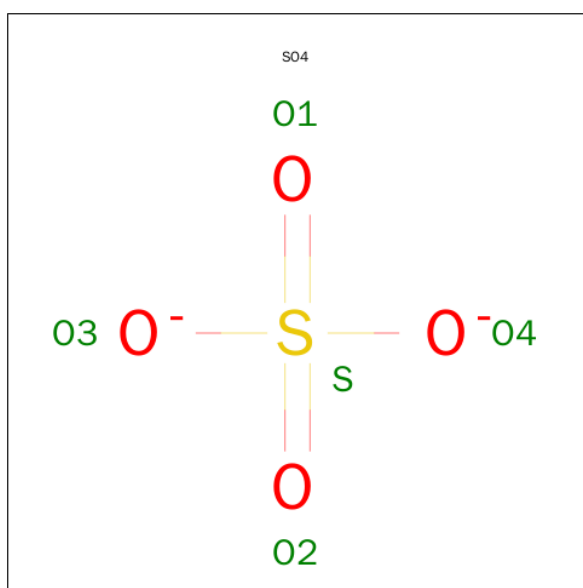
Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MSE	-	expression tag	UNP P39130
A	6	SER	-	expression tag	UNP P39130
A	447	GLU	-	expression tag	UNP P39130
A	448	GLY	-	expression tag	UNP P39130
A	449	HIS	-	expression tag	UNP P39130
A	450	HIS	-	expression tag	UNP P39130
A	451	HIS	-	expression tag	UNP P39130
A	452	HIS	-	expression tag	UNP P39130
A	453	HIS	-	expression tag	UNP P39130
A	454	HIS	-	expression tag	UNP P39130
B	5	MSE	-	expression tag	UNP P39130
B	6	SER	-	expression tag	UNP P39130
B	447	GLU	-	expression tag	UNP P39130
B	448	GLY	-	expression tag	UNP P39130
B	449	HIS	-	expression tag	UNP P39130
B	450	HIS	-	expression tag	UNP P39130
B	451	HIS	-	expression tag	UNP P39130
B	452	HIS	-	expression tag	UNP P39130
B	453	HIS	-	expression tag	UNP P39130
B	454	HIS	-	expression tag	UNP P39130
C	5	MSE	-	expression tag	UNP P39130

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	SER	-	expression tag	UNP P39130
C	447	GLU	-	expression tag	UNP P39130
C	448	GLY	-	expression tag	UNP P39130
C	449	HIS	-	expression tag	UNP P39130
C	450	HIS	-	expression tag	UNP P39130
C	451	HIS	-	expression tag	UNP P39130
C	452	HIS	-	expression tag	UNP P39130
C	453	HIS	-	expression tag	UNP P39130
C	454	HIS	-	expression tag	UNP P39130
D	5	MSE	-	expression tag	UNP P39130
D	6	SER	-	expression tag	UNP P39130
D	447	GLU	-	expression tag	UNP P39130
D	448	GLY	-	expression tag	UNP P39130
D	449	HIS	-	expression tag	UNP P39130
D	450	HIS	-	expression tag	UNP P39130
D	451	HIS	-	expression tag	UNP P39130
D	452	HIS	-	expression tag	UNP P39130
D	453	HIS	-	expression tag	UNP P39130
D	454	HIS	-	expression tag	UNP P39130

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

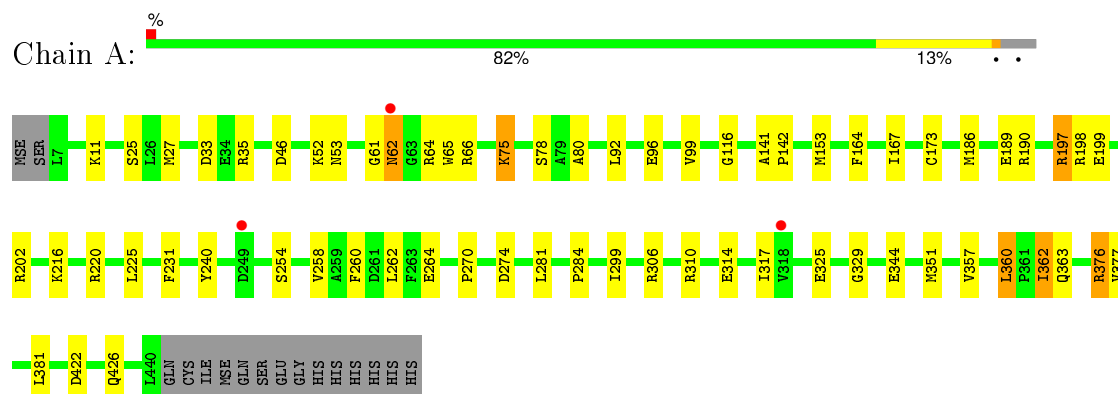
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total	O	0	0
			139	139		
4	B	154	Total	O	0	0
			154	154		
4	C	130	Total	O	0	0
			130	130		
4	D	112	Total	O	0	0
			112	112		

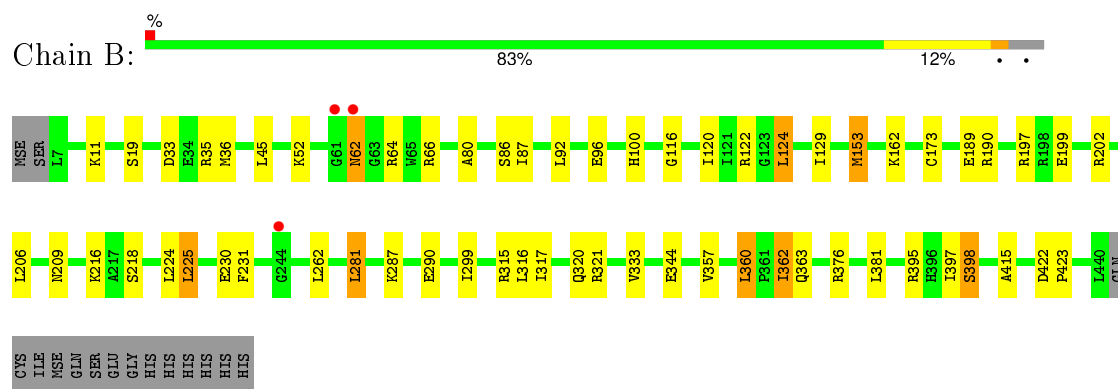
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

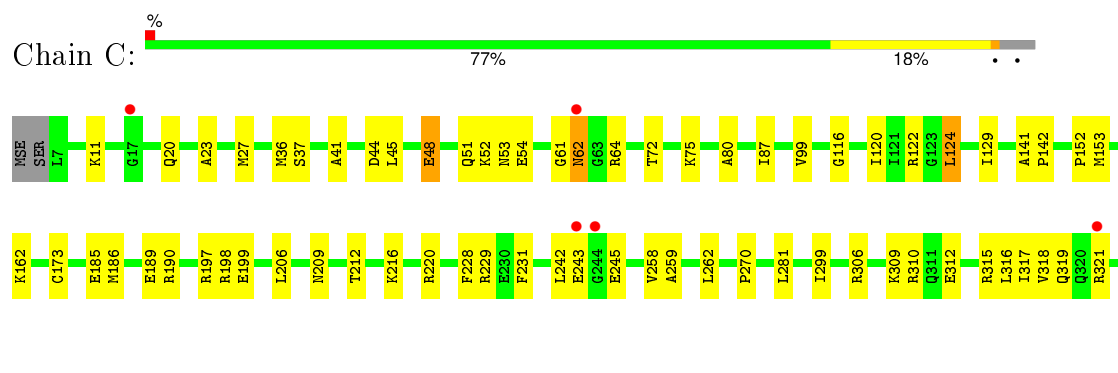
- Molecule 1: Putative glucosidase lplD, ALPHA-GALACTURONIDASE



- Molecule 1: Putative glucosidase lplD, ALPHA-GALACTURONIDASE

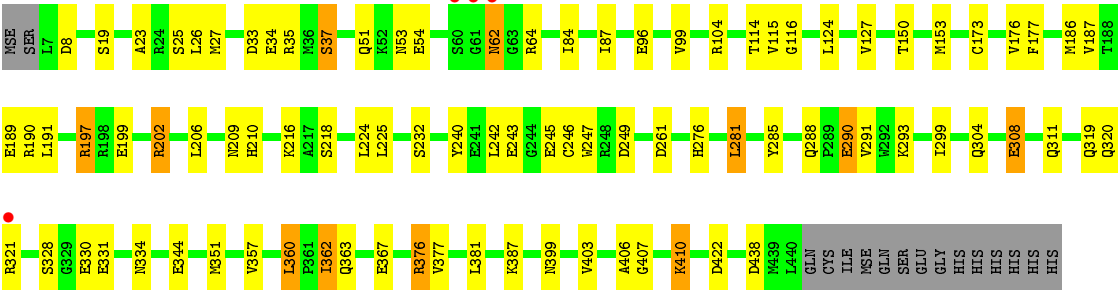
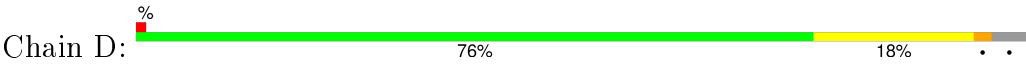


- Molecule 1: Putative glucosidase lplD, ALPHA-GALACTURONIDASE





● Molecule 1: Putative glucosidase lplD, ALPHA-GALACTURONIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.99Å 84.84Å 86.05Å 69.80° 68.10° 64.07°	Depositor
Resolution (Å)	50.00 – 2.20 38.10 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.5 (50.00-2.20) 87.9 (38.10-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.26 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.187 , 0.243 0.182 , 0.236	Depositor DCC
$R_{free}$ test set	4504 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.7	EDS
Estimated twinning fraction	0.065 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 90050 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14117	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 4.74% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, SO4

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	0/3449	0.60	0/4664
1	B	0.51	0/3444	0.62	1/4657 (0.0%)
1	C	0.48	0/3447	0.61	0/4661
1	D	0.49	0/3447	0.62	0/4661
All	All	0.49	0/13787	0.61	1/18643 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	LEU	CA-CB-CG	-5.24	103.26	115.30

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	3388	0	3366	60	0
1	B	3383	0	3366	56	0
1	C	3386	0	3368	73	0
1	D	3386	0	3368	64	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	10	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	139	0	0	3	0
4	B	154	0	0	4	0
4	C	130	0	0	2	0
4	D	112	0	0	2	0
All	All	14117	0	13468	234	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 9.

All (234) 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:B:64:ARG:HG3	1:B:64:ARG:HH11	1.11	1.08
1:C:306:ARG:HD3	1:C:310:ARG:CZ	1.86	1.03
1:B:316:LEU:HD23	1:B:321:ARG:NH1	1.72	1.03
1:D:362:ILE:HG13	1:D:363:GLN:HG2	1.46	0.96
1:A:216:LYS:HD3	1:B:376:ARG:HD2	1.46	0.95
1:A:64:ARG:HH11	1:A:64:ARG:HG3	1.29	0.95
1:B:316:LEU:HD23	1:B:321:ARG:HH12	1.29	0.95
1:D:64:ARG:HG3	1:D:64:ARG:HH11	1.32	0.94
1:B:64:ARG:HG3	1:B:64:ARG:NH1	1.87	0.89
1:A:376:ARG:HD2	1:B:216:LYS:HD2	1.53	0.88
1:A:62:ASN:HD22	1:A:62:ASN:N	1.76	0.83
1:B:62:ASN:N	1:B:62:ASN:HD22	1.76	0.82
1:C:316:LEU:HD23	1:C:321:ARG:NH1	1.93	0.82
1:A:202:ARG:HD2	1:B:344:GLU:OE1	1.83	0.79
1:A:306:ARG:HD3	1:A:310:ARG:CZ	2.13	0.79
1:C:357:VAL:HG11	1:C:360:LEU:HD22	1.65	0.78
1:B:100:HIS:CD2	1:B:299:ILE:HG12	2.19	0.78
1:C:344:GLU:OE1	1:D:202:ARG:CD	2.32	0.77
1:C:312:GLU:CG	1:C:315:ARG:HH12	1.97	0.77
1:A:306:ARG:HD3	1:A:310:ARG:NH1	1.99	0.77
1:B:316:LEU:CD2	1:B:321:ARG:NH1	2.47	0.77
1:D:27:MSE:HE1	1:D:53:ASN:HB3	1.67	0.77
1:B:316:LEU:CD2	1:B:321:ARG:HH12	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:GLU:HG3	1:C:315:ARG:HH12	1.51	0.76
1:A:216:LYS:CD	1:B:376:ARG:HD2	2.16	0.75
1:D:99:VAL:HG21	1:D:299:ILE:HD11	1.68	0.74
1:C:316:LEU:CD2	1:C:321:ARG:NH1	2.51	0.74
1:A:62:ASN:ND2	1:A:62:ASN:N	2.35	0.73
1:C:306:ARG:HD3	1:C:310:ARG:NH2	2.04	0.73
1:D:64:ARG:NH1	1:D:64:ARG:HG3	1.96	0.73
1:A:362:ILE:HG13	1:A:363:GLN:HG2	1.70	0.73
1:B:100:HIS:NE2	1:B:299:ILE:HG12	2.05	0.71
1:C:306:ARG:NE	1:C:310:ARG:NH2	2.39	0.70
1:B:96:GLU:HA	1:B:299:ILE:HG13	1.73	0.70
1:B:362:ILE:HG13	1:B:363:GLN:HG2	1.72	0.70
1:C:312:GLU:HA	1:C:315:ARG:NH1	2.06	0.70
1:A:64:ARG:HG2	1:A:65:TRP:CD1	2.26	0.70
1:A:64:ARG:HG3	1:A:64:ARG:NH1	2.03	0.70
1:B:315:ARG:HH11	1:B:315:ARG:HG2	1.57	0.69
1:B:362:ILE:O	1:B:363:GLN:HB2	1.91	0.69
1:A:357:VAL:HG11	1:A:360:LEU:HD22	1.76	0.67
1:A:189:GLU:OE1	1:A:240:TYR:HE1	1.78	0.66
1:D:304:GLN:O	1:D:308:GLU:HG2	1.96	0.66
1:D:308:GLU:HA	1:D:311:GLN:HE21	1.61	0.65
1:C:316:LEU:CD2	1:C:321:ARG:HH12	2.09	0.65
1:D:189:GLU:OE1	1:D:240:TYR:HE1	1.80	0.65
1:A:141:ALA:N	1:A:142:PRO:CD	2.61	0.65
1:D:357:VAL:HG11	1:D:360:LEU:HD22	1.80	0.64
1:A:11:LYS:HG2	1:A:80:ALA:HA	1.79	0.64
1:C:216:LYS:HD3	1:D:376:ARG:HD2	1.79	0.64
1:D:362:ILE:O	1:D:363:GLN:HB2	1.97	0.64
1:C:306:ARG:CD	1:C:310:ARG:NH2	2.61	0.63
1:D:104:ARG:NH2	1:D:438:ASP:OD2	2.30	0.63
1:B:64:ARG:HH11	1:B:64:ARG:CG	1.95	0.63
1:B:33:ASP:OD1	1:B:35:ARG:HB2	1.98	0.63
1:C:316:LEU:HD23	1:C:321:ARG:HH11	1.62	0.62
1:D:362:ILE:O	1:D:363:GLN:CB	2.48	0.62
1:B:357:VAL:HG11	1:B:360:LEU:HD22	1.82	0.62
1:C:357:VAL:CG1	1:C:360:LEU:HD22	2.30	0.61
1:D:19:SER:HB3	1:D:23:ALA:HB2	1.83	0.61
1:C:344:GLU:OE1	1:D:202:ARG:NE	2.34	0.61
1:C:64:ARG:HH11	1:C:64:ARG:HG3	1.65	0.61
1:C:197:ARG:HB3	1:C:199:GLU:OE1	2.00	0.60
1:B:315:ARG:NH1	1:B:315:ARG:HG2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:ASN:ND2	4:D:463:HOH:O	2.29	0.60
1:C:62:ASN:N	1:C:62:ASN:OD1	2.35	0.59
1:C:153:MSE:CE	1:C:173:CYS:HB2	2.32	0.59
1:D:218:SER:HA	1:D:224:LEU:HG	1.83	0.59
1:A:186:MSE:O	1:A:190:ARG:HG2	2.02	0.59
1:B:62:ASN:N	1:B:62:ASN:ND2	2.49	0.58
1:D:34:GLU:HA	1:D:64:ARG:CZ	2.33	0.57
1:D:308:GLU:HA	1:D:311:GLN:NE2	2.19	0.57
1:B:395:ARG:O	1:B:398:SER:HB2	2.04	0.57
1:C:116:GLY:O	1:C:120:ILE:HG12	2.05	0.57
1:A:381:LEU:HD21	1:B:381:LEU:HD21	1.85	0.57
1:A:96:GLU:HA	1:A:299:ILE:HG13	1.85	0.57
1:D:8:ASP:OD1	1:D:37:SER:HB3	2.05	0.56
1:A:426:GLN:C	1:C:426:GLN:HE22	2.08	0.56
1:C:344:GLU:OE1	1:D:202:ARG:HD3	2.04	0.56
1:A:351:MSE:SE	1:A:377:VAL:HG12	2.55	0.56
1:D:62:ASN:N	1:D:62:ASN:OD1	2.39	0.56
1:B:362:ILE:O	1:B:363:GLN:CB	2.54	0.56
1:A:426:GLN:HA	1:C:426:GLN:HE22	1.71	0.56
1:C:376:ARG:HD2	1:D:216:LYS:HD2	1.88	0.55
1:D:23:ALA:O	1:D:27:MSE:HG3	2.07	0.55
1:B:87:ILE:CD1	1:B:129:ILE:HG21	2.36	0.55
1:C:242:LEU:O	1:C:245:GLU:HB2	2.07	0.55
1:C:52:LYS:HB3	1:C:317:ILE:HD11	1.86	0.55
1:D:330:GLU:OE1	1:D:330:GLU:HA	2.07	0.55
1:A:62:ASN:H	1:A:62:ASN:ND2	2.05	0.55
1:A:99:VAL:HG21	1:A:299:ILE:HD11	1.89	0.55
1:C:51:GLN:O	1:C:54:GLU:HB3	2.07	0.55
1:B:64:ARG:CG	1:B:64:ARG:NH1	2.58	0.54
1:C:162:LYS:NZ	1:C:405:ASP:OD1	2.33	0.54
1:B:209:ASN:ND2	4:B:458:HOH:O	2.39	0.54
1:C:362:ILE:HG13	1:C:363:GLN:HG2	1.88	0.54
1:A:64:ARG:CG	1:A:64:ARG:NH1	2.70	0.54
1:A:52:LYS:HG2	1:A:317:ILE:CD1	2.38	0.54
1:D:261:ASP:OD2	1:D:285:TYR:OH	2.21	0.53
1:D:319:GLN:OE1	1:D:321:ARG:HD3	2.08	0.53
1:A:92:LEU:HD12	1:A:306:ARG:CZ	2.39	0.53
1:A:426:GLN:CA	1:C:426:GLN:HE22	2.21	0.53
1:A:362:ILE:O	1:A:363:GLN:HB2	2.09	0.53
1:C:362:ILE:O	1:C:363:GLN:HB2	2.09	0.53
1:A:116:GLY:HA2	1:A:422:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:MSE:HE1	1:D:53:ASN:CB	2.37	0.52
1:A:306:ARG:HD2	4:A:588:HOH:O	2.10	0.52
1:B:124:LEU:HD21	1:B:415:ALA:HB1	1.91	0.52
1:A:190:ARG:HD3	1:A:231:PHE:HD1	1.75	0.52
1:C:306:ARG:HD3	1:C:310:ARG:NE	2.20	0.51
1:C:44:ASP:O	1:C:45:LEU:C	2.48	0.51
1:A:344:GLU:OE1	1:B:202:ARG:HD2	2.09	0.51
1:B:100:HIS:CD2	1:B:299:ILE:CG1	2.93	0.51
1:B:52:LYS:HG2	1:B:317:ILE:CD1	2.40	0.51
1:C:306:ARG:CD	1:C:310:ARG:CZ	2.76	0.51
1:C:64:ARG:HG3	1:C:64:ARG:NH1	2.26	0.51
1:D:328:SER:OG	1:D:330:GLU:HG2	2.11	0.51
1:A:357:VAL:CG1	1:A:360:LEU:HD22	2.42	0.50
1:A:362:ILE:O	1:A:363:GLN:CB	2.60	0.50
1:C:23:ALA:O	1:C:27:MSE:HG3	2.11	0.50
1:C:61:GLY:HA2	1:C:325:GLU:OE2	2.12	0.50
1:A:27:MSE:HE1	1:A:53:ASN:HB3	1.94	0.49
1:D:186:MSE:O	1:D:190:ARG:HG2	2.12	0.49
1:A:426:GLN:HA	1:C:426:GLN:NE2	2.26	0.49
1:D:246:CYS:HB3	1:D:249:ASP:OD1	2.13	0.49
1:B:197:ARG:HB3	1:B:199:GLU:OE1	2.12	0.48
1:D:176:VAL:HG23	4:D:674:HOH:O	2.13	0.48
1:A:258:VAL:HB	1:A:274:ASP:CG	2.33	0.48
1:D:34:GLU:HA	1:D:64:ARG:NH2	2.28	0.48
1:D:153:MSE:CE	1:D:173:CYS:HB2	2.43	0.48
1:B:122:ARG:HD2	4:B:472:HOH:O	2.14	0.48
1:D:399:ASN:O	1:D:403:VAL:HG23	2.13	0.48
1:A:189:GLU:OE1	1:A:240:TYR:CE1	2.64	0.48
1:B:116:GLY:O	1:B:120:ILE:HG12	2.14	0.47
1:B:153:MSE:CE	1:B:173:CYS:HB2	2.43	0.47
1:D:406:ALA:O	1:D:410:LYS:N	2.48	0.47
1:B:357:VAL:CG1	1:B:360:LEU:HD22	2.44	0.47
1:B:206:LEU:HD23	1:B:206:LEU:N	2.29	0.47
1:C:206:LEU:HD23	1:C:206:LEU:N	2.29	0.47
1:C:258:VAL:O	1:C:262:LEU:HG	2.14	0.47
1:C:259:ALA:HA	1:C:270:PRO:HG2	1.97	0.47
1:A:11:LYS:NZ	1:A:78:SER:O	2.46	0.47
1:A:426:GLN:CA	1:C:426:GLN:NE2	2.78	0.47
1:C:124:LEU:HD21	1:C:415:ALA:HB1	1.96	0.47
1:C:319:GLN:OE1	1:C:321:ARG:CD	2.63	0.47
1:A:92:LEU:HD12	1:A:306:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:HD3	1:A:231:PHE:CD1	2.50	0.47
1:A:284:PRO:HG3	2:A:455:SO4:O4	2.15	0.47
1:C:312:GLU:CG	1:C:315:ARG:NH1	2.73	0.47
1:C:48:GLU:O	1:C:52:LYS:HG3	2.15	0.47
1:C:376:ARG:HD2	1:D:216:LYS:CD	2.45	0.46
1:C:27:MSE:HE1	1:C:53:ASN:HB3	1.98	0.46
1:D:210:HIS:HB3	1:D:276:HIS:HB3	1.98	0.46
1:B:262:LEU:HD21	1:B:281:LEU:HD21	1.97	0.46
1:D:26:LEU:HD22	1:D:84:ILE:HD13	1.97	0.46
1:A:153:MSE:CE	1:A:173:CYS:HB2	2.45	0.46
1:A:197:ARG:HB3	1:A:199:GLU:OE1	2.16	0.46
1:D:362:ILE:C	1:D:363:GLN:HG2	2.36	0.46
1:D:206:LEU:HD23	1:D:206:LEU:N	2.31	0.46
1:C:229:ARG:NH1	4:C:540:HOH:O	2.39	0.45
1:D:351:MSE:SE	1:D:377:VAL:HG12	2.66	0.45
1:C:72:THR:OG1	1:C:75:LYS:HB2	2.16	0.45
1:A:260:PHE:O	1:A:264:GLU:HG2	2.16	0.45
1:D:114:THR:HG22	1:D:115:VAL:HG13	1.99	0.45
1:D:127:VAL:HG11	1:D:407:GLY:C	2.37	0.45
1:C:75:LYS:HE2	1:C:75:LYS:HB2	1.64	0.45
1:B:36:MSE:HE1	1:B:333:VAL:HG13	1.99	0.45
1:D:33:ASP:OD1	1:D:35:ARG:HB2	2.16	0.45
1:C:318:VAL:HG12	1:C:319:GLN:HG3	1.99	0.45
1:C:122:ARG:HG2	1:C:152:PRO:HD3	1.98	0.45
1:D:189:GLU:OE1	1:D:240:TYR:CE1	2.66	0.45
1:D:290:GLU:CD	1:D:290:GLU:H	2.20	0.45
1:D:288:GLN:HB3	1:D:291:VAL:HB	1.99	0.45
1:C:87:ILE:CD1	1:C:129:ILE:HG21	2.47	0.45
1:D:87:ILE:O	1:D:150:THR:HG23	2.16	0.45
1:D:96:GLU:HA	1:D:299:ILE:HG13	1.99	0.45
1:B:360:LEU:HG	1:B:397:ILE:CD1	2.47	0.45
1:A:33:ASP:OD1	1:A:35:ARG:HB2	2.17	0.44
1:B:360:LEU:HG	1:B:397:ILE:HD12	1.99	0.44
1:C:351:MSE:SE	1:C:377:VAL:HG12	2.68	0.44
1:B:162:LYS:NZ	4:B:567:HOH:O	2.41	0.44
1:D:197:ARG:HB3	1:D:199:GLU:OE1	2.17	0.44
1:D:247:TRP:CE2	1:D:293:LYS:HG2	2.52	0.44
1:A:351:MSE:SE	1:A:377:VAL:CG1	3.16	0.44
1:C:319:GLN:HB2	1:C:321:ARG:HD3	1.98	0.44
1:B:287:LYS:NZ	4:B:552:HOH:O	2.46	0.43
1:A:426:GLN:C	1:C:426:GLN:NE2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:LYS:HE2	1:D:387:LYS:HB2	1.80	0.43
1:B:87:ILE:HD12	1:B:129:ILE:HG21	2.00	0.43
1:C:185:GLU:CD	1:C:242:LEU:HD22	2.38	0.43
1:C:36:MSE:HE1	1:C:333:VAL:HG13	2.00	0.43
1:D:242:LEU:O	1:D:245:GLU:HB2	2.17	0.43
1:A:141:ALA:N	1:A:142:PRO:HD2	2.31	0.43
1:A:61:GLY:HA2	1:A:325:GLU:OE2	2.19	0.43
1:C:381:LEU:HD21	1:D:381:LEU:HD21	2.00	0.43
1:C:348:ASN:ND2	1:C:367:GLU:OE2	2.46	0.43
1:D:357:VAL:CG1	1:D:360:LEU:HD22	2.47	0.43
1:D:281:LEU:N	1:D:281:LEU:HD12	2.34	0.43
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.84	0.43
1:D:177:PHE:CZ	1:D:331:GLU:HG3	2.54	0.43
1:C:99:VAL:HG21	1:C:299:ILE:HD11	2.01	0.43
1:B:62:ASN:H	1:B:62:ASN:HD22	1.62	0.43
1:C:399:ASN:O	1:C:403:VAL:HG23	2.19	0.43
1:B:422:ASP:HA	1:B:423:PRO:HD3	1.91	0.42
1:B:218:SER:HA	1:B:224:LEU:HG	2.02	0.42
1:A:344:GLU:CD	4:A:528:HOH:O	2.57	0.42
1:B:190:ARG:HD3	1:B:231:PHE:HD1	1.84	0.42
1:C:209:ASN:ND2	4:C:476:HOH:O	2.44	0.42
1:C:190:ARG:HD3	1:C:231:PHE:HD1	1.84	0.42
1:C:11:LYS:HG3	1:C:80:ALA:HA	2.02	0.42
1:A:52:LYS:HB3	1:A:317:ILE:HD11	2.02	0.42
1:D:116:GLY:N	1:D:422:ASP:OD2	2.52	0.42
1:A:52:LYS:NZ	1:A:314:GLU:OE2	2.33	0.42
1:C:11:LYS:HE3	1:C:41:ALA:HB2	2.00	0.42
1:C:186:MSE:SE	1:C:228:PHE:HA	2.70	0.42
1:D:187:VAL:O	1:D:191:LEU:HB2	2.20	0.41
1:B:45:LEU:HA	1:B:45:LEU:HD23	1.83	0.41
1:B:262:LEU:CD2	1:B:281:LEU:HD21	2.50	0.41
1:D:51:GLN:O	1:D:54:GLU:HB3	2.20	0.41
1:A:46:ASP:OD1	1:A:46:ASP:C	2.59	0.41
1:C:20:GLN:NE2	1:C:309:LYS:HB3	2.35	0.41
1:B:11:LYS:HG2	1:B:80:ALA:HA	2.03	0.41
1:C:262:LEU:HB2	1:C:270:PRO:HG3	2.02	0.41
1:D:206:LEU:HA	1:D:367:GLU:O	2.20	0.41
1:A:75:LYS:HE2	1:A:75:LYS:HB2	1.76	0.41
1:B:290:GLU:CD	1:B:290:GLU:H	2.24	0.41
1:A:262:LEU:HB2	1:A:270:PRO:HG2	2.01	0.41
1:D:319:GLN:O	1:D:320:GLN:C	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLY:N	4:A:500:HOH:O	2.44	0.41
1:C:373:THR:O	1:C:374:ARG:C	2.59	0.41
1:B:62:ASN:HB2	1:B:64:ARG:H	1.86	0.40
1:C:141:ALA:N	1:C:142:PRO:CD	2.84	0.40
1:B:116:GLY:HA2	1:B:422:ASP:OD1	2.20	0.40
1:A:164:PHE:CD2	1:A:167:ILE:HB	2.57	0.40

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	433/450 (96%)	419 (97%)	14 (3%)	0	100	100
1	B	432/450 (96%)	417 (96%)	15 (4%)	0	100	100
1	C	432/450 (96%)	415 (96%)	17 (4%)	0	100	100
1	D	432/450 (96%)	411 (95%)	21 (5%)	0	100	100
All	All	1729/1800 (96%)	1662 (96%)	67 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	357/363 (98%)	344 (96%)	13 (4%)	42	52
1	B	357/363 (98%)	343 (96%)	14 (4%)	39	48
1	C	358/363 (99%)	343 (96%)	15 (4%)	36	44
1	D	358/363 (99%)	340 (95%)	18 (5%)	30	35
All	All	1430/1452 (98%)	1370 (96%)	60 (4%)	36	44

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	62	ASN
1	A	66	ARG
1	A	75	LYS
1	A	197	ARG
1	A	198	ARG
1	A	220	ARG
1	A	225	LEU
1	A	254	SER
1	A	281	LEU
1	A	360	LEU
1	A	362	ILE
1	A	376	ARG
1	B	19	SER
1	B	62	ASN
1	B	66	ARG
1	B	86	SER
1	B	124	LEU
1	B	153	MSE
1	B	189	GLU
1	B	225	LEU
1	B	230	GLU
1	B	281	LEU
1	B	320	GLN
1	B	360	LEU
1	B	362	ILE
1	B	398	SER
1	C	37	SER
1	C	48	GLU
1	C	62	ASN
1	C	124	LEU
1	C	189	GLU
1	C	198	ARG

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Mol	Chain	Res	Type
1	C	212	THR
1	C	220	ARG
1	C	243	GLU
1	C	281	LEU
1	C	334	ASN
1	C	360	LEU
1	C	362	ILE
1	C	398	SER
1	C	426	GLN
1	D	25	SER
1	D	37	SER
1	D	62	ASN
1	D	124	LEU
1	D	197	ARG
1	D	202	ARG
1	D	225	LEU
1	D	232	SER
1	D	243	GLU
1	D	281	LEU
1	D	290	GLU
1	D	308	GLU
1	D	334	ASN
1	D	344	GLU
1	D	360	LEU
1	D	362	ILE
1	D	376	ARG
1	D	410	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	174	HIS
1	A	209	ASN
1	A	304	GLN
1	A	354	GLN
1	A	417	GLN
1	A	426	GLN
1	B	62	ASN
1	B	304	GLN
1	B	417	GLN
1	C	20	GLN

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Mol	Chain	Res	Type
1	C	209	ASN
1	C	304	GLN
1	C	417	GLN
1	C	426	GLN
1	D	174	HIS
1	D	311	GLN
1	D	417	GLN
1	D	434	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](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	$\# Z  > 2$
2	SO4	A	2	-	4,4,4	0.32	0	6,6,6	0.19	0
2	SO4	A	455	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	B	1	-	4,4,4	0.35	0	6,6,6	0.12	0
2	SO4	B	455	-	4,4,4	0.19	0	6,6,6	0.16	0
2	SO4	C	3	-	4,4,4	0.28	0	6,6,6	0.08	0
2	SO4	D	4	-	4,4,4	0.23	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	D	455	-	4,4,4	0.15	0	6,6,6	0.08	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	SO4	A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	A	455	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1	-	-	0/0/0/0	0/0/0/0
2	SO4	B	455	-	-	0/0/0/0	0/0/0/0
2	SO4	C	3	-	-	0/0/0/0	0/0/0/0
2	SO4	D	4	-	-	0/0/0/0	0/0/0/0
2	SO4	D	455	-	-	0/0/0/0	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	455	SO4	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	426/450 (94%)	-0.23	3 (0%) 89 88	17, 31, 48, 61	0
1	B	426/450 (94%)	-0.40	3 (0%) 89 88	18, 30, 47, 62	0
1	C	426/450 (94%)	-0.33	5 (1%) 81 80	19, 31, 50, 63	0
1	D	426/450 (94%)	-0.30	4 (0%) 85 85	20, 32, 49, 62	0
All	All	1704/1800 (94%)	-0.32	15 (0%) 85 85	17, 31, 49, 63	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	62	ASN	4.2
1	C	62	ASN	3.0
1	D	321	ARG	3.0
1	D	60	SER	2.9
1	B	61	GLY	2.8
1	D	61	GLY	2.7
1	A	62	ASN	2.6
1	C	244	GLY	2.5
1	B	244	GLY	2.4
1	B	62	ASN	2.3
1	C	243	GLU	2.3
1	A	318	VAL	2.2
1	A	249	ASP	2.2
1	C	17	GLY	2.1
1	C	321	ARG	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 [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. 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	455	5/5	0.87	0.18	1.89	92,92,93,93	0
3	MG	D	1	1/1	0.87	0.18	1.75	37,37,37,37	0
3	MG	C	1	1/1	0.90	0.14	0.85	34,34,34,34	0
2	SO4	A	2	5/5	0.99	0.10	-0.26	60,60,62,62	0
3	MG	A	1	1/1	0.90	0.14	-0.41	39,39,39,39	0
2	SO4	D	4	5/5	0.97	0.10	-0.67	66,67,68,69	0
3	MG	B	456	1/1	0.95	0.12	-0.70	32,32,32,32	0
2	SO4	C	3	5/5	0.98	0.08	-1.56	59,60,62,63	0
2	SO4	B	1	5/5	0.99	0.07	-2.08	49,52,53,53	0
2	SO4	B	455	5/5	0.96	0.17	-	71,71,72,72	0
2	SO4	D	455	5/5	0.91	0.12	-	92,93,93,94	0

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

There are no such residues in this entry.