



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:26 am GMT

PDB ID : 2XHY  
Title : Crystal Structure of E.coli BglA  
Authors : Totir, M.; Zubietta, C.; Echols, N.; May, A.P.; Gee, C.L.; Nanao, M.; Alber, T.  
Deposited on : 2010-06-24  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

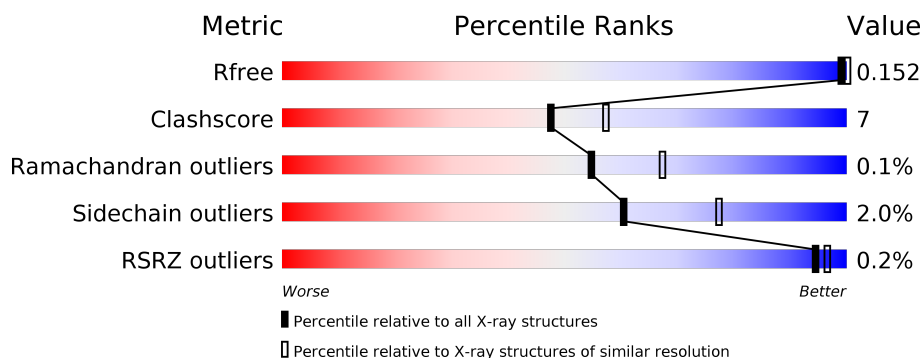
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	479	
1	B	479	
1	C	479	
1	D	479	

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
2	BR	B	1483	-	-	X	-
2	BR	D	1480	-	-	X	-
2	BR	D	1481	-	-	X	-
3	SO4	B	1485	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16976 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 6-PHOSPHO-BETA-GLUCOSIDASE BGLA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	1	0
			3847	2475	641	705	26			
1	B	468	Total	C	N	O	S	0	0	0
			3826	2460	639	702	25			
1	C	466	Total	C	N	O	S	0	1	0
			3809	2448	635	700	26			
1	D	464	Total	C	N	O	S	0	0	0
			3802	2445	634	698	25			

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	6	Total	Br	0	0
			6	6		
2	A	3	Total	Br	0	0
			3	3		
2	D	7	Total	Br	0	0
			7	7		
2	C	3	Total	Br	0	0
			3	3		

- 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	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		

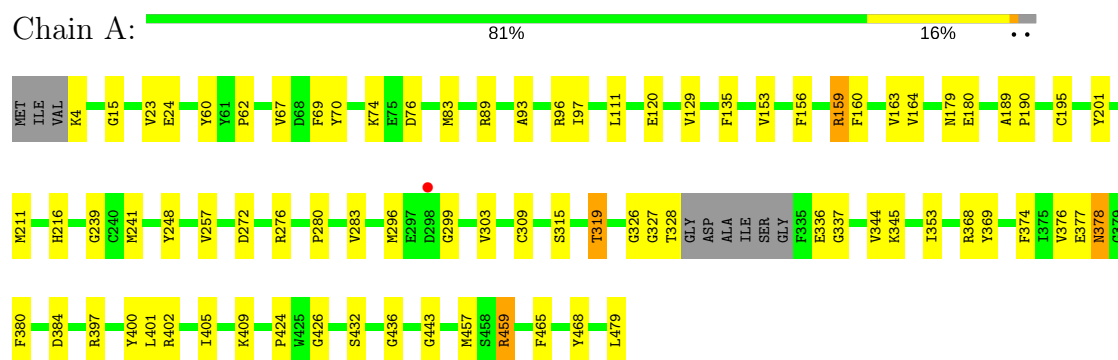
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	370	Total	O	0	0
			370	370		
4	B	399	Total	O	0	0
			399	399		
4	C	479	Total	O	0	0
			479	479		
4	D	400	Total	O	0	0
			400	400		

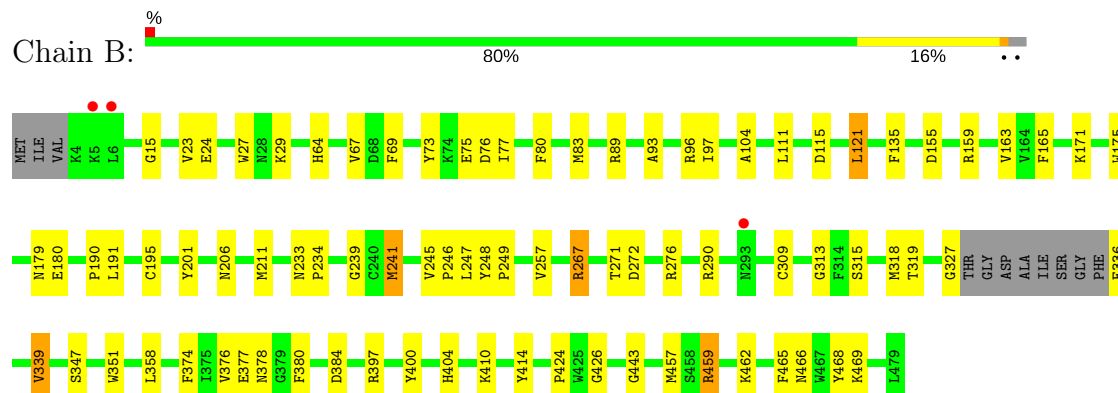
### 3 Residue-property plots

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.

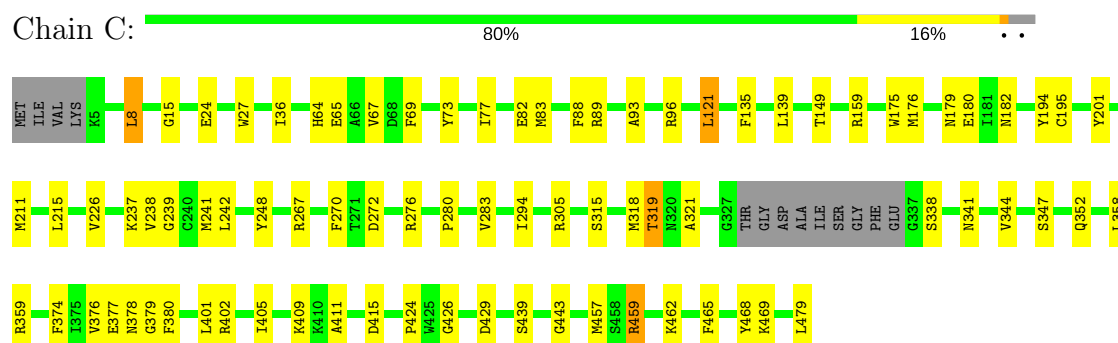
#### • Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE BGLA



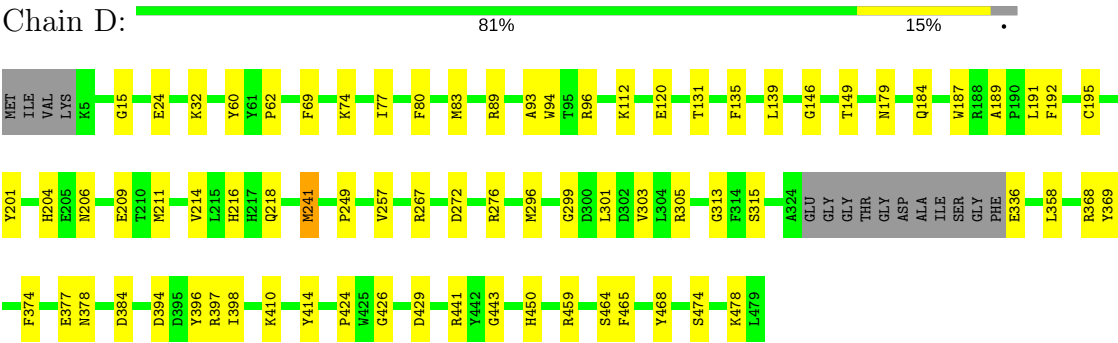
#### • Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE BGLA



#### • Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE BGLA



● Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE BGLA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.67Å 79.42Å 98.60Å 99.96° 107.21° 102.83°	Depositor
Resolution (Å)	22.94 – 2.30 47.35 – 2.79	Depositor EDS
% Data completeness (in resolution range)	92.7 (22.94-2.30) 81.4 (47.35-2.79)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.33 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6_289)	Depositor
R, $R_{free}$	0.171 , 0.236 0.151 , 0.152	Depositor DCC
$R_{free}$ test set	2218 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.900	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16976	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.99% 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: SO4, BR

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	0.24	0/3963	0.39	0/5361
1	B	0.23	0/3938	0.40	0/5327
1	C	0.24	0/3924	0.40	0/5311
1	D	0.24	0/3914	0.40	0/5297
All	All	0.24	0/15739	0.40	0/21296

There are no bond length outliers.

There are no bond angle outliers.

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	3847	0	3667	56	0
1	B	3826	0	3646	55	0
1	C	3809	0	3621	47	0
1	D	3802	0	3621	53	0
2	A	3	0	0	0	0
2	B	6	0	0	3	0
2	C	3	0	0	1	0
2	D	7	0	0	8	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	370	0	0	1	0
4	B	399	0	0	2	0
4	C	479	0	0	3	0
4	D	400	0	0	5	0
All	All	16976	0	14555	210	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 7.

All (210) 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:190:PRO:HD2	2:B:1483:BR:BR	2.39	0.76
1:D:93:ALA:HB3	1:D:96:ARG:HG3	1.69	0.74
1:A:93:ALA:HB3	1:A:96:ARG:HG3	1.73	0.71
1:B:272:ASP:O	1:B:276:ARG:HB2	1.91	0.71
1:C:315:SER:HB3	1:C:377:GLU:HB2	1.76	0.68
1:D:191:LEU:HB2	2:D:1484:BR:BR	2.49	0.68
1:C:93:ALA:HB3	1:C:96:ARG:HG3	1.76	0.67
1:B:267:ARG:HD2	1:B:267:ARG:N	2.10	0.67
1:C:226:VAL:HG13	4:C:2123:HOH:O	1.96	0.65
1:D:336:GLU:HG3	2:D:1481:BR:BR	2.52	0.65
2:D:1481:BR:BR	4:D:2292:HOH:O	2.69	0.65
1:B:410:LYS:O	1:B:414:TYR:HB3	1.99	0.63
1:D:187:TRP:HB3	1:D:211:MET:HE3	1.80	0.62
1:B:347:SER:HB3	1:B:351:TRP:H	1.66	0.61
1:C:315:SER:CB	1:C:377:GLU:HB2	2.31	0.60
1:B:239:GLY:HA2	1:B:309:CYS:HB3	1.82	0.60
1:A:24:GLU:HA	1:A:69:PHE:HB3	1.84	0.60
1:D:24:GLU:HA	1:D:69:PHE:HB3	1.84	0.60
1:B:245:VAL:O	1:B:267:ARG:NH1	2.35	0.59
1:C:8:LEU:HD21	1:C:409:LYS:HG2	1.84	0.59
1:D:384:ASP:CG	1:D:397:ARG:HH22	2.06	0.58
1:B:247:LEU:HG	1:B:267:ARG:HH12	1.69	0.58
1:A:272:ASP:O	1:A:276:ARG:HB2	2.04	0.58
1:C:135:PHE:HA	1:C:195:CYS:O	2.04	0.58
1:C:272:ASP:O	1:C:276:ARG:HB2	2.04	0.58
1:B:315:SER:CB	1:B:377:GLU:HB2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:MET:HG3	1:B:459:ARG:HH21	1.70	0.57
1:A:327:GLY:HA3	1:A:337:GLY:HA2	1.86	0.56
1:B:83:MET:HE3	1:B:465:PHE:HA	1.88	0.56
1:D:187:TRP:HB3	1:D:211:MET:CE	2.35	0.56
1:B:247:LEU:HG	1:B:267:ARG:NH1	2.20	0.56
1:A:83:MET:HE1	1:A:468:TYR:HD2	1.70	0.56
1:A:257:VAL:HG11	1:B:248:TYR:CE1	2.41	0.56
1:A:135:PHE:HA	1:A:195:CYS:O	2.06	0.55
1:B:249:PRO:HB3	1:B:257:VAL:HA	1.88	0.54
1:D:83:MET:CE	1:D:468:TYR:HB3	2.37	0.54
1:D:315:SER:CB	1:D:377:GLU:HB2	2.38	0.53
1:B:75:GLU:HG3	4:B:2102:HOH:O	2.08	0.53
1:D:206:ASN:HB3	1:D:209:GLU:HB3	1.89	0.53
1:D:272:ASP:O	1:D:276:ARG:HB2	2.09	0.53
1:C:24:GLU:HA	1:C:69:PHE:HB3	1.90	0.53
1:B:246:PRO:HD2	1:B:319:THR:HG22	1.91	0.53
1:D:135:PHE:HA	1:D:195:CYS:O	2.08	0.53
1:C:305:ARG:HD2	4:C:2140:HOH:O	2.08	0.53
1:B:23:VAL:HA	1:B:67:VAL:HG22	1.90	0.53
1:D:15:GLY:O	1:D:424:PRO:HD2	2.09	0.53
1:A:89:ARG:NH1	1:A:377:GLU:HG3	2.25	0.52
1:B:83:MET:CE	1:B:468:TYR:HB3	2.39	0.52
1:A:201:TYR:CE1	1:A:211:MET:HA	2.45	0.51
1:A:74:LYS:HG2	1:A:120:GLU:HG3	1.93	0.51
1:B:93:ALA:HB3	1:B:96:ARG:HG3	1.92	0.51
1:B:89:ARG:HD2	1:B:376:VAL:HB	1.91	0.51
1:B:426:GLY:O	1:B:443:GLY:HA2	2.10	0.51
1:D:410:LYS:HG3	2:D:1480:BR:BR	2.66	0.51
1:B:15:GLY:O	1:B:424:PRO:HD2	2.11	0.51
1:C:294:ILE:N	1:C:294:ILE:HD12	2.26	0.50
1:C:36:ILE:HB	1:C:194:TYR:CZ	2.45	0.50
1:A:70:TYR:CE1	1:A:96:ARG:NH2	2.79	0.50
1:B:384:ASP:CG	1:B:397:ARG:HH22	2.14	0.50
1:C:443:GLY:O	1:C:462:LYS:HD2	2.12	0.50
1:D:426:GLY:O	1:D:443:GLY:HA2	2.12	0.50
1:A:83:MET:CE	1:A:468:TYR:HB3	2.42	0.50
1:D:305:ARG:HG3	4:D:2255:HOH:O	2.10	0.50
1:D:83:MET:HE3	1:D:465:PHE:HA	1.93	0.50
1:B:24:GLU:HA	1:B:69:PHE:HB3	1.94	0.50
1:B:76:ASP:OD1	1:B:459:ARG:HD3	2.11	0.50
1:A:93:ALA:CB	1:A:96:ARG:HG3	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:MET:HG3	1:A:459:ARG:HH21	1.78	0.49
1:C:321:ALA:O	1:C:338:SER:HB2	2.12	0.49
1:A:89:ARG:HD2	1:A:376:VAL:HB	1.93	0.49
1:D:201:TYR:CE1	1:D:211:MET:HA	2.47	0.49
1:A:4:LYS:C	1:A:4:LYS:HD3	2.33	0.49
1:D:241:MET:HA	1:D:313:GLY:O	2.11	0.49
1:A:23:VAL:HA	1:A:67:VAL:HG22	1.95	0.49
1:B:135:PHE:HA	1:B:195:CYS:O	2.13	0.49
1:B:443:GLY:O	1:B:462:LYS:HD2	2.13	0.49
1:B:69:PHE:O	1:B:73:TYR:HB3	2.12	0.49
1:C:88:PHE:HD2	1:C:121:LEU:HD21	1.77	0.49
1:A:97:ILE:HD12	1:A:111:LEU:HD23	1.95	0.49
1:D:77:ILE:HA	1:D:80:PHE:CD2	2.48	0.49
1:D:429:ASP:OD2	1:D:441:ARG:HD3	2.13	0.48
1:B:380:PHE:HB2	1:B:400:TYR:CG	2.49	0.48
1:D:184:GLN:O	1:D:211:MET:HE2	2.13	0.48
1:D:315:SER:HB3	1:D:377:GLU:HB2	1.95	0.48
1:A:76:ASP:OD1	1:A:459:ARG:HD3	2.13	0.48
1:D:272:ASP:OD1	1:D:368:ARG:NH1	2.47	0.48
1:A:426:GLY:O	1:A:443:GLY:HA2	2.14	0.48
1:D:131:THR:HG21	1:D:179:ASN:HB2	1.96	0.48
1:D:60:TYR:CE2	1:D:62:PRO:HG3	2.48	0.48
1:C:280:PRO:O	1:C:283:VAL:HG12	2.13	0.48
1:C:83:MET:CE	1:C:468:TYR:HB3	2.44	0.48
1:D:93:ALA:CB	1:D:96:ARG:HG3	2.41	0.48
1:D:216:HIS:CE1	1:D:296:MET:HG2	2.48	0.48
1:D:368:ARG:HD3	1:D:369:TYR:CZ	2.49	0.47
1:A:299:GLY:O	1:A:303:VAL:HG23	2.14	0.47
1:D:394:ASP:HA	1:D:396:TYR:CZ	2.50	0.47
1:C:201:TYR:CE1	1:C:211:MET:HA	2.50	0.47
1:C:176:MET:HA	1:C:239:GLY:O	2.15	0.47
1:D:204:HIS:HE1	4:D:2199:HOH:O	1.97	0.47
1:D:299:GLY:O	1:D:303:VAL:HG23	2.15	0.47
1:A:239:GLY:HA2	1:A:309:CYS:HB3	1.97	0.47
1:B:201:TYR:CE1	1:B:211:MET:HA	2.50	0.47
1:C:67:VAL:HG11	1:C:429:ASP:O	2.15	0.47
1:A:83:MET:HE1	1:A:468:TYR:CD2	2.49	0.47
1:D:414:TYR:HB2	2:D:1480:BR:BR	2.70	0.46
1:D:206:ASN:ND2	2:D:1485:BR:BR	3.04	0.46
1:A:344:VAL:HG12	1:A:345:LYS:O	2.15	0.46
1:A:315:SER:CB	1:A:377:GLU:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ASP:OD1	1:B:171:LYS:HE3	2.15	0.46
1:C:175:TRP:HB2	1:C:238:VAL:HG22	1.97	0.46
1:A:153:VAL:HA	1:A:156:PHE:CD2	2.51	0.46
1:A:15:GLY:O	1:A:424:PRO:HD2	2.16	0.46
1:C:8:LEU:CD2	1:C:409:LYS:HG2	2.46	0.46
1:D:32:LYS:HD2	1:D:96:ARG:HG2	1.97	0.46
1:C:248:TYR:CE2	1:C:319:THR:HG21	2.50	0.46
1:D:214:VAL:O	1:D:218:GLN:HG3	2.16	0.46
1:A:353:ILE:HD11	1:A:380:PHE:HE1	1.81	0.45
1:A:378:ASN:O	1:A:424:PRO:HA	2.17	0.45
1:B:318:MET:HE1	1:B:351:TRP:CD2	2.51	0.45
1:C:347:SER:HB3	1:C:380:PHE:CE1	2.51	0.45
1:C:378:ASN:O	1:C:424:PRO:HA	2.17	0.45
1:D:410:LYS:O	1:D:414:TYR:HB3	2.17	0.45
1:D:146:GLY:O	1:D:149:THR:HG22	2.16	0.45
1:D:450:HIS:HB3	2:D:1482:BR:BR	2.70	0.45
1:C:402:ARG:HD3	1:C:479:LEU:O	2.15	0.45
1:C:379:GLY:HA2	1:C:401:LEU:HD21	1.99	0.45
1:A:409:LYS:HB3	4:A:2318:HOH:O	2.15	0.45
1:B:77:ILE:HD13	1:B:121:LEU:HD13	1.98	0.45
1:C:237:LYS:HA	4:C:2287:HOH:O	2.17	0.45
1:A:83:MET:CE	1:A:468:TYR:HD2	2.30	0.45
1:C:83:MET:HE1	1:C:468:TYR:HD2	1.82	0.45
1:B:89:ARG:NH1	1:B:377:GLU:HG3	2.32	0.44
1:D:474:SER:HB3	1:D:478:LYS:HD2	2.00	0.44
1:C:411:ALA:HA	1:C:415:ASP:OD1	2.17	0.44
1:D:249:PRO:HB3	1:D:257:VAL:HA	1.99	0.44
1:C:341:ASN:HB3	1:C:344:VAL:HG22	2.00	0.44
1:A:67:VAL:O	1:A:459:ARG:NH2	2.42	0.44
1:C:215:LEU:HD22	1:C:270:PHE:HE2	1.82	0.44
1:A:153:VAL:HA	1:A:156:PHE:HD2	1.82	0.44
1:A:216:HIS:NE2	1:A:296:MET:HG2	2.33	0.44
1:A:401:LEU:O	1:A:405:ILE:HG13	2.17	0.44
1:B:27:TRP:HB3	1:B:64:HIS:HA	2.00	0.44
1:D:378:ASN:O	1:D:424:PRO:HA	2.18	0.44
1:D:394:ASP:HA	1:D:396:TYR:CE2	2.52	0.44
1:B:400:TYR:CE2	1:B:404:HIS:CE1	3.06	0.44
1:B:206:ASN:HB3	2:B:1487:BR:BR	2.73	0.43
1:D:120:GLU:HG2	4:D:2120:HOH:O	2.17	0.43
1:A:179:ASN:O	1:A:180:GLU:C	2.57	0.43
1:A:189:ALA:HA	1:A:190:PRO:HD3	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:ASN:OD1	1:C:242:LEU:HD12	2.19	0.43
1:C:27:TRP:HB3	1:C:64:HIS:HA	2.00	0.43
1:A:280:PRO:O	1:A:283:VAL:HG12	2.19	0.43
1:B:336:GLU:HA	3:B:1485:SO4:O2	2.18	0.43
1:A:384:ASP:CG	1:A:397:ARG:HH22	2.22	0.43
1:C:318:MET:HE3	1:C:352:GLN:H	1.83	0.43
1:B:315:SER:HB2	1:B:377:GLU:HB2	2.01	0.43
1:C:179:ASN:O	1:C:180:GLU:C	2.57	0.43
1:B:191:LEU:HB2	2:B:1483:BR:BR	2.74	0.43
1:A:4:LYS:O	1:A:4:LYS:HD3	2.19	0.42
1:B:466:ASN:O	1:B:469:LYS:HB3	2.18	0.42
1:C:457:MET:HG3	1:C:459:ARG:HH21	1.83	0.42
1:A:160:PHE:O	1:A:164:VAL:HG22	2.19	0.42
1:B:290:ARG:HD3	4:B:2274:HOH:O	2.19	0.42
1:C:15:GLY:O	1:C:424:PRO:HD2	2.19	0.42
1:D:83:MET:HE2	1:D:468:TYR:HB3	2.01	0.42
1:C:426:GLY:O	1:C:443:GLY:HA2	2.20	0.42
1:D:112:LYS:HD3	4:D:2111:HOH:O	2.19	0.42
1:A:83:MET:HG3	1:A:465:PHE:CZ	2.55	0.42
1:C:83:MET:HE3	1:C:465:PHE:HA	2.02	0.42
1:A:402:ARG:HD3	1:A:479:LEU:O	2.20	0.42
1:A:257:VAL:HG11	1:B:248:TYR:CD1	2.54	0.42
1:B:327:GLY:HA2	1:B:339:VAL:HG23	2.02	0.42
1:C:359:ARG:HG3	1:C:411:ALA:HB2	2.02	0.42
1:C:89:ARG:NH1	1:C:377:GLU:HG3	2.35	0.42
1:D:83:MET:HE1	1:D:468:TYR:HD2	1.84	0.42
1:A:60:TYR:CE2	1:A:62:PRO:HG3	2.55	0.42
1:B:83:MET:HE1	1:B:468:TYR:HD2	1.85	0.42
1:B:104:ALA:HA	1:B:159:ARG:NH2	2.35	0.42
1:B:233:ASN:HA	1:B:234:PRO:HD2	1.87	0.42
1:C:376:VAL:O	1:C:377:GLU:HG3	2.19	0.42
1:D:74:LYS:HG2	1:D:120:GLU:HG3	2.01	0.41
1:D:94:TRP:HD1	1:D:94:TRP:O	2.03	0.41
1:C:77:ILE:CD1	1:C:121:LEU:HD13	2.50	0.41
1:A:328:THR:O	1:A:336:GLU:HA	2.20	0.41
1:A:377:GLU:O	1:A:378:ASN:HB2	2.20	0.41
1:B:159:ARG:O	1:B:163:VAL:HG23	2.19	0.41
1:B:77:ILE:HA	1:B:80:PHE:CD2	2.54	0.41
1:A:248:TYR:CE2	1:A:319:THR:HG21	2.54	0.41
1:B:29:LYS:HA	1:B:29:LYS:HD3	1.91	0.41
1:B:97:ILE:HD12	1:B:111:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:ARG:NH1	1:D:377:GLU:HG3	2.36	0.41
1:B:378:ASN:O	1:B:424:PRO:HA	2.20	0.41
1:B:179:ASN:O	1:B:180:GLU:C	2.59	0.41
1:C:439:SER:HB3	2:C:1480:BR:BR	2.76	0.41
1:A:159:ARG:O	1:A:163:VAL:HG23	2.21	0.40
1:D:189:ALA:HB3	1:D:192:PHE:CD2	2.55	0.40
1:A:432:SER:O	1:A:436:GLY:HA2	2.21	0.40
1:C:401:LEU:O	1:C:405:ILE:HG13	2.22	0.40
1:D:301:LEU:HB2	2:D:1487:BR:BR	2.76	0.40
1:A:344:VAL:HG13	1:A:353:ILE:O	2.21	0.40
1:A:380:PHE:HB2	1:A:400:TYR:CG	2.56	0.40
1:C:82:GLU:O	1:C:469:LYS:HE2	2.21	0.40
1:D:398:ILE:HD11	1:D:464:SER:HA	2.03	0.40
1:A:89:ARG:HA	1:A:129:VAL:O	2.22	0.40
1:A:344:VAL:HG12	1:A:345:LYS:N	2.35	0.40
1:B:165:PHE:HE1	1:B:175:TRP:CD2	2.39	0.40
1:A:368:ARG:HD3	1:A:369:TYR:CZ	2.57	0.40
1:A:83:MET:HE2	1:A:468:TYR:HB3	2.02	0.40
1:B:241:MET:HA	1:B:313:GLY:O	2.21	0.40
1:C:69:PHE:O	1:C:73:TYR:HB3	2.21	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	467/479 (98%)	447 (96%)	18 (4%)	2 (0%)	38	47
1	B	464/479 (97%)	446 (96%)	18 (4%)	0	100	100
1	C	463/479 (97%)	447 (96%)	16 (4%)	0	100	100
1	D	460/479 (96%)	439 (95%)	21 (5%)	0	100	100
All	All	1854/1916 (97%)	1779 (96%)	73 (4%)	2 (0%)	55	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	GLY
1	A	378	ASN

### 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	405/411 (98%)	400 (99%)	5 (1%)	75	87
1	B	402/411 (98%)	393 (98%)	9 (2%)	57	74
1	C	401/411 (98%)	389 (97%)	12 (3%)	46	63
1	D	401/411 (98%)	395 (98%)	6 (2%)	70	83
All	All	1609/1644 (98%)	1577 (98%)	32 (2%)	60	77

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	ARG
1	A	241	MET
1	A	319	THR
1	A	374	PHE
1	A	459	ARG
1	B	121	LEU
1	B	155	ASP
1	B	241	MET
1	B	267	ARG
1	B	271	THR
1	B	339	VAL
1	B	358	LEU
1	B	374	PHE
1	B	459	ARG
1	C	8	LEU
1	C	65	GLU
1	C	121	LEU
1	C	139	LEU

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Mol	Chain	Res	Type
1	C	149	THR
1	C	159	ARG
1	C	241	MET
1	C	267	ARG
1	C	319	THR
1	C	358	LEU
1	C	374	PHE
1	C	459	ARG
1	D	139	LEU
1	D	241	MET
1	D	267	ARG
1	D	358	LEU
1	D	374	PHE
1	D	459	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	378	ASN
1	B	170	HIS
1	B	450	HIS
1	D	204	HIS
1	D	293	ASN
1	D	370	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 24 ligands modelled in this entry, 19 are monoatomic - leaving 5 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	SO4	A	1481	-	4,4,4	0.15	0	6,6,6	0.15	0
3	SO4	B	1484	-	4,4,4	0.15	0	6,6,6	0.14	0
3	SO4	B	1485	-	4,4,4	0.15	0	6,6,6	0.14	0
3	SO4	C	1482	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	D	1486	-	4,4,4	0.16	0	6,6,6	0.16	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
3	SO4	A	1481	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1484	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1485	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1482	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1486	-	-	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
3	B	1485	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 [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	470/479 (98%)	-0.37	1 (0%) 94 96	14, 22, 36, 52	0
1	B	468/479 (97%)	-0.30	3 (0%) 89 92	13, 19, 34, 60	0
1	C	466/479 (97%)	-0.40	0 100 100	12, 17, 29, 47	0
1	D	464/479 (96%)	-0.43	0 100 100	13, 18, 30, 45	0
All	All	1868/1916 (97%)	-0.38	4 (0%) 94 96	12, 19, 33, 60	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	LEU	3.4
1	A	298	ASP	2.1
1	B	293	ASN	2.1
1	B	5	LYS	2.0

### 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. 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
3	SO4	B	1485	5/5	0.92	0.24	3.53	36,39,59,66	0
2	BR	B	1486	1/1	0.97	0.16	1.52	73,73,73,73	0
2	BR	B	1487	1/1	0.91	0.19	1.00	77,77,77,77	0
2	BR	D	1485	1/1	0.93	0.23	1.00	66,66,66,66	0
2	BR	D	1487	1/1	0.97	0.15	0.93	74,74,74,74	0
2	BR	A	1482	1/1	0.77	0.13	-0.11	79,79,79,79	0
3	SO4	A	1481	5/5	0.99	0.09	-1.62	22,23,27,28	0
3	SO4	C	1482	5/5	0.99	0.09	-2.40	15,17,18,19	0
3	SO4	B	1484	5/5	0.99	0.08	-2.59	18,19,24,28	0
3	SO4	D	1486	5/5	0.99	0.08	-3.62	19,19,22,24	0
2	BR	C	1480	1/1	0.95	0.06	-3.72	69,69,69,69	0
2	BR	C	1483	1/1	0.98	0.13	-	59,59,59,59	0
2	BR	D	1481	1/1	0.95	0.10	-	89,89,89,89	0
2	BR	A	1480	1/1	0.99	0.26	-	81,81,81,81	0
2	BR	B	1481	1/1	0.96	0.09	-	73,73,73,73	0
2	BR	B	1483	1/1	0.98	0.10	-	74,74,74,74	0
2	BR	C	1481	1/1	0.97	0.09	-	73,73,73,73	0
2	BR	D	1483	1/1	0.99	0.13	-	71,71,71,71	0
2	BR	B	1482	1/1	0.97	0.19	-	83,83,83,83	0
2	BR	D	1480	1/1	0.95	0.34	-	91,91,91,91	0
2	BR	B	1480	1/1	0.97	0.15	-	74,74,74,74	0
2	BR	D	1484	1/1	0.95	0.19	-	71,71,71,71	0
2	BR	D	1482	1/1	0.97	0.16	-	80,80,80,80	0
2	BR	A	1483	1/1	0.96	0.15	-	94,94,94,94	0

## 6.5 Other polymers

There are no such residues in this entry.