



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2021 – 06:05 PM EDT

PDB ID : 7K1R  
Title : X-ray Structure of an Enterobacter GH43 Beta-Xylosidase: EcXyl43 F507A mutant  
Authors : Briganti, L.; Capetti, C.C.M.; Polikarpov, I.  
Deposited on : 2020-09-08  
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

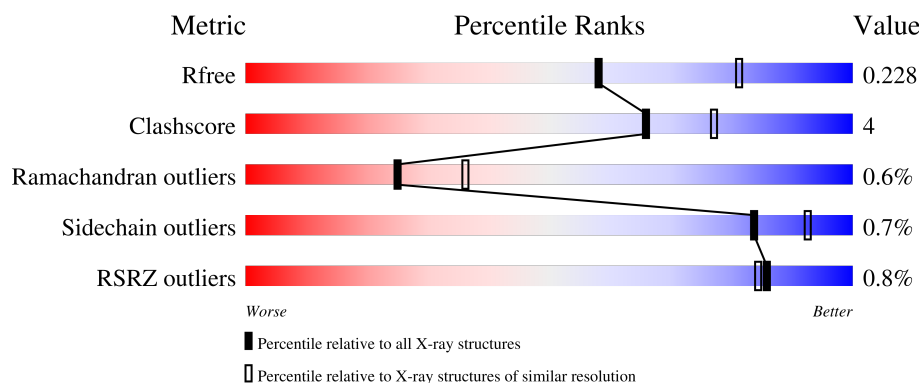
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

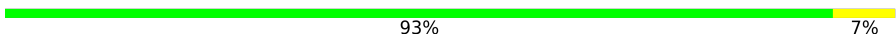



The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	536	
1	B	536	
1	C	536	
1	D	536	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18520 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 Beta xylosidase GH43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4295	2750	731	796	18			
1	B	532	Total	C	N	O	S	0	0	0
			4258	2729	726	785	18			
1	C	531	Total	C	N	O	S	0	0	0
			4277	2738	727	794	18			
1	D	534	Total	C	N	O	S	0	0	0
			4279	2740	729	792	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	GLY	UNK	conflict	UNP V5J3M5
A	507	ALA	PHE	engineered mutation	UNP V5J3M5
B	204	GLY	UNK	conflict	UNP V5J3M5
B	507	ALA	PHE	engineered mutation	UNP V5J3M5
C	204	GLY	UNK	conflict	UNP V5J3M5
C	507	ALA	PHE	engineered mutation	UNP V5J3M5
D	204	GLY	UNK	conflict	UNP V5J3M5
D	507	ALA	PHE	engineered mutation	UNP V5J3M5

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

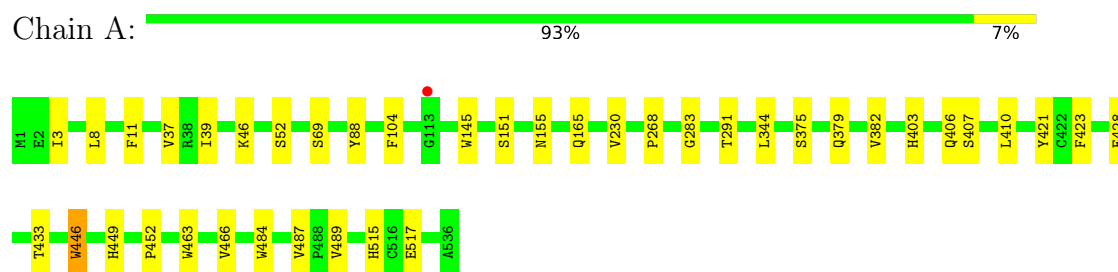
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	403	Total	O	0	0
			403	403		
4	B	350	Total	O	0	0
			350	350		
4	C	328	Total	O	0	0
			328	328		
4	D	314	Total	O	0	0
			314	314		

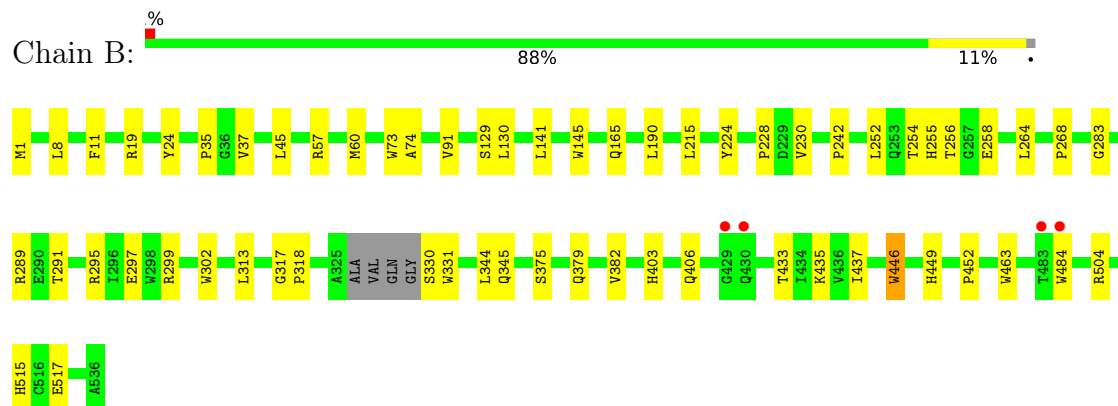
### 3 Residue-property plots [i](#)

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.

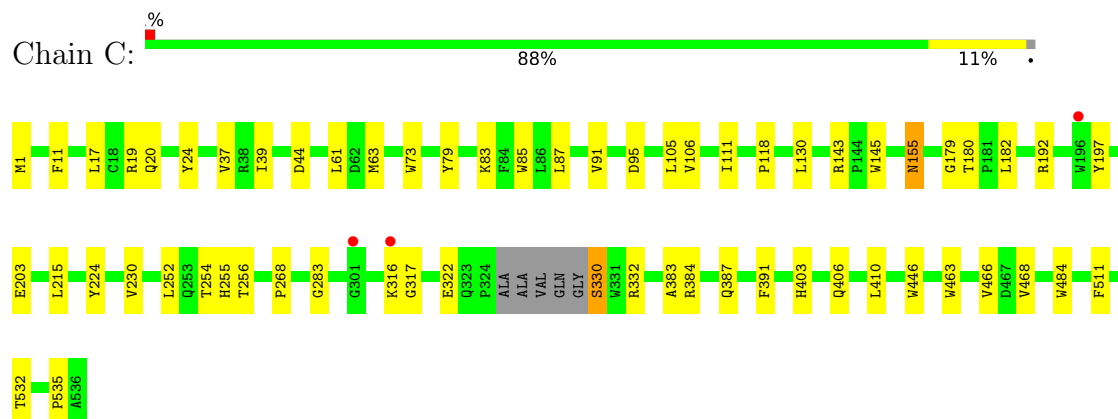
#### • Molecule 1: Beta xylosidase GH43



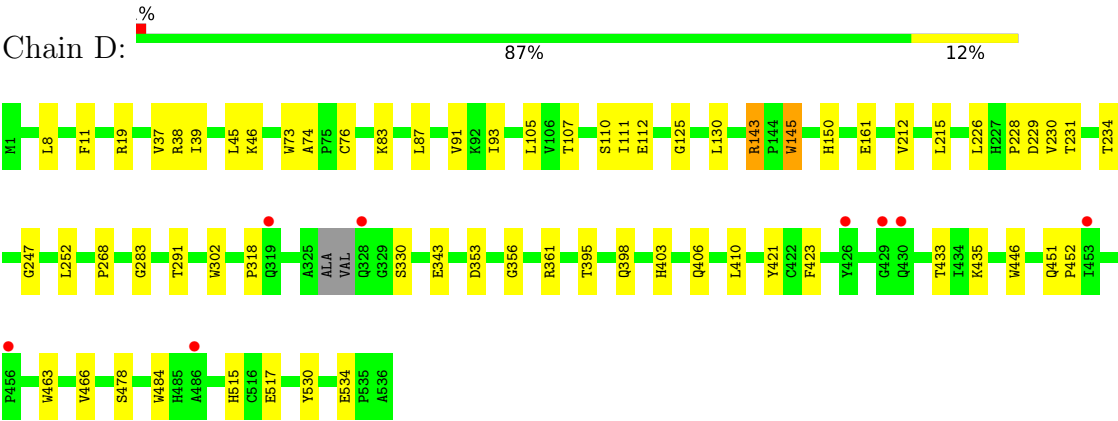
#### • Molecule 1: Beta xylosidase GH43



#### • Molecule 1: Beta xylosidase GH43



● Molecule 1: Beta xylosidase GH43



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.12Å 153.10Å 182.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.72 – 2.40 48.64 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (22.72-2.40) 99.9 (48.64-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, $R_{free}$	0.190 , 0.228 0.190 , 0.228	Depositor DCC
$R_{free}$ test set	4619 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 32.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18520	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: CA, GOL

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	0.25	0/4446	0.46	0/6076
1	B	0.24	0/4408	0.47	0/6024
1	C	0.25	0/4427	0.47	0/6047
1	D	0.24	0/4429	0.47	0/6051
All	All	0.25	0/17710	0.47	0/24198

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	4295	0	4032	22	0
1	B	4258	0	3994	36	0
1	C	4277	0	4017	35	0
1	D	4279	0	4013	41	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
3	B	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	6	0	8	1	0
4	A	403	0	0	2	0
4	B	350	0	0	4	0
4	C	328	0	0	4	0
4	D	314	0	0	8	0
All	All	18520	0	16072	133	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 4.

All (133) 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:143:ARG:NH1	4:C:701:HOH:O	2.05	0.85
1:D:463:TRP:HB2	1:D:478:SER:HB3	1.59	0.84
1:D:76:CYS:SG	4:D:724:HOH:O	2.42	0.77
1:B:375:SER:O	1:B:379:GLN:NE2	2.16	0.76
1:C:180:THR:HG22	1:C:182:LEU:H	1.50	0.76
1:A:165:GLN:NE2	4:A:702:HOH:O	2.22	0.72
1:C:155:ASN:O	1:C:155:ASN:ND2	2.26	0.68
1:D:268:PRO:HB2	1:D:283:GLY:HA3	1.77	0.66
1:B:242:PRO:HG2	1:B:313:LEU:HD21	1.78	0.66
1:D:330:SER:OG	4:D:701:HOH:O	2.14	0.65
1:B:289:ARG:HH12	3:B:601:GOL:H31	1.61	0.65
1:C:332:ARG:HB2	1:C:532:THR:HG22	1.78	0.65
1:D:361:ARG:HH12	1:D:398:GLN:HE21	1.47	0.63
1:C:330:SER:N	4:C:708:HOH:O	2.33	0.61
1:A:375:SER:HB2	1:D:93:ILE:HD11	1.81	0.61
1:B:504:ARG:NH2	4:B:707:HOH:O	2.33	0.61
1:D:110:SER:OG	1:D:112:GLU:OE2	2.19	0.60
1:A:8:LEU:HB2	1:A:291:THR:HB	1.82	0.60
1:D:229:ASP:O	1:D:231:THR:N	2.34	0.59
1:B:268:PRO:HB2	1:B:283:GLY:HA3	1.84	0.59
1:C:20:GLN:NE2	4:C:704:HOH:O	2.35	0.59
1:C:95:ASP:OD1	4:C:702:HOH:O	2.16	0.58
1:C:268:PRO:HB2	1:C:283:GLY:HA3	1.86	0.58
1:B:57:ARG:NH1	4:B:709:HOH:O	2.37	0.57
1:B:19:ARG:HB3	1:B:252:LEU:HD21	1.88	0.56
1:A:151:SER:HA	1:A:155:ASN:HD22	1.71	0.55
1:D:74:ALA:HB2	3:D:601:GOL:H31	1.89	0.55
1:C:384:ARG:NH2	1:C:387:GLN:OE1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ILE:HB	1:A:52:SER:HB3	1.87	0.55
1:A:344:LEU:HD22	1:A:382:VAL:HG12	1.88	0.55
1:B:141:LEU:HD11	1:B:190:LEU:HG	1.89	0.54
1:B:1:MET:HE2	1:B:318:PRO:HD2	1.90	0.54
1:B:24:TYR:OH	1:B:255:HIS:ND1	2.41	0.54
1:C:330:SER:HB3	1:C:535:PRO:HD2	1.90	0.53
1:D:39:ILE:HG21	1:D:111:ILE:HD11	1.91	0.53
1:C:20:GLN:HG3	1:C:79:TYR:CZ	2.44	0.53
1:C:1:MET:SD	1:C:317:GLY:HA3	2.50	0.52
1:A:433:THR:HB	1:A:452:PRO:HB2	1.92	0.52
1:C:180:THR:HB	1:C:203:GLU:OE1	2.10	0.52
1:A:403:HIS:CE1	1:A:406:GLN:HG3	2.45	0.51
1:A:69:SER:O	1:A:69:SER:OG	2.28	0.51
1:D:45:LEU:HD12	1:D:318:PRO:HG3	1.91	0.51
1:A:268:PRO:HB2	1:A:283:GLY:HA3	1.92	0.51
1:D:361:ARG:HH22	1:D:398:GLN:HE22	1.59	0.51
1:B:254:THR:OG1	1:B:256:THR:OG1	2.26	0.50
1:B:403:HIS:CE1	1:B:406:GLN:HG3	2.46	0.50
1:D:215:LEU:HG	1:D:226:LEU:HD23	1.92	0.50
1:C:463:TRP:HB3	1:C:484:TRP:CH2	2.47	0.49
1:B:433:THR:HB	1:B:452:PRO:HB2	1.95	0.49
1:B:437:ILE:HD13	1:B:446:TRP:HB3	1.94	0.49
1:C:391:PHE:CZ	1:C:468:VAL:HG21	2.49	0.48
1:A:463:TRP:HB3	1:A:484:TRP:CH2	2.49	0.48
1:D:38:ARG:NH2	4:D:704:HOH:O	2.24	0.48
1:C:1:MET:CE	1:C:44:ASP:HB2	2.43	0.48
1:C:61:LEU:HG	1:C:63:MET:HG3	1.96	0.48
1:A:410:LEU:HD21	1:A:466:VAL:HG12	1.96	0.48
1:C:254:THR:OG1	1:C:256:THR:OG1	2.28	0.47
1:B:8:LEU:HB2	1:B:291:THR:HB	1.96	0.47
1:A:428:GLU:OE2	4:A:701:HOH:O	2.20	0.47
1:D:451:GLN:NE2	4:D:732:HOH:O	2.47	0.47
1:D:231:THR:HG21	1:D:234:THR:HG22	1.97	0.47
1:D:395:THR:OG1	1:D:530:TYR:O	2.22	0.47
1:C:106:VAL:HG12	1:C:118:PRO:HA	1.96	0.47
1:C:87:LEU:HD11	1:C:130:LEU:HB2	1.96	0.47
1:D:361:ARG:HH22	1:D:398:GLN:NE2	2.13	0.46
1:D:410:LEU:HD21	1:D:466:VAL:HG12	1.98	0.46
1:B:297:GLU:OE2	1:B:299:ARG:NH2	2.39	0.46
1:D:73:TRP:CE2	1:D:91:VAL:HG21	2.51	0.46
1:B:258:GLU:OE2	1:B:295:ARG:NH1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:TRP:HB3	1:B:484:TRP:CH2	2.51	0.45
1:B:35:PRO:O	1:B:345:GLN:NE2	2.50	0.45
1:D:403:HIS:CE1	1:D:406:GLN:HG3	2.51	0.45
1:C:403:HIS:CE1	1:C:406:GLN:HG3	2.51	0.45
1:D:343:GLU:HA	4:D:704:HOH:O	2.16	0.45
1:D:433:THR:HB	1:D:452:PRO:HB2	1.98	0.45
1:C:87:LEU:HD23	1:C:105:LEU:HB2	1.99	0.44
1:B:1:MET:HE2	1:B:317:GLY:HA3	1.99	0.44
1:A:3:ILE:HG12	1:A:46:LYS:HB2	1.98	0.44
1:A:515:HIS:NE2	1:A:517:GLU:HB3	2.32	0.44
1:B:435:LYS:HE3	1:B:452:PRO:HB3	1.98	0.44
1:B:57:ARG:HB2	1:B:60:MET:HG3	1.99	0.44
1:B:74:ALA:HB2	3:B:601:GOL:H11	1.99	0.44
1:A:446:TRP:HB2	1:A:449:HIS:ND1	2.33	0.44
1:B:344:LEU:HD22	1:B:382:VAL:HG12	1.99	0.44
1:B:299:ARG:NH1	4:B:714:HOH:O	2.39	0.43
1:C:39:ILE:HG21	1:C:111:ILE:HD11	2.00	0.43
1:C:215:LEU:HB3	1:C:224:TYR:HB3	2.00	0.43
1:B:330:SER:OG	1:B:331:TRP:N	2.49	0.43
1:C:83:LYS:HE2	1:C:85:TRP:CZ2	2.53	0.43
1:D:463:TRP:HB3	1:D:484:TRP:CH2	2.54	0.43
1:B:228:PRO:HD3	1:B:302:TRP:CE2	2.54	0.43
1:C:383:ALA:HB1	1:C:511:PHE:HB3	2.01	0.43
1:D:8:LEU:HB2	1:D:291:THR:HB	2.01	0.43
1:D:212:VAL:HG23	1:D:247:GLY:HA2	2.01	0.43
1:A:515:HIS:HE2	1:A:517:GLU:HB3	1.84	0.42
1:D:19:ARG:HB3	1:D:252:LEU:HD21	2.01	0.42
1:A:407:SER:HB2	1:A:423:PHE:CD1	2.55	0.42
1:B:437:ILE:HD11	1:B:449:HIS:CE1	2.54	0.42
1:D:83:LYS:HE3	1:D:107:THR:HG21	1.99	0.42
1:D:73:TRP:CD2	1:D:91:VAL:HG21	2.54	0.42
1:B:45:LEU:HD12	1:B:318:PRO:HG3	2.01	0.42
1:B:515:HIS:HE2	1:B:517:GLU:HB3	1.85	0.42
1:C:316:LYS:HD3	1:C:316:LYS:HA	1.88	0.42
1:D:161:GLU:OE2	4:D:702:HOH:O	2.22	0.42
1:D:515:HIS:HE2	1:D:517:GLU:HB3	1.85	0.42
1:D:421:TYR:CZ	1:D:423:PHE:HB3	2.55	0.42
1:D:534:GLU:HG2	4:D:701:HOH:O	2.20	0.42
1:C:1:MET:HE2	1:C:322:GLU:HG2	2.02	0.42
1:D:435:LYS:HE3	1:D:452:PRO:HB3	2.02	0.42
1:A:421:TYR:CE1	1:A:423:PHE:HB3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:TYR:HH	1:C:255:HIS:HD1	1.63	0.41
1:D:87:LEU:HD23	1:D:105:LEU:HB2	2.03	0.41
1:B:73:TRP:CD2	1:B:91:VAL:HG21	2.55	0.41
1:B:130:LEU:HD12	1:B:130:LEU:HA	1.92	0.41
1:B:264:LEU:HD13	1:B:289:ARG:HD2	2.02	0.41
1:D:145:TRP:HB2	1:D:150:HIS:NE2	2.36	0.41
1:C:19:ARG:HG2	1:C:252:LEU:HD11	2.02	0.41
1:D:46:LYS:NZ	4:D:712:HOH:O	2.35	0.41
1:A:487:VAL:O	1:A:489:VAL:N	2.51	0.41
1:B:165:GLN:N	4:B:701:HOH:O	2.53	0.41
1:D:125:GLY:HA3	1:D:143:ARG:O	2.20	0.41
1:C:17:LEU:HG	1:C:252:LEU:HD22	2.04	0.40
1:C:73:TRP:CD2	1:C:91:VAL:HG21	2.56	0.40
1:C:192:ARG:HD2	1:C:197:TYR:CE1	2.56	0.40
1:A:375:SER:O	1:A:379:GLN:NE2	2.36	0.40
1:C:155:ASN:HD21	1:C:179:GLY:HA3	1.86	0.40
1:D:228:PRO:HD3	1:D:302:TRP:CE2	2.56	0.40
1:B:215:LEU:HB3	1:B:224:TYR:HB3	2.03	0.40
1:B:435:LYS:HD3	1:B:449:HIS:CE1	2.56	0.40
1:D:353:ASP:HA	1:D:356:GLY:O	2.22	0.40
1:C:410:LEU:HD21	1:C:466:VAL:HG12	2.03	0.40
1:D:87:LEU:HD11	1:D:130:LEU:HB2	2.04	0.40
1:A:88:TYR:CZ	1:A:104:PHE:HB2	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	534/536 (100%)	515 (96%)	16 (3%)	3 (1%)	25 36
1	B	528/536 (98%)	504 (96%)	21 (4%)	3 (1%)	25 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	527/536 (98%)	505 (96%)	19 (4%)	3 (1%)	25	36
1	D	530/536 (99%)	507 (96%)	20 (4%)	3 (1%)	25	36
All	All	2119/2144 (99%)	2031 (96%)	76 (4%)	12 (1%)	25	36

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	37	VAL
1	B	11	PHE
1	B	37	VAL
1	C	37	VAL
1	D	37	VAL
1	C	11	PHE
1	D	11	PHE
1	D	230	VAL
1	B	230	VAL
1	C	230	VAL
1	A	230	VAL

### 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	456/459 (99%)	454 (100%)	2 (0%)	91	96
1	B	451/459 (98%)	448 (99%)	3 (1%)	84	92
1	C	457/459 (100%)	453 (99%)	4 (1%)	78	90
1	D	454/459 (99%)	451 (99%)	3 (1%)	84	92
All	All	1818/1836 (99%)	1806 (99%)	12 (1%)	84	92

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	TRP
1	A	446	TRP
1	B	129	SER
1	B	145	TRP
1	B	446	TRP
1	C	145	TRP
1	C	155	ASN
1	C	330	SER
1	C	446	TRP
1	D	143	ARG
1	D	145	TRP
1	D	446	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	155	ASN
1	D	155	ASN
1	D	398	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	GOL	B	601	-	5,5,5	0.91	0	5,5,5	0.94	0
3	GOL	D	601	-	5,5,5	0.85	0	5,5,5	1.05	1 (20%)

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	GOL	B	601	-	-	4/4/4/4	-
3	GOL	D	601	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	D	601	GOL	C3-C2-C1	-2.01	103.91	111.70

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	GOL	O1-C1-C2-C3
3	B	601	GOL	C1-C2-C3-O3
3	D	601	GOL	O1-C1-C2-O2
3	D	601	GOL	O1-C1-C2-C3
3	D	601	GOL	C1-C2-C3-O3
3	B	601	GOL	O1-C1-C2-O2
3	D	601	GOL	O2-C2-C3-O3
3	B	601	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	601	GOL	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	536/536 (100%)	-0.20	1 (0%)	95 94	29, 37, 47, 56	0
1	B	532/536 (99%)	-0.19	4 (0%)	86 84	31, 41, 52, 66	0
1	C	531/536 (99%)	-0.25	3 (0%)	89 88	31, 42, 58, 65	0
1	D	534/536 (99%)	-0.04	8 (1%)	73 72	32, 44, 57, 70	0
All	All	2133/2144 (99%)	-0.17	16 (0%)	86 84	29, 41, 56, 70	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	483	THR	2.8
1	A	113	GLY	2.8
1	D	486	ALA	2.8
1	D	429	GLY	2.5
1	B	430	GLN	2.5
1	B	429	GLY	2.5
1	D	456	PRO	2.4
1	D	430	GLN	2.4
1	D	328	GLN	2.4
1	C	301	GLY	2.3
1	C	316	LYS	2.1
1	B	484	TRP	2.1
1	D	426	TYR	2.1
1	D	453	ILE	2.1
1	D	319	GLN	2.1
1	C	196	TRP	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 monosaccharides 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
3	GOL	B	601	6/6	0.77	0.28	38,38,38,38	0
2	CA	C	601	1/1	0.79	0.20	52,52,52,52	0
2	CA	B	602	1/1	0.80	0.34	60,60,60,60	0
3	GOL	D	601	6/6	0.88	0.18	40,40,40,40	0
2	CA	A	601	1/1	0.94	0.28	51,51,51,51	0
2	CA	D	602	1/1	0.95	0.34	65,65,65,65	0

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

There are no such residues in this entry.