



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 09:40 PM JST

PDB ID : 7XSY  
Title : Ligand free structure of branching enzyme isoform 3 (BE3) from *Crocospaera subtropica* ATCC 51142  
Authors : Tamura, T.; Suzuki, E.; Suzuki, R.  
Deposited on : 2022-05-15  
Resolution : 2.50 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.

The types of validation reports are described at

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

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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 : 2.36  
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) : 2.36

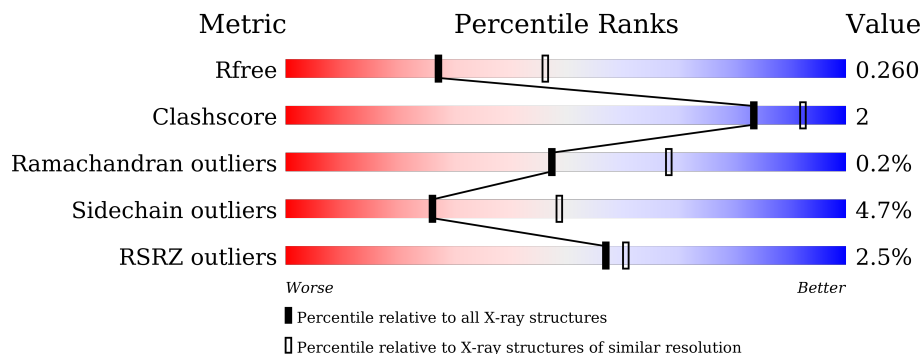
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	667	 88% 7% . .
1	B	667	 86% 9% 5%
1	C	667	 85% 9% . 5%
1	D	667	 84% 9% . 6%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21274 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 1,4-alpha-glucan branching enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	639	5260	3359	913	964	24	0	0	0
1	B	635	5232	3344	907	957	24	0	0	0
1	C	633	5211	3330	904	953	24	0	0	0
1	D	630	5181	3314	897	946	24	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP B1WZK4
A	-18	GLY	-	expression tag	UNP B1WZK4
A	-17	SER	-	expression tag	UNP B1WZK4
A	-16	SER	-	expression tag	UNP B1WZK4
A	-15	HIS	-	expression tag	UNP B1WZK4
A	-14	HIS	-	expression tag	UNP B1WZK4
A	-13	HIS	-	expression tag	UNP B1WZK4
A	-12	HIS	-	expression tag	UNP B1WZK4
A	-11	HIS	-	expression tag	UNP B1WZK4
A	-10	HIS	-	expression tag	UNP B1WZK4
A	-9	SER	-	expression tag	UNP B1WZK4
A	-8	SER	-	expression tag	UNP B1WZK4
A	-7	GLY	-	expression tag	UNP B1WZK4
A	-6	LEU	-	expression tag	UNP B1WZK4
A	-5	VAL	-	expression tag	UNP B1WZK4
A	-4	PRO	-	expression tag	UNP B1WZK4
A	-3	ARG	-	expression tag	UNP B1WZK4
A	-2	GLY	-	expression tag	UNP B1WZK4
A	-1	SER	-	expression tag	UNP B1WZK4
A	0	HIS	-	expression tag	UNP B1WZK4
B	-19	MET	-	initiating methionine	UNP B1WZK4

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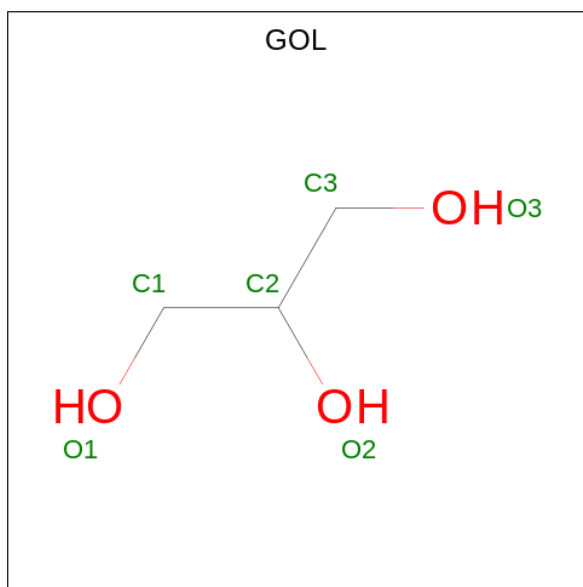
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP B1WZK4
B	-17	SER	-	expression tag	UNP B1WZK4
B	-16	SER	-	expression tag	UNP B1WZK4
B	-15	HIS	-	expression tag	UNP B1WZK4
B	-14	HIS	-	expression tag	UNP B1WZK4
B	-13	HIS	-	expression tag	UNP B1WZK4
B	-12	HIS	-	expression tag	UNP B1WZK4
B	-11	HIS	-	expression tag	UNP B1WZK4
B	-10	HIS	-	expression tag	UNP B1WZK4
B	-9	SER	-	expression tag	UNP B1WZK4
B	-8	SER	-	expression tag	UNP B1WZK4
B	-7	GLY	-	expression tag	UNP B1WZK4
B	-6	LEU	-	expression tag	UNP B1WZK4
B	-5	VAL	-	expression tag	UNP B1WZK4
B	-4	PRO	-	expression tag	UNP B1WZK4
B	-3	ARG	-	expression tag	UNP B1WZK4
B	-2	GLY	-	expression tag	UNP B1WZK4
B	-1	SER	-	expression tag	UNP B1WZK4
B	0	HIS	-	expression tag	UNP B1WZK4
C	-19	MET	-	initiating methionine	UNP B1WZK4
C	-18	GLY	-	expression tag	UNP B1WZK4
C	-17	SER	-	expression tag	UNP B1WZK4
C	-16	SER	-	expression tag	UNP B1WZK4
C	-15	HIS	-	expression tag	UNP B1WZK4
C	-14	HIS	-	expression tag	UNP B1WZK4
C	-13	HIS	-	expression tag	UNP B1WZK4
C	-12	HIS	-	expression tag	UNP B1WZK4
C	-11	HIS	-	expression tag	UNP B1WZK4
C	-10	HIS	-	expression tag	UNP B1WZK4
C	-9	SER	-	expression tag	UNP B1WZK4
C	-8	SER	-	expression tag	UNP B1WZK4
C	-7	GLY	-	expression tag	UNP B1WZK4
C	-6	LEU	-	expression tag	UNP B1WZK4
C	-5	VAL	-	expression tag	UNP B1WZK4
C	-4	PRO	-	expression tag	UNP B1WZK4
C	-3	ARG	-	expression tag	UNP B1WZK4
C	-2	GLY	-	expression tag	UNP B1WZK4
C	-1	SER	-	expression tag	UNP B1WZK4
C	0	HIS	-	expression tag	UNP B1WZK4
D	-19	MET	-	initiating methionine	UNP B1WZK4
D	-18	GLY	-	expression tag	UNP B1WZK4
D	-17	SER	-	expression tag	UNP B1WZK4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP B1WZK4
D	-15	HIS	-	expression tag	UNP B1WZK4
D	-14	HIS	-	expression tag	UNP B1WZK4
D	-13	HIS	-	expression tag	UNP B1WZK4
D	-12	HIS	-	expression tag	UNP B1WZK4
D	-11	HIS	-	expression tag	UNP B1WZK4
D	-10	HIS	-	expression tag	UNP B1WZK4
D	-9	SER	-	expression tag	UNP B1WZK4
D	-8	SER	-	expression tag	UNP B1WZK4
D	-7	GLY	-	expression tag	UNP B1WZK4
D	-6	LEU	-	expression tag	UNP B1WZK4
D	-5	VAL	-	expression tag	UNP B1WZK4
D	-4	PRO	-	expression tag	UNP B1WZK4
D	-3	ARG	-	expression tag	UNP B1WZK4
D	-2	GLY	-	expression tag	UNP B1WZK4
D	-1	SER	-	expression tag	UNP B1WZK4
D	0	HIS	-	expression tag	UNP B1WZK4

- 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	0
			6	3	3		

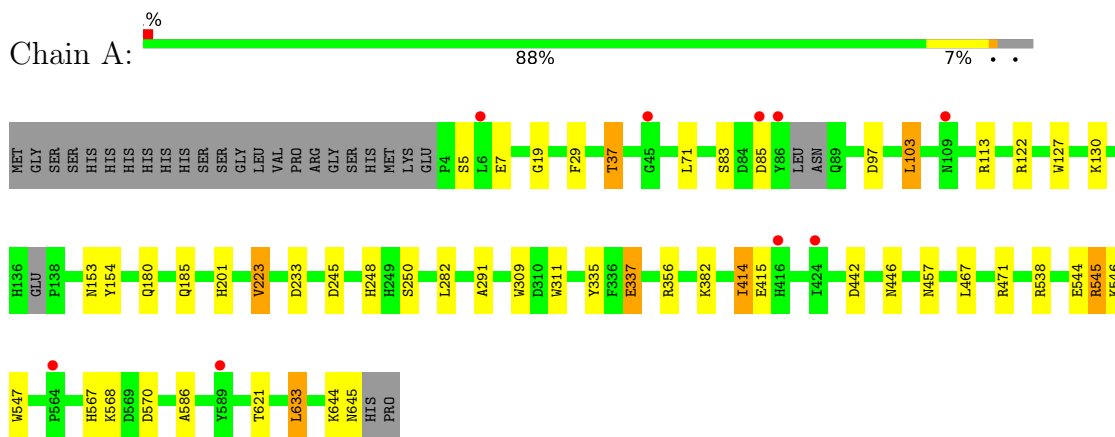
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	111	Total 111	O 111	0	0
3	B	74	Total 74	O 74	0	0
3	C	101	Total 101	O 101	0	0
3	D	92	Total 92	O 92	0	0

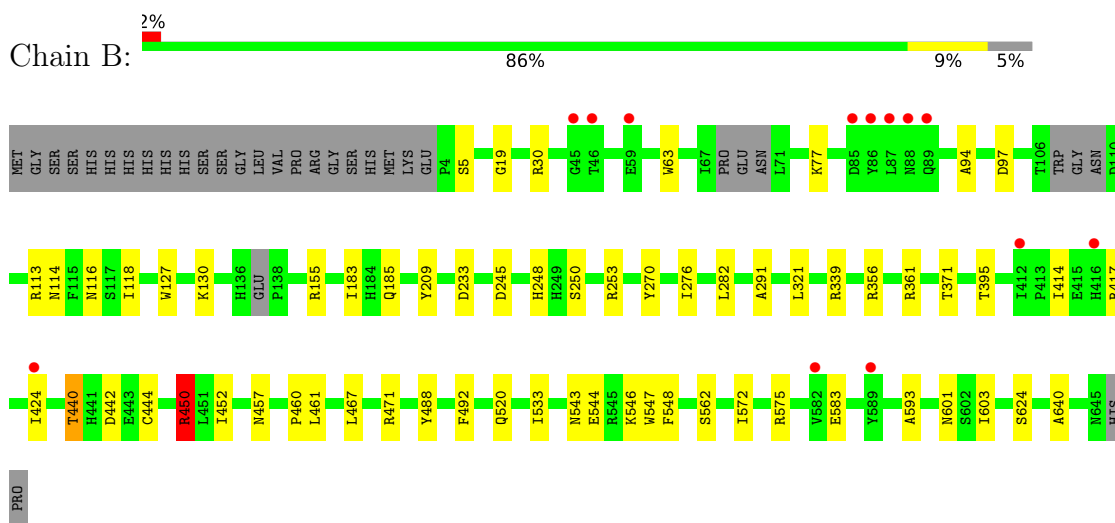
### 3 Residue-property plots [i](#)

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.

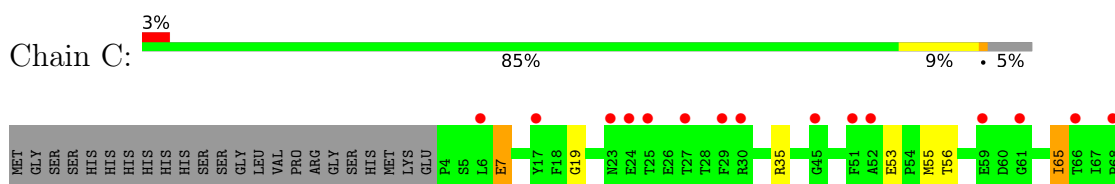
- Molecule 1: 1,4-alpha-glucan branching enzyme

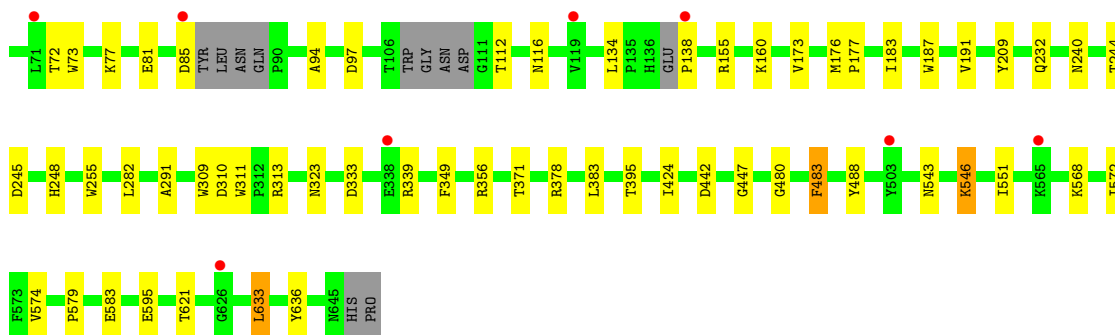


- Molecule 1: 1,4-alpha-glucan branching enzyme

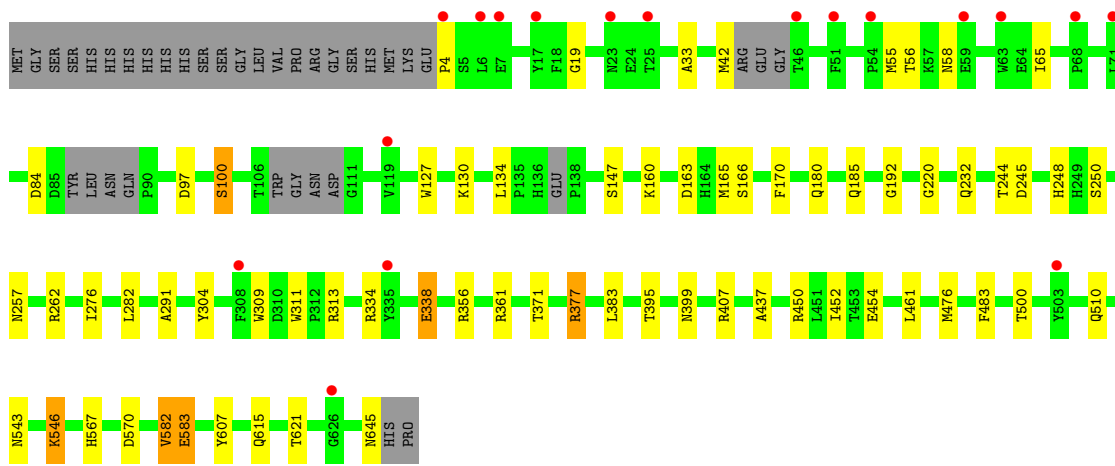
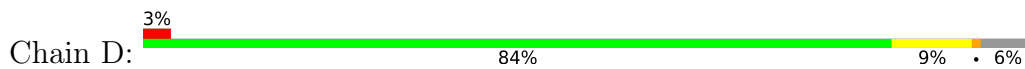


- Molecule 1: 1,4-alpha-glucan branching enzyme





• Molecule 1: 1,4-alpha-glucan branching enzyme





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.05Å 149.91Å 162.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.06 – 2.50 48.06 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.06-2.50) 99.9 (48.06-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.27 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.197 , 0.261 0.202 , 0.260	Depositor DCC
$R_{free}$ test set	6476 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtrriage
Anisotropy	0.028	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21274	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7318e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

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	0.68	0/5433	0.85	0/7390
1	B	0.68	0/5402	0.84	2/7344 (0.0%)
1	C	0.68	0/5381	0.83	1/7315 (0.0%)
1	D	0.67	0/5350	0.84	0/7272
All	All	0.68	0/21566	0.84	3/29321 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	450	ARG	CG-CD-NE	5.53	123.41	111.80
1	C	138	PRO	N-CA-CB	5.20	109.54	103.30
1	B	488	TYR	CB-CA-C	5.14	120.69	110.40

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	5260	0	4881	19	0
1	B	5232	0	4866	26	0
1	C	5211	0	4848	26	0
1	D	5181	0	4816	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	6	0	8	0	0
2	C	6	0	8	1	0
3	A	111	0	0	0	0
3	B	74	0	0	0	0
3	C	101	0	0	0	0
3	D	92	0	0	0	0
All	All	21274	0	19427	97	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 2.

All (97) 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:543:ASN:O	1:C:546:LYS:HD2	1.91	0.69
1:B:414:ILE:HD11	1:B:546:LYS:HG2	1.84	0.59
1:B:127:TRP:CD2	1:B:130:LYS:HG3	2.38	0.59
1:C:155:ARG:HG2	1:C:209:TYR:CD1	2.38	0.58
1:D:97:ASP:O	1:D:100:SER:OG	2.21	0.58
1:C:309:TRP:CE2	1:C:311:TRP:HB3	2.41	0.56
1:D:309:TRP:CE2	1:D:311:TRP:HB3	2.42	0.55
1:B:19:GLY:HA2	1:B:97:ASP:OD2	2.07	0.55
1:C:55:MET:CE	1:C:65:ILE:HG22	2.35	0.55
1:D:437:ALA:HB2	1:D:476:MET:HE2	1.88	0.55
1:A:127:TRP:CE3	1:A:130:LYS:HA	2.44	0.53
1:D:127:TRP:CD1	1:D:130:LYS:HD2	2.43	0.53
1:B:543:ASN:O	1:B:546:LYS:HD2	2.10	0.52
1:B:155:ARG:HG2	1:B:209:TYR:CD1	2.45	0.51
1:A:414:ILE:HG22	1:A:546:LYS:HG3	1.93	0.50
1:B:276:ILE:HG21	1:B:361:ARG:HD2	1.93	0.49
1:C:77:LYS:HD2	1:C:94:ALA:HB1	1.95	0.49
1:C:323:ASN:HB3	1:C:349:PHE:CD1	2.48	0.48
1:B:492:PHE:CZ	1:D:232:GLN:HG3	2.48	0.48
1:C:55:MET:HE2	1:C:65:ILE:HG22	1.94	0.48
1:B:291:ALA:O	1:B:371:THR:HA	2.13	0.47
1:A:335:TYR:CE2	1:A:337:GLU:HA	2.50	0.47
1:B:414:ILE:HD11	1:B:546:LYS:CG	2.45	0.47
1:C:77:LYS:HE2	1:C:116:ASN:OD1	2.14	0.47
1:C:245:ASP:HB3	1:C:248:HIS:O	2.15	0.47
1:D:19:GLY:HA2	1:D:97:ASP:OD2	2.14	0.46
1:B:543:ASN:O	1:B:546:LYS:CD	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:MET:O	1:C:177:PRO:C	2.54	0.46
1:C:447:GLY:HA2	1:C:488:TYR:CE1	2.50	0.46
1:C:240:ASN:HA	1:C:244:THR:O	2.15	0.46
1:A:19:GLY:HA2	1:A:97:ASP:OD2	2.16	0.46
1:D:180:GLN:OE1	1:D:192:GLY:HA3	2.16	0.46
1:D:276:ILE:HG21	1:D:361:ARG:HD2	1.98	0.46
1:A:245:ASP:HB3	1:A:248:HIS:O	2.16	0.46
1:C:155:ARG:HG2	1:C:209:TYR:CG	2.50	0.46
1:C:72:THR:HG22	1:C:73:TRP:CD1	2.51	0.45
1:A:586:ALA:HB2	1:A:633:LEU:HD22	1.98	0.45
1:B:114:ASN:ND2	1:B:116:ASN:OD1	2.47	0.45
1:D:134:LEU:CD2	1:D:220:GLY:CA	2.95	0.45
1:D:55:MET:CG	1:D:65:ILE:HB	2.47	0.45
1:D:567:HIS:ND1	1:D:570:ASP:OD2	2.46	0.45
1:A:414:ILE:N	1:A:414:ILE:HD13	2.32	0.44
1:B:30:ARG:HA	1:B:63:TRP:O	2.17	0.44
1:D:543:ASN:O	1:D:546:LYS:HD2	2.18	0.44
1:D:65:ILE:HD12	1:D:65:ILE:HA	1.90	0.44
1:D:58:ASN:C	1:D:58:ASN:OD1	2.56	0.43
1:B:601:ASN:OD1	1:B:603:ILE:HG12	2.18	0.43
1:C:19:GLY:HA2	1:C:97:ASP:OD2	2.18	0.43
1:B:492:PHE:CE2	1:D:232:GLN:HG3	2.53	0.43
1:C:595:GLU:HG2	1:C:621:THR:CG2	2.48	0.43
1:D:163:ASP:O	1:D:166:SER:HB3	2.18	0.43
1:A:153:ASN:HA	1:A:201:HIS:O	2.18	0.43
1:A:223:VAL:O	1:A:291:ALA:HA	2.19	0.43
1:A:545:ARG:HB3	1:A:547:TRP:CD1	2.54	0.43
1:D:127:TRP:CG	1:D:130:LYS:HD2	2.54	0.43
1:B:440:THR:HG22	1:B:442:ASP:H	1.84	0.42
1:B:444:CYS:HB3	1:B:450:ARG:HD3	2.01	0.42
1:B:572:ILE:O	1:B:640:ALA:HA	2.18	0.42
1:B:245:ASP:HB3	1:B:248:HIS:O	2.19	0.42
1:C:574:VAL:CG1	1:C:633:LEU:HD21	2.50	0.42
1:B:547:TRP:HA	1:B:575:ARG:O	2.20	0.42
1:D:291:ALA:O	1:D:371:THR:HA	2.20	0.42
1:D:304:TYR:CE2	1:D:377:ARG:HD3	2.54	0.42
1:B:467:LEU:O	1:B:471:ARG:HG3	2.19	0.42
1:C:7:GLU:HA	1:C:7:GLU:OE1	2.19	0.42
1:B:457:ASN:O	1:B:460:PRO:HD2	2.20	0.42
1:A:19:GLY:O	1:A:29:PHE:HA	2.19	0.42
1:A:446:ASN:HA	1:C:255:TRP:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ALA:O	1:C:371:THR:HA	2.20	0.42
1:A:103:LEU:HD22	1:A:180:GLN:HG3	2.01	0.41
1:C:551:ILE:HG12	1:C:572:ILE:HD13	2.02	0.41
1:A:154:TYR:CZ	1:A:201:HIS:HB2	2.55	0.41
1:D:483:PHE:CD2	1:D:500:THR:HG22	2.55	0.41
1:A:567:HIS:ND1	1:A:570:ASP:OD2	2.52	0.41
1:D:134:LEU:HD23	1:D:220:GLY:CA	2.50	0.41
1:A:309:TRP:CE2	1:A:311:TRP:HB3	2.55	0.41
1:D:248:HIS:CG	1:D:262:ARG:HB3	2.55	0.41
1:A:37:THR:HG21	1:A:83:SER:OG	2.20	0.41
1:B:548:PHE:CZ	1:B:575:ARG:HD3	2.55	0.41
1:C:187:TRP:CE2	2:C:701:GOL:H2	2.56	0.41
1:D:165:MET:SD	1:D:170:PHE:HB2	2.60	0.41
1:C:480:GLY:HA2	1:C:483:PHE:CE1	2.56	0.41
1:B:452:ILE:HD13	1:B:461:LEU:HD22	2.03	0.41
1:D:510:GLN:HB3	1:D:607:TYR:O	2.21	0.41
1:D:55:MET:HG2	1:D:65:ILE:HB	2.03	0.41
1:B:593:ALA:HA	1:B:624:SER:OG	2.20	0.40
1:C:55:MET:HE3	1:C:65:ILE:HG22	2.01	0.40
1:D:407:ARG:HB3	1:D:454:GLU:OE2	2.20	0.40
1:D:582:VAL:HG13	1:D:583:GLU:N	2.36	0.40
1:A:467:LEU:O	1:A:471:ARG:HG3	2.21	0.40
1:C:323:ASN:HB3	1:C:349:PHE:CE1	2.56	0.40
1:B:77:LYS:HE2	1:B:94:ALA:HB1	2.04	0.40
1:B:270:TYR:CD1	1:B:270:TYR:C	2.95	0.40
1:C:579:PRO:HB3	1:C:636:TYR:CZ	2.56	0.40
1:D:245:ASP:HB3	1:D:248:HIS:O	2.21	0.40
1:D:257:ASN:ND2	1:D:309:TRP:HB3	2.35	0.40
1:A:644:LYS:O	1:A:645:ASN:C	2.59	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	633/667 (95%)	607 (96%)	26 (4%)	0	100	100
1	B	627/667 (94%)	603 (96%)	24 (4%)	0	100	100
1	C	625/667 (94%)	593 (95%)	31 (5%)	1 (0%)	47	68
1	D	620/667 (93%)	579 (93%)	37 (6%)	4 (1%)	25	43
All	All	2505/2668 (94%)	2382 (95%)	118 (5%)	5 (0%)	47	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	84	ASP
1	D	338	GLU
1	D	399	ASN
1	C	65	ILE
1	D	33	ALA

### 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	553/579 (96%)	527 (95%)	26 (5%)	26	49
1	B	551/579 (95%)	529 (96%)	22 (4%)	31	56
1	C	549/579 (95%)	520 (95%)	29 (5%)	22	43
1	D	545/579 (94%)	519 (95%)	26 (5%)	25	48
All	All	2198/2316 (95%)	2095 (95%)	103 (5%)	26	49

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	7	GLU
1	A	37	THR
1	A	71	LEU
1	A	85	ASP
1	A	103	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	113	ARG
1	A	122	ARG
1	A	185	GLN
1	A	223	VAL
1	A	233	ASP
1	A	250	SER
1	A	282	LEU
1	A	337	GLU
1	A	356	ARG
1	A	382	LYS
1	A	414	ILE
1	A	415	GLU
1	A	442	ASP
1	A	457	ASN
1	A	538	ARG
1	A	544	GLU
1	A	545	ARG
1	A	568	LYS
1	A	621	THR
1	A	633	LEU
1	B	5	SER
1	B	113	ARG
1	B	118	ILE
1	B	183	ILE
1	B	185	GLN
1	B	233	ASP
1	B	250	SER
1	B	253	ARG
1	B	282	LEU
1	B	321	LEU
1	B	339	ARG
1	B	356	ARG
1	B	395	THR
1	B	417	ARG
1	B	424	ILE
1	B	440	THR
1	B	450	ARG
1	B	520	GLN
1	B	533	ILE
1	B	544	GLU
1	B	562	SER
1	B	583	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	7	GLU
1	C	35	ARG
1	C	53	GLU
1	C	56	THR
1	C	81	GLU
1	C	85	ASP
1	C	112	THR
1	C	134	LEU
1	C	160	LYS
1	C	173	VAL
1	C	183	ILE
1	C	191	VAL
1	C	232	GLN
1	C	282	LEU
1	C	310	ASP
1	C	313	ARG
1	C	333	ASP
1	C	339	ARG
1	C	356	ARG
1	C	378	ARG
1	C	383	LEU
1	C	395	THR
1	C	424	ILE
1	C	442	ASP
1	C	483	PHE
1	C	546	LYS
1	C	568	LYS
1	C	583	GLU
1	C	633	LEU
1	D	4	PRO
1	D	42	MET
1	D	56	THR
1	D	100	SER
1	D	147	SER
1	D	160	LYS
1	D	185	GLN
1	D	244	THR
1	D	250	SER
1	D	282	LEU
1	D	313	ARG
1	D	334	ARG
1	D	338	GLU

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Mol	Chain	Res	Type
1	D	356	ARG
1	D	377	ARG
1	D	383	LEU
1	D	395	THR
1	D	450	ARG
1	D	452	ILE
1	D	461	LEU
1	D	546	LYS
1	D	582	VAL
1	D	583	GLU
1	D	615	GLN
1	D	621	THR
1	D	645	ASN

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

Mol	Chain	Res	Type
1	B	131	HIS

### 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](#)

2 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	701	-	5,5,5	0.17	0	5,5,5	0.40	0
2	GOL	C	701	-	5,5,5	0.19	0	5,5,5	0.41	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	701	-	-	4/4/4/4	-
2	GOL	C	701	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	701	GOL	O1-C1-C2-C3
2	C	701	GOL	O1-C1-C2-O2
2	A	701	GOL	O1-C1-C2-C3
2	A	701	GOL	C1-C2-C3-O3
2	A	701	GOL	O1-C1-C2-O2
2	A	701	GOL	O2-C2-C3-O3
2	C	701	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	GOL	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	639/667 (95%)	0.01	9 (1%) 75 77	26, 42, 77, 108	0
1	B	635/667 (95%)	0.11	13 (2%) 65 68	31, 47, 80, 104	0
1	C	633/667 (94%)	0.16	23 (3%) 42 46	28, 46, 80, 106	0
1	D	630/667 (94%)	0.08	18 (2%) 51 55	27, 48, 87, 114	0
All	All	2537/2668 (95%)	0.09	63 (2%) 57 61	26, 45, 82, 114	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	416	HIS	5.1
1	B	85	ASP	4.7
1	C	66	THR	4.6
1	C	68	PRO	4.2
1	D	17	TYR	3.7
1	A	6	LEU	3.6
1	C	29	PHE	3.5
1	B	45	GLY	3.5
1	A	85	ASP	3.4
1	A	109	ASN	3.4
1	D	119	VAL	3.4
1	D	4	PRO	3.2
1	A	564	PRO	3.2
1	C	52	ALA	3.2
1	A	86	TYR	3.1
1	B	86	TYR	3.1
1	C	30	ARG	3.1
1	C	61	GLY	3.0
1	D	308	PHE	3.0
1	B	89	GLN	3.0
1	C	59	GLU	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	6	LEU	2.9
1	B	582	VAL	2.9
1	D	503	TYR	2.9
1	D	59	GLU	2.9
1	C	51	PHE	2.9
1	C	626	GLY	2.8
1	D	25	THR	2.8
1	B	88	ASN	2.8
1	D	68	PRO	2.8
1	D	71	LEU	2.7
1	B	416	HIS	2.7
1	B	424	ILE	2.6
1	D	63	TRP	2.6
1	C	565	LYS	2.6
1	C	23	ASN	2.6
1	D	7	GLU	2.6
1	C	503	TYR	2.6
1	A	589	TYR	2.5
1	C	24	GLU	2.5
1	C	27	THR	2.5
1	B	87	LEU	2.4
1	C	45	GLY	2.4
1	B	589	TYR	2.4
1	C	17	TYR	2.4
1	D	54	PRO	2.4
1	B	46	THR	2.4
1	C	6	LEU	2.4
1	D	626	GLY	2.3
1	C	119	VAL	2.3
1	A	424	ILE	2.3
1	A	45	GLY	2.3
1	C	25	THR	2.3
1	D	46	THR	2.3
1	D	51	PHE	2.2
1	C	338	GLU	2.2
1	B	412	ILE	2.2
1	C	138	PRO	2.1
1	C	71	LEU	2.1
1	C	85	ASP	2.1
1	D	23	ASN	2.1
1	D	335	TYR	2.0
1	B	59	GLU	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(Å <sup>2</sup> )	Q<0.9
2	GOL	A	701	6/6	0.89	0.12	59,66,68,68	0
2	GOL	C	701	6/6	0.91	0.20	43,48,54,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.