



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 02:56 PM JST

PDB ID : 7YP4  
Title : Crystal structure of elaiophylin glycosyltransferase in apo-form  
Authors : Xu, T.; Liu, Q.; Gan, Q.; Liu, J.  
Deposited on : 2022-08-02  
Resolution : 3.10 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

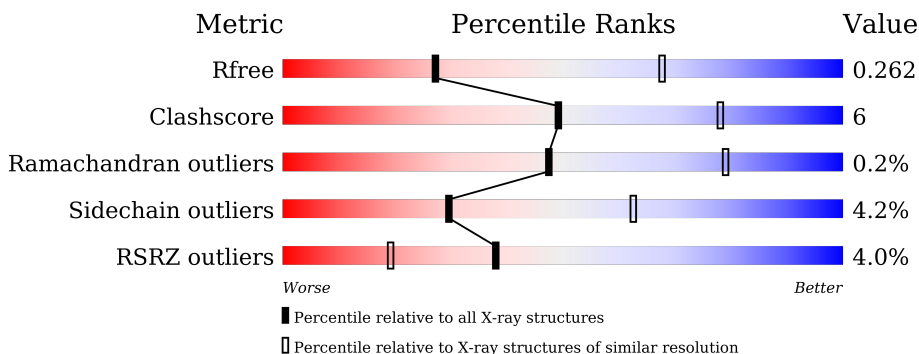
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	437	 78% 14% • 7%
1	B	437	 77% 16% • 5%
1	C	437	 10% 73% 15% • 10%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 9604 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 Glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	407	Total 3192	C 2033	N 559	O 588	S 12	0	0	0
1	B	416	Total 3259	C 2074	N 572	O 600	S 13	0	0	0
1	C	394	Total 3092	C 1970	N 545	O 565	S 12	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

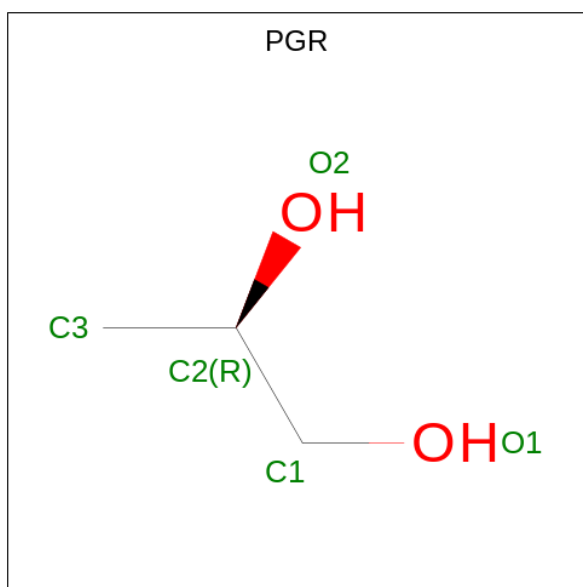
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP E5L4T5
A	-18	GLY	-	expression tag	UNP E5L4T5
A	-17	SER	-	expression tag	UNP E5L4T5
A	-16	SER	-	expression tag	UNP E5L4T5
A	-15	HIS	-	expression tag	UNP E5L4T5
A	-14	HIS	-	expression tag	UNP E5L4T5
A	-13	HIS	-	expression tag	UNP E5L4T5
A	-12	HIS	-	expression tag	UNP E5L4T5
A	-11	HIS	-	expression tag	UNP E5L4T5
A	-10	HIS	-	expression tag	UNP E5L4T5
A	-9	SER	-	expression tag	UNP E5L4T5
A	-8	SER	-	expression tag	UNP E5L4T5
A	-7	GLY	-	expression tag	UNP E5L4T5
A	-6	LEU	-	expression tag	UNP E5L4T5
A	-5	VAL	-	expression tag	UNP E5L4T5
A	-4	PRO	-	expression tag	UNP E5L4T5
A	-3	ARG	-	expression tag	UNP E5L4T5
A	-2	GLY	-	expression tag	UNP E5L4T5
A	-1	SER	-	expression tag	UNP E5L4T5
A	0	HIS	-	expression tag	UNP E5L4T5
B	-19	MET	-	initiating methionine	UNP E5L4T5
B	-18	GLY	-	expression tag	UNP E5L4T5
B	-17	SER	-	expression tag	UNP E5L4T5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP E5L4T5
B	-15	HIS	-	expression tag	UNP E5L4T5
B	-14	HIS	-	expression tag	UNP E5L4T5
B	-13	HIS	-	expression tag	UNP E5L4T5
B	-12	HIS	-	expression tag	UNP E5L4T5
B	-11	HIS	-	expression tag	UNP E5L4T5
B	-10	HIS	-	expression tag	UNP E5L4T5
B	-9	SER	-	expression tag	UNP E5L4T5
B	-8	SER	-	expression tag	UNP E5L4T5
B	-7	GLY	-	expression tag	UNP E5L4T5
B	-6	LEU	-	expression tag	UNP E5L4T5
B	-5	VAL	-	expression tag	UNP E5L4T5
B	-4	PRO	-	expression tag	UNP E5L4T5
B	-3	ARG	-	expression tag	UNP E5L4T5
B	-2	GLY	-	expression tag	UNP E5L4T5
B	-1	SER	-	expression tag	UNP E5L4T5
B	0	HIS	-	expression tag	UNP E5L4T5
C	-19	MET	-	initiating methionine	UNP E5L4T5
C	-18	GLY	-	expression tag	UNP E5L4T5
C	-17	SER	-	expression tag	UNP E5L4T5
C	-16	SER	-	expression tag	UNP E5L4T5
C	-15	HIS	-	expression tag	UNP E5L4T5
C	-14	HIS	-	expression tag	UNP E5L4T5
C	-13	HIS	-	expression tag	UNP E5L4T5
C	-12	HIS	-	expression tag	UNP E5L4T5
C	-11	HIS	-	expression tag	UNP E5L4T5
C	-10	HIS	-	expression tag	UNP E5L4T5
C	-9	SER	-	expression tag	UNP E5L4T5
C	-8	SER	-	expression tag	UNP E5L4T5
C	-7	GLY	-	expression tag	UNP E5L4T5
C	-6	LEU	-	expression tag	UNP E5L4T5
C	-5	VAL	-	expression tag	UNP E5L4T5
C	-4	PRO	-	expression tag	UNP E5L4T5
C	-3	ARG	-	expression tag	UNP E5L4T5
C	-2	GLY	-	expression tag	UNP E5L4T5
C	-1	SER	-	expression tag	UNP E5L4T5
C	0	HIS	-	expression tag	UNP E5L4T5

- Molecule 2 is R-1,2-PROPANEDIOL (three-letter code: PGR) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			5	3	2		
2	A	1	Total	C	O	0	0
			5	3	2		
2	A	1	Total	C	O	0	0
			5	3	2		
2	B	1	Total	C	O	0	0
			5	3	2		
2	B	1	Total	C	O	0	0
			5	3	2		
2	B	1	Total	C	O	0	0
			5	3	2		
2	C	1	Total	C	O	0	0
			5	3	2		

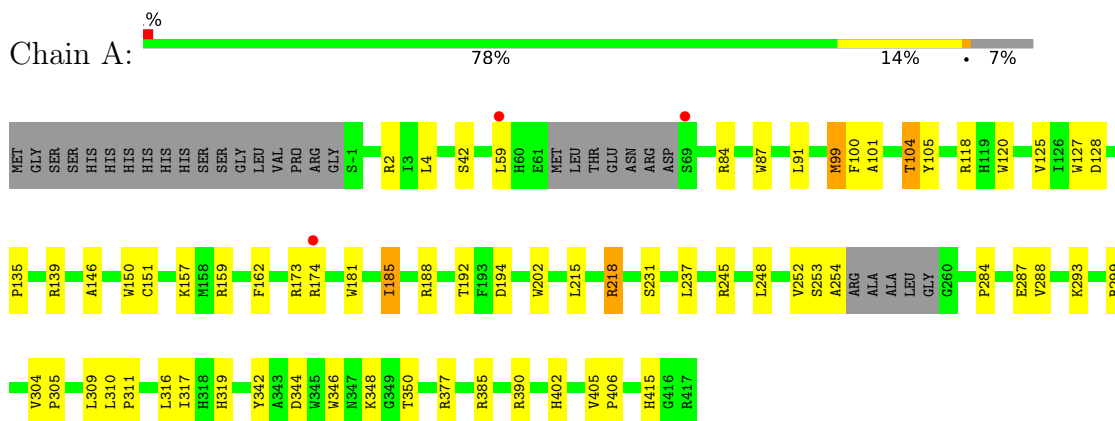
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	11	Total	O	0	0
			11	11		

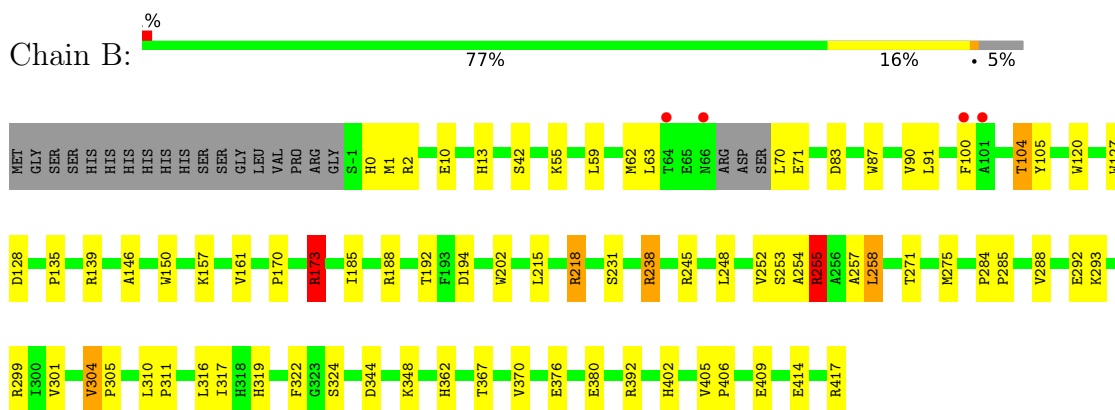
### 3 Residue-property plots [i](#)

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.

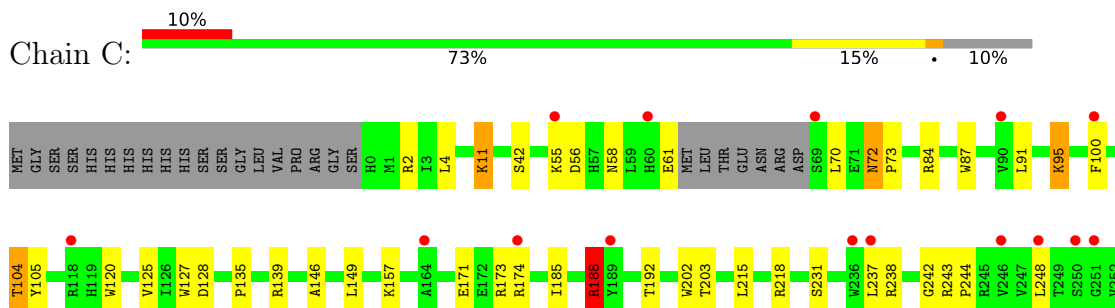
- Molecule 1: Glycosyltransferase

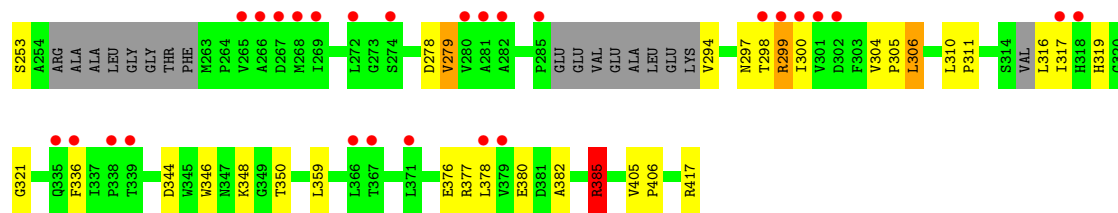


- Molecule 1: Glycosyltransferase



- Molecule 1: Glycosyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.37Å 131.21Å 225.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.69 – 3.10 65.61 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (65.69-3.10) 99.7 (65.61-3.10)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 3.13Å)	Xtrriage
Refinement program	REFMAC 5.8.0352	Depositor
R, $R_{free}$	0.214 , 0.265 0.218 , 0.262	Depositor DCC
$R_{free}$ test set	1850 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.0	Xtrriage
Anisotropy	0.360	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 76.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9604	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: PGR

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	0.46	0/3280	0.76	0/4484
1	B	0.44	0/3348	0.75	0/4577
1	C	0.39	0/3177	0.72	0/4342
All	All	0.43	0/9805	0.75	0/13403

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	8
1	C	0	10
All	All	0	27

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ARG	Sidechain
1	A	174	ARG	Sidechain
1	A	188	ARG	Sidechain
1	A	218	ARG	Sidechain
1	A	245	ARG	Sidechain
1	A	299	ARG	Sidechain
1	A	385	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	390	ARG	Sidechain
1	A	84	ARG	Sidechain
1	B	173	ARG	Sidechain
1	B	218	ARG	Sidechain
1	B	238	ARG	Sidechain
1	B	245	ARG	Sidechain
1	B	255	ARG	Sidechain
1	B	299	ARG	Sidechain
1	B	392	ARG	Sidechain
1	B	417	ARG	Sidechain
1	C	139	ARG	Sidechain
1	C	173	ARG	Sidechain
1	C	174	ARG	Sidechain
1	C	188	ARG	Sidechain
1	C	218	ARG	Sidechain
1	C	238	ARG	Sidechain
1	C	299	ARG	Sidechain
1	C	385	ARG	Sidechain
1	C	417	ARG	Sidechain
1	C	84	ARG	Sidechain

## 5.2 Too-close contacts

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	3192	0	3129	38	0
1	B	3259	0	3201	38	0
1	C	3092	0	3032	38	0
2	A	15	0	24	3	0
2	B	15	0	24	3	0
2	C	5	0	8	1	0
3	A	15	0	0	0	0
3	B	11	0	0	1	0
All	All	9604	0	9418	112	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 6.

All (112) 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:A:304:VAL:HG11	1:A:309:LEU:HD22	1.37	1.03
1:A:173:ARG:HH21	1:A:173:ARG:HG2	1.45	0.81
1:B:258:LEU:HD22	1:B:258:LEU:O	1.84	0.76
1:A:139:ARG:HH22	1:A:194:ASP:HB3	1.61	0.66
1:A:100:PHE:O	1:A:104:THR:OG1	2.15	0.65
1:C:100:PHE:O	1:C:104:THR:OG1	2.14	0.65
1:B:100:PHE:O	1:B:104:THR:OG1	2.14	0.64
1:C:188:ARG:HH21	1:C:188:ARG:HB2	1.63	0.62
1:A:231:SER:HB2	1:A:305:PRO:HB3	1.80	0.62
1:A:99:MET:SD	1:C:95:LYS:HB3	2.39	0.62
1:A:304:VAL:CG1	1:A:309:LEU:HD22	2.22	0.62
1:A:157:LYS:HD2	1:A:215:LEU:HD21	1.82	0.61
1:A:101:ALA:HB1	2:A:502:PGR:H31	1.82	0.61
1:A:159:ARG:NH1	1:A:162:PHE:CE2	2.69	0.60
1:A:252:VAL:HG23	2:A:503:PGR:H31	1.82	0.59
1:C:306:LEU:HD13	1:C:310:LEU:HG	1.83	0.59
1:B:231:SER:HB2	1:B:305:PRO:HB3	1.85	0.58
1:C:58:ASN:HD22	1:C:61:GLU:HB2	1.69	0.58
1:C:11:LYS:HD3	1:C:11:LYS:H	1.69	0.57
1:A:87:TRP:CZ2	1:A:91:LEU:HD22	2.41	0.56
1:A:173:ARG:HG2	1:A:173:ARG:NH2	2.17	0.56
1:B:59:LEU:CD2	1:B:63:LEU:HD13	2.36	0.56
1:C:377:ARG:HH21	1:C:377:ARG:HG2	1.71	0.55
1:A:252:VAL:CG2	2:A:503:PGR:H31	2.36	0.55
1:C:87:TRP:CZ2	1:C:91:LEU:HD22	2.42	0.55
1:C:294:VAL:HG13	1:C:300:ILE:HD11	1.88	0.54
1:A:59:LEU:O	1:A:59:LEU:HD23	2.07	0.54
1:C:299:ARG:HG3	1:C:299:ARG:HH11	1.72	0.53
1:C:127:TRP:CD2	1:C:135:PRO:HD3	2.44	0.53
1:B:252:VAL:HG23	2:B:503:PGR:H2	1.89	0.53
1:B:87:TRP:CZ2	1:B:91:LEU:HD22	2.43	0.53
1:A:127:TRP:CD2	1:A:135:PRO:HD3	2.44	0.53
1:C:279:VAL:HG13	1:C:298:THR:HA	1.90	0.52
1:B:139:ARG:HH22	1:B:194:ASP:HB2	1.74	0.52
1:B:253:SER:O	1:B:255:ARG:N	2.31	0.52
1:A:139:ARG:NH2	1:A:194:ASP:HB3	2.23	0.52
1:B:127:TRP:CD2	1:B:135:PRO:HD3	2.44	0.52
1:A:346:TRP:O	1:A:350:THR:HG23	2.10	0.51
1:C:376:GLU:O	1:C:380:GLU:HG2	2.11	0.51
1:C:321:GLY:HA3	2:C:501:PGR:C3	2.40	0.50
1:A:218:ARG:NH1	1:A:415:HIS:NE2	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:TRP:O	1:C:350:THR:HG23	2.11	0.50
1:C:149:LEU:HD13	1:C:203:THR:HG23	1.94	0.50
1:A:377:ARG:HH21	1:A:377:ARG:HG3	1.77	0.49
1:A:284:PRO:O	1:A:288:VAL:HG23	2.13	0.48
1:B:238:ARG:HG3	1:B:238:ARG:HH21	1.77	0.48
1:C:157:LYS:HD3	1:C:215:LEU:HD21	1.96	0.48
1:B:59:LEU:HD23	1:B:59:LEU:O	2.13	0.47
1:B:218:ARG:NH1	1:B:414:GLU:OE2	2.47	0.47
1:C:72:ASN:ND2	1:C:73:PRO:HD2	2.29	0.47
1:C:231:SER:HB2	1:C:305:PRO:HB3	1.96	0.47
1:A:237:LEU:HD11	1:A:309:LEU:HD12	1.97	0.47
1:B:1:MET:HE2	1:B:409:GLU:HG2	1.96	0.46
1:B:2:ARG:HG2	1:B:120:TRP:CZ2	2.50	0.46
1:A:248:LEU:HD12	1:A:317:ILE:HB	1.98	0.46
1:C:310:LEU:N	1:C:311:PRO:CD	2.79	0.46
1:A:253:SER:O	1:A:254:ALA:HB3	2.15	0.46
1:B:0:HIS:HB3	3:B:601:HOH:O	2.16	0.46
1:A:402:HIS:CD2	1:B:402:HIS:CD2	3.04	0.45
1:A:310:LEU:N	1:A:311:PRO:CD	2.80	0.45
1:B:253:SER:C	1:B:255:ARG:H	2.18	0.45
1:B:310:LEU:N	1:B:311:PRO:CD	2.79	0.45
1:A:344:ASP:OD2	1:A:348:LYS:HE3	2.17	0.45
1:A:405:VAL:N	1:A:406:PRO:HD2	2.32	0.45
1:B:170:PRO:HG2	1:B:173:ARG:HG3	1.99	0.45
1:C:317:ILE:HD13	1:C:336:PHE:HB3	1.98	0.45
1:C:248:LEU:HD12	1:C:317:ILE:HB	1.99	0.45
1:B:376:GLU:O	1:B:380:GLU:HG2	2.17	0.44
1:C:2:ARG:HG2	1:C:120:TRP:CZ2	2.52	0.44
1:A:2:ARG:HG2	1:A:120:TRP:CZ2	2.52	0.44
1:C:405:VAL:N	1:C:406:PRO:HD2	2.32	0.44
1:B:10:GLU:HB2	1:B:13:HIS:CD2	2.53	0.44
1:C:188:ARG:O	1:C:188:ARG:HG3	2.15	0.44
1:B:405:VAL:N	1:B:406:PRO:HD2	2.32	0.44
1:B:146:ALA:HB2	1:B:202:TRP:CE2	2.53	0.44
1:B:271:THR:HG22	1:B:275:MET:CE	2.48	0.44
1:C:55:LYS:HD2	1:C:56:ASP:H	1.83	0.44
1:B:322:PHE:H	2:B:502:PGR:H2	1.82	0.43
1:C:242:GLY:N	1:C:278:ASP:OD2	2.51	0.43
1:B:301:VAL:HG21	1:B:304:VAL:CG1	2.49	0.43
1:B:248:LEU:HD12	1:B:317:ILE:HB	2.00	0.43
1:B:344:ASP:OD2	1:B:348:LYS:HE3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:LEU:HG	1:C:378:LEU:HD21	1.99	0.43
1:A:173:ARG:NH2	1:A:173:ARG:CG	2.82	0.43
1:B:157:LYS:HD3	1:B:215:LEU:HD21	2.01	0.43
1:C:146:ALA:HB2	1:C:202:TRP:CE2	2.54	0.43
1:C:279:VAL:HG13	1:C:297:ASN:O	2.19	0.42
1:C:310:LEU:HD11	1:C:316:LEU:HD22	2.00	0.42
1:C:382:ALA:HA	1:C:385:ARG:HH22	1.83	0.42
1:A:287:GLU:HA	1:A:287:GLU:OE1	2.19	0.42
1:B:284:PRO:O	1:B:288:VAL:HG23	2.19	0.42
1:B:71:GLU:OE2	1:B:362:HIS:NE2	2.53	0.42
1:B:90:VAL:HG21	1:B:161:VAL:HG12	2.01	0.42
1:B:367:THR:OG1	1:B:370:VAL:HG23	2.20	0.42
1:A:146:ALA:HB2	1:A:202:TRP:CE2	2.55	0.42
1:B:70:LEU:HD11	1:B:257:ALA:O	2.19	0.41
1:B:150:TRP:CZ3	2:B:502:PGR:H12	2.55	0.41
1:B:319:HIS:CD2	1:B:319:HIS:H	2.37	0.41
1:A:342:TYR:CD1	1:A:342:TYR:C	2.93	0.41
1:C:319:HIS:CD2	1:C:319:HIS:H	2.38	0.41
1:C:378:LEU:O	1:C:385:ARG:NH1	2.53	0.41
1:A:150:TRP:CZ3	1:A:151:CYS:HB3	2.55	0.41
1:A:181:TRP:O	1:A:185:ILE:HG13	2.20	0.41
1:B:284:PRO:O	1:B:285:PRO:C	2.58	0.41
1:C:382:ALA:HA	1:C:385:ARG:NH2	2.35	0.41
1:A:310:LEU:HD11	1:A:316:LEU:HD22	2.03	0.41
1:A:319:HIS:H	1:A:319:HIS:CD2	2.39	0.41
1:B:316:LEU:HD21	1:B:324:SER:HB3	2.03	0.41
1:A:4:LEU:HB3	1:A:125:VAL:HG22	2.03	0.40
1:C:4:LEU:HB3	1:C:125:VAL:HG22	2.04	0.40
1:C:317:ILE:CD1	1:C:336:PHE:HB3	2.51	0.40
1:C:344:ASP:OD2	1:C:348:LYS:HE3	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	401/437 (92%)	388 (97%)	13 (3%)	0	100	100
1	B	412/437 (94%)	391 (95%)	20 (5%)	1 (0%)	47	79
1	C	384/437 (88%)	367 (96%)	16 (4%)	1 (0%)	41	73
All	All	1197/1311 (91%)	1146 (96%)	49 (4%)	2 (0%)	47	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	253	SER
1	B	254	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	342/366 (93%)	334 (98%)	8 (2%)	50	77
1	B	348/366 (95%)	332 (95%)	16 (5%)	27	59
1	C	331/366 (90%)	312 (94%)	19 (6%)	20	52
All	All	1021/1098 (93%)	978 (96%)	43 (4%)	30	62

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	SER
1	A	99	MET
1	A	104	THR
1	A	105	TYR
1	A	128	ASP
1	A	185	ILE
1	A	192	THR
1	A	293	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	42	SER
1	B	55	LYS
1	B	62	MET
1	B	83	ASP
1	B	104	THR
1	B	105	TYR
1	B	128	ASP
1	B	173	ARG
1	B	185	ILE
1	B	188	ARG
1	B	192	THR
1	B	255	ARG
1	B	258	LEU
1	B	292	GLU
1	B	293	LYS
1	B	304	VAL
1	C	11	LYS
1	C	42	SER
1	C	70	LEU
1	C	72	ASN
1	C	95	LYS
1	C	104	THR
1	C	105	TYR
1	C	128	ASP
1	C	171	GLU
1	C	185	ILE
1	C	188	ARG
1	C	192	THR
1	C	237	LEU
1	C	243	ARG
1	C	244	PRO
1	C	279	VAL
1	C	304	VAL
1	C	306	LEU
1	C	385	ARG

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	13	HIS
1	B	119	HIS
1	B	228	ASN

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Mol	Chain	Res	Type
1	B	402	HIS
1	C	103	GLN
1	C	119	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](#)

7 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	PGR	B	503	-	3,4,4	0.27	0	1,4,4	0.84	0
2	PGR	B	502	-	3,4,4	0.26	0	1,4,4	0.12	0
2	PGR	A	501	-	3,4,4	0.19	0	1,4,4	0.32	0
2	PGR	B	501	-	3,4,4	0.26	0	1,4,4	0.34	0
2	PGR	A	503	-	3,4,4	0.34	0	1,4,4	0.06	0
2	PGR	A	502	-	3,4,4	0.54	0	1,4,4	0.43	0
2	PGR	C	501	-	3,4,4	0.20	0	1,4,4	0.66	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	PGR	B	503	-	-	0/2/2/2	-
2	PGR	B	502	-	-	2/2/2/2	-
2	PGR	A	501	-	-	2/2/2/2	-
2	PGR	B	501	-	-	2/2/2/2	-
2	PGR	A	503	-	-	1/2/2/2	-
2	PGR	A	502	-	-	0/2/2/2	-
2	PGR	C	501	-	-	2/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PGR	O1-C1-C2-C3
2	B	501	PGR	O1-C1-C2-O2
2	B	502	PGR	O1-C1-C2-O2
2	C	501	PGR	O1-C1-C2-C3
2	C	501	PGR	O1-C1-C2-O2
2	B	501	PGR	O1-C1-C2-C3
2	B	502	PGR	O1-C1-C2-C3
2	A	501	PGR	O1-C1-C2-O2
2	A	503	PGR	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	503	PGR	1	0
2	B	502	PGR	2	0
2	A	503	PGR	2	0
2	A	502	PGR	1	0
2	C	501	PGR	1	0

## 5.7 Other polymers [\(i\)](#)

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	407/437 (93%)	0.18	3 (0%) 87 75	34, 63, 120, 169	0
1	B	416/437 (95%)	0.24	4 (0%) 82 67	37, 73, 133, 181	0
1	C	394/437 (90%)	0.70	42 (10%) 6 2	61, 118, 177, 225	0
All	All	1217/1311 (92%)	0.37	49 (4%) 38 19	34, 81, 159, 225	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	SER	6.3
1	C	338	PRO	4.7
1	C	339	THR	4.5
1	C	366	LEU	4.3
1	C	367	THR	4.3
1	C	272	LEU	4.2
1	C	269	ILE	4.2
1	C	301	VAL	4.1
1	C	100	PHE	4.1
1	C	268	MET	3.9
1	C	280	VAL	3.9
1	C	300	ILE	3.6
1	C	336	PHE	3.4
1	C	317	ILE	3.3
1	C	69	SER	3.3
1	C	246	VAL	3.1
1	C	267	ASP	3.1
1	C	237	LEU	3.1
1	C	250	SER	3.0
1	C	248	LEU	2.8
1	C	55	LYS	2.8
1	B	100	PHE	2.8
1	C	299	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	274	SER	2.7
1	C	251	GLY	2.7
1	C	282	ALA	2.6
1	C	335	GLN	2.6
1	B	101	ALA	2.6
1	C	265	VAL	2.5
1	C	189	TYR	2.5
1	C	236	TRP	2.5
1	B	66	ASN	2.5
1	C	285	PRO	2.4
1	C	298	THR	2.4
1	A	59	LEU	2.4
1	C	281	ALA	2.3
1	C	378	LEU	2.3
1	A	174	ARG	2.3
1	C	371	LEU	2.3
1	C	118	ARG	2.3
1	C	90	VAL	2.3
1	C	302	ASP	2.2
1	C	379	VAL	2.2
1	C	266	ALA	2.2
1	C	164	ALA	2.1
1	C	60	HIS	2.1
1	C	174	ARG	2.1
1	C	318	HIS	2.0
1	B	64	THR	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
2	PGR	C	501	5/5	0.59	0.24	124,151,153,159	0
2	PGR	B	503	5/5	0.90	0.29	85,87,98,100	0
2	PGR	B	501	5/5	0.90	0.29	59,72,76,77	0
2	PGR	A	503	5/5	0.91	0.19	72,73,80,82	0
2	PGR	A	502	5/5	0.95	0.47	58,59,62,65	0
2	PGR	B	502	5/5	0.96	0.42	68,68,70,84	0
2	PGR	A	501	5/5	0.98	0.34	52,60,63,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.