



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2024 – 06:50 AM EDT

PDB ID : 3TWK  
Title : Crystal structure of arabidopsis thaliana FPG  
Authors : Duclos, S.; Aller, P.; Wallace, S.S.; Doublié, S.  
Deposited on : 2011-09-22  
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

<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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

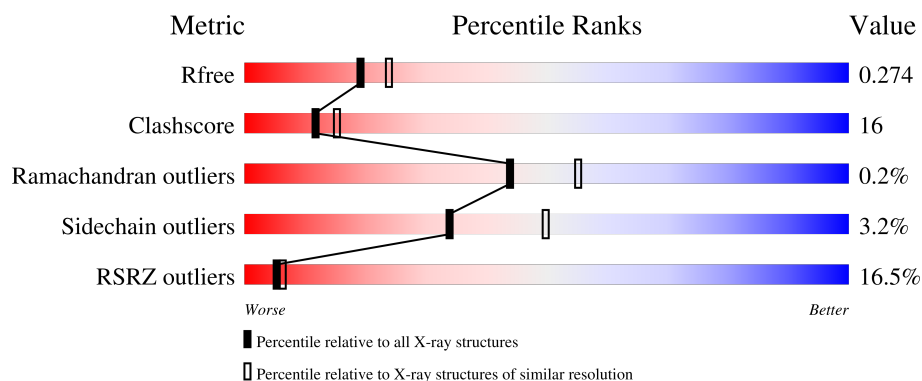
# 1 Overall quality at a glance

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))
$R_{free}$	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (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 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	297	
1	B	297	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	301	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4843 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 Formamidopyrimidine-DNA glycosylase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	Se	3	0	0
			2303	1476	392	430	3	2			
1	B	286	Total	C	N	O	S	Se	0	0	0
			2257	1446	389	417	3	2			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	CYS	-	expression tag	UNP Q9SBB4
A	283	VAL	-	expression tag	UNP Q9SBB4
A	284	ASP	-	expression tag	UNP Q9SBB4
A	285	LYS	-	expression tag	UNP Q9SBB4
A	286	LEU	-	expression tag	UNP Q9SBB4
A	287	ALA	-	expression tag	UNP Q9SBB4
A	288	ALA	-	expression tag	UNP Q9SBB4
A	289	ALA	-	expression tag	UNP Q9SBB4
A	290	LEU	-	expression tag	UNP Q9SBB4
A	291	GLU	-	expression tag	UNP Q9SBB4
A	292	HIS	-	expression tag	UNP Q9SBB4
A	293	HIS	-	expression tag	UNP Q9SBB4
A	294	HIS	-	expression tag	UNP Q9SBB4
A	295	HIS	-	expression tag	UNP Q9SBB4
A	296	HIS	-	expression tag	UNP Q9SBB4
A	297	HIS	-	expression tag	UNP Q9SBB4
B	282	CYS	-	expression tag	UNP Q9SBB4
B	283	VAL	-	expression tag	UNP Q9SBB4
B	284	ASP	-	expression tag	UNP Q9SBB4
B	285	LYS	-	expression tag	UNP Q9SBB4
B	286	LEU	-	expression tag	UNP Q9SBB4
B	287	ALA	-	expression tag	UNP Q9SBB4
B	288	ALA	-	expression tag	UNP Q9SBB4
B	289	ALA	-	expression tag	UNP Q9SBB4
B	290	LEU	-	expression tag	UNP Q9SBB4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	291	GLU	-	expression tag	UNP Q9SBB4
B	292	HIS	-	expression tag	UNP Q9SBB4
B	293	HIS	-	expression tag	UNP Q9SBB4
B	294	HIS	-	expression tag	UNP Q9SBB4
B	295	HIS	-	expression tag	UNP Q9SBB4
B	296	HIS	-	expression tag	UNP Q9SBB4
B	297	HIS	-	expression tag	UNP Q9SBB4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

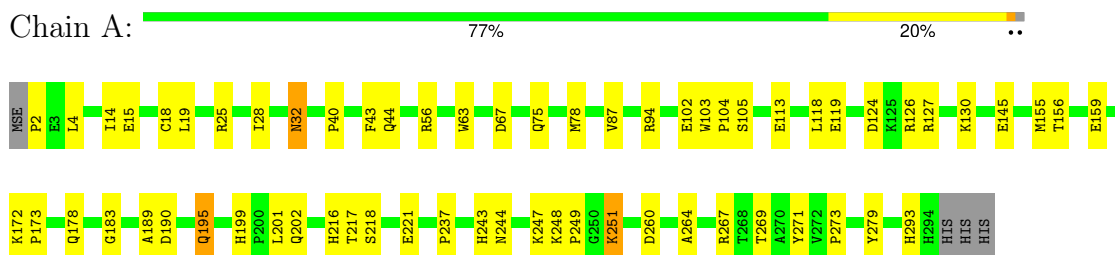
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	207	Total	O	0	0
			207	207		
3	B	64	Total	O	0	0
			64	64		

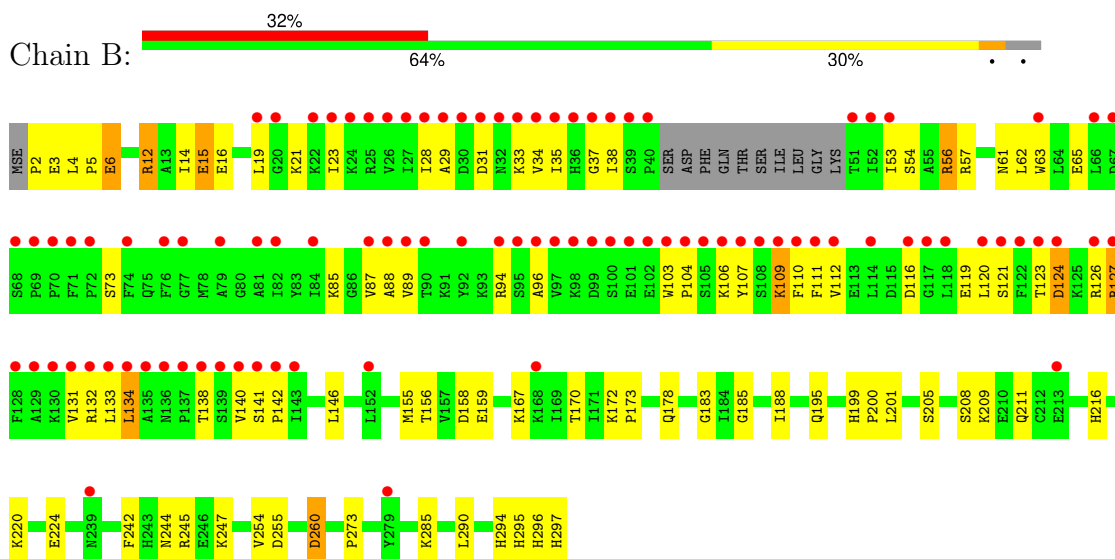
### 3 Residue-property plots

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: Formamidopyrimidine-DNA glycosylase 1



- Molecule 1: Formamidopyrimidine-DNA glycosylase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.05Å 93.05Å 157.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.30) 100.0 (50.00-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.27 (at 2.27Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.222 , 0.273 0.225 , 0.274	Depositor DCC
$R_{free}$ test set	3166 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4843	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 3.94% 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

### 5.1 Standard geometry

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	0.41	0/2351	0.63	0/3171
1	B	0.34	0/2306	0.57	0/3110
All	All	0.38	0/4657	0.60	0/6281

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

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	2303	0	2343	52	1
1	B	2257	0	2287	98	0
2	A	12	0	16	5	0
3	A	207	0	0	9	1
3	B	64	0	0	7	0
All	All	4843	0	4646	144	1

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 16.

All (144) 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:2:PRO:N	2:A:301:GOL:HO2	1.60	0.98
1:B:199:HIS:HD2	1:B:201:LEU:H	1.04	0.96
1:A:202:GLN:HE22	1:A:279:TYR:H	0.97	0.95
1:A:199:HIS:HD2	1:A:201:LEU:H	1.10	0.95
1:B:178:GLN:HE22	1:B:183:GLY:H	1.19	0.91
1:A:28:ILE:H	1:A:44:GLN:HE21	1.11	0.89
1:B:54:SER:HB3	1:B:65:GLU:HB3	1.53	0.89
1:B:170:THR:HG23	1:B:173:PRO:HD2	1.55	0.86
1:A:178:GLN:HE22	1:A:183:GLY:H	1.24	0.85
1:A:199:HIS:CD2	1:A:201:LEU:H	1.98	0.79
1:B:21:LYS:HD2	1:B:116:ASP:HB2	1.68	0.75
1:B:87:VAL:HG12	1:B:88:ALA:H	1.52	0.74
1:B:178:GLN:NE2	1:B:183:GLY:H	1.84	0.74
3:A:598:HOH:O	1:B:170:THR:HG21	1.88	0.74
1:A:78:MSE:HA	2:A:301:GOL:H12	1.70	0.73
1:A:267:ARG:HD2	3:A:532:HOH:O	1.88	0.73
1:A:260:ASP:OD2	1:A:273:PRO:HG2	1.88	0.73
1:B:170:THR:HG23	1:B:173:PRO:CD	2.19	0.72
1:B:199:HIS:CD2	1:B:201:LEU:H	1.97	0.71
1:B:2:PRO:HA	1:B:6:GLU:HG3	1.71	0.71
1:A:217:THR:O	1:A:221:GLU:HG3	1.90	0.71
1:B:220:LYS:O	1:B:224:GLU:HG3	1.91	0.71
1:B:34:VAL:HG11	1:B:109:LYS:HG2	1.73	0.69
1:B:156:THR:OG1	1:B:159:GLU:HG3	1.92	0.69
1:B:34:VAL:HG11	1:B:109:LYS:CG	2.24	0.67
1:A:156:THR:OG1	1:A:159:GLU:HG3	1.94	0.67
1:B:15:GLU:HA	1:B:19:LEU:HG	1.77	0.66
1:A:102:GLU:HG3	1:A:105:SER:HA	1.78	0.65
1:A:249:PRO:HG2	1:B:296:HIS:CD2	2.31	0.65
1:B:87:VAL:HG12	1:B:88:ALA:N	2.11	0.64
1:A:15:GLU:HA	1:A:19:LEU:HD13	1.79	0.64
1:B:195:GLN:HG3	3:B:361:HOH:O	1.98	0.64
1:A:178:GLN:NE2	1:A:183:GLY:H	1.94	0.63
1:B:4:LEU:C	1:B:4:LEU:HD23	2.19	0.63
1:A:244:ASN:HD22	1:A:247:LYS:HE2	1.64	0.62
1:B:56:ARG:O	1:B:62:LEU:HD12	2.01	0.61
1:A:190:ASP:OD1	1:A:269:THR:HG23	2.01	0.61
1:A:216:HIS:HD2	3:A:425:HOH:O	1.83	0.61
1:A:244:ASN:ND2	1:A:247:LYS:HE2	2.16	0.60
1:B:12:ARG:O	1:B:16:GLU:HG3	2.01	0.60
1:A:202:GLN:HE22	1:A:279:TYR:N	1.82	0.59
1:B:123:THR:HG22	1:B:124:ASP:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:MSE:SE	1:A:126:ARG:NH1	2.87	0.57
1:A:271:TYR:OH	1:B:294:HIS:HE1	1.88	0.57
1:B:89:VAL:HG13	1:B:96:ALA:CB	2.35	0.57
1:B:242:PHE:O	1:B:245:ARG:HG2	2.05	0.56
1:B:285:LYS:HE3	3:B:362:HOH:O	2.05	0.56
1:B:3:GLU:HG2	1:B:185:GLY:HA3	1.88	0.55
1:B:134:LEU:N	1:B:134:LEU:HD22	2.22	0.55
1:B:172:LYS:HB3	1:B:173:PRO:HD3	1.88	0.55
1:B:120:LEU:HD23	1:B:121:SER:N	2.22	0.54
1:B:140:VAL:HG12	1:B:141:SER:N	2.23	0.54
1:B:155:MSE:O	1:B:216:HIS:HE1	1.91	0.54
1:A:2:PRO:N	2:A:301:GOL:O2	2.33	0.54
1:B:260:ASP:OD2	1:B:273:PRO:HG2	2.08	0.53
1:B:242:PHE:HA	1:B:245:ARG:HD2	1.90	0.53
1:B:89:VAL:HG13	1:B:96:ALA:HB1	1.91	0.53
1:B:110:PHE:O	1:B:121:SER:HA	2.09	0.53
1:A:293:HIS:HD2	1:B:170:THR:HG22	1.73	0.53
1:A:293:HIS:CD2	1:B:170:THR:H	2.26	0.53
1:A:78:MSE:CA	2:A:301:GOL:H12	2.38	0.52
1:B:106:LYS:O	1:B:106:LYS:HD3	2.09	0.52
1:B:133:LEU:O	1:B:134:LEU:HD13	2.08	0.52
1:B:133:LEU:C	1:B:134:LEU:HD13	2.30	0.52
1:B:138:THR:HG22	1:B:138:THR:O	2.09	0.52
1:B:3:GLU:O	1:B:6:GLU:HG2	2.09	0.52
1:B:104:PRO:HG3	1:B:111:PHE:CE1	2.44	0.52
1:B:28:ILE:HG22	1:B:35:ILE:HD11	1.90	0.52
1:A:293:HIS:CD2	1:B:170:THR:HG22	2.46	0.51
1:B:31:ASP:OD2	1:B:34:VAL:HG23	2.10	0.51
1:B:34:VAL:O	1:B:131:VAL:HG22	2.10	0.51
1:A:87:VAL:HG23	1:A:118:LEU:HD13	1.91	0.51
1:B:254:VAL:O	1:B:254:VAL:HG13	2.11	0.51
1:B:120:LEU:HD23	1:B:120:LEU:C	2.30	0.51
1:B:38:ILE:CD1	1:B:133:LEU:HD23	2.41	0.50
1:B:23:ILE:HG23	1:B:112:VAL:HG23	1.92	0.50
1:B:216:HIS:HD2	3:B:327:HOH:O	1.94	0.50
1:B:170:THR:OG1	1:B:201:LEU:HA	2.12	0.49
1:B:56:ARG:HG2	1:B:56:ARG:NH1	2.27	0.49
1:B:199:HIS:HE1	3:B:301:HOH:O	1.94	0.49
1:A:248:LYS:O	1:A:251:LYS:HG2	2.12	0.49
1:B:111:PHE:HZ	1:B:119:GLU:OE1	1.96	0.49
1:B:56:ARG:HG2	1:B:56:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:THR:O	1:B:173:PRO:HD2	2.12	0.49
1:B:53:ILE:O	1:B:53:ILE:HG13	2.13	0.48
1:B:103:TRP:HA	1:B:104:PRO:C	2.33	0.48
1:B:4:LEU:HB3	1:B:5:PRO:HD3	1.94	0.48
1:A:94:ARG:HG2	3:A:530:HOH:O	2.12	0.48
1:B:15:GLU:HB2	1:B:19:LEU:HD11	1.96	0.48
1:B:199:HIS:CD2	1:B:200:PRO:HD2	2.49	0.48
1:A:40:PRO:O	1:A:44:GLN:HG3	2.14	0.48
1:B:208:SER:OG	1:B:211:GLN:HB2	2.14	0.48
1:A:271:TYR:OH	1:B:294:HIS:CE1	2.67	0.47
1:A:103:TRP:HA	1:A:104:PRO:C	2.34	0.47
1:B:19:LEU:HD12	3:B:313:HOH:O	2.13	0.47
1:A:75:GLN:HB3	1:A:130:LYS:HB2	1.96	0.47
1:A:32:ASN:HD22	1:A:32:ASN:C	2.18	0.47
1:B:31:ASP:HB3	1:B:34:VAL:HB	1.97	0.47
1:A:155:MSE:O	1:A:216:HIS:HE1	1.98	0.47
2:A:302:GOL:H11	3:A:607:HOH:O	2.14	0.47
1:B:73:SER:OG	1:B:132:ARG:HB2	2.15	0.47
1:B:56:ARG:HB3	1:B:63:TRP:CE2	2.49	0.47
1:A:25:ARG:HD2	3:A:597:HOH:O	2.15	0.46
1:A:267:ARG:HH11	1:A:267:ARG:HG2	1.80	0.46
1:A:14:ILE:O	1:A:18:CYS:HB2	2.16	0.46
1:A:172:LYS:HB3	1:A:173:PRO:CD	2.44	0.46
1:B:6:GLU:H	1:B:6:GLU:CD	2.18	0.46
1:B:3:GLU:H	1:B:6:GLU:CG	2.29	0.46
1:A:94:ARG:HD3	3:A:536:HOH:O	2.15	0.46
1:B:12:ARG:NH1	3:B:321:HOH:O	2.48	0.46
1:A:264:ALA:HB3	3:A:533:HOH:O	2.15	0.46
1:A:124:ASP:OD2	1:A:127:ARG:HA	2.15	0.45
1:A:145:GLU:OE1	1:B:33:LYS:HE3	2.15	0.45
1:A:113:GLU:HG3	1:A:119:GLU:HG2	1.97	0.45
1:B:167:LYS:O	1:B:205:SER:HB3	2.17	0.45
1:B:57:ARG:HG3	1:B:61:ASN:O	2.17	0.45
1:B:33:LYS:HD3	1:B:127:ARG:HD3	1.99	0.45
1:A:199:HIS:HE1	3:A:419:HOH:O	1.99	0.45
1:B:142:PRO:O	1:B:146:LEU:HD13	2.18	0.44
1:B:156:THR:HG23	1:B:159:GLU:OE1	2.18	0.44
1:B:85:LYS:HD3	1:B:103:TRP:CD1	2.53	0.44
1:B:37:GLY:O	1:B:38:ILE:HB	2.18	0.43
1:B:123:THR:CG2	1:B:124:ASP:N	2.80	0.43
1:B:107:TYR:O	1:B:109:LYS:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:HIS:HD2	1:B:201:LEU:N	1.90	0.43
1:B:290:LEU:O	1:B:294:HIS:HD2	2.00	0.43
1:A:56:ARG:HB2	1:A:63:TRP:CE2	2.54	0.43
1:B:19:LEU:HD22	1:B:53:ILE:C	2.39	0.43
1:A:4:LEU:HD23	1:A:4:LEU:C	2.39	0.42
1:A:237:PRO:O	1:A:243:HIS:HE1	2.03	0.41
1:A:172:LYS:HE3	1:A:189:ALA:HB3	2.01	0.41
1:B:6:GLU:HB3	1:B:94:ARG:NH2	2.34	0.41
1:A:267:ARG:HG2	1:A:267:ARG:NH1	2.36	0.41
1:B:29:ALA:O	1:B:35:ILE:HD11	2.20	0.41
1:A:195:GLN:HB3	1:A:218:SER:HB2	2.01	0.41
1:B:87:VAL:CG1	1:B:88:ALA:H	2.27	0.41
1:B:126:ARG:O	1:B:127:ARG:CG	2.69	0.41
1:B:170:THR:CG2	1:B:173:PRO:HG2	2.50	0.41
1:B:244:ASN:ND2	1:B:247:LYS:NZ	2.68	0.41
1:B:103:TRP:CH2	1:B:121:SER:HB3	2.56	0.41
1:B:209:LYS:HA	3:B:358:HOH:O	2.21	0.41
1:B:3:GLU:OE1	1:B:188:ILE:HG13	2.20	0.40
1:B:12:ARG:HG3	1:B:12:ARG:HH11	1.85	0.40
1:B:14:ILE:HD12	1:B:62:LEU:HD21	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASP:OD1	3:A:606:HOH:O[6_465]	2.19	0.01

## 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	291/297 (98%)	284 (98%)	7 (2%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	282/297 (95%)	259 (92%)	22 (8%)	1 (0%)	30	39
All	All	573/594 (96%)	543 (95%)	29 (5%)	1 (0%)	44	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	124	ASP

### 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	250/251 (100%)	246 (98%)	4 (2%)	58	74
1	B	244/251 (97%)	232 (95%)	12 (5%)	21	31
All	All	494/502 (98%)	478 (97%)	16 (3%)	34	50

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	43	PHE
1	A	195	GLN
1	A	251	LYS
1	B	6	GLU
1	B	12	ARG
1	B	15	GLU
1	B	56	ARG
1	B	109	LYS
1	B	127	ARG
1	B	134	LEU
1	B	158	ASP
1	B	255	ASP
1	B	260	ASP
1	B	295	HIS

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Mol	Chain	Res	Type
1	B	297	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	44	GLN
1	A	178	GLN
1	A	199	HIS
1	A	202	GLN
1	A	216	HIS
1	A	235	GLN
1	A	243	HIS
1	A	244	ASN
1	A	292	HIS
1	A	293	HIS
1	A	294	HIS
1	B	61	ASN
1	B	136	ASN
1	B	178	GLN
1	B	199	HIS
1	B	216	HIS
1	B	243	HIS
1	B	244	ASN
1	B	294	HIS
1	B	295	HIS
1	B	296	HIS
1	B	297	HIS

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

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	302	-	5,5,5	0.30	0	5,5,5	0.25	0
2	GOL	A	301	-	5,5,5	0.27	0	5,5,5	0.13	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	302	-	-	2/4/4/4	-
2	GOL	A	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	GOL	O1-C1-C2-C3
2	A	302	GOL	O1-C1-C2-C3
2	A	301	GOL	O1-C1-C2-O2
2	A	302	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	GOL	1	0
2	A	301	GOL	4	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	291/297 (97%)	-0.14	0 100 100	14, 26, 51, 60	1 (0%)
1	B	284/297 (95%)	1.37	95 (33%) 1 1	17, 47, 92, 102	0
All	All	575/594 (96%)	0.60	95 (16%) 5 6	14, 35, 88, 102	1 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	34	VAL	6.4
1	B	40	PRO	5.6
1	B	35	ILE	5.3
1	B	51	THR	5.1
1	B	134	LEU	5.0
1	B	27	ILE	4.9
1	B	111	PHE	4.8
1	B	23	ILE	4.7
1	B	28	ILE	4.7
1	B	97	VAL	4.6
1	B	39	SER	4.5
1	B	87	VAL	4.5
1	B	100	SER	4.4
1	B	133	LEU	4.4
1	B	104	PRO	4.3
1	B	279	TYR	4.3
1	B	129	ALA	4.1
1	B	126	ARG	4.0
1	B	29	ALA	4.0
1	B	123	THR	3.8
1	B	107	TYR	3.7
1	B	128	PHE	3.7
1	B	30	ASP	3.7
1	B	26	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	127	ARG	3.6
1	B	53	ILE	3.6
1	B	112	VAL	3.6
1	B	122	PHE	3.6
1	B	138	THR	3.6
1	B	103	TRP	3.5
1	B	105	SER	3.4
1	B	139	SER	3.4
1	B	114	LEU	3.4
1	B	143	ILE	3.3
1	B	135	ALA	3.2
1	B	137	PRO	3.2
1	B	132	ARG	3.1
1	B	88	ALA	3.1
1	B	142	PRO	3.1
1	B	110	PHE	3.1
1	B	131	VAL	3.1
1	B	66	LEU	3.1
1	B	116	ASP	3.1
1	B	120	LEU	3.0
1	B	108	SER	3.0
1	B	89	VAL	3.0
1	B	71	PHE	3.0
1	B	36	HIS	3.0
1	B	99	ASP	2.9
1	B	140	VAL	2.9
1	B	20	GLY	2.9
1	B	239	ASN	2.9
1	B	213	GLU	2.9
1	B	96	ALA	2.8
1	B	102	GLU	2.8
1	B	98	LYS	2.8
1	B	90	THR	2.8
1	B	38	ILE	2.8
1	B	117	GLY	2.8
1	B	52	ILE	2.8
1	B	76	PHE	2.8
1	B	63	TRP	2.8
1	B	152	LEU	2.8
1	B	82	ILE	2.7
1	B	130	LYS	2.7
1	B	101	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	33	LYS	2.7
1	B	32	ASN	2.6
1	B	72	PRO	2.6
1	B	68	SER	2.6
1	B	70	PRO	2.6
1	B	67	ASP	2.6
1	B	69	PRO	2.6
1	B	124	ASP	2.6
1	B	79	ALA	2.5
1	B	84	ILE	2.5
1	B	19	LEU	2.5
1	B	31	ASP	2.4
1	B	74	PHE	2.4
1	B	25	ARG	2.4
1	B	118	LEU	2.4
1	B	136	ASN	2.3
1	B	95	SER	2.3
1	B	141	SER	2.3
1	B	109	LYS	2.3
1	B	106	LYS	2.2
1	B	121	SER	2.2
1	B	37	GLY	2.2
1	B	168	LYS	2.2
1	B	24	LYS	2.2
1	B	77	GLY	2.2
1	B	92	TYR	2.1
1	B	22	LYS	2.1
1	B	81	ALA	2.0
1	B	94	ARG	2.0

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

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

## 6.3 Carbohydrates ⓘ

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	GOL	A	301	6/6	0.80	0.19	61,62,63,64	0
2	GOL	A	302	6/6	0.84	0.14	47,52,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.