



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:30 am BST

PDB ID : 6IJ7  
Title : Crystal Structure of Arabidopsis thaliana UGT89C1  
Authors : Zong, G.; Wang, X.  
Deposited on : 2018-10-09  
Resolution : 2.70 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 : 2.11  
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) : 2.11

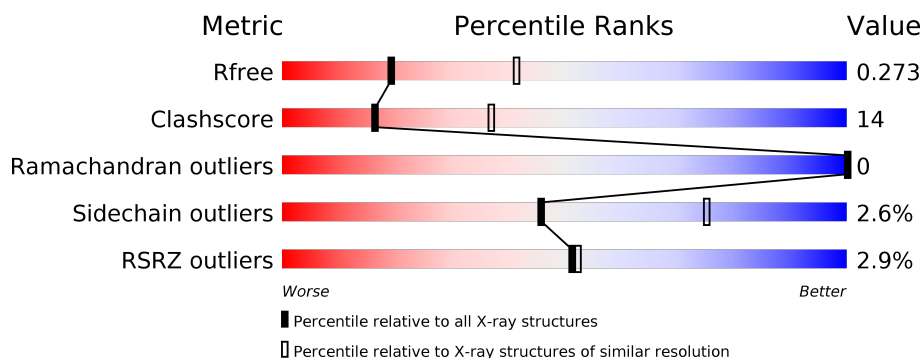
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	435	<div> <div>3%</div> <div>65%</div> <div>26%</div> <div>8%</div> </div>
1	B	435	<div> <div>3%</div> <div>67%</div> <div>24%</div> <div>7%</div> </div>

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	B	501	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6411 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 Rhamnosyltransferase protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3150	2028	534	575	13			
1	B	405	Total	C	N	O	S	0	0	0
			3174	2039	541	581	13			

- 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	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

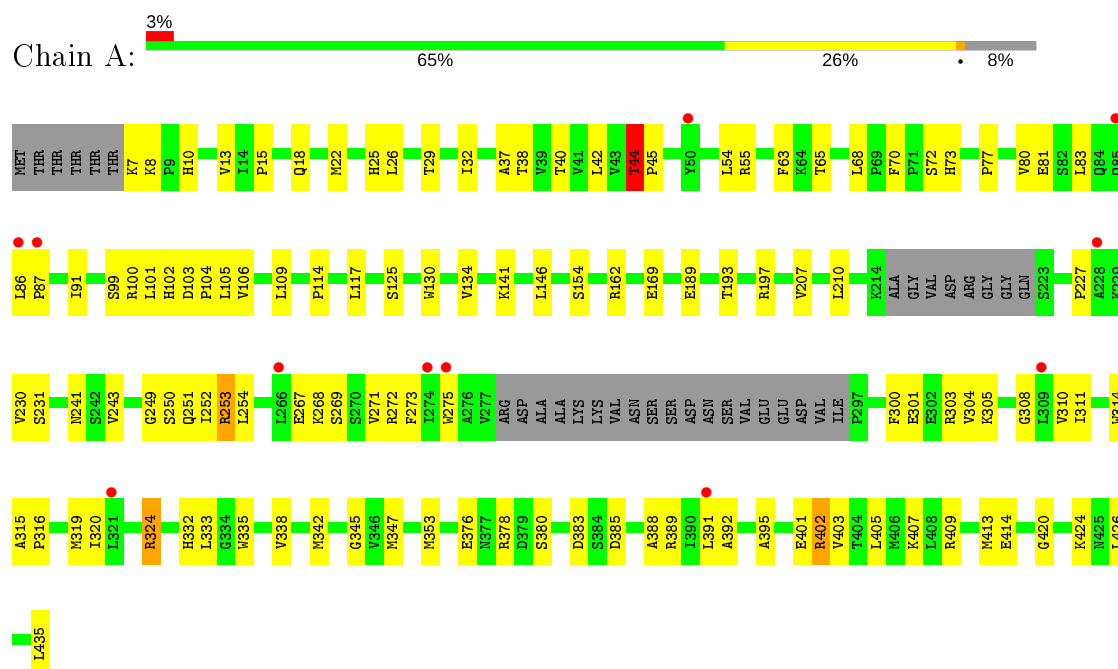
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	17	Total O 17 17	0	0
4	B	18	Total O 18 18	0	0

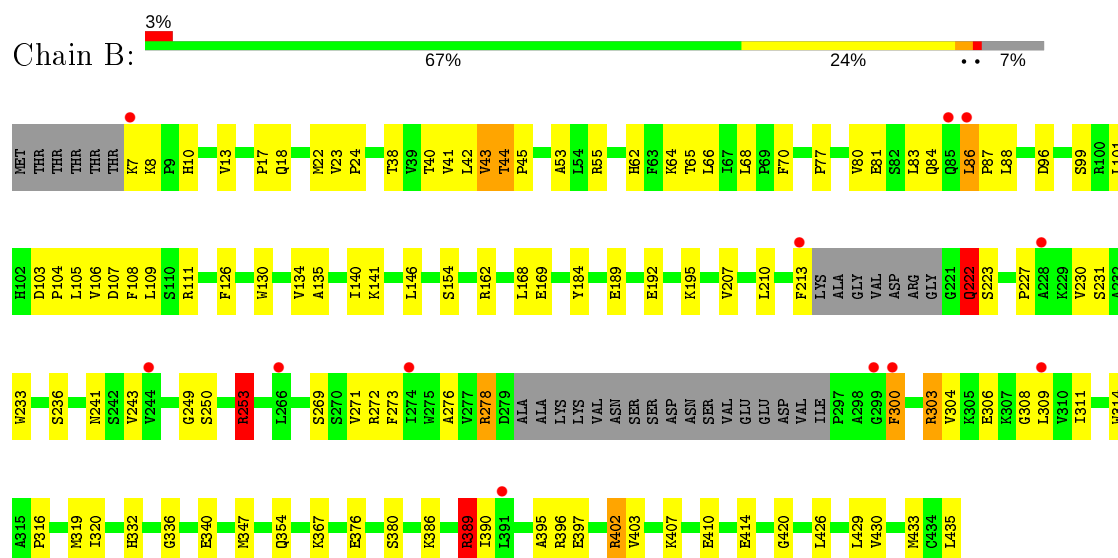
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Rhamnosyltransferase protein



#### • Molecule 1: Rhamnosyltransferase protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.65Å 80.65Å 340.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.36 – 2.70 47.36 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.36-2.70) 99.9 (47.36-2.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.217 , 0.260 0.226 , 0.273	Depositor DCC
$R_{free}$ test set	1500 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.4	Xtriage
Anisotropy	0.596	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 32.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.477 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6411	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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, EDO

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	0.50	0/3230	0.70	2/4393 (0.0%)
1	B	0.49	1/3255 (0.0%)	0.75	5/4428 (0.1%)
All	All	0.50	1/6485 (0.0%)	0.72	7/8821 (0.1%)

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	1
1	B	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	VAL	C-N	-5.29	1.21	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	389	ARG	NE-CZ-NH1	-14.22	113.19	120.30
1	B	389	ARG	NE-CZ-NH2	11.19	125.89	120.30
1	A	253	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	44	THR	C-N-CD	5.90	140.79	128.40
1	B	253	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	B	86	LEU	CA-CB-CG	5.72	128.45	115.30
1	B	410	GLU	CA-CB-CG	5.12	124.67	113.40



There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300	PHE	Peptide
1	B	222	GLN	Peptide
1	B	300	PHE	Peptide

## 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	3150	0	3161	92	1
1	B	3174	0	3178	95	1
2	A	18	0	24	3	0
2	B	6	0	8	5	0
3	A	16	0	24	0	0
3	B	12	0	18	3	0
4	A	17	0	0	3	0
4	B	18	0	0	4	0
All	All	6411	0	6413	183	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 14.

All (183) 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:249:GLY:H	2:A:501:GOL:H11	1.32	0.94
1:A:193:THR:HG22	1:B:189:GLU:HG2	1.60	0.83
1:B:222:GLN:OE1	1:B:223:SER:N	2.11	0.83
1:A:7:LYS:N	4:A:601:HOH:O	2.13	0.81
1:B:249:GLY:H	2:B:501:GOL:H32	1.48	0.79
1:B:269:SER:OG	1:B:271:VAL:HG12	1.83	0.78
1:A:402:ARG:HH11	1:A:402:ARG:HG3	1.52	0.74
1:A:227:PRO:HG3	1:A:314:TRP:HZ3	1.53	0.74
1:B:40:THR:HG22	1:B:64:LYS:HB2	1.71	0.73
1:B:108:PHE:HD2	1:B:109:LEU:HD12	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ASP:HB3	1:B:111:ARG:NH1	2.06	0.69
1:A:333:LEU:CD1	1:A:338:VAL:HG22	2.23	0.69
1:A:268:LYS:HG2	1:A:385:ASP:OD1	1.94	0.68
1:B:300:PHE:CD2	1:B:304:VAL:HG21	2.28	0.68
1:A:13:VAL:HG12	1:A:15:PRO:HD3	1.77	0.65
1:B:107:ASP:HB3	1:B:111:ARG:HH12	1.61	0.65
1:B:253:ARG:HH21	1:B:278:ARG:HH12	1.44	0.64
1:A:353:MET:CE	1:A:378:ARG:HA	2.28	0.64
1:A:324:ARG:NH2	4:A:604:HOH:O	2.30	0.64
1:B:7:LYS:HG2	1:B:8:LYS:H	1.63	0.63
1:A:332:HIS:HB2	2:A:501:GOL:H12	1.80	0.63
1:B:227:PRO:HG3	1:B:314:TRP:HZ3	1.64	0.62
1:B:241:ASN:ND2	1:B:395:ALA:O	2.32	0.62
1:A:304:VAL:HG13	1:A:305:LYS:HG2	1.82	0.61
1:A:207:VAL:HG12	1:A:210:LEU:HD21	1.82	0.61
1:A:55:ARG:NH1	1:A:65:THR:OG1	2.34	0.61
1:A:333:LEU:HD11	1:A:338:VAL:HG22	1.82	0.60
1:A:68:LEU:HD13	1:A:104:PRO:HB2	1.83	0.60
1:A:101:LEU:HA	1:A:104:PRO:HG2	1.84	0.59
1:A:402:ARG:HG3	1:A:402:ARG:NH1	2.18	0.59
1:A:114:PRO:HA	1:A:117:LEU:HD12	1.84	0.59
1:A:189:GLU:O	1:A:193:THR:HG23	2.02	0.59
1:B:253:ARG:NH2	4:B:603:HOH:O	2.34	0.59
1:A:403:VAL:O	1:A:407:LYS:HG3	2.03	0.58
1:B:273:PHE:CZ	1:B:308:GLY:HA3	2.38	0.58
1:B:241:ASN:OD1	1:B:402:ARG:NH2	2.33	0.58
1:B:402:ARG:HG2	1:B:402:ARG:HH11	1.69	0.58
1:A:72:SER:O	1:A:100:ARG:NH1	2.36	0.57
1:B:84:GLN:NE2	4:B:602:HOH:O	2.33	0.57
1:B:249:GLY:H	2:B:501:GOL:C3	2.15	0.57
1:B:195:LYS:NZ	3:B:503:EDO:H22	2.19	0.57
1:B:396:ARG:NE	4:B:604:HOH:O	2.38	0.56
1:B:103:ASP:O	1:B:106:VAL:HG12	2.04	0.56
1:B:250:SER:N	2:B:501:GOL:H11	2.20	0.56
1:A:388:ALA:HA	1:A:391:LEU:HD12	1.87	0.56
1:B:68:LEU:HD13	1:B:104:PRO:HB2	1.86	0.56
1:A:273:PHE:CZ	1:A:308:GLY:HA3	2.41	0.56
1:A:252:ILE:HD13	1:A:378:ARG:HG3	1.88	0.56
1:B:126:PHE:HA	1:B:168:LEU:HD13	1.88	0.55
1:A:241:ASN:ND2	1:A:395:ALA:O	2.38	0.55
1:A:345:GLY:O	1:A:402:ARG:NH2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:VAL:O	1:B:407:LYS:HG3	2.06	0.55
1:B:376:GLU:HB3	1:B:380:SER:OG	2.06	0.55
1:B:222:GLN:OE1	1:B:222:GLN:C	2.45	0.55
1:A:70:PHE:CG	1:A:81:GLU:HG2	2.42	0.55
1:B:101:LEU:HA	1:B:104:PRO:HG2	1.87	0.55
1:A:311:ILE:HD11	1:A:315:ALA:HB2	1.89	0.55
1:A:249:GLY:N	2:A:501:GOL:H11	2.14	0.54
1:B:10:HIS:NE2	1:B:40:THR:HG23	2.22	0.54
1:A:141:LYS:NZ	1:A:435:LEU:O	2.24	0.54
1:A:32:ILE:HG22	1:A:37:ALA:HB3	1.88	0.54
1:B:105:LEU:HD23	1:B:134:VAL:HG11	1.90	0.54
1:B:414:GLU:O	1:B:420:GLY:HA3	2.08	0.54
1:A:10:HIS:HA	1:A:38:THR:O	2.07	0.54
1:A:311:ILE:HD11	1:A:315:ALA:CB	2.38	0.54
1:A:353:MET:HE1	1:A:378:ARG:HA	1.88	0.54
1:A:54:LEU:HD23	1:A:63:PHE:CE1	2.43	0.53
1:A:13:VAL:HG21	1:A:29:THR:HG22	1.89	0.53
1:B:42:LEU:HD23	1:B:66:LEU:HD23	1.89	0.53
1:B:10:HIS:HA	1:B:38:THR:O	2.07	0.53
1:B:332:HIS:HB2	2:B:501:GOL:H31	1.91	0.53
1:A:99:SER:HA	1:A:130:TRP:CD1	2.44	0.53
1:B:99:SER:HA	1:B:130:TRP:CD1	2.44	0.52
1:B:207:VAL:HG12	1:B:210:LEU:HD21	1.90	0.52
1:A:42:LEU:HD22	1:A:105:LEU:HD13	1.91	0.52
1:A:22:MET:HE2	1:A:26:LEU:HD11	1.90	0.52
1:A:162:ARG:HD2	1:A:169:GLU:OE2	2.09	0.52
1:A:342:MET:HA	1:A:405:LEU:HD11	1.92	0.52
1:A:7:LYS:O	1:A:8:LYS:HD2	2.10	0.51
1:B:44:THR:HG21	1:B:81:GLU:HB3	1.92	0.51
1:A:193:THR:O	1:A:197:ARG:HB2	2.11	0.51
1:A:109:LEU:O	1:A:117:LEU:HD21	2.11	0.50
1:A:105:LEU:HD23	1:A:134:VAL:HG11	1.93	0.50
1:A:333:LEU:HD12	1:A:338:VAL:HG22	1.92	0.50
1:B:55:ARG:NH1	1:B:65:THR:OG1	2.44	0.50
1:B:300:PHE:HD2	1:B:304:VAL:HG21	1.76	0.50
1:B:233:TRP:O	1:B:236:SER:HB3	2.11	0.50
1:B:231:SER:HB2	1:B:319:MET:CE	2.42	0.50
1:A:250:SER:HB3	1:A:251:GLN:HA	1.94	0.50
1:B:23:VAL:HG22	1:B:24:PRO:HD3	1.93	0.49
1:A:243:VAL:HG22	1:A:272:ARG:HB3	1.93	0.49
1:B:184:TYR:OH	1:B:192:GLU:OE2	2.18	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ARG:HD2	1:B:169:GLU:OE2	2.12	0.49
1:B:13:VAL:HG22	1:B:41:VAL:HG22	1.95	0.49
1:A:77:PRO:HG2	1:A:80:VAL:HG21	1.94	0.49
1:A:347:MET:HA	1:A:347:MET:HE3	1.93	0.49
1:B:241:ASN:ND2	1:B:397:GLU:HG3	2.27	0.49
1:B:17:PRO:HA	1:B:22:MET:HE1	1.95	0.49
1:B:222:GLN:CD	1:B:223:SER:H	2.16	0.48
1:B:108:PHE:CD2	1:B:109:LEU:HD12	2.44	0.48
1:B:402:ARG:HG2	1:B:402:ARG:NH1	2.27	0.48
1:A:383:ASP:OD1	4:A:602:HOH:O	2.20	0.48
1:B:230:VAL:HG12	1:B:309:LEU:HD21	1.94	0.48
1:B:70:PHE:CG	1:B:81:GLU:HG2	2.49	0.48
1:A:230:VAL:HG21	1:A:316:PRO:HG3	1.95	0.47
1:A:271:VAL:HG11	1:A:392:ALA:HA	1.96	0.47
1:B:243:VAL:HG22	1:B:272:ARG:HB3	1.96	0.47
1:B:86:LEU:HB2	1:B:87:PRO:HD2	1.96	0.47
1:A:25:HIS:O	1:A:29:THR:HG23	2.15	0.47
1:B:53:ALA:HB1	1:B:213:PHE:HE2	1.79	0.47
1:B:402:ARG:HH11	1:B:402:ARG:CG	2.27	0.47
1:A:207:VAL:HG13	1:A:426:LEU:HD21	1.95	0.47
1:B:306:GLU:OE2	1:B:306:GLU:HA	2.14	0.47
1:A:13:VAL:HG11	1:A:29:THR:HG21	1.97	0.47
1:B:38:THR:HG23	1:B:62:HIS:HA	1.96	0.46
1:B:347:MET:HE3	1:B:347:MET:HA	1.97	0.46
1:B:195:LYS:CE	3:B:503:EDO:H22	2.45	0.46
1:A:193:THR:HG22	1:B:189:GLU:CG	2.39	0.46
1:A:353:MET:HE2	1:A:378:ARG:HA	1.95	0.46
1:B:7:LYS:HG2	1:B:8:LYS:N	2.28	0.46
1:B:276:ALA:HA	1:B:311:ILE:HG23	1.99	0.45
1:B:45:PRO:HD3	1:B:68:LEU:O	2.16	0.45
1:A:83:LEU:HD23	1:A:86:LEU:HD21	1.98	0.45
1:B:41:VAL:HG12	1:B:43:VAL:HG13	1.99	0.45
1:A:102:HIS:HD2	1:A:103:ASP:OD1	1.99	0.45
1:B:367:LYS:HZ1	3:B:502:EDO:C1	2.30	0.45
1:B:8:LYS:HA	1:B:8:LYS:HD3	1.58	0.45
1:A:301:GLU:O	1:A:304:VAL:HG12	2.18	0.44
1:A:86:LEU:HB2	1:A:87:PRO:HD2	1.99	0.44
1:A:193:THR:CG2	1:B:189:GLU:HG2	2.41	0.44
1:A:83:LEU:HD11	1:A:91:ILE:HD12	2.00	0.44
1:B:250:SER:H	2:B:501:GOL:H32	1.82	0.44
1:B:386:LYS:O	1:B:390:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ARG:CD	4:B:604:HOH:O	2.65	0.44
1:B:42:LEU:HD21	1:B:68:LEU:HG	1.99	0.44
1:B:40:THR:HA	1:B:64:LYS:O	2.17	0.44
1:A:227:PRO:HG3	1:A:314:TRP:CZ3	2.42	0.44
1:A:267:GLU:HG3	1:A:305:LYS:HG2	2.00	0.44
1:B:207:VAL:CG1	1:B:210:LEU:HD21	2.47	0.43
1:B:83:LEU:HA	1:B:86:LEU:HD23	2.00	0.43
1:B:141:LYS:NZ	1:B:435:LEU:O	2.46	0.43
1:B:429:LEU:O	1:B:433:MET:HG3	2.18	0.43
1:A:102:HIS:O	1:A:106:VAL:HG13	2.19	0.43
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.83	0.43
1:A:275:TRP:HB3	1:A:310:VAL:HG22	2.00	0.43
1:B:10:HIS:CE1	1:B:40:THR:HG23	2.54	0.43
1:A:420:GLY:O	1:A:424:LYS:HG3	2.19	0.42
1:A:426:LEU:HA	1:A:426:LEU:HD23	1.85	0.42
1:A:335:TRP:CE3	1:A:335:TRP:HA	2.54	0.42
1:B:253:ARG:HE	1:B:278:ARG:NH2	2.18	0.42
1:B:303:ARG:NE	1:B:303:ARG:O	2.52	0.42
1:A:231:SER:HB2	1:A:319:MET:HE1	2.00	0.42
1:A:376:GLU:HB2	1:A:380:SER:OG	2.19	0.42
1:B:316:PRO:O	1:B:320:ILE:HG13	2.19	0.42
1:A:230:VAL:HG23	1:A:319:MET:HE1	2.00	0.42
1:A:83:LEU:HD11	1:A:91:ILE:CD1	2.50	0.42
1:B:135:ALA:HB1	1:B:140:ILE:O	2.19	0.42
1:A:231:SER:HB2	1:A:319:MET:CE	2.50	0.42
1:A:83:LEU:HA	1:A:86:LEU:CD2	2.49	0.42
1:A:414:GLU:O	1:A:420:GLY:HA3	2.19	0.42
1:B:231:SER:HB2	1:B:319:MET:HE2	2.02	0.42
1:A:409:ARG:O	1:A:413:MET:HG2	2.19	0.41
1:B:300:PHE:CE2	1:B:304:VAL:HG21	2.55	0.41
1:A:154:SER:OG	1:A:193:THR:OG1	2.38	0.41
1:B:88:LEU:HD11	1:B:354:GLN:OE1	2.21	0.41
1:A:193:THR:HG22	1:B:189:GLU:HB3	2.02	0.41
1:A:10:HIS:NE2	1:A:40:THR:HG22	2.36	0.41
1:B:146:LEU:HD23	1:B:146:LEU:HA	1.70	0.41
1:A:207:VAL:CG1	1:A:426:LEU:HD21	2.50	0.41
1:A:44:THR:HG23	1:A:45:PRO:CD	2.50	0.41
1:A:72:SER:OG	1:A:73:HIS:N	2.53	0.41
1:B:253:ARG:HH21	1:B:278:ARG:NH1	2.16	0.41
1:B:426:LEU:O	1:B:430:VAL:HG13	2.21	0.41
1:A:347:MET:HE1	1:A:401:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:GLY:O	1:B:340:GLU:HG3	2.21	0.41
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.71	0.40
1:B:253:ARG:NH2	1:B:278:ARG:HH12	2.15	0.40
1:A:207:VAL:CG1	1:A:210:LEU:HD21	2.50	0.40
1:A:268:LYS:HG2	1:A:385:ASP:CG	2.41	0.40
1:A:316:PRO:O	1:A:320:ILE:HG13	2.22	0.40
1:B:103:ASP:HA	1:B:106:VAL:HG12	2.02	0.40
1:B:311:ILE:HD11	1:B:314:TRP:O	2.21	0.40
1:B:77:PRO:HG2	1:B:80:VAL:HG21	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:389:ARG:NH1	1:B:389:ARG:NH2[6_655]	2.13	0.07

## 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	396/435 (91%)	381 (96%)	15 (4%)	0	100	100
1	B	399/435 (92%)	381 (96%)	18 (4%)	0	100	100
All	All	795/870 (91%)	762 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	349/377 (93%)	341 (98%)	8 (2%)	50	78
1	B	352/377 (93%)	342 (97%)	10 (3%)	43	73
All	All	701/754 (93%)	683 (97%)	18 (3%)	46	75

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	44	THR
1	A	125	SER
1	A	253	ARG
1	A	269	SER
1	A	303	ARG
1	A	324	ARG
1	A	402	ARG
1	B	18	GLN
1	B	44	THR
1	B	96	ASP
1	B	154	SER
1	B	222	GLN
1	B	253	ARG
1	B	278	ARG
1	B	303	ARG
1	B	389	ARG
1	B	402	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	102	HIS
1	B	73	HIS
1	B	85	GLN
1	B	251	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

11 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	$\# Z  > 2$
3	EDO	A	507	-	3,3,3	0.41	0	2,2,2	0.88	0
3	EDO	B	502	-	3,3,3	0.49	0	2,2,2	0.65	0
3	EDO	A	506	-	3,3,3	0.52	0	2,2,2	0.71	0
2	GOL	A	503	-	5,5,5	0.32	0	5,5,5	0.46	0
3	EDO	B	503	-	3,3,3	0.48	0	2,2,2	0.76	0
3	EDO	A	505	-	3,3,3	0.49	0	2,2,2	0.68	0
2	GOL	A	502	-	5,5,5	0.28	0	5,5,5	0.58	0
2	GOL	A	501	-	5,5,5	0.55	0	5,5,5	0.95	0
3	EDO	B	504	-	3,3,3	0.50	0	2,2,2	0.86	0
3	EDO	A	504	-	3,3,3	0.38	0	2,2,2	0.53	0
2	GOL	B	501	-	5,5,5	0.49	0	5,5,5	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	507	-	-	1/1/1/1	-
3	EDO	B	502	-	-	1/1/1/1	-
3	EDO	A	506	-	-	1/1/1/1	-
2	GOL	A	503	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	503	-	-	1/1/1/1	-
3	EDO	A	505	-	-	1/1/1/1	-
2	GOL	A	502	-	-	2/4/4/4	-
2	GOL	A	501	-	-	0/4/4/4	-
3	EDO	B	504	-	-	1/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
2	GOL	B	501	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	GOL	O1-C1-C2-C3
2	B	501	GOL	O1-C1-C2-C3
2	B	501	GOL	O1-C1-C2-O2
2	A	502	GOL	O1-C1-C2-C3
2	B	501	GOL	C1-C2-C3-O3
2	A	503	GOL	O1-C1-C2-O2
2	A	502	GOL	O1-C1-C2-O2
3	A	507	EDO	O1-C1-C2-O2
3	B	502	EDO	O1-C1-C2-O2
3	B	504	EDO	O1-C1-C2-O2
2	B	501	GOL	O2-C2-C3-O3
3	A	506	EDO	O1-C1-C2-O2
3	A	505	EDO	O1-C1-C2-O2
3	B	503	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	EDO	1	0
3	B	503	EDO	2	0
2	A	501	GOL	3	0
2	B	501	GOL	5	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	402/435 (92%)	0.35	11 (2%) 54 55	40, 63, 97, 119	0
1	B	405/435 (93%)	0.37	12 (2%) 50 51	40, 64, 97, 121	0
All	All	807/870 (92%)	0.36	23 (2%) 51 52	40, 64, 98, 121	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	GLN	4.0
1	B	213	PHE	3.8
1	A	275	TRP	3.7
1	A	309	LEU	3.4
1	B	391	LEU	3.3
1	B	274	ILE	3.2
1	A	86	LEU	3.1
1	B	228	ALA	3.1
1	A	228	ALA	3.0
1	B	299	GLY	3.0
1	A	274	ILE	2.9
1	B	309	LEU	2.8
1	B	86	LEU	2.7
1	B	7	LYS	2.5
1	A	87	PRO	2.5
1	A	321	LEU	2.5
1	A	85	GLN	2.3
1	A	50	TYR	2.2
1	B	300	PHE	2.2
1	A	266	LEU	2.1
1	B	244	VAL	2.1
1	A	391	LEU	2.1
1	B	266	LEU	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	EDO	B	503	4/4	0.79	0.34	53,53,53,53	0
3	EDO	B	502	4/4	0.80	0.18	66,66,66,66	0
3	EDO	A	505	4/4	0.85	0.24	64,64,64,64	0
2	GOL	A	502	6/6	0.86	0.21	64,65,65,66	0
3	EDO	A	507	4/4	0.89	0.26	54,54,54,54	0
2	GOL	B	501	6/6	0.89	0.23	59,60,60,61	0
2	GOL	A	501	6/6	0.90	0.24	56,57,57,58	0
3	EDO	A	506	4/4	0.92	0.26	54,54,54,54	0
3	EDO	A	504	4/4	0.93	0.18	57,57,57,57	0
3	EDO	B	504	4/4	0.93	0.30	55,55,55,55	0
2	GOL	A	503	6/6	0.95	0.19	65,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.