



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:22 AM GMT

PDB ID : 3EDF  
Title : Structural base for cyclodextrin hydrolysis  
Authors : Buedenbender, S.; Schulz, G.E.  
Deposited on : 2008-09-03  
Resolution : 1.65 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

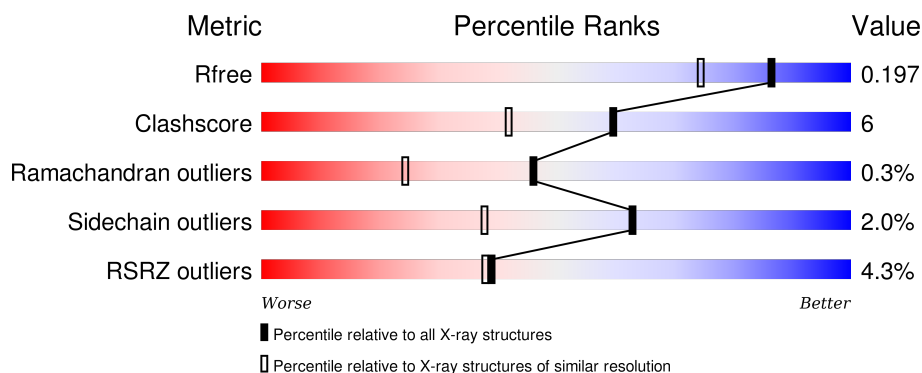
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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))
$R_{free}$	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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. 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	601	<div> <div>4%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	B	601	<div> <div>4%</div> <div>88%</div> <div>11%</div> <div>..</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
3	CE6	A	700[B]	X	-	-	-
3	CE6	B	700[B]	X	-	-	-
5	GOL	A	801	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11344 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 Cyclomaltoextrinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	20	0
			4847	3060	874	889	24			
1	B	597	Total	C	N	O	S	0	29	0
			4901	3098	887	891	25			

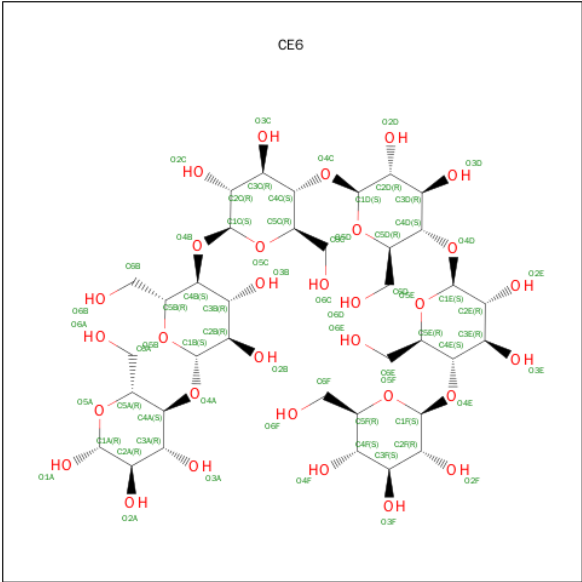
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	PRO	THR	ENGINEERED	UNP Q8KKG0
A	340	GLN	GLU	ENGINEERED	UNP Q8KKG0
B	49	PRO	THR	ENGINEERED	UNP Q8KKG0
B	340	GLN	GLU	ENGINEERED	UNP Q8KKG0

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

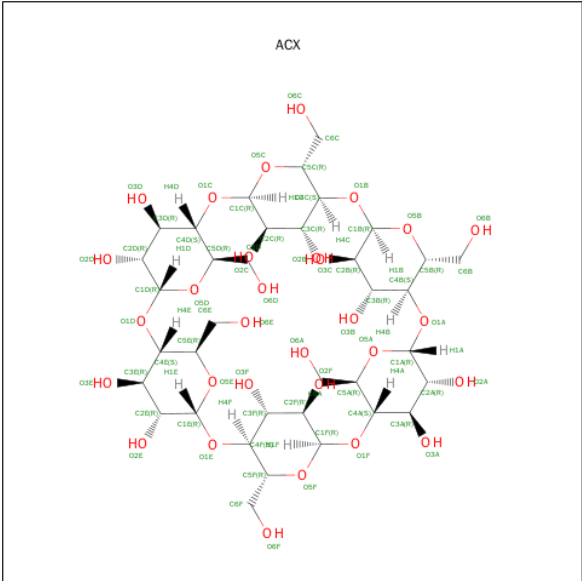
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is SUGAR (CELLOHEXAOSE) (three-letter code: CE6) (formula: C<sub>36</sub>H<sub>62</sub>O<sub>31</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			67	36	31		
3	B	1	Total	C	O	0	1
			67	36	31		

- Molecule 4 is SUGAR (ALPHA-CYCLODEXTRIN (CYCLOHEXA-AMYLOSE)) (three-letter code: ACX) (formula: C<sub>36</sub>H<sub>60</sub>O<sub>30</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			66	36	30		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	1
			66	36	30		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

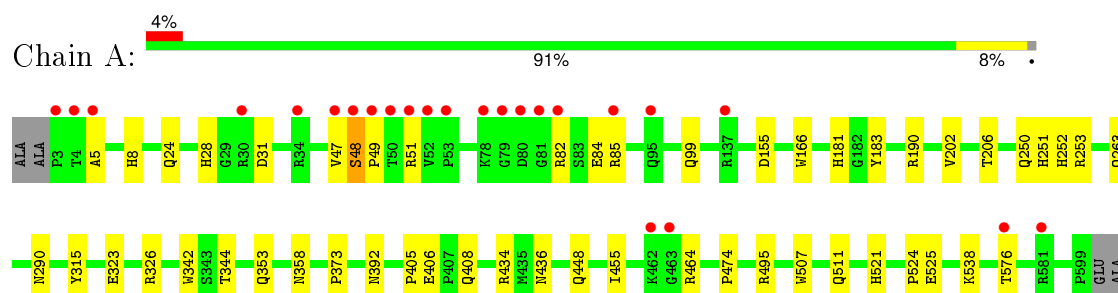
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	685	Total	O	0	0
			685	685		
6	B	617	Total	O	0	0
			617	617		

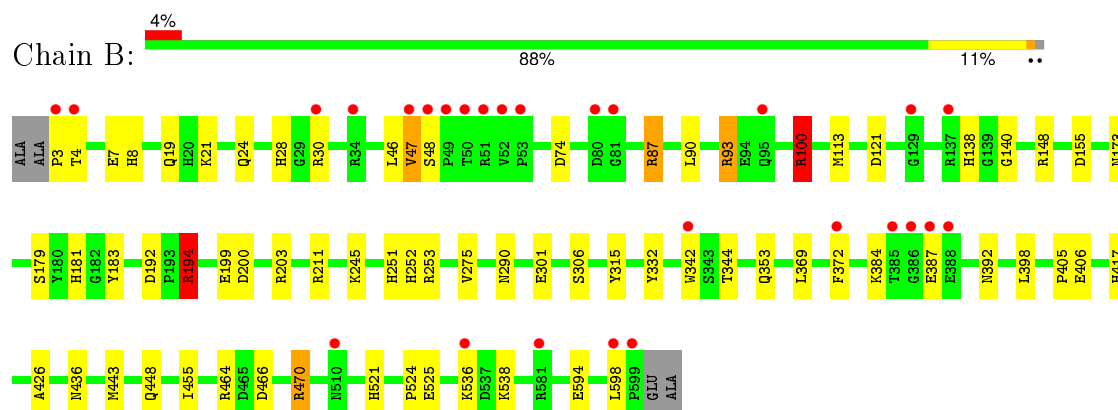
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Cyclomaltodextrinase



#### • Molecule 1: Cyclomaltodextrinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.54Å 111.11Å 106.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.57 – 1.65 19.57 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.57-1.65) 99.9 (19.57-1.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.167 , 0.201 0.164 , 0.197	Depositor DCC
$R_{free}$ test set	3038 reflections (2.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.0	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.6	EDS
Estimated twinning fraction	0.009 for -h,l,k 0.010 for -k,-h,l 0.007 for l,-k,h 0.000 for l,h,k 0.000 for k,l,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 151899 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11344	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, CA, ACX, CE6

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	0.75	0/5075	0.75	1/6878 (0.0%)
1	B	0.73	1/5165 (0.0%)	0.94	12/6997 (0.2%)
All	All	0.74	1/10240 (0.0%)	0.85	13/13875 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	100	ARG	CG-CD	5.33	1.65	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	470[A]	ARG	NE-CZ-NH2	20.76	130.68	120.30
1	B	470[B]	ARG	NE-CZ-NH2	20.76	130.68	120.30
1	B	470[A]	ARG	NE-CZ-NH1	-16.84	111.88	120.30
1	B	470[B]	ARG	NE-CZ-NH1	-16.84	111.88	120.30
1	B	194	ARG	NE-CZ-NH1	-14.90	112.85	120.30
1	B	93	ARG	NE-CZ-NH1	-12.07	114.26	120.30
1	B	194	ARG	NE-CZ-NH2	11.13	125.87	120.30
1	B	100	ARG	NE-CZ-NH1	9.77	125.18	120.30
1	B	93	ARG	NE-CZ-NH2	9.48	125.04	120.30
1	B	470[A]	ARG	CD-NE-CZ	7.47	134.06	123.60
1	B	470[B]	ARG	CD-NE-CZ	7.47	134.06	123.60
1	B	100	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	190	ARG	NE-CZ-NH1	5.14	122.87	120.30

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	4847	0	4647	40	0
1	B	4901	0	4698	73	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	67	0	62	1	0
3	B	67	0	60	9	0
4	A	66	0	60	2	0
4	B	66	0	60	2	0
5	A	12	0	16	0	0
5	B	12	0	16	0	0
6	A	685	0	0	14	0
6	B	617	0	0	8	0
All	All	11344	0	9619	113	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 (113) 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:B:464[B]:ARG:HD2	3:B:700[B]:CE6:O6A	1.17	1.28
1:B:342[B]:TRP:CZ3	3:B:700[B]:CE6:C5A	2.13	1.25
1:B:344[B]:THR:OG1	1:B:372[B]:PHE:CE2	1.95	1.18
1:B:342[B]:TRP:CZ3	3:B:700[B]:CE6:H5A	1.64	1.06
1:B:47:VAL:HG12	1:B:48:SER:H	1.23	1.01
1:B:464[B]:ARG:CD	3:B:700[B]:CE6:O6A	2.11	0.97
1:B:344[B]:THR:OG1	1:B:372[B]:PHE:HE2	1.45	0.92
1:B:253:ARG:NH1	3:B:700[B]:CE6:O3A	2.03	0.92
1:B:464[B]:ARG:HD2	3:B:700[B]:CE6:HO6A	1.17	0.91
1:B:138:HIS:HD2	1:B:140:GLY:H	1.18	0.91
1:B:342[B]:TRP:CE2	1:B:372[B]:PHE:HE1	1.89	0.90
1:B:342[B]:TRP:CH2	3:B:700[B]:CE6:H5A	2.10	0.87
1:B:466:ASP:O	1:B:470[B]:ARG:HD2	1.75	0.86
1:B:342[B]:TRP:CZ2	1:B:372[B]:PHE:HE1	1.94	0.85
1:B:47:VAL:HG12	1:B:48:SER:N	1.91	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344[B]:THR:OG1	1:B:372[B]:PHE:CD2	2.21	0.83
1:B:93:ARG:CD	1:B:301:GLU:OE2	2.25	0.82
1:B:93:ARG:HD2	1:B:301:GLU:OE2	1.81	0.80
1:B:342[B]:TRP:CE2	1:B:372[B]:PHE:CE1	2.69	0.79
1:B:406[A]:GLU:OE1	6:B:1409:HOH:O	2.00	0.79
1:B:138:HIS:CD2	1:B:140:GLY:H	2.01	0.79
1:B:74:ASP:OD1	1:B:87[A]:ARG:HG2	1.85	0.77
1:B:192:ASP:OD2	1:B:194:ARG:CD	2.33	0.77
1:B:192:ASP:OD2	1:B:194:ARG:HD2	1.85	0.76
1:B:181:HIS:HD2	1:B:183:TYR:H	1.34	0.76
1:B:417:HIS:O	1:B:470[A]:ARG:HD2	1.85	0.75
1:A:181:HIS:HD2	1:A:183:TYR:H	1.35	0.75
1:B:113:MET:SD	1:B:470[A]:ARG:HG2	2.27	0.74
1:A:47:VAL:O	1:A:48:SER:HB3	1.89	0.72
1:B:93:ARG:HD3	1:B:301:GLU:OE2	1.89	0.72
1:B:251:HIS:HD2	1:B:315:TYR:OH	1.72	0.72
1:B:466:ASP:O	1:B:470[A]:ARG:HD3	1.92	0.70
1:B:138:HIS:HD2	1:B:140:GLY:N	1.90	0.70
1:A:8:HIS:HD2	1:A:28:HIS:ND1	1.90	0.69
4:A:701[A]:ACX:H5F	6:A:1006:HOH:O	1.92	0.69
1:B:8:HIS:HD2	1:B:28:HIS:ND1	1.92	0.67
1:A:353:GLN:HE21	1:A:405:PRO:HD2	1.58	0.67
1:B:466:ASP:O	1:B:470[B]:ARG:CD	2.42	0.66
1:A:251:HIS:HD2	1:A:315:TYR:OH	1.78	0.66
1:B:155:ASP:OD2	1:B:211:ARG:HD3	1.96	0.65
1:B:353:GLN:HE21	1:B:405:PRO:HD2	1.63	0.63
1:B:342[B]:TRP:CZ2	1:B:372[B]:PHE:CE1	2.84	0.63
1:B:417:HIS:O	1:B:470[B]:ARG:NH1	2.33	0.62
1:B:192:ASP:OD2	1:B:194:ARG:HD3	1.98	0.62
1:B:384:LYS:HB3	1:B:387:GLU:HG3	1.82	0.60
1:B:93:ARG:HD3	1:B:301:GLU:CD	2.22	0.60
1:A:47:VAL:O	1:A:48:SER:CB	2.50	0.60
1:B:306[B]:SER:OG	6:B:1496:HOH:O	2.16	0.59
1:A:525:GLU:OE2	1:B:252:HIS:HE1	1.86	0.59
1:A:181:HIS:CD2	1:A:183:TYR:H	2.19	0.59
1:B:342[B]:TRP:HH2	1:B:464[B]:ARG:NH1	2.01	0.58
1:A:576[A]:THR:HG23	6:A:1095:HOH:O	2.05	0.56
1:B:47:VAL:CG1	1:B:48:SER:N	2.63	0.56
1:B:100:ARG:HD2	1:B:332:TYR:CD1	2.41	0.56
1:B:342[A]:TRP:CH2	1:B:464[A]:ARG:NH1	2.74	0.56
1:A:495[A]:ARG:NE	6:A:895:HOH:O	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:GLN:HE22	1:A:538:LYS:HZ2	1.54	0.55
1:B:200:ASP:OD1	1:B:203[A]:ARG:NH2	2.40	0.55
1:A:434:ARG:NH2	6:A:1054:HOH:O	2.40	0.55
1:A:252:HIS:HD2	6:B:1200:HOH:O	1.91	0.54
1:A:323[A]:GLU:OE2	1:A:326[A]:ARG:NH2	2.35	0.54
1:B:181:HIS:HE1	6:B:1563:HOH:O	1.90	0.54
6:A:828:HOH:O	1:B:252:HIS:HD2	1.92	0.53
4:B:701[A]:ACX:H6F2	4:B:701[A]:ACX:H3E	1.90	0.53
1:A:252:HIS:HE1	1:B:525:GLU:OE2	1.93	0.52
1:A:202:VAL:O	1:A:206[B]:THR:HG23	2.10	0.52
1:A:8:HIS:HE1	6:A:1379:HOH:O	1.93	0.51
1:B:406[A]:GLU:CD	6:B:1409:HOH:O	2.47	0.50
1:A:342:TRP:CG	3:A:700[B]:CE6:H3A	2.47	0.50
1:A:495[A]:ARG:NH2	6:A:1058:HOH:O	2.45	0.50
1:A:392:ASN:HA	1:A:524:PRO:HG2	1.94	0.49
1:B:342[B]:TRP:CH2	1:B:464[B]:ARG:NH1	2.80	0.49
1:B:19:GLN:O	1:B:21:LYS:NZ	2.43	0.49
1:B:181:HIS:CD2	1:B:183:TYR:H	2.21	0.49
1:A:353:GLN:NE2	1:A:406:GLU:H	2.10	0.49
1:B:24:GLN:NE2	1:B:290:ASN:HD22	2.10	0.49
1:B:3:PRO:HB3	1:B:7:GLU:HB2	1.95	0.48
1:A:344[B]:THR:HG23	1:A:373:PRO:HA	1.95	0.47
1:A:24:GLN:NE2	1:A:290:ASN:HD22	2.12	0.47
1:A:511:GLN:HE22	1:A:538:LYS:NZ	2.11	0.47
1:A:464[A]:ARG:HD2	4:A:701[A]:ACX:H3F	1.95	0.47
1:B:342[A]:TRP:HH2	1:B:464[A]:ARG:HH12	1.62	0.46
1:A:455[A]:ILE:HD11	1:A:474:PRO:CG	2.45	0.46
1:A:344[B]:THR:HG22	6:A:1169:HOH:O	2.15	0.46
1:A:250[B]:GLN:HG2	1:B:525:GLU:CD	2.36	0.46
1:A:263:GLN:NE2	6:A:1328:HOH:O	2.48	0.46
1:B:253:ARG:NH1	3:B:700[B]:CE6:HO3A	2.12	0.45
1:A:155:ASP:HB2	6:A:1052:HOH:O	2.17	0.45
1:B:417:HIS:HB2	1:B:470[B]:ARG:NH2	2.31	0.45
1:B:275:VAL:HG11	4:B:701[A]:ACX:H6C2	1.98	0.44
1:A:507:TRP:O	1:A:511:GLN:HG2	2.17	0.44
1:B:405:PRO:HB2	1:B:406[A]:GLU:HG3	2.00	0.44
1:A:99:GLN:NE2	6:A:1290:HOH:O	2.50	0.43
1:A:31:ASP:HB2	1:A:82:ARG:HH21	1.84	0.43
1:B:538:LYS:HZ1	1:B:594[B]:GLU:CD	2.22	0.43
1:B:426:ALA:HB2	6:B:1321:HOH:O	2.19	0.42
3:B:700[B]:CE6:H4B	3:B:700[B]:CE6:H5C	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ASN:O	1:B:179:SER:HB2	2.19	0.42
1:B:398:LEU:HD11	1:B:443:MET:SD	2.60	0.41
1:B:121:ASP:HB2	1:B:148:ARG:HD3	2.02	0.41
1:B:392:ASN:HA	1:B:524:PRO:HG2	2.02	0.41
1:A:358:ASN:ND2	6:A:1029:HOH:O	2.53	0.41
1:A:48:SER:HA	1:A:49:PRO:HD3	1.91	0.41
1:A:408:GLN:HB2	6:A:1063:HOH:O	2.22	0.40
1:A:166:TRP:CD1	1:A:166:TRP:C	2.93	0.40
1:A:206[B]:THR:HG21	6:A:1003:HOH:O	2.21	0.40
1:B:536[A]:LYS:HE3	6:B:1518:HOH:O	2.20	0.40
1:B:199:GLU:HG3	6:B:1590:HOH:O	2.20	0.40
1:A:82:ARG:NH1	1:A:84:GLU:OE2	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	615/601 (102%)	598 (97%)	15 (2%)	2 (0%)	46	24
1	B	624/601 (104%)	611 (98%)	12 (2%)	1 (0%)	52	30
All	All	1239/1202 (103%)	1209 (98%)	27 (2%)	3 (0%)	46	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	B	47	VAL
1	A	5	ALA

### 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	512/493 (104%)	506 (99%)	6 (1%)	78	60
1	B	521/493 (106%)	505 (97%)	16 (3%)	47	16
All	All	1033/986 (105%)	1011 (98%)	22 (2%)	63	34

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	85	ARG
1	A	253	ARG
1	A	436	ASN
1	A	448	GLN
1	A	521	HIS
1	B	4	THR
1	B	30[A]	ARG
1	B	30[B]	ARG
1	B	46	LEU
1	B	87[A]	ARG
1	B	87[B]	ARG
1	B	90	LEU
1	B	100	ARG
1	B	194	ARG
1	B	245	LYS
1	B	369	LEU
1	B	436	ASN
1	B	448	GLN
1	B	455	ILE
1	B	521	HIS
1	B	598	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	24	GLN
1	A	99	GLN
1	A	111	GLN
1	A	181	HIS
1	A	217	GLN
1	A	241	ASN
1	A	251	HIS
1	A	252	HIS
1	A	257	GLN
1	A	263	GLN
1	A	353	GLN
1	A	358	ASN
1	A	448	GLN
1	A	498	GLN
1	A	511	GLN
1	B	8	HIS
1	B	24	GLN
1	B	111	GLN
1	B	138	HIS
1	B	181	HIS
1	B	217	GLN
1	B	241	ASN
1	B	251	HIS
1	B	252	HIS
1	B	257	GLN
1	B	296	ASN
1	B	353	GLN
1	B	358	ASN
1	B	448	GLN
1	B	498	GLN
1	B	511	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	CE6	A	700[B]	-	72,72,72	0.56	0	107,107,107	1.13	7 (6%)
4	ACX	A	701[A]	-	72,72,72	0.53	0	108,108,108	1.02	6 (5%)
5	GOL	A	800	-	5,5,5	0.51	0	5,5,5	0.34	0
5	GOL	A	801	-	5,5,5	0.47	0	5,5,5	0.48	0
3	CE6	B	700[B]	-	72,72,72	0.55	0	107,107,107	1.23	8 (7%)
4	ACX	B	701[A]	-	72,72,72	0.64	0	108,108,108	1.10	7 (6%)
5	GOL	B	800	-	5,5,5	0.47	0	5,5,5	0.11	0
5	GOL	B	801	-	5,5,5	0.28	0	5,5,5	0.48	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	CE6	A	700[B]	-	6/6/30/30	0/32/152/152	0/6/6/6
4	ACX	A	701[A]	-	-	0/36/156/156	0/0/7/7
5	GOL	A	800	-	-	0/4/4/4	0/0/0/0
5	GOL	A	801	-	-	0/4/4/4	0/0/0/0
3	CE6	B	700[B]	-	6/6/30/30	0/32/152/152	0/6/6/6
4	ACX	B	701[A]	-	-	0/36/156/156	0/0/7/7
5	GOL	B	800	-	-	0/4/4/4	0/0/0/0
5	GOL	B	801	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.



All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701[A]	ACX	C3D-C4D-C5D	-2.68	104.78	110.84
4	A	701[A]	ACX	C1B-O1B-C4C	-2.13	112.43	118.01
3	A	700[B]	CE6	O5D-C1D-C2D	-2.07	106.03	110.28
4	B	701[A]	ACX	O5E-C5E-C4E	2.03	114.04	109.75
3	B	700[B]	CE6	C2D-C3D-C4D	2.05	114.11	109.60
3	B	700[B]	CE6	C1F-C2F-C3F	2.10	114.12	109.97
3	B	700[B]	CE6	C1C-O5C-C5C	2.16	117.95	113.75
4	B	701[A]	ACX	O2E-C2E-C1E	2.17	114.78	110.02
3	A	700[B]	CE6	C3F-C4F-C5F	2.22	114.07	110.20
4	A	701[A]	ACX	O3D-C3D-C4D	2.24	115.17	109.87
3	B	700[B]	CE6	O4B-C4B-C3B	2.34	113.21	107.17
4	B	701[A]	ACX	C2D-C3D-C4D	2.36	114.77	109.60
3	B	700[B]	CE6	O5E-C5E-C6E	2.39	112.39	106.36
3	A	700[B]	CE6	C1C-O5C-C5C	2.41	118.43	113.75
3	A	700[B]	CE6	O5C-C5C-C4C	2.61	115.26	109.75
3	B	700[B]	CE6	C1F-O5F-C5F	2.61	118.82	113.75
4	B	701[A]	ACX	O1E-C4F-C3F	2.74	114.23	107.17
4	B	701[A]	ACX	O1F-C4A-C5A	2.83	116.75	109.32
4	A	701[A]	ACX	O5C-C5C-C4C	2.83	115.72	109.75
3	A	700[B]	CE6	O5F-C5F-C4F	2.98	115.28	109.68
4	A	701[A]	ACX	C1C-O5C-C5C	3.02	119.61	113.75
3	A	700[B]	CE6	C1F-O5F-C5F	3.07	119.70	113.75
4	B	701[A]	ACX	C1F-O5F-C5F	3.11	119.77	113.75
3	A	700[B]	CE6	O4B-C4B-C3B	3.28	115.63	107.17
4	B	701[A]	ACX	C1E-O5E-C5E	3.31	120.17	113.75
3	B	700[B]	CE6	O5E-C5E-C4E	3.41	116.96	109.75
4	A	701[A]	ACX	O1C-C4D-C3D	3.50	116.20	107.17
3	B	700[B]	CE6	C1E-O5E-C5E	5.45	124.32	113.75

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	700[B]	CE6	C1B
3	A	700[B]	CE6	C1C
3	A	700[B]	CE6	C1D
3	A	700[B]	CE6	C1E
3	A	700[B]	CE6	C1F
3	A	700[B]	CE6	C1A
3	B	700[B]	CE6	C1B
3	B	700[B]	CE6	C1C
3	B	700[B]	CE6	C1D
3	B	700[B]	CE6	C1E

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Mol	Chain	Res	Type	Atom
3	B	700[B]	CE6	C1F
3	B	700[B]	CE6	C1A

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	700[B]	CE6	1	0
4	A	701[A]	ACX	2	0
3	B	700[B]	CE6	9	0
4	B	701[A]	ACX	2	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 ⓘ

### 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	597/601 (99%)	-0.13	24 (4%)	42 41	10, 15, 31, 54	0
1	B	597/601 (99%)	-0.04	27 (4%)	37 35	11, 17, 35, 57	0
All	All	1194/1202 (99%)	-0.09	51 (4%)	39 38	10, 16, 34, 57	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	PRO	17.3
1	B	3	PRO	14.3
1	A	4	THR	9.2
1	B	4	THR	7.4
1	B	48	SER	6.5
1	B	51	ARG	6.3
1	A	81	GLY	6.2
1	A	51	ARG	6.1
1	B	50	THR	5.9
1	A	79	GLY	5.0
1	B	49	PRO	4.9
1	A	50	THR	4.9
1	A	48	SER	4.9
1	A	80	ASP	4.5
1	B	53	PRO	4.4
1	B	386	GLY	4.4
1	A	49	PRO	4.0
1	B	47	VAL	3.7
1	A	53	PRO	3.7
1	B	581	ARG	3.7
1	A	30	ARG	3.6
1	B	30[A]	ARG	3.6
1	B	599	PRO	3.5
1	B	81	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	463	GLY	3.4
1	A	581	ARG	3.3
1	A	95	GLN	3.2
1	A	52	VAL	3.2
1	B	95	GLN	3.1
1	B	80	ASP	2.9
1	A	5	ALA	2.9
1	B	598	LEU	2.9
1	A	47	VAL	2.9
1	A	34	ARG	2.9
1	B	388[A]	GLU	2.8
1	B	385	THR	2.8
1	B	137[A]	ARG	2.7
1	B	342[A]	TRP	2.7
1	B	34	ARG	2.6
1	B	387	GLU	2.6
1	B	536[A]	LYS	2.4
1	A	462	LYS	2.4
1	A	82	ARG	2.3
1	A	576[A]	THR	2.3
1	B	52	VAL	2.3
1	A	137	ARG	2.2
1	B	372[A]	PHE	2.2
1	B	129	GLY	2.2
1	A	85	ARG	2.1
1	B	510	ASN	2.1
1	A	78	LYS	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	A	801	6/6	0.86	0.13	3.25	30,32,34,35	0
3	CE6	B	700[B]	67/67	0.93	0.15	0.67	13,18,41,41	67
5	GOL	A	800	6/6	0.97	0.08	0.57	14,15,16,16	0
5	GOL	B	801	6/6	0.95	0.09	0.40	27,30,32,32	0
3	CE6	A	700[B]	67/67	0.94	0.10	0.20	9,15,26,27	67
4	ACX	A	701[A]	66/66	0.95	0.09	0.01	8,17,24,28	66
4	ACX	B	701[A]	66/66	0.93	0.10	-0.22	9,16,21,22	66
5	GOL	B	800	6/6	0.96	0.07	-0.51	18,20,20,21	0
2	CA	B	602	1/1	0.99	0.07	-0.83	15,15,15,15	0
2	CA	A	602	1/1	0.99	0.04	-1.67	12,12,12,12	0
2	CA	B	603	1/1	0.99	0.05	-1.81	19,19,19,19	0
2	CA	A	603	1/1	1.00	0.03	-2.39	15,15,15,15	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.