



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2018 – 12:46 AM EDT

PDB ID : 2C4U  
Title : Crystal structure of the apo form of the 5'-Fluoro-5'-deoxyadenosine synthase enzyme from *Streptomyces cattleya*  
Authors : McEwan, A.R.; Deng, H.; Robinson, D.A.; DeLaurentis, W.; McGlinchey, R.P.; O'Hagan, D.; Naismith, J.H.  
Deposited on : 2005-10-22  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031021  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031021

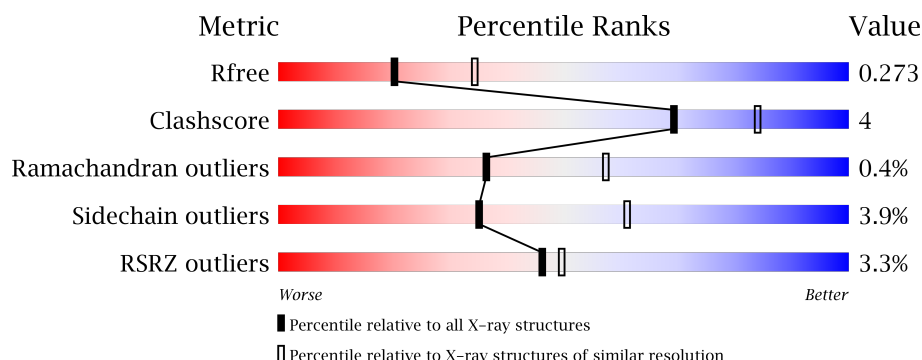
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	299	<div> <div>3%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>
1	B	299	<div> <div>%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	C	299	<div> <div>3%</div> <div>84%</div> <div>13%</div> <div>.</div> </div>
1	D	299	<div> <div>7%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	E	299	<div> <div>4%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	299	<div><div><div>%</div><div><div></div></div><div>86%</div><div>11%</div><div></div></div></div>

## 2 Entry composition [i](#)

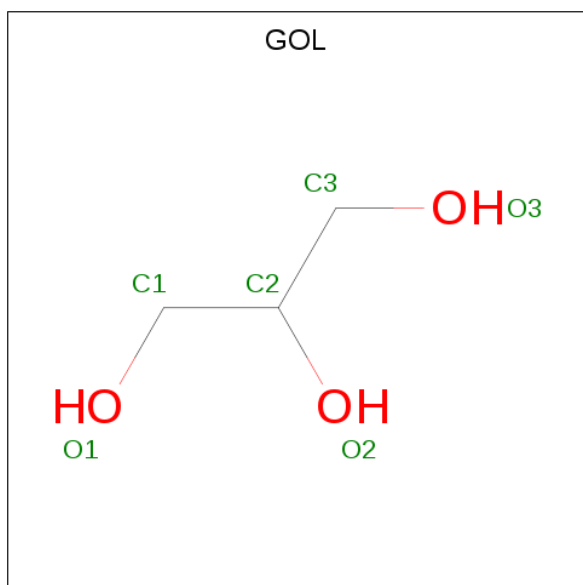
There are 3 unique types of molecules in this entry. The entry contains 13825 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 5'-FLUORO-5'-DEOXYADENOSINE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	1	0
			2225	1413	378	426	8			
1	B	291	Total	C	N	O	S	0	1	0
			2225	1413	378	426	8			
1	C	291	Total	C	N	O	S	0	1	0
			2225	1413	378	426	8			
1	D	291	Total	C	N	O	S	0	1	0
			2225	1413	378	426	8			
1	E	291	Total	C	N	O	S	0	1	0
			2225	1413	378	426	8			
1	F	291	Total	C	N	O	S	0	1	0
			2225	1413	378	426	8			

- 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 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0

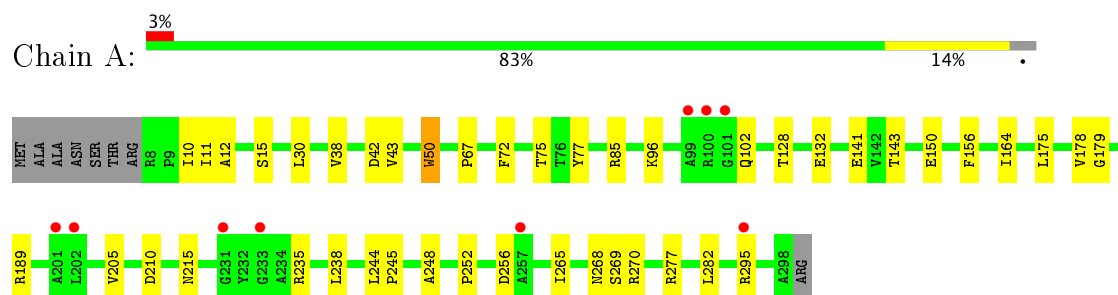
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	85	Total O 85 85	0	0
3	B	88	Total O 88 88	0	0
3	C	61	Total O 61 61	0	0
3	D	38	Total O 38 38	0	0
3	E	82	Total O 82 82	0	0
3	F	55	Total O 55 55	0	0

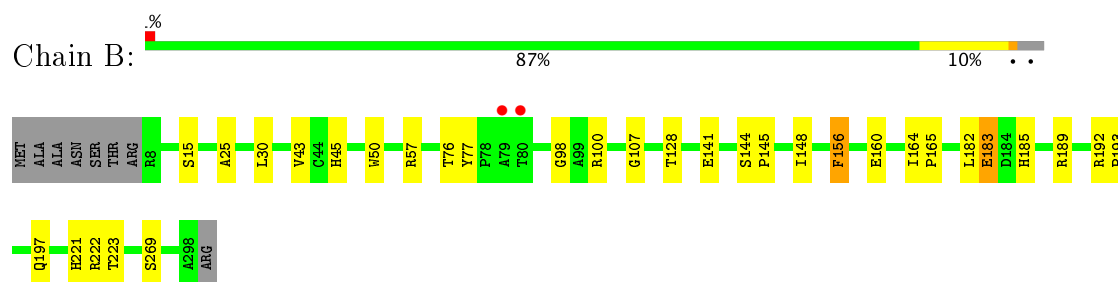
### 3 Residue-property plots [i](#)

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.

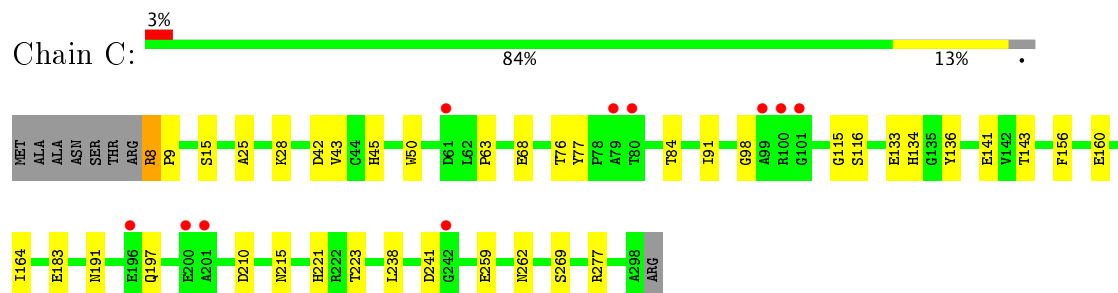
#### • Molecule 1: 5'-FLUORO-5'-DEOXYADENOSINE SYNTHASE



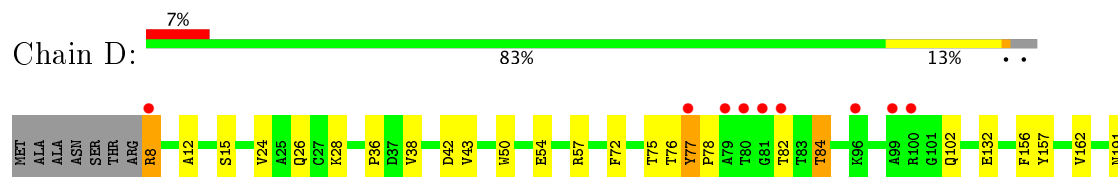
#### • Molecule 1: 5'-FLUORO-5'-DEOXYADENOSINE SYNTHASE

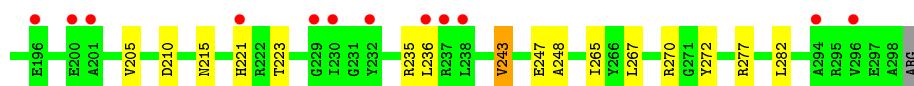


#### • Molecule 1: 5'-FLUORO-5'-DEOXYADENOSINE SYNTHASE

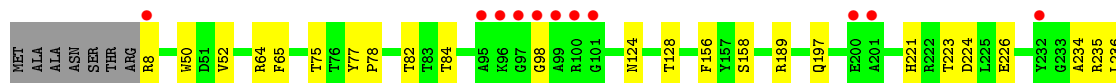
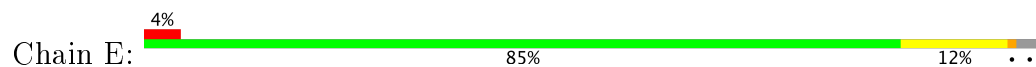


#### • Molecule 1: 5'-FLUORO-5'-DEOXYADENOSINE SYNTHASE

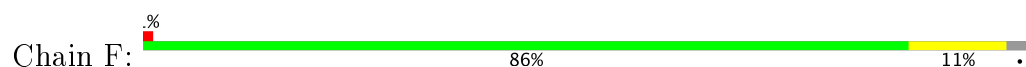




• Molecule 1: 5'-FLUORO-5'-DEOXYADENOSINE SYNTHASE



• Molecule 1: 5'-FLUORO-5'-DEOXYADENOSINE SYNTHASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.91Å 128.06Å 146.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.23 – 2.50 73.25 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (96.23-2.50) 99.3 (73.25-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.215 , 0.273 0.237 , 0.273	Depositor DCC
$R_{free}$ test set	3413 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtrriage
Anisotropy	0.224	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13825	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3352e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.60	0/2284	0.66	0/3117
1	B	0.63	0/2284	0.68	0/3117
1	C	0.57	0/2284	0.65	0/3117
1	D	0.59	0/2284	0.68	0/3117
1	E	0.64	0/2284	0.68	0/3117
1	F	0.58	0/2284	0.67	0/3117
All	All	0.60	0/13704	0.67	0/18702

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	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	75	THR	Peptide

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2225	0	2167	22	0
1	B	2225	0	2167	17	0
1	C	2225	0	2167	21	0
1	D	2225	0	2167	21	0
1	E	2225	0	2167	18	0
1	F	2225	0	2167	15	0
2	A	18	0	24	3	0
2	B	6	0	8	0	0
2	C	12	0	16	3	0
2	D	12	0	16	0	0
2	E	6	0	8	0	0
2	F	12	0	16	0	0
3	A	85	0	0	0	0
3	B	88	0	0	2	0
3	C	61	0	0	0	0
3	D	38	0	0	1	0
3	E	82	0	0	0	0
3	F	55	0	0	0	0
All	All	13825	0	13090	107	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 4.

All (107) 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:50:TRP:HE1	2:A:1299:GOL:H2	1.30	0.94
1:B:221:HIS:HD2	1:B:223:THR:H	1.29	0.80
1:A:175:LEU:O	1:A:178:VAL:HG22	1.87	0.74
1:E:128:THR:HG23	1:E:189:ARG:HG3	1.70	0.73
2:A:1301:GOL:H2	1:C:50:TRP:HE1	1.58	0.69
1:E:64:ARG:NH2	1:E:98:GLY:H	1.92	0.67
1:C:28:LYS:NZ	2:C:1299:GOL:H32	2.10	0.67
1:E:237:ARG:HH12	1:E:245:PRO:HB3	1.62	0.65
1:A:42:ASP:HB2	2:C:1299:GOL:H31	1.78	0.65
1:C:28:LYS:HZ2	2:C:1299:GOL:H32	1.62	0.62
1:A:210:ASP:HB3	1:A:215:ASN:HB2	1.82	0.61
1:E:221:HIS:HD2	1:E:223:THR:HG23	1.67	0.60
1:B:221:HIS:CD2	1:B:223:THR:H	2.17	0.60
1:E:236:LEU:O	1:E:247:GLU:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:GLU:HA	1:C:164:ILE:HD12	1.85	0.57
1:E:268:ASN:C	1:E:270:ARG:H	2.07	0.56
1:D:210:ASP:HB3	1:D:215:ASN:HB2	1.87	0.56
1:E:221:HIS:CD2	1:E:223:THR:HG23	2.41	0.56
1:E:254:PHE:O	1:E:278:ASN:HB2	2.06	0.56
1:A:248:ALA:HB3	1:A:265:ILE:HD12	1.90	0.54
1:F:221:HIS:CD2	1:F:223:THR:H	2.25	0.54
1:A:50:TRP:NE1	2:A:1299:GOL:H2	2.12	0.54
1:E:268:ASN:O	1:E:270:ARG:N	2.39	0.53
1:A:43:VAL:HA	1:C:25:ALA:HB2	1.91	0.53
1:A:10:ILE:HD12	1:A:67:PRO:HG2	1.91	0.52
1:D:236:LEU:O	1:D:247:GLU:HA	2.09	0.52
1:D:267:LEU:HA	1:D:272:TYR:O	2.11	0.50
1:F:175:LEU:O	1:F:178:VAL:HG22	2.11	0.50
1:B:128:THR:HG23	1:B:189:ARG:HG3	1.93	0.50
1:B:141:GLU:HB2	1:B:182:LEU:HD21	1.94	0.49
1:A:10:ILE:HD12	1:A:67:PRO:CG	2.43	0.49
1:A:150:GLU:HG3	1:B:107:GLY:HA2	1.95	0.49
1:A:252:PRO:HD2	1:A:256:ASP:OD2	2.12	0.49
1:B:57:ARG:NH1	3:B:2018:HOH:O	2.46	0.49
1:B:98:GLY:HA2	1:B:269:SER:O	2.13	0.49
1:D:76:THR:O	1:D:76:THR:HG23	2.12	0.49
1:D:12:ALA:HB3	1:D:72:PHE:CD1	2.48	0.48
1:E:64:ARG:HH22	1:E:98:GLY:H	1.60	0.48
1:B:148:ILE:HG22	1:B:165:PRO:HG3	1.95	0.48
1:B:25:ALA:HB2	1:C:43:VAL:HA	1.96	0.48
1:B:222:ARG:NH2	3:B:2057:HOH:O	2.46	0.48
1:B:30:LEU:HD13	1:B:164:ILE:HD11	1.96	0.48
1:E:82:THR:OG1	1:E:84:THR:HG22	2.13	0.48
1:C:221:HIS:HD2	1:C:223:THR:HG23	1.80	0.47
1:D:36:PRO:HB3	1:E:8:ARG:HD2	1.96	0.47
1:D:221:HIS:HD2	1:D:223:THR:H	1.62	0.47
1:C:98:GLY:HA2	1:C:269:SER:O	2.15	0.47
1:C:91:ILE:HA	1:C:136:TYR:HA	1.97	0.46
1:C:91:ILE:O	1:C:115:GLY:HA2	2.16	0.46
1:D:54:GLU:HG3	1:D:57:ARG:NH2	2.31	0.46
1:C:259:GLU:O	1:C:262:ASN:HB2	2.15	0.46
1:D:75:THR:HB	1:D:162:VAL:HG11	1.97	0.46
1:C:8:ARG:NE	1:C:8:ARG:N	2.63	0.46
1:C:68:GLU:HB3	1:C:116:SER:HB3	1.97	0.46
1:E:75:THR:HG21	1:E:158:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASN:C	1:A:270:ARG:H	2.20	0.45
1:E:238:LEU:HA	1:E:295:ARG:O	2.17	0.45
1:E:251:THR:HB	1:E:252:PRO:CD	2.45	0.45
1:D:43:VAL:HA	1:F:25:ALA:HB2	1.98	0.45
1:F:75:THR:HG21	1:F:158:SER:HB3	1.99	0.44
1:B:183:GLU:OE2	1:B:185:HIS:HB2	2.16	0.44
1:A:11:ILE:HD12	1:A:38:VAL:HG21	2.00	0.44
1:C:28:LYS:NZ	1:C:42:ASP:OD2	2.48	0.43
1:D:277:ARG:HD2	1:D:282:LEU:HA	2.00	0.43
1:E:78:PRO:HD2	1:E:124:ASN:HD22	1.83	0.43
1:A:128:THR:HG23	1:A:189:ARG:HG3	1.99	0.43
1:C:141:GLU:HG2	1:C:143:THR:HG23	2.01	0.43
1:C:63:PRO:HG2	1:C:134:HIS:CE1	2.53	0.43
1:F:160:GLU:HA	1:F:164:ILE:HD12	2.00	0.43
1:B:156:PHE:O	1:B:160:GLU:HG2	2.19	0.43
1:A:141:GLU:O	1:A:179:GLY:HA3	2.19	0.43
1:A:277:ARG:HG3	1:A:282:LEU:HB2	2.00	0.42
1:D:24:VAL:HG23	3:D:2007:HOH:O	2.19	0.42
1:F:11:ILE:HD11	1:F:167:ALA:HA	2.01	0.42
1:D:54:GLU:HG3	1:D:57:ARG:HH22	1.83	0.42
1:C:8:ARG:HA	1:C:9:PRO:HD3	1.91	0.42
1:A:30:LEU:HD13	1:A:164:ILE:HD11	2.00	0.42
1:D:8:ARG:HD2	1:F:36:PRO:HB3	2.01	0.42
1:F:153:GLU:HA	1:F:154:PRO:HD3	1.95	0.42
1:B:192:ARG:HA	1:B:193:PRO:HD2	1.92	0.42
1:A:238:LEU:HA	1:A:295:ARG:O	2.19	0.42
1:D:15:SER:HA	1:D:75:THR:O	2.19	0.42
1:F:164:ILE:HB	1:F:165:PRO:HD3	2.01	0.42
1:A:15:SER:HA	1:A:75:THR:O	2.20	0.42
1:A:12:ALA:HB3	1:A:72:PHE:CD1	2.55	0.42
1:D:77:TYR:CD1	1:D:157:TYR:HB3	2.55	0.42
1:F:162:VAL:C	1:F:165:PRO:HD2	2.40	0.42
1:A:244:LEU:HA	1:A:245:PRO:HD3	1.95	0.41
1:C:262:ASN:O	1:C:277:ARG:HA	2.20	0.41
1:B:15:SER:O	1:B:45:HIS:HA	2.20	0.41
1:B:76:THR:O	1:B:76:THR:HG23	2.21	0.41
1:C:76:THR:O	1:C:76:THR:HG23	2.20	0.41
1:C:210:ASP:HB3	1:C:215:ASN:HB2	2.02	0.41
1:D:82:THR:OG1	1:D:84:THR:CG2	2.69	0.41
1:F:248:ALA:HB3	1:F:265:ILE:HD12	2.03	0.41
1:F:91:ILE:O	1:F:115:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ARG:HG3	1:A:143:THR:HG22	2.02	0.41
1:B:144:SER:HA	1:B:145:PRO:HD3	1.95	0.41
1:F:243:VAL:O	1:F:245:PRO:HD3	2.21	0.41
1:D:248:ALA:HB3	1:D:265:ILE:HD12	2.03	0.41
1:C:15:SER:O	1:C:45:HIS:HA	2.20	0.41
1:D:77:TYR:O	1:D:78:PRO:C	2.60	0.40
1:D:26:GLN:HG2	1:E:65:PHE:CD2	2.57	0.40
1:F:221:HIS:HD2	1:F:223:THR:H	1.67	0.40
1:F:237:ARG:HB3	1:F:297:GLU:HG3	2.03	0.40
1:D:28:LYS:HZ1	1:D:42:ASP:CG	2.24	0.40
1:E:234:ALA:O	1:E:249:PRO:HA	2.22	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	290/299 (97%)	273 (94%)	15 (5%)	2 (1%)	24	42
1	B	290/299 (97%)	280 (97%)	9 (3%)	1 (0%)	43	64
1	C	290/299 (97%)	272 (94%)	18 (6%)	0	100	100
1	D	290/299 (97%)	273 (94%)	16 (6%)	1 (0%)	43	64
1	E	290/299 (97%)	277 (96%)	11 (4%)	2 (1%)	24	42
1	F	290/299 (97%)	274 (94%)	15 (5%)	1 (0%)	43	64
All	All	1740/1794 (97%)	1649 (95%)	84 (5%)	7 (0%)	36	57

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	LYS

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Mol	Chain	Res	Type
1	E	269	SER
1	A	269	SER
1	F	43	VAL
1	E	252	PRO
1	B	43	VAL
1	D	243	VAL

### 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	232/237 (98%)	225 (97%)	7 (3%)	44	71
1	B	232/237 (98%)	226 (97%)	6 (3%)	49	76
1	C	232/237 (98%)	222 (96%)	10 (4%)	32	56
1	D	232/237 (98%)	219 (94%)	13 (6%)	23	43
1	E	232/237 (98%)	222 (96%)	10 (4%)	32	56
1	F	232/237 (98%)	224 (97%)	8 (3%)	40	67
All	All	1392/1422 (98%)	1338 (96%)	54 (4%)	35	61

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	TRP
1	A	77	TYR
1	A	102	GLN
1	A	132	GLU
1	A	156	PHE
1	A	205	VAL
1	A	235	ARG
1	B	50	TRP
1	B	77	TYR
1	B	100	ARG
1	B	156	PHE
1	B	183	GLU

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Mol	Chain	Res	Type
1	B	197	GLN
1	C	8	ARG
1	C	77	TYR
1	C	84	THR
1	C	133	GLU
1	C	156	PHE
1	C	183	GLU
1	C	191	ASN
1	C	197	GLN
1	C	238	LEU
1	C	241	ASP
1	D	8	ARG
1	D	38	VAL
1	D	50	TRP
1	D	77	TYR
1	D	84	THR
1	D	102	GLN
1	D	132	GLU
1	D	156	PHE
1	D	191	ASN
1	D	205	VAL
1	D	235	ARG
1	D	243	VAL
1	D	270	ARG
1	E	50	TRP
1	E	52	VAL
1	E	77	TYR
1	E	156	PHE
1	E	197	GLN
1	E	224	ASP
1	E	226	GLU
1	E	235	ARG
1	E	256	ASP
1	E	270	ARG
1	F	50	TRP
1	F	76	THR
1	F	77	TYR
1	F	151	GLN
1	F	156	PHE
1	F	192	ARG
1	F	241	ASP
1	F	270	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	221	HIS
1	B	221	HIS
1	C	221	HIS
1	C	287	HIS
1	D	102	GLN
1	D	151	GLN
1	D	197	GLN
1	D	221	HIS
1	E	151	GLN
1	E	185	HIS
1	E	197	GLN
1	E	221	HIS
1	F	151	GLN
1	F	185	HIS
1	F	221	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 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	$\# Z  > 2$
2	GOL	A	1299	-	5,5,5	0.41	0	5,5,5	0.72	0
2	GOL	A	1300	-	5,5,5	0.46	0	5,5,5	0.43	0
2	GOL	A	1301	-	5,5,5	0.34	0	5,5,5	0.45	0
2	GOL	B	1299	-	5,5,5	0.52	0	5,5,5	0.46	0
2	GOL	C	1299	-	5,5,5	0.41	0	5,5,5	0.85	0
2	GOL	C	1300	-	5,5,5	0.45	0	5,5,5	0.25	0
2	GOL	D	1299	-	5,5,5	0.36	0	5,5,5	0.63	0
2	GOL	D	1300	-	5,5,5	0.32	0	5,5,5	0.49	0
2	GOL	E	1299	-	5,5,5	0.16	0	5,5,5	0.54	0
2	GOL	F	1299	-	5,5,5	0.43	0	5,5,5	0.36	0
2	GOL	F	1300	-	5,5,5	0.37	0	5,5,5	0.39	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	1299	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1300	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1301	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1299	-	-	0/4/4/4	0/0/0/0
2	GOL	C	1299	-	-	0/4/4/4	0/0/0/0
2	GOL	C	1300	-	-	0/4/4/4	0/0/0/0
2	GOL	D	1299	-	-	0/4/4/4	0/0/0/0
2	GOL	D	1300	-	-	0/4/4/4	0/0/0/0
2	GOL	E	1299	-	-	0/4/4/4	0/0/0/0
2	GOL	F	1299	-	-	0/4/4/4	0/0/0/0
2	GOL	F	1300	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1299	GOL	2	0
2	A	1301	GOL	1	0
2	C	1299	GOL	3	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	291/299 (97%)	0.12	9 (3%)	49	52	3, 15, 36, 49	0
1	B	291/299 (97%)	-0.05	2 (0%)	87	88	3, 12, 26, 36	0
1	C	291/299 (97%)	0.14	10 (3%)	45	48	5, 13, 30, 39	0
1	D	291/299 (97%)	0.33	21 (7%)	15	16	2, 16, 37, 50	0
1	E	291/299 (97%)	0.17	12 (4%)	37	40	2, 13, 34, 45	0
1	F	291/299 (97%)	0.05	4 (1%)	75	77	3, 13, 27, 36	0
All	All	1746/1794 (97%)	0.13	58 (3%)	46	50	2, 13, 33, 50	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	201	ALA	7.6
1	D	80	THR	5.4
1	D	79	ALA	5.4
1	A	201	ALA	5.0
1	A	100	ARG	4.9
1	E	95	ALA	4.6
1	E	201	ALA	4.6
1	F	100	ARG	4.4
1	E	98	GLY	4.1
1	E	101	GLY	4.0
1	E	100	ARG	3.9
1	E	99	ALA	3.8
1	D	200	GLU	3.8
1	D	238	LEU	3.8
1	D	229	GLY	3.6
1	E	97	GLY	3.4
1	D	296	VAL	3.4
1	A	101	GLY	3.4
1	D	196	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	230	ILE	3.3
1	E	269	SER	3.2
1	D	232	TYR	3.1
1	D	8	ARG	3.1
1	D	96	LYS	2.8
1	C	100	ARG	2.7
1	D	81	GLY	2.7
1	B	79	ALA	2.7
1	E	200	GLU	2.6
1	D	77	TYR	2.6
1	E	96	LYS	2.6
1	C	196	GLU	2.6
1	A	202	LEU	2.4
1	C	242	GLY	2.4
1	D	100	ARG	2.4
1	D	82	THR	2.3
1	C	61[A]	ASP	2.3
1	C	201	ALA	2.3
1	F	196	GLU	2.3
1	D	237	ARG	2.3
1	F	227	LYS	2.2
1	C	79	ALA	2.2
1	C	101	GLY	2.2
1	C	200	GLU	2.2
1	D	294	ALA	2.2
1	A	295	ARG	2.2
1	C	80	THR	2.2
1	E	232	TYR	2.2
1	A	257	ALA	2.2
1	B	80	THR	2.2
1	A	99	ALA	2.1
1	D	99	ALA	2.1
1	E	8	ARG	2.1
1	F	183	GLU	2.1
1	A	233	GLY	2.1
1	C	99	ALA	2.0
1	D	221	HIS	2.0
1	D	236	LEU	2.0
1	A	231	GLY	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. 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	1301	6/6	0.81	0.30	47,47,47,48	0
2	GOL	C	1300	6/6	0.81	0.23	29,30,30,31	0
2	GOL	D	1300	6/6	0.88	0.25	24,28,29,31	0
2	GOL	D	1299	6/6	0.89	0.14	10,13,16,19	0
2	GOL	F	1300	6/6	0.91	0.22	20,22,22,23	0
2	GOL	A	1299	6/6	0.92	0.14	30,30,31,31	0
2	GOL	F	1299	6/6	0.92	0.15	12,13,14,17	0
2	GOL	E	1299	6/6	0.92	0.14	10,11,13,16	0
2	GOL	C	1299	6/6	0.93	0.16	11,13,15,15	0
2	GOL	A	1300	6/6	0.98	0.11	8,12,13,13	0
2	GOL	B	1299	6/6	0.98	0.09	6,8,10,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.