



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:35 am BST

PDB ID : 2WYL  
Title : Apo structure of a metallo- $\beta$ -lactamase  
Authors : Garces, F.; Fernandez, F.J.; Playa-Soler, E.; Aguilar, J.; Baldoma, L.; Coll, M.; Badia, J.; Vega, M.C.  
Deposited on : 2009-11-16  
Resolution : 2.59 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

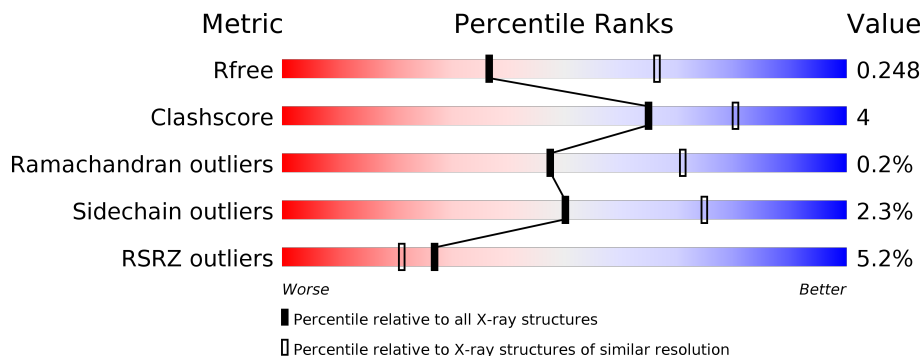
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	360	 4% 73% 11% 16%
1	B	360	 6% 79% 16%
1	C	360	 3% 72% 10% 17%
1	D	360	 3% 74% 9% 17%
1	E	360	 6% 73% 10% 16%
1	F	360	 4% 74% 10% 16%

## 2 Entry composition [i](#)

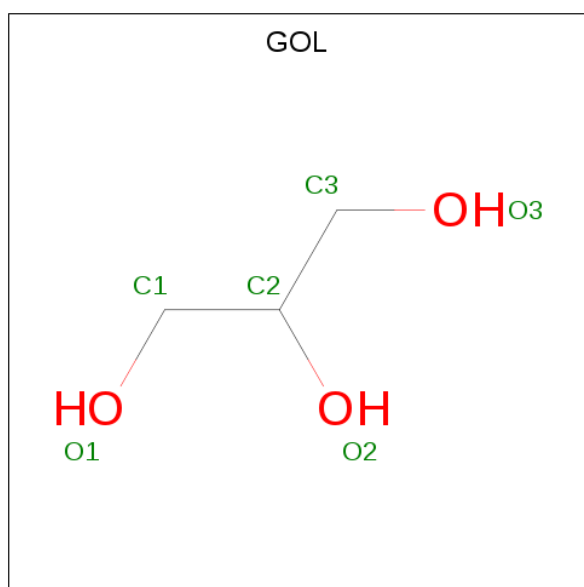
There are 4 unique types of molecules in this entry. The entry contains 15043 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-ASCORBATE-6-PHOSPHATE LACTONASE ULAG.

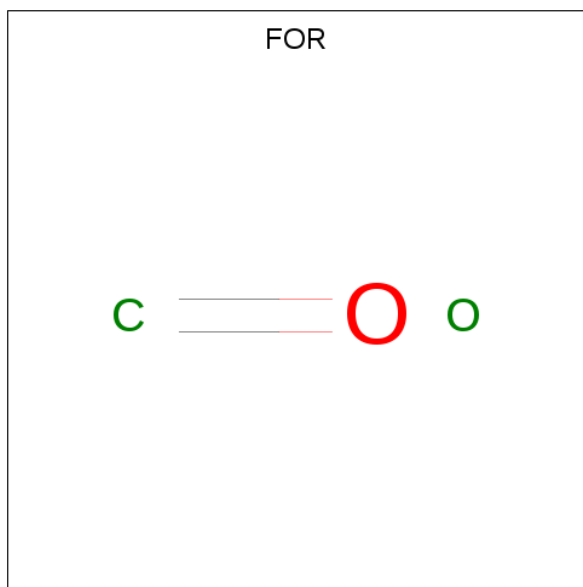
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	304	Total 2438	C 1564	N 417	O 443	S 6	Se 8	0	0	0
1	B	302	Total 2425	C 1555	N 414	O 442	S 6	Se 8	0	1	0
1	C	299	Total 2403	C 1541	N 411	O 437	S 6	Se 8	0	1	0
1	D	300	Total 2406	C 1545	N 409	O 438	S 6	Se 8	0	0	0
1	E	302	Total 2435	C 1566	N 415	O 440	S 6	Se 8	0	1	0
1	F	302	Total 2430	C 1561	N 415	O 440	S 6	Se 8	0	0	0

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

- Molecule 3 is FORMYL GROUP (three-letter code: FOR) (formula: CH<sub>2</sub>O).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	59	Total	O	0	0
			59	59		
4	C	72	Total	O	0	0
			72	72		
4	D	86	Total	O	0	0
			86	86		
4	E	49	Total	O	0	0
			49	49		
4	F	45	Total	O	0	0
			45	45		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.61Å 178.56Å 112.42Å 90.00° 103.82° 90.00°	Depositor
Resolution (Å)	14.94 – 2.59 14.94 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.5 (14.94-2.59) 98.5 (14.94-2.59)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	12.57 (at 2.58Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.198 , 0.248 0.200 , 0.248	Depositor DCC
$R_{free}$ test set	3037 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.1	Xtrriage
Anisotropy	0.154	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	15043	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

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

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

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	0.40	0/2506	0.47	0/3393
1	B	0.33	0/2495	0.46	0/3380
1	C	0.38	1/2473 (0.0%)	0.46	0/3348
1	D	0.38	0/2474	0.47	0/3350
1	E	0.33	0/2507	0.45	0/3395
1	F	0.35	0/2499	0.45	0/3384
All	All	0.36	1/14954 (0.0%)	0.46	0/20250

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	161	CYS	CB-SG	-5.55	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2438	0	2325	27	0
1	B	2425	0	2322	7	0
1	C	2403	0	2297	28	0
1	D	2406	0	2293	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2435	0	2338	22	0
1	F	2430	0	2327	23	0
2	A	18	0	24	2	0
2	B	12	0	16	0	0
2	C	24	0	32	1	0
2	D	24	0	32	0	0
2	E	24	0	32	0	0
2	F	18	0	24	1	0
3	C	2	0	0	0	0
3	F	2	0	0	0	0
4	A	71	0	0	0	0
4	B	59	0	0	0	0
4	C	72	0	0	0	0
4	D	86	0	0	0	0
4	E	49	0	0	0	0
4	F	45	0	0	0	0
All	All	15043	0	14062	119	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 (119) 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:40:MSE:HE1	1:A:246:LEU:HD11	1.64	0.80
1:A:247:GLY:HA3	1:A:265:MSE:HE1	1.62	0.80
1:C:23:TRP:HE1	2:C:1339:GOL:H12	1.48	0.78
1:C:265:MSE:HA	1:C:265:MSE:HE2	1.66	0.77
1:A:40:MSE:CE	1:A:246:LEU:HD11	2.17	0.74
1:D:98:THR:CG2	1:D:284:ILE:HD12	2.20	0.72
1:C:260:MSE:SE	1:C:265:MSE:HE3	2.40	0.72
1:C:229:TYR:HD1	1:C:260:MSE:CE	2.07	0.67
1:F:247:GLY:HA3	1:F:265:MSE:HE1	1.78	0.64
1:F:265:MSE:HA	1:F:265:MSE:HE2	1.80	0.64
1:F:278:ILE:HG12	1:F:313:PHE:HB3	1.79	0.64
1:E:148:VAL:HG21	1:E:163:VAL:HG22	1.80	0.63
1:C:247:GLY:HA3	1:C:265:MSE:HE1	1.82	0.62
1:F:40:MSE:HG2	1:F:315:TRP:HH2	1.65	0.61
1:A:175:ILE:HG12	1:A:216:THR:HG22	1.84	0.60
1:D:98:THR:HG23	1:D:284:ILE:HD12	1.84	0.60
1:A:265:MSE:HA	1:A:265:MSE:HE2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ILE:HG12	1:B:313:PHE:HB3	1.84	0.59
1:D:98:THR:HG22	1:D:284:ILE:HA	1.85	0.58
1:A:117:HIS:HE1	1:A:226:ASP:H	1.51	0.57
1:E:175:ILE:HG12	1:E:216:THR:HG22	1.86	0.57
1:E:229:TYR:HD1	1:E:260:MSE:HE3	1.69	0.57
1:C:229:TYR:HD1	1:C:260:MSE:HE3	1.69	0.57
1:C:303:LYS:HG2	1:C:304:ASP:N	2.19	0.57
1:E:229:TYR:HD1	1:E:260:MSE:CE	2.16	0.57
1:D:132:MSE:HE3	1:D:156:VAL:HG22	1.86	0.57
1:D:259:LYS:HE3	1:D:281:HIS:CD2	2.41	0.56
1:D:114:LEU:HG	1:D:142:ILE:HB	1.89	0.55
1:F:175:ILE:HG12	1:F:216:THR:HG22	1.89	0.55
1:E:132:MSE:CE	1:E:156:VAL:HG22	2.38	0.54
1:C:260:MSE:SE	1:C:265:MSE:CE	3.06	0.54
1:F:124:ASP:H	2:F:1339:GOL:H2	1.74	0.53
1:D:132:MSE:CE	1:D:156:VAL:HG22	2.39	0.53
1:F:260:MSE:SE	1:F:265:MSE:HE3	2.59	0.52
1:F:260:MSE:HE2	1:F:264:ASP:HB3	1.91	0.52
1:E:278:ILE:HG12	1:E:313:PHE:HB3	1.92	0.51
1:C:278:ILE:HG12	1:C:313:PHE:HB3	1.93	0.51
1:C:299:TRP:O	1:C:303:LYS:HB3	2.10	0.51
1:B:1:MSE:HA	1:B:1:MSE:HE2	1.94	0.50
1:F:114:LEU:HD21	1:F:177:ILE:HD13	1.93	0.49
1:D:183:PHE:HB2	1:D:230:SER:HB2	1.95	0.49
1:E:114:LEU:HG	1:E:142:ILE:HB	1.94	0.49
1:E:183:PHE:CE1	1:E:232:TYR:HB2	2.47	0.49
1:F:40:MSE:HG2	1:F:315:TRP:CH2	2.47	0.49
1:A:114:LEU:HG	1:A:142:ILE:HB	1.95	0.49
1:B:114:LEU:HG	1:B:142:ILE:HB	1.94	0.49
1:F:260:MSE:HE1	1:F:268:MSE:HB2	1.95	0.49
1:F:58:VAL:HG22	1:F:112:ALA:HB3	1.95	0.49
1:A:274:ALA:O	1:A:310:PHE:HB3	2.13	0.48
1:F:148:VAL:HG21	1:F:163:VAL:HG22	1.94	0.48
1:C:175:ILE:HG12	1:C:216:THR:HG22	1.95	0.48
1:A:40:MSE:HE2	1:A:48:ILE:HD12	1.96	0.48
1:B:260:MSE:HE2	1:B:265:MSE:SE	2.64	0.47
1:A:205:MSE:HE1	1:A:209:ALA:HB3	1.97	0.47
1:A:111:ASP:O	1:A:140:PRO:HD2	2.13	0.47
1:C:148:VAL:HG21	1:C:163:VAL:HG22	1.95	0.47
1:F:229:TYR:HD1	1:F:260:MSE:HE3	1.80	0.47
1:E:58:VAL:HG22	1:E:112:ALA:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:TYR:CD1	1:E:260:MSE:HE3	2.50	0.47
1:D:260:MSE:SE	1:D:265:MSE:HE2	2.66	0.46
1:A:260:MSE:HE2	1:A:264:ASP:HB3	1.97	0.46
1:C:248:SER:O	1:C:260:MSE:HB2	2.17	0.45
1:C:265:MSE:CE	1:C:265:MSE:HA	2.41	0.45
1:E:40:MSE:HG2	1:E:315:TRP:HH2	1.81	0.45
1:C:260:MSE:HE1	1:C:268:MSE:HB2	1.97	0.45
1:D:136:ALA:C	1:D:138:ASP:H	2.20	0.45
1:E:205:MSE:CG	1:E:206:ASP:H	2.29	0.45
1:E:270:GLU:OE2	1:F:336:ARG:NH2	2.44	0.45
1:A:183:PHE:CE1	1:A:232:TYR:HB2	2.52	0.45
1:A:117:HIS:HB3	1:A:209:ALA:HB2	1.98	0.45
1:D:278:ILE:HG12	1:D:313:PHE:HB3	1.98	0.45
1:F:40:MSE:HE2	1:F:321:PHE:HB3	1.98	0.45
1:A:24:LEU:HD11	1:A:41:TRP:CD1	2.52	0.45
1:A:278:ILE:HG12	1:A:313:PHE:HB3	1.99	0.45
1:E:132:MSE:HE1	1:E:156:VAL:HG22	1.97	0.45
1:E:117:HIS:CE1	1:E:119:HIS:HB3	2.52	0.45
1:A:259:LYS:HE3	1:A:281:HIS:CE1	2.52	0.44
1:A:260:MSE:HE1	1:A:268:MSE:HB2	1.99	0.44
1:C:252:ASN:HB3	1:C:256:ILE:O	2.17	0.44
1:F:117:HIS:HD1	1:F:119:HIS:HB2	1.83	0.44
1:A:335:PRO:HD2	2:A:1339:GOL:H31	2.00	0.44
1:B:98[A]:THR:OG1	1:B:284:ILE:HD12	2.18	0.44
1:C:229:TYR:CD1	1:C:260:MSE:HE3	2.50	0.44
1:C:111:ASP:O	1:C:140:PRO:HD2	2.16	0.44
1:C:159:GLU:HG3	1:C:159:GLU:H	1.32	0.44
1:F:98:THR:HG22	1:F:284:ILE:HD12	2.00	0.44
1:C:136:ALA:C	1:C:138:ASP:H	2.21	0.43
1:E:260:MSE:HE1	1:E:268:MSE:HB2	2.00	0.43
1:C:125:VAL:HG22	1:C:154:TRP:CZ2	2.54	0.43
1:A:132:MSE:HE3	1:A:156:VAL:HG22	2.00	0.43
1:C:58:VAL:HG22	1:C:112:ALA:HB3	2.00	0.43
1:A:336:ARG:NH2	1:D:270:GLU:OE2	2.42	0.43
1:E:146:THR:CG2	1:E:208:ARG:HA	2.49	0.43
1:D:110:ILE:HG23	1:D:139:VAL:HG21	2.01	0.43
1:F:98:THR:CG2	1:F:284:ILE:HD12	2.49	0.42
1:C:10:GLU:H	1:C:10:GLU:CD	2.21	0.42
1:F:114:LEU:HG	1:F:142:ILE:HB	2.00	0.42
1:E:205:MSE:HG2	1:E:206:ASP:H	1.84	0.42
1:F:111:ASP:O	1:F:140:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:MSE:SE	1:A:265:MSE:HE3	2.70	0.42
1:C:13:ILE:HG22	1:D:13:ILE:HG22	2.01	0.42
1:D:176:GLU:HB3	1:D:215:LYS:HB2	2.01	0.42
1:C:333:HIS:HB2	1:F:305:ARG:HG2	2.01	0.42
1:E:59:CYS:SG	1:E:62:PHE:HB2	2.60	0.42
1:B:58:VAL:HG13	1:B:114:LEU:HD13	2.01	0.41
1:C:17:PHE:CD2	1:D:17:PHE:CD2	3.07	0.41
1:C:114:LEU:HD21	1:C:177:ILE:HD13	2.01	0.41
1:E:132:MSE:HE3	1:E:156:VAL:HG22	2.03	0.41
1:A:160:ARG:HE	1:A:160:ARG:HB3	1.74	0.41
1:A:132:MSE:CE	1:A:156:VAL:HG22	2.51	0.41
1:A:1:MSE:HE2	1:A:5:LYS:HG2	2.03	0.41
1:B:286:SER:HB2	1:E:334:TYR:CG	2.56	0.41
1:C:137:ASP:HA	1:C:160:ARG:NH1	2.36	0.41
1:D:4:VAL:HG23	1:D:5:LYS:HD2	2.02	0.41
1:A:148:VAL:HG21	1:A:163:VAL:HG22	2.03	0.41
1:D:146:THR:HG22	1:D:207:ASP:O	2.20	0.41
1:F:183:PHE:CE1	1:F:232:TYR:HB2	2.56	0.41
1:A:123:ILE:HG13	2:A:1340:GOL:H32	2.03	0.40
1:E:98:THR:CG2	1:E:284:ILE:HD12	2.51	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	298/360 (83%)	289 (97%)	8 (3%)	1 (0%)	41 64
1	B	297/360 (82%)	289 (97%)	8 (3%)	0	100 100
1	C	294/360 (82%)	284 (97%)	10 (3%)	0	100 100
1	D	294/360 (82%)	284 (97%)	9 (3%)	1 (0%)	41 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	297/360 (82%)	284 (96%)	13 (4%)	0	100	100
1	F	296/360 (82%)	288 (97%)	7 (2%)	1 (0%)	41	64
All	All	1776/2160 (82%)	1718 (97%)	55 (3%)	3 (0%)	47	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	LYS
1	D	137	ASP
1	F	91	LEU

### 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	259/297 (87%)	258 (100%)	1 (0%)	91	97
1	B	259/297 (87%)	254 (98%)	5 (2%)	57	79
1	C	256/297 (86%)	249 (97%)	7 (3%)	44	71
1	D	256/297 (86%)	246 (96%)	10 (4%)	32	58
1	E	260/297 (88%)	251 (96%)	9 (4%)	36	62
1	F	259/297 (87%)	255 (98%)	4 (2%)	65	83
All	All	1549/1782 (87%)	1513 (98%)	36 (2%)	50	75

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	PHE
1	B	185	ARG
1	B	248	SER
1	B	280	PHE
1	B	306	LEU
1	B	315	TRP
1	C	10	GLU

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Mol	Chain	Res	Type
1	C	159	GLU
1	C	173	LYS
1	C	181	ASP
1	C	258	ASP
1	C	280	PHE
1	C	303	LYS
1	D	5	LYS
1	D	98	THR
1	D	138	ASP
1	D	158	LYS
1	D	159	GLU
1	D	248	SER
1	D	275	LYS
1	D	280	PHE
1	D	315	TRP
1	D	338	PHE
1	E	14	LEU
1	E	68	LYS
1	E	91	LEU
1	E	117	HIS
1	E	184	ASP
1	E	259	LYS
1	E	260	MSE
1	E	280	PHE
1	E	322	THR
1	F	10	GLU
1	F	181	ASP
1	F	258	ASP
1	F	280	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	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](#)

22 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	C	1340	-	5,5,5	0.40	0	5,5,5	0.28	0
2	GOL	F	1340	-	5,5,5	0.38	0	5,5,5	0.27	0
2	GOL	C	1341	-	5,5,5	0.37	0	5,5,5	0.26	0
2	GOL	B	1338	-	5,5,5	0.37	0	5,5,5	0.29	0
3	FOR	F	1338	-	0,1,1	0.00	-	-	-	-
2	GOL	A	1340	-	5,5,5	0.39	0	5,5,5	0.25	0
2	GOL	E	1342	-	5,5,5	0.38	0	5,5,5	0.20	0
2	GOL	F	1339	-	5,5,5	0.38	0	5,5,5	0.23	0
2	GOL	D	1342	-	5,5,5	0.39	0	5,5,5	0.32	0
2	GOL	E	1340	-	5,5,5	0.35	0	5,5,5	0.31	0
2	GOL	D	1340	-	5,5,5	0.36	0	5,5,5	0.27	0
2	GOL	B	1339	-	5,5,5	0.38	0	5,5,5	0.27	0
2	GOL	C	1339	-	5,5,5	0.37	0	5,5,5	0.21	0
2	GOL	A	1339	-	5,5,5	0.38	0	5,5,5	0.24	0
2	GOL	A	1341	-	5,5,5	0.36	0	5,5,5	0.29	0
3	FOR	C	1337	-	0,1,1	0.00	-	-	-	-
2	GOL	D	1343	-	5,5,5	0.42	0	5,5,5	0.25	0
2	GOL	C	1338	-	5,5,5	0.37	0	5,5,5	0.34	0
2	GOL	E	1341	-	5,5,5	0.35	0	5,5,5	0.32	0
2	GOL	F	1341	-	5,5,5	0.37	0	5,5,5	0.27	0
2	GOL	D	1341	-	5,5,5	0.37	0	5,5,5	0.32	0
2	GOL	E	1339	-	5,5,5	0.36	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	B	1338	-	-	0/4/4/4	-
2	GOL	E	1340	-	-	0/4/4/4	-
2	GOL	C	1340	-	-	0/4/4/4	-
2	GOL	A	1340	-	-	0/4/4/4	-
2	GOL	D	1341	-	-	4/4/4/4	-
2	GOL	D	1343	-	-	2/4/4/4	-
2	GOL	F	1340	-	-	2/4/4/4	-
2	GOL	D	1340	-	-	1/4/4/4	-
2	GOL	E	1342	-	-	0/4/4/4	-
2	GOL	C	1338	-	-	2/4/4/4	-
2	GOL	B	1339	-	-	2/4/4/4	-
2	GOL	C	1339	-	-	2/4/4/4	-
2	GOL	E	1341	-	-	0/4/4/4	-
2	GOL	F	1341	-	-	2/4/4/4	-
2	GOL	C	1341	-	-	3/4/4/4	-
2	GOL	A	1339	-	-	2/4/4/4	-
2	GOL	A	1341	-	-	1/4/4/4	-
2	GOL	F	1339	-	-	4/4/4/4	-
2	GOL	D	1342	-	-	3/4/4/4	-
2	GOL	E	1339	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1342	GOL	C1-C2-C3-O3
2	C	1339	GOL	C1-C2-C3-O3
2	A	1339	GOL	O1-C1-C2-C3
2	C	1338	GOL	O1-C1-C2-C3
2	D	1341	GOL	C1-C2-C3-O3
2	E	1339	GOL	O1-C1-C2-O2
2	E	1339	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	1339	GOL	O1-C1-C2-O2
2	D	1341	GOL	O2-C2-C3-O3
2	F	1340	GOL	C1-C2-C3-O3
2	C	1341	GOL	C1-C2-C3-O3
2	F	1339	GOL	O1-C1-C2-C3
2	F	1339	GOL	C1-C2-C3-O3
2	B	1339	GOL	C1-C2-C3-O3
2	A	1341	GOL	C1-C2-C3-O3
2	D	1343	GOL	C1-C2-C3-O3
2	F	1341	GOL	C1-C2-C3-O3
2	D	1341	GOL	O1-C1-C2-C3
2	C	1341	GOL	O2-C2-C3-O3
2	C	1339	GOL	O2-C2-C3-O3
2	D	1343	GOL	O2-C2-C3-O3
2	C	1338	GOL	O1-C1-C2-O2
2	F	1341	GOL	O2-C2-C3-O3
2	F	1339	GOL	O1-C1-C2-O2
2	C	1341	GOL	O1-C1-C2-C3
2	D	1341	GOL	O1-C1-C2-O2
2	D	1342	GOL	O2-C2-C3-O3
2	B	1339	GOL	O2-C2-C3-O3
2	E	1339	GOL	O2-C2-C3-O3
2	D	1340	GOL	C1-C2-C3-O3
2	F	1339	GOL	O2-C2-C3-O3
2	F	1340	GOL	O2-C2-C3-O3
2	D	1342	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1340	GOL	1	0
2	F	1339	GOL	1	0
2	C	1339	GOL	1	0
2	A	1339	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	296/360 (82%)	0.14	14 (4%) 31 25	16, 30, 41, 59	0
1	B	294/360 (81%)	0.24	21 (7%) 16 11	18, 31, 44, 58	0
1	C	291/360 (80%)	-0.01	11 (3%) 40 33	16, 26, 40, 54	0
1	D	292/360 (81%)	-0.03	9 (3%) 49 42	14, 25, 37, 56	0
1	E	294/360 (81%)	0.35	22 (7%) 14 10	21, 35, 49, 54	0
1	F	294/360 (81%)	0.23	15 (5%) 28 22	19, 31, 45, 54	0
All	All	1761/2160 (81%)	0.15	92 (5%) 27 21	14, 30, 46, 59	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	338	PHE	7.1
1	B	186	THR	7.1
1	B	72	GLY	6.8
1	D	338	PHE	6.8
1	A	72	GLY	6.6
1	B	91	LEU	6.6
1	B	185	ARG	6.3
1	A	338	PHE	6.2
1	E	91	LEU	6.0
1	A	73	ASN	5.4
1	E	338	PHE	5.3
1	C	204	GLY	5.3
1	A	91	LEU	5.2
1	A	232	TYR	5.0
1	D	339	ASP	5.0
1	E	232	TYR	4.8
1	D	183	PHE	4.7
1	B	184	ASP	4.6
1	C	184	ASP	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	232	TYR	4.5
1	E	136	ALA	4.5
1	F	91	LEU	4.5
1	E	185	ARG	4.5
1	E	72	GLY	4.4
1	C	232	TYR	4.4
1	A	90	LYS	4.1
1	B	169	VAL	4.1
1	B	232	TYR	4.1
1	A	184	ASP	4.0
1	E	137	ASP	4.0
1	F	185	ARG	3.8
1	A	185	ARG	3.8
1	E	138	ASP	3.8
1	A	337	GLY	3.7
1	A	137	ASP	3.7
1	E	159	GLU	3.6
1	B	337	GLY	3.5
1	F	72	GLY	3.5
1	F	90	LYS	3.5
1	F	119	HIS	3.4
1	C	337	GLY	3.4
1	E	54	GLY	3.3
1	E	90	LYS	3.3
1	B	159	GLU	3.3
1	C	72	GLY	3.2
1	B	204	GLY	3.2
1	F	138	ASP	3.2
1	F	232	TYR	3.2
1	D	204	GLY	3.1
1	D	207	ASP	3.0
1	A	5	LYS	3.0
1	B	137	ASP	3.0
1	F	120	ASN	3.0
1	B	5	LYS	3.0
1	F	184	ASP	3.0
1	E	183	PHE	2.8
1	A	208	ARG	2.8
1	D	72	GLY	2.8
1	B	92	GLN	2.7
1	B	183	PHE	2.6
1	C	119	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	119	HIS	2.5
1	F	137	ASP	2.5
1	E	184	ASP	2.5
1	F	337	GLY	2.5
1	D	228	HIS	2.4
1	B	208	ARG	2.4
1	B	32	GLN	2.4
1	E	158	LYS	2.4
1	F	208	ARG	2.4
1	E	153	GLY	2.4
1	C	241	GLN	2.4
1	F	92	GLN	2.3
1	B	153	GLY	2.3
1	C	120	ASN	2.2
1	B	138	ASP	2.2
1	E	119	HIS	2.2
1	E	208	ARG	2.2
1	C	137	ASP	2.2
1	F	158	LYS	2.2
1	E	120	ASN	2.2
1	C	208	ARG	2.1
1	D	120	ASN	2.1
1	B	2	SER	2.1
1	E	117	HIS	2.1
1	A	241	GLN	2.1
1	E	145	LYS	2.1
1	C	145	LYS	2.0
1	B	207	ASP	2.0
1	E	241	GLN	2.0
1	A	204	GLY	2.0
1	E	30	GLN	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(Å <sup>2</sup> )	Q<0.9
3	FOR	F	1338	2/2	0.62	0.29	34,34,34,34	0
2	GOL	C	1341	6/6	0.71	0.29	46,46,46,46	0
3	FOR	C	1337	2/2	0.71	0.26	35,35,35,35	0
2	GOL	F	1341	6/6	0.72	0.27	68,68,68,68	0
2	GOL	A	1341	6/6	0.74	0.37	44,44,44,45	0
2	GOL	E	1342	6/6	0.78	0.23	58,58,58,58	0
2	GOL	D	1341	6/6	0.83	0.31	38,38,38,38	0
2	GOL	C	1339	6/6	0.86	0.23	46,46,46,46	0
2	GOL	E	1341	6/6	0.86	0.27	40,40,41,41	0
2	GOL	C	1338	6/6	0.87	0.23	40,41,41,42	0
2	GOL	E	1340	6/6	0.89	0.26	45,46,46,46	0
2	GOL	E	1339	6/6	0.90	0.23	53,53,53,53	0
2	GOL	D	1342	6/6	0.91	0.17	34,34,34,34	0
2	GOL	D	1343	6/6	0.92	0.16	26,27,27,27	0
2	GOL	D	1340	6/6	0.92	0.20	33,33,34,34	0
2	GOL	A	1339	6/6	0.92	0.15	34,34,34,34	0
2	GOL	F	1339	6/6	0.93	0.18	36,37,37,37	0
2	GOL	F	1340	6/6	0.94	0.16	52,53,53,53	0
2	GOL	B	1339	6/6	0.94	0.17	40,41,41,41	0
2	GOL	A	1340	6/6	0.94	0.18	31,32,32,32	0
2	GOL	B	1338	6/6	0.96	0.12	33,34,34,34	0
2	GOL	C	1340	6/6	0.97	0.12	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.