



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 18, 2016 – 11:18 AM EDT

PDB ID : 5ILQ
Title : Crystal structure of truncated unliganded Aspartate Transcarbamoylase from Plasmodium falciparum
Authors : Lunev, S.; Bosch, S.S.; Batista, F.D.A.; Wrenger, C.; Groves, M.R.
Deposited on : 2016-03-04
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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) : rb-20027790

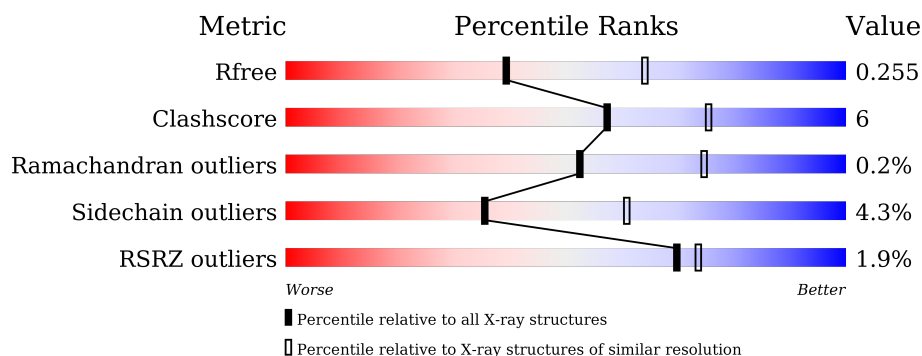
1 Overall quality at a glance

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 ≥ 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	349	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>10%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	349	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>•</div> <div>7%</div> </div> </div>
1	C	349	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>•</div> <div>7%</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
2	GOL	B	401	-	-	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 7907 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 Aspartate carbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2563	1637	422	496	8			
1	B	324	Total	C	N	O	S	0	0	0
			2612	1669	430	505	8			
1	C	325	Total	C	N	O	S	0	0	0
			2623	1678	431	506	8			

There are 30 discrepancies between the modelled and reference sequences:

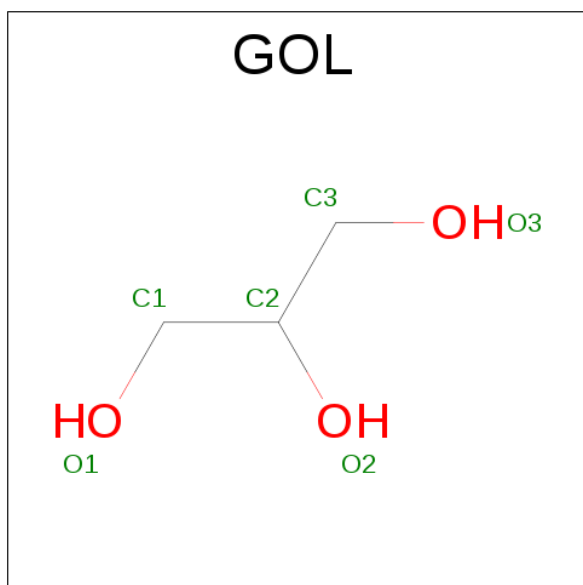
Chain	Residue	Modelled	Actual	Comment	Reference
A	376	SER	-	expression tag	UNP Q8IDP8
A	377	ALA	-	expression tag	UNP Q8IDP8
A	378	TRP	-	expression tag	UNP Q8IDP8
A	379	SER	-	expression tag	UNP Q8IDP8
A	380	HIS	-	expression tag	UNP Q8IDP8
A	381	PRO	-	expression tag	UNP Q8IDP8
A	382	GLN	-	expression tag	UNP Q8IDP8
A	383	PHE	-	expression tag	UNP Q8IDP8
A	384	GLU	-	expression tag	UNP Q8IDP8
A	385	LYS	-	expression tag	UNP Q8IDP8
B	376	SER	-	expression tag	UNP Q8IDP8
B	377	ALA	-	expression tag	UNP Q8IDP8
B	378	TRP	-	expression tag	UNP Q8IDP8
B	379	SER	-	expression tag	UNP Q8IDP8
B	380	HIS	-	expression tag	UNP Q8IDP8
B	381	PRO	-	expression tag	UNP Q8IDP8
B	382	GLN	-	expression tag	UNP Q8IDP8
B	383	PHE	-	expression tag	UNP Q8IDP8
B	384	GLU	-	expression tag	UNP Q8IDP8
B	385	LYS	-	expression tag	UNP Q8IDP8
C	376	SER	-	expression tag	UNP Q8IDP8
C	377	ALA	-	expression tag	UNP Q8IDP8
C	378	TRP	-	expression tag	UNP Q8IDP8

Continued on next page...

Continued from previous page...

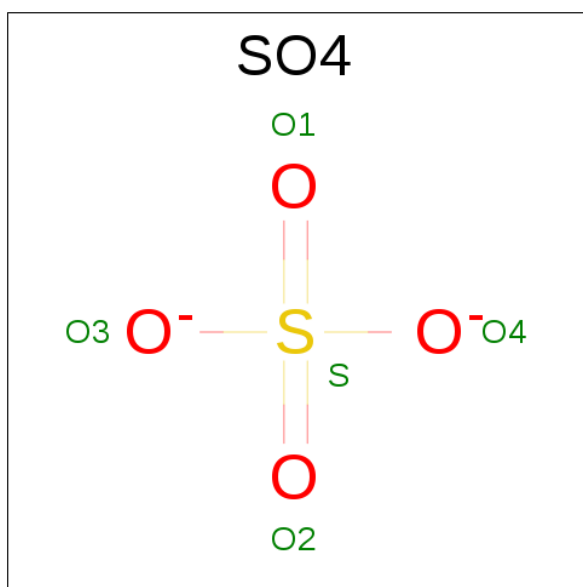
Chain	Residue	Modelled	Actual	Comment	Reference
C	379	SER	-	expression tag	UNP Q8IDP8
C	380	HIS	-	expression tag	UNP Q8IDP8
C	381	PRO	-	expression tag	UNP Q8IDP8
C	382	GLN	-	expression tag	UNP Q8IDP8
C	383	PHE	-	expression tag	UNP Q8IDP8
C	384	GLU	-	expression tag	UNP Q8IDP8
C	385	LYS	-	expression tag	UNP Q8IDP8

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



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	38	Total	O	0	0
			38	38		
4	C	25	Total	O	0	0
			25	25		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.98Å 103.80Å 87.11Å 90.00° 117.68° 90.00°	Depositor
Resolution (Å)	45.03 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.1 (45.03-2.50) 95.3 (20.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.208 , 0.250 0.211 , 0.255	Depositor DCC
R_{free} test set	2354 reflections (5.49%)	DCC
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.044 for -h-l,k,h 0.044 for l,k,-h-l 0.048 for h,-k,-h-l 0.049 for -h-l,-k,l 0.078 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7907	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, SO4

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	0.93	0/2609	1.03	13/3524 (0.4%)
1	B	0.97	2/2661 (0.1%)	1.04	11/3597 (0.3%)
1	C	0.91	0/2673	1.00	9/3613 (0.2%)
All	All	0.93	2/7943 (0.0%)	1.03	33/10734 (0.3%)

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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	372	SER	CB-OG	-5.17	1.35	1.42
1	B	282	GLU	CG-CD	5.07	1.59	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	LEU	CA-CB-CG	12.11	143.16	115.30
1	C	126	LEU	CA-CB-CG	11.73	142.28	115.30
1	A	111	ARG	NE-CZ-NH1	-9.51	115.55	120.30
1	C	237	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	B	237	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	A	363	ARG	NE-CZ-NH2	7.57	124.08	120.30
1	C	363	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	C	208	ARG	NE-CZ-NH1	7.21	123.90	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	A	237	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	C	237	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	B	159	ARG	NE-CZ-NH2	6.57	123.58	120.30
1	A	111	ARG	NE-CZ-NH2	6.55	123.58	120.30
1	A	237	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	C	90	ASP	CB-CG-OD1	6.38	124.05	118.30
1	C	295	ARG	NE-CZ-NH2	6.21	123.41	120.30
1	B	208	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	B	208	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	208	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	B	363	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	A	159	ARG	NE-CZ-NH2	5.81	123.20	120.30
1	A	363	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	C	363	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	B	115	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	B	237	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	208	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	109	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	B	205	ILE	CB-CA-C	-5.38	100.83	111.60
1	A	205	ILE	N-CA-CB	5.33	123.06	110.80
1	A	126	LEU	CB-CA-C	5.32	120.31	110.20
1	C	208	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	205	ILE	CB-CA-C	-5.11	101.38	111.60
1	A	90	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	375	SER	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	2563	0	2570	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2612	0	2620	41	0
1	C	2623	0	2629	26	0
2	A	12	0	16	4	0
2	B	6	0	8	3	0
3	C	5	0	0	0	0
4	A	23	0	0	0	0
4	B	38	0	0	1	0
4	C	25	0	0	1	0
All	All	7907	0	7843	94	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 (94) 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)
2:B:401:GOL:O1	4:B:501:HOH:O	1.58	1.19
1:B:125:VAL:O	2:B:401:GOL:H31	1.81	0.81
1:B:146:PHE:O	1:B:150:SER:HB3	1.85	0.77
1:A:67:ASP:HB2	2:A:402:GOL:H11	1.67	0.76
1:A:146:PHE:O	1:A:150:SER:HB3	1.87	0.75
1:C:146:PHE:O	1:C:150:SER:HB3	1.87	0.73
1:B:375:SER:HB2	1:B:376:SER:HA	1.70	0.72
1:B:215:ASN:H	1:B:289:HIS:HD2	1.41	0.69
1:C:107:SER:OG	4:C:501:HOH:O	2.11	0.69
1:B:52:MET:CE	1:B:380:HIS:CE1	2.76	0.68
1:A:215:ASN:H	1:A:289:HIS:HD2	1.43	0.66
1:B:52:MET:HE3	1:B:380:HIS:CE1	2.30	0.65
1:C:205:ILE:HD12	1:C:214:LEU:HD22	1.77	0.64
1:B:375:SER:CB	1:B:376:SER:HA	2.29	0.62
1:B:56:LYS:NZ	1:B:373:SER:HB3	2.14	0.62
1:C:337:VAL:HG22	1:C:339:GLU:OE1	2.01	0.61
1:A:124:LYS:HD3	1:C:119:LEU:HD22	1.83	0.60
1:A:48:LEU:HG	1:A:52:MET:HE2	1.84	0.60
1:C:45:LYS:HB3	1:C:46:ILE:HG12	1.82	0.59
1:B:48:LEU:HG	1:B:52:MET:HE2	1.85	0.59
1:B:163:LYS:HB3	1:B:184:THR:HG23	1.86	0.58
1:B:312:ASN:OD1	1:B:312:ASN:N	2.35	0.58
1:C:227:THR:CG2	1:C:292:TYR:OH	2.52	0.57
1:A:202:PHE:O	1:A:205:ILE:HG13	2.03	0.57
1:C:215:ASN:H	1:C:289:HIS:HD2	1.53	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:VAL:HG22	1:A:339:GLU:OE1	2.05	0.57
1:B:52:MET:HE1	1:B:380:HIS:ND1	2.19	0.57
1:B:373:SER:HA	1:B:374:THR:HG22	1.86	0.56
1:C:163:LYS:HB3	1:C:184:THR:HG23	1.87	0.56
1:C:48:LEU:HG	1:C:52:MET:HE2	1.86	0.56
1:B:202:PHE:O	1:B:205:ILE:HG13	2.06	0.56
1:A:163:LYS:HB3	1:A:184:THR:HG23	1.87	0.55
1:B:52:MET:HE1	1:B:380:HIS:CE1	2.41	0.55
1:B:119:LEU:HD22	1:C:124:LYS:HD3	1.88	0.55
1:A:337:VAL:HG23	1:A:338:ASN:H	1.71	0.55
1:A:119:LEU:HD22	1:B:124:LYS:HD3	1.88	0.55
1:B:227:THR:CG2	1:B:292:TYR:OH	2.55	0.55
1:B:375:SER:OG	1:B:376:SER:HB2	2.08	0.54
1:A:227:THR:CG2	1:A:292:TYR:OH	2.56	0.53
1:A:312:ASN:OD1	1:A:312:ASN:N	2.42	0.53
1:C:163:LYS:H	1:C:163:LYS:HD3	1.72	0.53
1:C:52:MET:CE	1:C:380:HIS:CE1	2.92	0.53
1:B:281:LEU:HD13	1:B:314:PHE:HD1	1.75	0.52
1:B:163:LYS:HD3	1:B:163:LYS:H	1.75	0.52
1:B:125:VAL:O	2:B:401:GOL:C3	2.56	0.51
1:C:281:LEU:HD13	1:C:314:PHE:HD1	1.76	0.51
1:A:52:MET:CE	1:A:380:HIS:CE1	2.95	0.50
1:B:334:LEU:HB3	1:B:335:PRO:HA	1.94	0.49
1:B:56:LYS:HZ1	1:B:373:SER:HB3	1.76	0.49
1:C:66:VAL:O	1:C:237:ARG:NH2	2.39	0.49
1:A:114:PHE:CZ	1:A:363:ARG:HD3	2.48	0.48
1:C:312:ASN:OD1	1:C:312:ASN:N	2.47	0.48
1:A:334:LEU:HB3	1:A:335:PRO:HA	1.96	0.48
1:A:52:MET:HE3	1:A:380:HIS:CE1	2.49	0.47
1:C:334:LEU:HB3	1:C:335:PRO:HA	1.96	0.47
1:B:68:ASP:OD2	1:B:208:ARG:NH2	2.47	0.47
1:B:45:LYS:HB3	1:B:46:ILE:HG12	1.98	0.46
1:A:68:ASP:H	2:A:402:GOL:H12	1.80	0.46
1:C:52:MET:HE3	1:C:380:HIS:CE1	2.51	0.46
1:A:57:ASN:O	2:A:401:GOL:O3	2.34	0.45
1:C:68:ASP:OD2	1:C:208:ARG:NH2	2.49	0.45
1:B:215:ASN:H	1:B:289:HIS:CD2	2.28	0.45
1:B:375:SER:CB	1:B:376:SER:CA	2.93	0.45
1:A:66:VAL:O	1:A:237:ARG:NH2	2.43	0.45
1:A:109:ARG:HE	1:B:148:ILE:HD13	1.82	0.45
1:C:159:ARG:HG3	1:C:181:GLY:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:PHE:CZ	1:C:363:ARG:HD3	2.52	0.45
1:C:52:MET:HE1	1:C:380:HIS:CE1	2.53	0.44
1:C:185:GLY:HA3	1:C:226:ARG:HB3	1.97	0.44
1:A:185:GLY:HA3	1:A:226:ARG:HB3	2.00	0.44
1:A:68:ASP:OD2	1:A:208:ARG:NH2	2.50	0.44
1:B:159:ARG:HG3	1:B:181:GLY:O	2.17	0.44
1:C:68:ASP:CG	1:C:208:ARG:HH22	2.21	0.44
1:A:68:ASP:CG	1:A:208:ARG:HH22	2.22	0.43
1:A:68:ASP:H	2:A:402:GOL:C1	2.32	0.43
1:A:163:LYS:CB	1:A:184:THR:HG23	2.48	0.43
1:C:163:LYS:HG2	1:C:164:LYS:N	2.33	0.43
1:A:215:ASN:H	1:A:289:HIS:CD2	2.29	0.42
1:A:325:ARG:HB2	1:A:328:THR:CG2	2.49	0.42
1:A:159:ARG:HG3	1:A:181:GLY:O	2.18	0.42
1:B:46:ILE:HG22	1:B:47:ASP:N	2.34	0.42
1:C:46:ILE:HG22	1:C:47:ASP:N	2.34	0.42
1:A:334:LEU:HD13	1:B:148:ILE:HD11	2.01	0.42
1:B:56:LYS:HE2	1:B:374:THR:HG22	2.02	0.42
1:B:163:LYS:HG2	1:B:164:LYS:N	2.35	0.42
1:B:163:LYS:CB	1:B:184:THR:HG23	2.49	0.42
1:B:66:VAL:O	1:B:237:ARG:NH2	2.44	0.42
1:B:373:SER:CA	1:B:374:THR:HG22	2.50	0.41
1:B:185:GLY:HA3	1:B:226:ARG:HB3	2.01	0.41
1:A:368:TYR:O	1:A:372:SER:OG	2.34	0.41
1:B:376:SER:O	1:B:380:HIS:NE2	2.54	0.41
1:B:68:ASP:CG	1:B:208:ARG:HH22	2.23	0.41
1:A:161:PRO:O	1:A:183:GLY:HA3	2.21	0.40
1:B:161:PRO:O	1:B:183:GLY:HA3	2.22	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	312/349 (89%)	300 (96%)	12 (4%)	0	100	100
1	B	320/349 (92%)	309 (97%)	10 (3%)	1 (0%)	46	68
1	C	321/349 (92%)	309 (96%)	11 (3%)	1 (0%)	46	68
All	All	953/1047 (91%)	918 (96%)	33 (4%)	2 (0%)	52	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	338	ASN
1	B	337	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	298/328 (91%)	285 (96%)	13 (4%)	35	60
1	B	303/328 (92%)	289 (95%)	14 (5%)	33	57
1	C	304/328 (93%)	292 (96%)	12 (4%)	39	66
All	All	905/984 (92%)	866 (96%)	39 (4%)	35	61

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ARG
1	A	126	LEU
1	A	150	SER
1	A	163	LYS
1	A	164	LYS
1	A	172	SER
1	A	205	ILE
1	A	227	THR
1	A	249	SER
1	A	282	GLU
1	A	312	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	352	TYR
1	A	372	SER
1	B	44	TYR
1	B	45	LYS
1	B	111	ARG
1	B	150	SER
1	B	163	LYS
1	B	164	LYS
1	B	172	SER
1	B	205	ILE
1	B	227	THR
1	B	248	LYS
1	B	249	SER
1	B	282	GLU
1	B	312	ASN
1	B	352	TYR
1	C	111	ARG
1	C	150	SER
1	C	163	LYS
1	C	164	LYS
1	C	172	SER
1	C	248	LYS
1	C	249	SER
1	C	282	GLU
1	C	312	ASN
1	C	352	TYR
1	C	375	SER
1	C	382	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	A	179	ASN
1	A	243	ASN
1	A	289	HIS
1	A	312	ASN
1	B	80	GLN
1	B	165	ASN
1	B	179	ASN
1	B	243	ASN
1	B	289	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	312	ASN
1	C	165	ASN
1	C	179	ASN
1	C	199	HIS
1	C	224	ASN
1	C	243	ASN
1	C	289	HIS
1	C	312	ASN

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](#)

4 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	401	-	5,5,5	1.00	0	5,5,5	1.11	0
2	GOL	A	402	-	5,5,5	0.85	0	5,5,5	1.34	1 (20%)
2	GOL	B	401	-	5,5,5	0.62	0	5,5,5	1.56	1 (20%)
3	SO4	C	401	-	4,4,4	0.84	0	6,6,6	0.51	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	401	-	-	0/4/4/4	0/0/0/0
2	GOL	A	402	-	-	0/4/4/4	0/0/0/0
2	GOL	B	401	-	-	0/4/4/4	0/0/0/0
3	SO4	C	401	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	GOL	O1-C1-C2	2.56	122.98	109.97
2	B	401	GOL	O3-C3-C2	3.08	125.57	109.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	GOL	1	0
2	A	402	GOL	3	0
2	B	401	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, 95th 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 ²)	Q<0.9
1	A	318/349 (91%)	-0.05	7 (2%) 65 69	37, 62, 107, 143	0
1	B	324/349 (92%)	-0.16	4 (1%) 81 83	34, 57, 103, 137	0
1	C	325/349 (93%)	-0.08	7 (2%) 65 69	37, 66, 104, 124	0
All	All	967/1047 (92%)	-0.10	18 (1%) 70 73	34, 62, 105, 143	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	138	LYS	6.5
1	C	139	GLY	4.3
1	B	378	TRP	3.8
1	C	323	ASN	3.4
1	A	135	SER	3.3
1	A	139	GLY	3.1
1	C	374	THR	3.1
1	A	134	THR	2.9
1	A	383	PHE	2.9
1	A	130	ASP	2.9
1	B	377	ALA	2.6
1	C	337	VAL	2.4
1	B	313	ALA	2.4
1	C	46	ILE	2.2
1	C	248	LYS	2.2
1	A	138	LYS	2.1
1	A	321	LEU	2.1
1	B	50	LYS	2.0

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

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

6.3 Carbohydrates [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, 95th 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(\AA^2)	Q<0.9
2	GOL	B	401	6/6	0.89	0.19	2.56	42,53,59,59	0
3	SO4	C	401	5/5	0.99	0.14	1.20	42,43,56,64	0
2	GOL	A	402	6/6	0.89	0.12	-0.64	52,59,66,68	0
2	GOL	A	401	6/6	0.84	0.15	-1.00	51,70,74,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.