

Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2022 – 05:58 pm BST

PDB ID	:	7ZST
Title	:	Crystal Structure of truncated aspartate transcarbamoylase from Plasmodium
		falciparum in complex with FLA-01
Authors	:	Wang, C.; Zhang, B.; Groves, M.R.
Deposited on	:	2022-05-08
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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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		
		0.40	9%		
1	А	349	69%	19%	• 9%
			6%		
1	В	349	72%	18%	• 6%
			20%		
1	С	349	67%	19%	•• 10%



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15668 atoms, of which 7833 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1 Λ	317	Total	С	Η	Ν	0	S	70	0	0	
1	I A	517	5125	1629	2571	422	495	8	19	0	0
1 D	200	Total	С	Η	Ν	0	S	81	0	0	
1	I D	529	5315	1690	2662	436	519	8	01	0	0
1 C	215	Total	С	Η	Ν	0	S	77	0	0	
	U	515	5110	1626	2568	417	491	8	11	0	0

• Molecule 1 is a protein called Aspartate carbamoyltransferase.

Chain	Residue	Modelled	Actual	Comment	Reference
А	376	SER	-	expression tag	UNP A0A5K1K910
А	377	ALA	-	expression tag	UNP A0A5K1K910
А	378	TRP	-	expression tag	UNP A0A5K1K910
А	379	SER	-	expression tag	UNP A0A5K1K910
А	380	HIS	-	expression tag	UNP A0A5K1K910
А	381	PRO	-	expression tag	UNP A0A5K1K910
А	382	GLN	-	expression tag	UNP A0A5K1K910
А	383	PHE	-	expression tag	UNP A0A5K1K910
А	384	GLU	-	expression tag	UNP A0A5K1K910
А	385	LYS	-	expression tag	UNP A0A5K1K910
В	376	SER	-	expression tag	UNP A0A5K1K910
В	377	ALA	-	expression tag	UNP A0A5K1K910
В	378	TRP	-	expression tag	UNP A0A5K1K910
В	379	SER	-	expression tag	UNP A0A5K1K910
В	380	HIS	-	expression tag	UNP A0A5K1K910
В	381	PRO	-	expression tag	UNP A0A5K1K910
В	382	GLN	-	expression tag	UNP A0A5K1K910
В	383	PHE	-	expression tag	UNP A0A5K1K910
В	384	GLU	-	expression tag	UNP A0A5K1K910
В	385	LYS	-	expression tag	UNP A0A5K1K910
С	376	SER	-	expression tag	UNP A0A5K1K910
С	377	ALA	-	expression tag	UNP A0A5K1K910
С	378	TRP	-	expression tag	UNP A0A5K1K910

There are 30 discrepancies between the modelled and reference sequences:



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Chain	Residue	Modelled	Actual	Comment	Reference
С	379	SER	-	expression tag	UNP A0A5K1K910
С	380	HIS	-	expression tag	UNP A0A5K1K910
С	381	PRO	-	expression tag	UNP A0A5K1K910
С	382	GLN	-	expression tag	UNP A0A5K1K910
С	383	PHE	-	expression tag	UNP A0A5K1K910
С	384	GLU	-	expression tag	UNP A0A5K1K910
C	385	LYS	-	expression tag	UNP A0A5K1K910

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf			
2	А	1	Total C H O	2	0			
	11	1	14 3 8 3	-				
0	А	٨	Δ	۸	1	Total C H O	2	0
2		1	14 3 8 3		U			

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





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Na 1 1	0	0

• Molecule 5 is 2-azanyl- {N}-(2-methoxyethyl)-5-phenyl-thiophene-3-carboxamide (three-letter code: JUF) (formula: $C_{14}H_{16}N_2O_2S$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	В	1	Total 35	C 14	Н 16	N 2	0 2	S 1	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	13	Total O 13 13	0	0
6	В	18	Total O 18 18	0	0
6	С	13	Total O 13 13	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Aspartate carbamoyltransferase







4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants	119.28Å 89.73Å 137.05Å	Depositor
a, b, c, α , β , γ	90.00° 109.22° 90.00°	Depositor
Bosolution (Å)	49.50 - 2.50	Depositor
Resolution (A)	49.46 - 2.50	EDS
% Data completeness	99.9 (49.50-2.50)	Depositor
(in resolution range)	99.8 (49.46-2.50)	EDS
R_{merge}	0.03	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.01 (at 2.51 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
P. P.	0.236 , 0.282	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.241 , 0.284	DCC
R_{free} test set	2446 reflections $(5.17%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	49.6	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$ L > = 0.46, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15668	wwPDB-VP
Average B, all atoms $(Å^2)$	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: JUF, NA, SO4, 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).

Mal	Chain	Bond lengths		Bond angles	
MIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.74	0/2599	0.91	1/3510~(0.0%)
1	В	0.80	0/2699	0.95	1/3646~(0.0%)
1	С	0.73	0/2587	0.88	0/3494
All	All	0.76	0/7885	0.92	2/10650~(0.0%)

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	А	0	2
1	В	0	1
1	С	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	363	ARG	NE-CZ-NH1	-7.47	116.56	120.30
1	А	208	ARG	NE-CZ-NH2	-6.79	116.91	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Group
1	А	128	ILE	Peptide
1	А	380	HIS	Peptide



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Mol	Chain	Res	Type	Group
1	В	139	GLY	Peptide
1	С	128	ILE	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	А	2554	2571	2562	46	2
1	В	2653	2662	2655	54	0
1	С	2542	2568	2561	60	0
2	А	12	16	16	1	0
3	А	5	0	0	0	0
3	В	5	0	0	1	0
4	А	1	0	0	0	0
5	В	19	16	0	2	0
6	А	13	0	0	1	0
6	В	18	0	0	0	0
6	С	13	0	0	1	0
All	All	7835	7833	7794	150	2

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 10.

All (150) 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:337:VAL:HG23	1:A:338:ASN:H	1.22	1.00
1:A:137:TYR:O	1:A:139:GLY:N	1.96	0.97
1:B:92:LYS:NZ	1:C:96:ASN:OD1	2.11	0.84
1:A:288:VAL:O	1:A:328:THR:HG22	1.79	0.82
1:C:288:VAL:O	1:C:328:THR:HG22	1.79	0.82
1:A:69:GLU:HG2	6:A:512:HOH:O	1.79	0.82
1:B:288:VAL:O	1:B:328:THR:HG22	1.81	0.79
1:A:140:GLU:OE2	1:C:109:ARG:NH1	2.18	0.77
1:A:337:VAL:HG23	1:A:338:ASN:N	2.03	0.72
1:A:337:VAL:CG2	1:A:338:ASN:H	2.03	0.71



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:185:GLY:HA3	1:A:226:ARG:HD2	1.74	0.70
1:A:137:TYR:C	1:A:139:GLY:H	1.94	0.68
1:C:332:HIS:NE2	1:C:339:GLU:OE2	2.18	0.68
1:B:49:ASP:OD1	1:B:49:ASP:N	2.22	0.68
1:B:110:THR:OG1	5:B:401:JUF:N2	2.29	0.66
1:B:163:LYS:HB3	1:B:184:THR:HG23	1.79	0.65
1:B:297:GLN:O	1:B:299:GLU:O	2.16	0.64
1:C:296:ILE:HG21	1:C:312:ASN:HB3	1.79	0.64
1:C:286:GLU:O	1:C:288:VAL:N	2.28	0.63
1:C:296:ILE:HD12	1:C:312:ASN:HD22	1.63	0.62
1:C:126:LEU:HD13	1:C:126:LEU:H	1.65	0.62
1:A:350:SER:HB2	1:A:352:TYR:CE1	2.36	0.61
1:C:325:ARG:HB2	1:C:328:THR:HG23	1.82	0.61
1:B:299:GLU:O	1:B:300:ARG:HB2	2.01	0.60
1:C:324:THR:OG1	1:C:349:LYS:NZ	2.34	0.60
1:B:325:ARG:HB2	1:B:328:THR:HG23	1.84	0.60
1:A:124:LYS:HD3	1:C:119:LEU:HD22	1.84	0.60
1:B:337:VAL:O	1:B:338:ASN:HB2	2.03	0.58
1:A:109:ARG:HE	1:B:148:ILE:HG21	1.69	0.57
1:A:325:ARG:HB2	1:A:328:THR:HG23	1.86	0.57
1:B:334:LEU:HD13	1:C:148:ILE:HD11	1.87	0.57
1:C:185:GLY:HA3	1:C:226:ARG:HB3	1.87	0.57
1:C:204:PHE:HA	1:C:207:ASP:OD2	2.06	0.56
1:B:149:LEU:HD23	1:B:156:ILE:HD13	1.87	0.56
1:C:163:LYS:HB3	1:C:184:THR:HG23	1.87	0.56
1:C:209:ASN:HB3	1:C:212:LYS:HG3	1.87	0.56
1:B:373:SER:O	1:B:375:SER:N	2.39	0.55
1:C:233:LYS:NZ	6:C:401:HOH:O	2.39	0.55
1:B:324:THR:OG1	1:B:349:LYS:NZ	2.35	0.55
1:B:350:SER:HB2	1:B:352:TYR:CE2	2.41	0.55
1:B:193:LEU:C	1:B:193:LEU:HD12	2.28	0.55
1:C:327:ASP:O	1:C:329:LYS:NZ	2.36	0.55
1:C:163:LYS:CB	1:C:184:THR:HG23	2.37	0.54
1:C:149:LEU:HD23	1:C:156:ILE:HD13	1.89	0.54
1:B:302:THR:HB	1:B:303:ASP:OD1	2.08	0.54
1:B:337:VAL:O	1:B:337:VAL:HG12	2.08	0.54
1:C:337:VAL:O	1:C:338:ASN:HB2	2.08	0.53
1:C:163:LYS:HG2	1:C:164:LYS:N	2.24	0.53
1:C:209:ASN:HB3	1:C:212:LYS:CG	2.39	0.53
1:C:281:LEU:HD13	1:C:314:PHE:CD1	2.44	0.52
1:A:193:LEU:HD12	1:A:193:LEU:C	2.30	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:58:LYS:NZ	1:C:65:ASP:O	2.30	0.52
1:C:352:TYR:N	1:C:352:TYR:CD2	2.76	0.51
1:B:312:ASN:OD1	1:B:312:ASN:N	2.42	0.51
1:C:163:LYS:HG2	1:C:164:LYS:H	1.74	0.51
1:B:163:LYS:CB	1:B:184:THR:HG23	2.40	0.51
1:B:163:LYS:HG2	1:B:164:LYS:H	1.76	0.51
1:B:308:ASN:N	1:B:308:ASN:OD1	2.44	0.51
1:B:62:ASN:HB2	1:B:186:GLU:OE1	2.11	0.50
1:B:109:ARG:NE	1:C:148:ILE:HG21	2.25	0.50
1:C:193:LEU:C	1:C:193:LEU:HD12	2.31	0.50
1:A:62:ASN:HD22	1:A:186:GLU:HG2	1.76	0.50
1:C:51:ILE:HD12	1:C:51:ILE:N	2.26	0.50
1:A:324:THR:HB	1:A:328:THR:HG21	1.92	0.50
1:C:243:ASN:N	1:C:243:ASN:HD22	2.10	0.49
1:A:133:SER:O	1:A:136:PHE:O	2.30	0.49
1:B:282:GLU:H	1:B:282:GLU:CD	2.16	0.49
1:B:126:LEU:HD12	1:B:126:LEU:H	1.78	0.48
1:B:179:ASN:ND2	1:B:181:GLY:H	2.10	0.48
1:C:51:ILE:N	1:C:51:ILE:CD1	2.76	0.48
1:B:109:ARG:HH12	1:C:140:GLU:CD	2.16	0.48
1:B:109:ARG:HB3	5:B:401:JUF:C4	2.43	0.48
1:A:334:LEU:HD13	1:B:148:ILE:HD11	1.96	0.47
1:C:114:PHE:CE2	1:C:363:ARG:HD3	2.49	0.47
1:C:208:ARG:NH1	1:C:237:ARG:O	2.46	0.47
1:C:62:ASN:HB2	1:C:186:GLU:OE1	2.14	0.47
1:A:173:SER:O	2:A:401:GOL:H11	2.14	0.47
1:B:324:THR:HB	1:B:328:THR:HG21	1.96	0.46
1:C:350:SER:HB2	1:C:352:TYR:CE2	2.51	0.46
1:A:97:LYS:HB2	1:A:123:SER:OG	2.16	0.46
1:B:97:LYS:HB2	1:B:123:SER:OG	2.16	0.46
1:A:71:LEU:HD23	1:A:238:TYR:OH	2.16	0.45
1:C:324:THR:HB	1:C:328:THR:HG21	1.98	0.45
1:C:100:CYS:SG	1:C:126:LEU:CD2	3.04	0.45
1:B:109:ARG:HE	1:C:148:ILE:HG21	1.82	0.45
1:A:62:ASN:ND2	1:A:186:GLU:HG2	2.32	0.45
1:C:48:LEU:H	1:C:51:ILE:HD13	1.81	0.45
1:C:161:PRO:O	1:C:183:GLY:HA3	2.17	0.45
1:C:283:GLU:O	1:C:286:GLU:HG3	2.17	0.45
1:A:62:ASN:HB2	1:A:186:GLU:OE1	2.17	0.45
1:B:214:LEU:O	1:B:240:VAL:HA	2.17	0.44
1:C:45:LYS:O	1:C:46:ILE:HD13	2.18	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:312:ASN:N	1:C:312:ASN:OD1	2.49	0.44
1:A:100:CYS:O	1:A:156:ILE:HA	2.17	0.44
1:A:163:LYS:HG2	1:A:164:LYS:HD2	1.98	0.44
1:B:163:LYS:HG2	1:B:164:LYS:N	2.31	0.44
1:A:94:LEU:HB3	1:A:121:LEU:HB3	1.99	0.44
1:A:160:ASP:O	1:A:182:ASN:HA	2.17	0.44
1:B:161:PRO:O	1:B:183:GLY:N	2.50	0.44
1:B:221:ASP:OD1	1:B:221:ASP:C	2.55	0.44
1:A:221:ASP:OD1	1:A:221:ASP:C	2.56	0.44
1:A:195:PHE:CZ	1:A:205:ILE:HD12	2.53	0.44
1:C:183:GLY:O	1:C:226:ARG:NH1	2.51	0.44
1:A:111:ARG:HG2	1:A:111:ARG:HH21	1.83	0.43
1:B:133:SER:O	1:B:136:PHE:O	2.36	0.43
1:C:281:LEU:HA	1:C:281:LEU:HD12	1.84	0.43
1:C:100:CYS:SG	1:C:126:LEU:HD22	2.58	0.43
1:C:221:ASP:OD1	1:C:221:ASP:C	2.57	0.43
1:C:161:PRO:O	1:C:183:GLY:CA	2.67	0.43
1:A:255:ASP:N	1:A:255:ASP:OD1	2.52	0.42
1:C:161:PRO:O	1:C:183:GLY:N	2.52	0.42
1:C:318:ASN:OD1	1:C:347:ASN:ND2	2.47	0.42
1:B:61:ILE:HG13	1:B:170:VAL:HG21	2.01	0.42
1:C:179:ASN:ND2	1:C:181:GLY:H	2.17	0.42
1:C:217:ALA:HB2	1:C:288:VAL:HG11	2.02	0.42
1:A:118:ILE:HD11	1:A:157:ILE:HD13	2.02	0.42
1:A:161:PRO:O	1:A:183:GLY:N	2.52	0.42
1:B:94:LEU:HB3	1:B:121:LEU:HB3	2.02	0.42
1:C:160:ASP:O	1:C:182:ASN:HA	2.18	0.42
1:A:135:SER:O	1:A:138:LYS:HG2	2.19	0.42
1:B:124:LYS:HG2	3:B:402:SO4:O4	2.19	0.42
1:B:168:ILE:O	1:B:171:SER:OG	2.22	0.42
1:B:282:GLU:CD	1:B:282:GLU:N	2.73	0.42
1:A:137:TYR:C	1:A:139:GLY:N	2.61	0.42
1:B:161:PRO:O	1:B:183:GLY:HA3	2.20	0.42
1:A:214:LEU:O	1:A:240:VAL:HA	2.20	0.42
1:A:161:PRO:O	1:A:183:GLY:HA3	2.19	0.41
1:A:161:PRO:O	1:A:183:GLY:CA	2.69	0.41
1:A:315:ILE:HG21	1:A:341:LYS:HE3	2.03	0.41
1:B:114:PHE:CE2	1:B:363:ARG:HD3	2.55	0.41
1:A:143:GLU:HA	1:A:172:SER:OG	2.20	0.41
1:A:47:ASP:O	1:A:51:ILE:HG13	2.21	0.41
1:C:71:LEU:HD23	1:C:238:TYR:OH	2.20	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
1:A:185:GLY:HA3	1:A:226:ARG:CD	2.49	0.41
1:A:215:ASN:H	1:A:289:HIS:CD2	2.38	0.41
1:B:299:GLU:O	1:B:300:ARG:CB	2.68	0.41
1:C:97:LYS:HB2	1:C:123:SER:OG	2.21	0.41
1:B:100:CYS:O	1:B:156:ILE:HA	2.20	0.41
1:A:281:LEU:HD11	1:A:314:PHE:HA	2.02	0.40
1:B:118:ILE:HD11	1:B:157:ILE:HD13	2.02	0.40
1:A:217:ALA:HB2	1:A:288:VAL:HG11	2.03	0.40
1:A:123:SER:O	1:B:124:LYS:NZ	2.53	0.40
1:B:195:PHE:CZ	1:B:205:ILE:HD12	2.57	0.40
1:B:71:LEU:HD23	1:B:238:TYR:OH	2.21	0.40
1:B:133:SER:O	1:B:137:TYR:HD2	2.03	0.40
1:C:50:LYS:O	1:C:53:THR:HG22	2.21	0.40
1:B:161:PRO:O	1:B:183:GLY:CA	2.70	0.40
1:B:215:ASN:H	1:B:289:HIS:CD2	2.39	0.40
1:C:82:GLU:HG3	1:C:361:TYR:CE2	2.57	0.40
1:C:118:ILE:HD11	1:C:157:ILE:HD13	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ASP:OD2	1:A:379:SER:HG[2_555]	1.19	0.41
1:A:49:ASP:OD2	1:A:379:SER:OG[2_555]	2.17	0.03

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	Perce	ntiles
1	А	311/349~(89%)	292 (94%)	16 (5%)	3~(1%)	15	28
1	В	325/349~(93%)	299 (92%)	22 (7%)	4 (1%)	13	24



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	С	311/349~(89%)	286~(92%)	20~(6%)	5(2%)	9 17
All	All	947/1047~(90%)	877~(93%)	58~(6%)	12 (1%)	12 21

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	138	LYS
1	А	286	GLU
1	В	374	THR
1	С	248	LYS
1	С	286	GLU
1	С	338	ASN
1	В	286	GLU
1	С	208	ARG
1	В	338	ASN
1	В	302	THR
1	А	337	VAL
1	С	225	GLY

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	А	297/328~(90%)	278~(94%)	19 (6%)	17 33		
1	В	308/328~(94%)	288 (94%)	20~(6%)	17 33		
1	С	295/328~(90%)	278 (94%)	17 (6%)	20 38		
All	All	900/984~(92%)	844 (94%)	56~(6%)	18 35		

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	69	GLU
1	А	87	ASN
1	А	111	ARG



Mol	Chain	Res	Type
1	А	113	SER
1	А	126	LEU
1	А	129	THR
1	А	163	LYS
1	А	184	THR
1	А	187	HIS
1	А	214	LEU
1	А	248	LYS
1	А	249	SER
1	А	254	LYS
1	А	255	ASP
1	А	271	SER
1	А	272	ASP
1	А	319	LYS
1	А	338	ASN
1	А	352	TYR
1	В	49	ASP
1	В	126	LEU
1	В	129	THR
1	В	163	LYS
1	В	189	THR
1	В	214	LEU
1	В	233	LYS
1	В	248	LYS
1	В	249	SER
1	В	281	LEU
1	В	299	GLU
1	В	300	ARG
1	В	302	THR
1	В	303	ASP
1	В	306	GLU
1	В	308	ASN
1	В	319	LYS
1	В	339	GLU
1	В	352	TYR
1	В	373	SER
1	С	44	TYR
1	С	48	LEU
1	С	51	ILE
1	С	53	THR
1	С	126	LEU
1	С	129	THR



Mol	Chain	Res	Type
1	С	138	LYS
1	С	163	LYS
1	С	187	HIS
1	С	199	HIS
1	С	208	ARG
1	С	243	ASN
1	С	281	LEU
1	С	337	VAL
1	С	338	ASN
1	С	339	GLU
1	С	352	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	87	ASN
1	А	127	ASN
1	А	165	ASN
1	А	179	ASN
1	А	243	ASN
1	А	268	ASN
1	А	280	ASN
1	А	289	HIS
1	A	338	ASN
1	В	62	ASN
1	В	87	ASN
1	В	165	ASN
1	В	179	ASN
1	В	243	ASN
1	В	268	ASN
1	В	280	ASN
1	В	289	HIS
1	В	323	ASN
1	В	338	ASN
1	С	62	ASN
1	С	165	ASN
1	С	179	ASN
1	С	243	ASN
1	С	268	ASN
1	С	289	HIS
1	С	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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).

Mal	Turne	Chain	Dog	Tink	Bo	ond leng	$_{\rm sths}$	B	ond ang	gles
	I Type Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	SO4	В	402	-	4,4,4	0.46	0	6,6,6	0.27	0
3	SO4	А	403	-	4,4,4	0.28	0	6,6,6	0.08	0
2	GOL	А	402	-	5,5,5	0.19	0	5,5,5	0.39	0
5	JUF	В	401	-	18,20,20	0.63	0	16,26,26	0.76	0
2	GOL	А	401	-	5,5,5	0.18	0	5,5,5	0.23	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	А	402	-	-	2/4/4/4	-
5	JUF	В	401	-	-	6/11/13/13	0/2/2/2
2	GOL	А	401	-	-	4/4/4/4	-

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
2	А	402	GOL	C1-C2-C3-O3
2	А	402	GOL	O2-C2-C3-O3
5	В	401	JUF	C5-C4-N1-C3
5	В	401	JUF	O2-C4-N1-C3
5	В	401	JUF	C6-C7-C8-C9
5	В	401	JUF	C6-C7-C8-C13
5	В	401	JUF	S1-C7-C8-C9
5	В	401	JUF	S1-C7-C8-C13
2	А	401	GOL	O1-C1-C2-C3
2	А	401	GOL	C1-C2-C3-O3
2	A	401	GOL	O1-C1-C2-O2
2	А	401	GOL	O2-C2-C3-O3

All (12) torsion outliers are listed below:

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	402	SO4	1	0
5	В	401	JUF	2	0
2	А	401	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	317/349~(90%)	0.93	32 (10%) 7 6	32, 58, 91, 102	0
1	В	329/349~(94%)	0.71	20 (6%) 21 22	33, 51, 77, 104	0
1	С	315/349~(90%)	1.33	69 (21%) 0 0	37, 73, 104, 127	0
All	All	961/1047~(91%)	0.98	121 (12%) 3 3	32, 58, 96, 127	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	214	LEU	7.4
1	А	379	SER	6.9
1	С	284	GLY	6.8
1	С	314	PHE	6.0
1	С	46	ILE	5.9
1	С	281	LEU	5.4
1	С	273	ASP	5.0
1	С	328	THR	4.9
1	С	326	ASP	4.9
1	С	206	LEU	4.9
1	С	222	LEU	4.8
1	А	48	LEU	4.8
1	А	247	CYS	4.7
1	А	248	LYS	4.7
1	С	349	LYS	4.7
1	А	381	PRO	4.7
1	С	285	LEU	4.7
1	С	72	LEU	4.6
1	С	201	TYR	4.5
1	С	207	ASP	4.2
1	В	314	PHE	4.0
1	В	376	SER	4.0
1	С	48	LEU	3.9



Mol	Chain	Res	Type	RSRZ
1	А	382	GLN	3.9
1	С	79	LYS	3.9
1	С	238	TYR	3.9
1	А	282	GLU	3.8
1	С	208	ARG	3.8
1	С	223	LYS	3.7
1	С	231	LEU	3.6
1	А	83	LYS	3.6
1	А	314	PHE	3.6
1	А	281	LEU	3.6
1	С	323	ASN	3.6
1	А	315	ILE	3.5
1	С	204	PHE	3.5
1	С	217	ALA	3.5
1	С	256	ILE	3.4
1	С	352	TYR	3.4
1	А	296	ILE	3.3
1	С	322	GLU	3.3
1	С	330	ILE	3.2
1	С	291	ILE	3.2
1	В	319	LYS	3.1
1	С	130	ASP	3.1
1	А	278	PHE	3.1
1	В	374	THR	3.1
1	С	315	ILE	3.1
1	А	250	LEU	3.0
1	А	279	ASP	3.0
1	А	87	ASN	3.0
1	С	318	ASN	3.0
1	В	282	GLU	3.0
1	С	216	ILE	3.0
1	A	108	THR	3.0
1	С	215	ASN	2.9
1	С	296	ILE	2.9
1	A	277	TYR	2.9
1	A	273	ASP	2.9
1	В	248	LYS	2.9
1	С	240	VAL	2.8
1	С	331	LEU	2.7
1	С	236	SER	2.7
1	A	245	VAL	2.7
1	В	126	LEU	2.7



Mol	Chain	Res	Type	RSRZ
1	В	321	LEU	2.7
1	А	100	CYS	2.7
1	В	100	CYS	2.7
1	А	110	THR	2.7
1	С	337	VAL	2.7
1	С	274	SER	2.7
1	С	202	PHE	2.6
1	С	244	PHE	2.6
1	С	289	HIS	2.6
1	В	48	LEU	2.6
1	В	315	ILE	2.6
1	С	290	ILE	2.6
1	С	340	ILE	2.6
1	А	249	SER	2.6
1	С	50	LYS	2.5
1	С	242	PHE	2.5
1	А	283	GLU	2.5
1	С	316	LEU	2.5
1	С	205	ILE	2.5
1	С	220	GLY	2.5
1	С	264	LEU	2.5
1	С	313	ALA	2.5
1	С	277	TYR	2.5
1	С	288	VAL	2.4
1	С	263	ASN	2.4
1	С	348	PRO	2.3
1	С	270	TYR	2.3
1	С	253	PRO	2.3
1	С	272	ASP	2.3
1	В	101	SER	2.3
1	А	76	TYR	2.3
1	С	347	ASN	2.3
1	В	337	VAL	2.2
1	А	101	SER	2.2
1	В	109	ARG	2.2
1	С	293	MET	2.2
1	А	148	ILE	2.2
1	А	93	TYR	2.2
1	А	223	LYS	2.2
1	С	292	TYR	2.2
1	В	102	VAL	2.2
1	С	129	THR	2.2



Mol	Chain	Res	Type	RSRZ
1	В	266	LYS	2.1
1	А	102	VAL	2.1
1	С	344	VAL	2.1
1	В	296	ILE	2.1
1	С	320	THR	2.1
1	В	125	VAL	2.1
1	С	227	THR	2.1
1	С	259	THR	2.1
1	А	112	CYS	2.1
1	В	112	CYS	2.1
1	В	322	GLU	2.0
1	С	276	LYS	2.0
1	А	328	THR	2.0
1	С	351	VAL	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 monosaccharides 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^{th} 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	$B-factors(Å^2)$	Q<0.9
2	GOL	А	402	6/6	0.68	0.27	30,82,83,84	2
5	JUF	В	401	19/19	0.81	0.26	85,90,94,95	0
4	NA	А	404	1/1	0.83	0.22	36,36,36,36	0
2	GOL	А	401	6/6	0.83	0.22	30,74,75,77	2
3	SO4	А	403	5/5	0.94	0.16	67,76,81,82	0
3	SO4	В	402	5/5	0.94	0.21	51,53,54,57	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers



as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers (i)

There are no such residues in this entry.

