



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2018 – 05:44 PM EST

PDB ID : 5ILN  
Title : Crystal structure of Aspartate Transcarbamoylase from Plasmodium falciparum (PfATC) with bound citrate  
Authors : Lunev, S.; Bosch, S.S.; Batista, F.D.A.; Wrenger, C.; Groves, M.R.  
Deposited on : 2016-03-04  
Resolution : 2.21 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030736

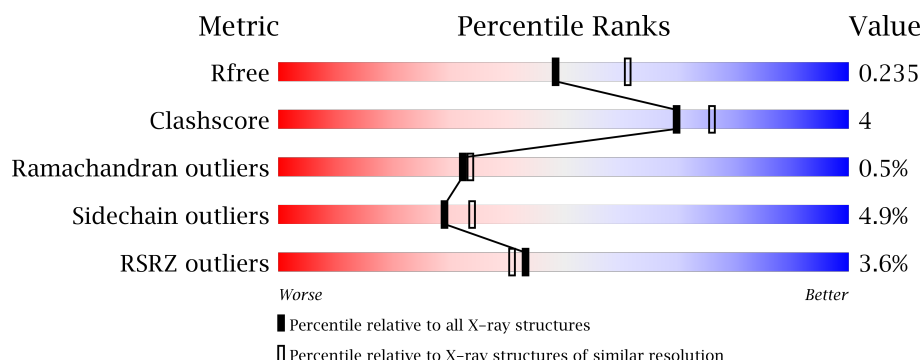
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.21 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))
$R_{free}$	100719	4744 (2.24-2.20)
Clashscore	112137	5509 (2.24-2.20)
Ramachandran outliers	110173	5427 (2.24-2.20)
Sidechain outliers	110143	5428 (2.24-2.20)
RSRZ outliers	101464	4776 (2.24-2.20)

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	385	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>15%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	385	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	385	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>••</div> <div>11%</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	A	401	-	-	-	X
2	GOL	C	402	-	-	-	X
3	PO4	A	402	-	-	-	X
4	FLC	C	401	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8418 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	331	Total	C	N	O	S	0	0	0
			2681	1715	440	517	9			
1	B	335	Total	C	N	O	S	0	0	0
			2727	1743	448	528	8			
1	C	343	Total	C	N	O	S	0	0	0
			2792	1784	457	542	9			

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

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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<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



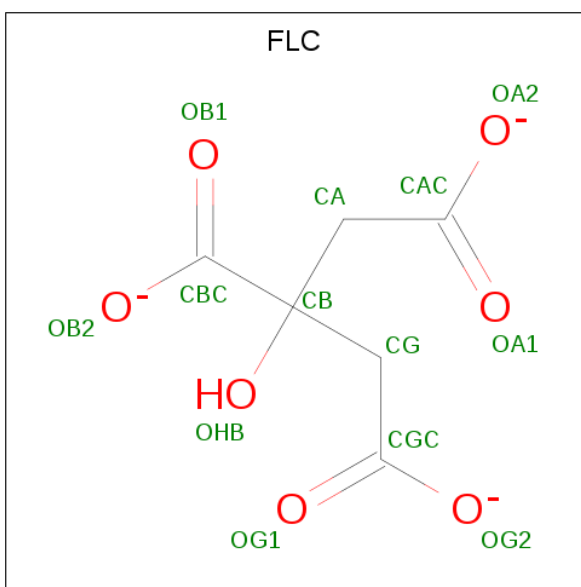
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			13	6	7		

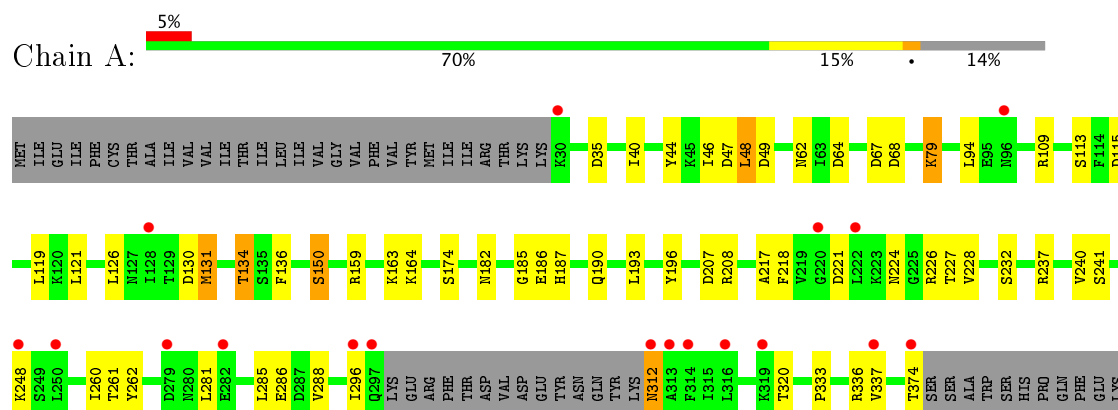
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	42	Total 42	O 42	0	0
5	B	54	Total 54	O 54	0	0
5	C	70	Total 70	O 70	0	0

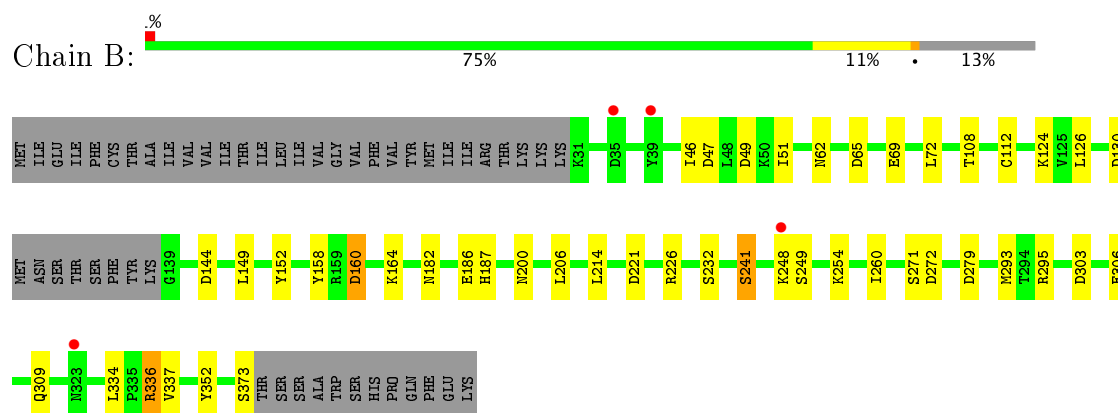
### 3 Residue-property plots [i](#)

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.

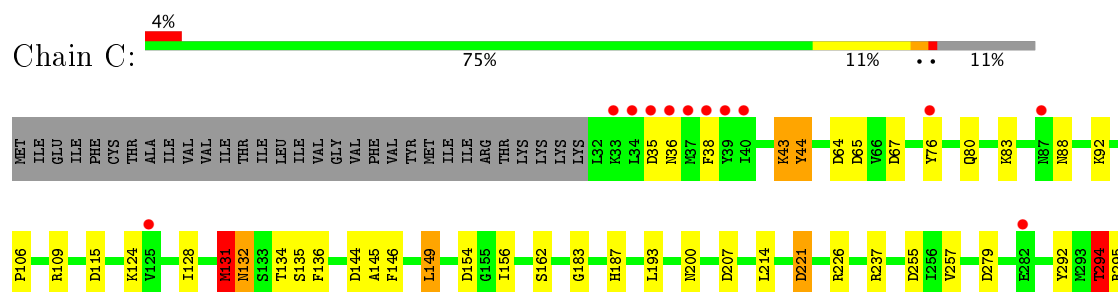
#### • Molecule 1: Aspartate carbamoyltransferase



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.45Å 107.29Å 87.32Å 90.00° 117.46° 90.00°	Depositor
Resolution (Å)	45.10 – 2.21 45.10 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.6 (45.10-2.21) 97.6 (45.10-2.21)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.180 , 0.234 0.186 , 0.235	Depositor DCC
$R_{free}$ test set	3470 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.0	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for -h-l,k,h 0.011 for l,k,-h-l 0.021 for h,-k,-h-l 0.023 for -h-l,-k,l 0.027 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8418	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GOL, FLC, CSO

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	1.10	2/2712 (0.1%)	1.14	18/3656 (0.5%)
1	B	1.15	3/2759 (0.1%)	1.14	12/3720 (0.3%)
1	C	1.15	2/2827 (0.1%)	1.13	14/3814 (0.4%)
All	All	1.13	7/8298 (0.1%)	1.14	44/11190 (0.4%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	241	SER	CB-OG	-6.67	1.33	1.42
1	C	294	THR	CB-CG2	-6.52	1.30	1.52
1	B	152	TYR	CE2-CZ	6.00	1.46	1.38
1	B	272	ASP	CB-CG	5.79	1.64	1.51
1	C	292	TYR	CB-CG	5.52	1.59	1.51
1	A	150	SER	CB-OG	-5.33	1.35	1.42
1	A	237	ARG	C-O	5.23	1.33	1.23

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ASP	CB-CG-OD1	8.90	126.31	118.30
1	C	131	MET	CG-SD-CE	-8.88	85.98	100.20
1	C	295	ARG	NE-CZ-NH1	8.10	124.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	A	47	ASP	CB-CG-OD1	7.14	124.73	118.30
1	B	336	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	C	64	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	C	154	ASP	CB-CG-OD2	6.83	124.45	118.30
1	A	68	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	130	ASP	CB-CG-OD1	-6.62	112.34	118.30
1	B	279	ASP	CB-CA-C	-6.26	97.88	110.40
1	B	144	ASP	CB-CG-OD1	6.23	123.90	118.30
1	A	208	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	65	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	C	144	ASP	CB-CG-OD1	6.08	123.77	118.30
1	B	206	LEU	CB-CG-CD2	6.06	121.30	111.00
1	A	150	SER	CB-CA-C	-6.04	98.62	110.10
1	A	208	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	B	226	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	115	ASP	CB-CG-OD1	5.74	123.46	118.30
1	B	160	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	303	ASP	CB-CG-OD1	5.72	123.44	118.30
1	A	44	TYR	N-CA-C	-5.61	95.84	111.00
1	C	154	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	A	67	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	131	MET	CA-CB-CG	5.55	122.73	113.30
1	B	226	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	207	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	130	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	C	65	ASP	CB-CG-OD2	5.45	123.21	118.30
1	C	237	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	47	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	C	144	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	A	115	ASP	CB-CG-OD2	-5.37	113.46	118.30
1	C	109	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	A	79	LYS	CB-CA-C	-5.34	99.71	110.40
1	C	326	ASP	CB-CG-OD1	5.30	123.07	118.30
1	C	221	ASP	CB-CG-OD1	5.24	123.02	118.30
1	C	279	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	A	48	LEU	CB-CG-CD1	5.17	119.79	111.00
1	C	67	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	35	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	159	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	A	64	ASP	CB-CG-OD1	5.08	122.88	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	131	MET	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	2681	0	2709	32	0
1	B	2727	0	2742	14	0
1	C	2792	0	2800	24	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	12	0	16	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	C	13	0	5	4	0
5	A	42	0	0	5	0
5	B	54	0	0	3	0
5	C	70	0	0	1	0
All	All	8418	0	8288	70	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 (70) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:CSO:OD	1:B:112:CSO:SG	1.96	1.23
4:C:401:FLC:OA1	5:C:501:HOH:O	1.80	1.00
1:C:187:HIS:HE1	4:C:401:FLC:OA2	1.69	0.75
1:C:38:PHE:CE2	1:C:76:TYR:CE1	2.80	0.69
1:A:182:ASN:O	1:A:226:ARG:NH2	2.27	0.67
1:A:185:GLY:HA2	1:A:226:ARG:HD3	1.77	0.66
1:A:134:THR:HG21	1:A:136:PHE:CD2	2.33	0.63
1:B:306:GLU:O	1:B:309:GLN:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:PRO:HG3	1:C:131:MET:HE1	1.80	0.62
1:A:79:LYS:HE3	1:A:196:TYR:OH	1.99	0.62
4:C:401:FLC:CBC	4:C:401:FLC:OG1	2.50	0.59
1:B:187:HIS:HD2	5:B:506:HOH:O	1.85	0.59
1:C:187:HIS:CE1	4:C:401:FLC:OA2	2.54	0.59
1:A:218:PHE:CD1	1:A:228:VAL:HG13	2.38	0.59
1:C:334:LEU:HB3	1:C:335:PRO:HA	1.83	0.58
1:A:221:ASP:OD2	1:A:224:ASN:HB2	2.03	0.58
1:A:217:ALA:HB2	1:A:288:VAL:HG11	1.85	0.58
1:A:46:ILE:HD12	1:A:48:LEU:HD13	1.86	0.57
1:B:62:ASN:HA	1:B:186:GLU:CG	2.34	0.56
1:C:38:PHE:CZ	1:C:76:TYR:HE1	2.25	0.54
1:C:338:ASN:HD22	1:C:338:ASN:H	1.56	0.54
1:B:62:ASN:OD1	1:B:186:GLU:HG2	2.08	0.54
1:A:109:ARG:HD2	5:A:515:HOH:O	2.07	0.53
1:B:46:ILE:HD13	1:B:72:LEU:HD13	1.88	0.53
1:C:44:TYR:OH	1:C:207:ASP:OD1	2.26	0.53
1:A:232:SER:HB3	1:A:260:ILE:HD11	1.90	0.52
1:C:106:PRO:HG3	1:C:131:MET:CE	2.40	0.52
1:B:160:ASP:O	1:B:182:ASN:HA	2.09	0.52
1:C:221:ASP:H	1:C:294:THR:CG2	2.23	0.52
1:A:281:LEU:HD13	1:A:320:THR:HG21	1.92	0.51
1:C:183:GLY:O	1:C:226:ARG:HD3	2.11	0.51
1:C:106:PRO:CG	1:C:131:MET:HE1	2.41	0.51
1:C:36:ASN:OD1	1:C:80:GLN:NE2	2.42	0.51
1:A:62:ASN:OD1	1:A:186:GLU:HG3	2.11	0.51
1:B:62:ASN:HA	1:B:186:GLU:HG3	1.92	0.51
1:C:35:ASP:OD1	1:C:83:LYS:NZ	2.29	0.50
1:C:38:PHE:CZ	1:C:76:TYR:CE1	2.99	0.50
1:A:119:LEU:HD12	1:B:126:LEU:HD21	1.93	0.49
1:A:312:ASN:N	1:A:312:ASN:HD22	2.09	0.49
1:A:186:GLU:OE1	5:A:501:HOH:O	2.20	0.48
1:A:150:SER:HB3	1:A:174:SER:OG	2.13	0.48
1:C:132:ASN:N	1:C:132:ASN:HD22	2.12	0.47
1:C:38:PHE:CE2	1:C:76:TYR:CD1	3.02	0.47
1:A:190:GLN:NE2	5:A:504:HOH:O	2.48	0.47
1:C:145:ALA:O	1:C:149:LEU:HB2	2.15	0.47
1:A:281:LEU:HB3	1:A:285:LEU:HD22	1.96	0.47
1:C:43:LYS:N	1:C:43:LYS:HD3	2.30	0.47
1:B:158:TYR:CE1	1:B:160:ASP:HB2	2.50	0.46
1:B:51:ILE:CD1	1:B:69:GLU:HB3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:THR:CG2	1:A:136:PHE:H	2.29	0.45
1:A:109:ARG:O	1:A:113:SER:HB2	2.17	0.45
1:C:146:PHE:HE1	1:C:156:ILE:HG21	1.82	0.45
1:C:38:PHE:CE2	1:C:76:TYR:HE1	2.32	0.44
1:A:134:THR:HG22	1:A:136:PHE:H	1.82	0.44
1:A:46:ILE:CD1	1:A:48:LEU:HD13	2.47	0.43
1:A:79:LYS:NZ	5:A:506:HOH:O	2.50	0.43
1:B:221:ASP:OD2	5:B:501:HOH:O	2.21	0.43
1:C:128:ILE:HG21	1:C:136:PHE:CE1	2.52	0.43
1:B:232:SER:HB3	1:B:260:ILE:HD11	2.01	0.43
1:A:240:VAL:HG12	1:A:241:SER:N	2.33	0.43
1:A:164:LYS:HA	5:A:530:HOH:O	2.19	0.42
1:A:227:THR:HG21	1:A:333:PRO:HG3	2.02	0.42
1:A:261:THR:O	1:A:262:TYR:C	2.58	0.42
1:C:193:LEU:HA	1:C:362:VAL:HG21	2.02	0.41
1:B:293:MET:HE3	5:B:527:HOH:O	2.20	0.41
1:A:94:LEU:HB3	1:A:121:LEU:HB3	2.02	0.41
1:A:126:LEU:HD22	1:C:115:ASP:HB3	2.02	0.41
1:A:134:THR:HG21	1:A:136:PHE:HD2	1.84	0.40
1:A:109:ARG:CZ	1:A:109:ARG:HB2	2.51	0.40
1:A:193:LEU:HD12	1:A:193:LEU:C	2.42	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	325/385 (84%)	306 (94%)	18 (6%)	1 (0%)	44	49
1	B	329/385 (86%)	318 (97%)	9 (3%)	2 (1%)	28	28
1	C	339/385 (88%)	319 (94%)	18 (5%)	2 (1%)	28	28
All	All	993/1155 (86%)	943 (95%)	45 (4%)	5 (0%)	32	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	VAL
1	C	88	ASN
1	C	337	VAL
1	B	337	VAL
1	B	334	LEU

### 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	309/360 (86%)	297 (96%)	12 (4%)	37	45
1	B	313/360 (87%)	297 (95%)	16 (5%)	28	32
1	C	321/360 (89%)	303 (94%)	18 (6%)	25	27
All	All	943/1080 (87%)	897 (95%)	46 (5%)	29	34

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	A	49	ASP
1	A	131	MET
1	A	134	THR
1	A	163	LYS
1	A	187	HIS
1	A	248	LYS
1	A	286	GLU
1	A	296	ILE
1	A	312	ASN
1	A	336	ARG
1	A	374	THR
1	B	49	ASP
1	B	108	THR
1	B	124	LYS
1	B	149	LEU

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Mol	Chain	Res	Type
1	B	164	LYS
1	B	200	ASN
1	B	214	LEU
1	B	241	SER
1	B	248	LYS
1	B	249	SER
1	B	254	LYS
1	B	271	SER
1	B	295	ARG
1	B	336	ARG
1	B	352	TYR
1	B	373	SER
1	C	43	LYS
1	C	44	TYR
1	C	92	LYS
1	C	124	LYS
1	C	132	ASN
1	C	134	THR
1	C	135	SER
1	C	149	LEU
1	C	162	SER
1	C	200	ASN
1	C	214	LEU
1	C	255	ASP
1	C	257	VAL
1	C	294	THR
1	C	335	PRO
1	C	338	ASN
1	C	352	TYR
1	C	372	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	127	ASN
1	A	318	ASN
1	B	87	ASN
1	B	187	HIS
1	B	190	GLN
1	B	338	ASN
1	B	358	ASN

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Mol	Chain	Res	Type
1	C	36	ASN
1	C	41	ASN
1	C	80	GLN
1	C	132	ASN
1	C	187	HIS
1	C	200	ASN
1	C	243	ASN
1	C	251	ASN
1	C	338	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CSO	A	112	1	4,6,7	1.42	0	1,6,8	1.32	0
1	CSO	A	247	1	4,6,7	0.79	0	1,6,8	2.25	1 (100%)
1	CSO	B	112	1	4,6,7	1.47	1 (25%)	1,6,8	1.10	0
1	CSO	B	247	1	4,6,7	1.88	1 (25%)	1,6,8	1.91	0
1	CSO	C	112	1	4,6,7	1.68	1 (25%)	1,6,8	0.95	0
1	CSO	C	247	1	4,6,7	0.61	0	1,6,8	0.85	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
1	CSO	A	112	1	-	0/1/5/7	0/0/0/0
1	CSO	A	247	1	-	0/1/5/7	0/0/0/0
1	CSO	B	112	1	-	0/1/5/7	0/0/0/0
1	CSO	B	247	1	-	0/1/5/7	0/0/0/0
1	CSO	C	112	1	-	0/1/5/7	0/0/0/0
1	CSO	C	247	1	-	0/1/5/7	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	CSO	CB-CA	2.32	1.59	1.53
1	B	247	CSO	CA-C	2.65	1.53	1.50
1	C	112	CSO	CA-C	3.10	1.54	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	CSO	O-C-CA	-2.25	118.80	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	112	CSO	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	0.89	0	5,5,5	0.98	0
3	PO4	A	402	-	4,4,4	1.02	0	6,6,6	0.72	0
2	GOL	B	401	-	5,5,5	0.75	0	5,5,5	0.81	0
3	PO4	B	402	-	4,4,4	0.71	0	6,6,6	0.85	0
4	FLC	C	401	-	3,12,12	2.25	2 (66%)	3,17,17	3.76	1 (33%)
2	GOL	C	402	-	5,5,5	0.33	0	5,5,5	0.70	0
2	GOL	C	403	-	5,5,5	0.51	0	5,5,5	0.42	0
3	PO4	C	404	-	4,4,4	1.11	0	6,6,6	0.82	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
3	PO4	A	402	-	-	0/0/0/0	0/0/0/0
2	GOL	B	401	-	-	0/4/4/4	0/0/0/0
3	PO4	B	402	-	-	0/0/0/0	0/0/0/0
4	FLC	C	401	-	-	0/6/16/16	0/0/0/0
2	GOL	C	402	-	-	0/4/4/4	0/0/0/0
2	GOL	C	403	-	-	0/4/4/4	0/0/0/0
3	PO4	C	404	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	FLC	CG-CB	-2.68	1.50	1.54
4	C	401	FLC	OHB-CB	2.77	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	FLC	CB-CG-CGC	-6.45	104.87	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	FLC	4	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	329/385 (85%)	-0.11	18 (5%) 26 24	36, 51, 85, 117	0
1	B	333/385 (86%)	-0.08	4 (1%) 79 77	31, 47, 74, 92	0
1	C	341/385 (88%)	-0.06	14 (4%) 38 36	31, 44, 86, 114	0
All	All	1003/1155 (86%)	-0.09	36 (3%) 43 41	31, 47, 81, 117	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	313	ALA	6.7
1	C	38	PHE	5.4
1	C	37	MET	5.4
1	A	248	LYS	4.7
1	C	39	TYR	4.0
1	C	40	ILE	3.8
1	C	33	LYS	3.6
1	A	319	LYS	3.2
1	A	314	PHE	3.1
1	A	297	GLN	2.9
1	B	248	LYS	2.9
1	C	35	ASP	2.9
1	A	374	THR	2.7
1	A	316	LEU	2.6
1	A	250	LEU	2.5
1	A	30	LYS	2.5
1	B	323	ASN	2.5
1	C	374	THR	2.4
1	C	34	LEU	2.4
1	C	76	TYR	2.4
1	A	296	ILE	2.4
1	A	282	GLU	2.3
1	A	312	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	128	ILE	2.3
1	C	319	LYS	2.2
1	A	222	LEU	2.2
1	A	337	VAL	2.2
1	A	279	ASP	2.2
1	C	87	ASN	2.2
1	C	282	GLU	2.2
1	B	35	ASP	2.1
1	C	36	ASN	2.1
1	C	125	VAL	2.1
1	B	39	TYR	2.0
1	A	96	ASN	2.0
1	A	220	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSO	C	247	7/8	0.96	0.09	-	45,51,54,55	0
1	CSO	A	247	7/8	0.87	0.35	-	90,105,112,115	0
1	CSO	B	112	7/8	0.97	0.22	-	40,43,46,53	0
1	CSO	A	112	7/8	0.95	0.18	-	38,40,49,53	0
1	CSO	C	112	7/8	0.95	0.20	-	35,38,40,50	0
1	CSO	B	247	7/8	0.94	0.17	-	51,57,61,64	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	401	6/6	0.66	0.22	13.83	58,74,81,83	0
3	PO4	A	402	5/5	0.88	0.23	4.05	55,63,75,76	5
2	GOL	C	402	6/6	0.96	0.14	3.31	42,53,53,55	0
3	PO4	B	402	5/5	0.83	0.22	1.78	57,61,74,80	5
3	PO4	C	404	5/5	1.00	0.15	-0.45	41,41,48,50	0
4	FLC	C	401	13/13	0.90	0.11	-1.12	37,47,54,54	0
2	GOL	C	403	6/6	0.68	0.21	-	82,88,93,93	0
2	GOL	B	401	6/6	0.82	0.23	-	57,69,72,85	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.