Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2023 – 09:01 PM EDT

PDB ID	:	3FOC
Title	:	Tryptophanyl-tRNA synthetase from Giardia lamblia
Authors	:	Arakaki, T.L.; Merritt, E.A.; Medical Structural Genomics of Pathogenic Protozoa (MSGPP)
Deposited on	:	2008-12-29
Resolution	:	2.09 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 ⓘ 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 ⓘ) were used in the production of this report:

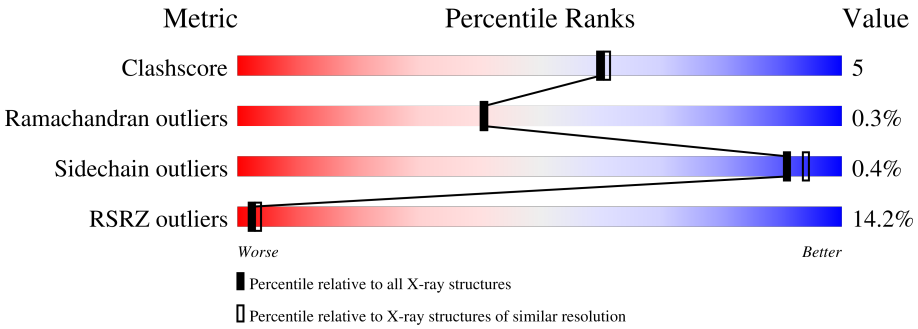
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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
1	A	451	13% 79% 10% 10%
1	B	451	12% 81% 7% 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6885 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 Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	8	0
			3260	2097	545	604	14			
1	B	399	Total	C	N	O	S	0	13	0
			3244	2096	544	591	13			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP A8B8N3
A	-20	ALA	-	expression tag	UNP A8B8N3
A	-19	HIS	-	expression tag	UNP A8B8N3
A	-18	HIS	-	expression tag	UNP A8B8N3
A	-17	HIS	-	expression tag	UNP A8B8N3
A	-16	HIS	-	expression tag	UNP A8B8N3
A	-15	HIS	-	expression tag	UNP A8B8N3
A	-14	HIS	-	expression tag	UNP A8B8N3
A	-13	MET	-	expression tag	UNP A8B8N3
A	-12	GLY	-	expression tag	UNP A8B8N3
A	-11	THR	-	expression tag	UNP A8B8N3
A	-10	LEU	-	expression tag	UNP A8B8N3
A	-9	GLU	-	expression tag	UNP A8B8N3
A	-8	ALA	-	expression tag	UNP A8B8N3
A	-7	GLN	-	expression tag	UNP A8B8N3
A	-6	THR	-	expression tag	UNP A8B8N3
A	-5	GLN	-	expression tag	UNP A8B8N3
A	-4	GLY	-	expression tag	UNP A8B8N3
A	-3	PRO	-	expression tag	UNP A8B8N3
A	-2	GLY	-	expression tag	UNP A8B8N3
A	-1	SER	-	expression tag	UNP A8B8N3
A	0	MET	-	expression tag	UNP A8B8N3
A	384	THR	ALA	SEE REMARK 999	UNP A8B8N3
B	-21	MET	-	expression tag	UNP A8B8N3
B	-20	ALA	-	expression tag	UNP A8B8N3

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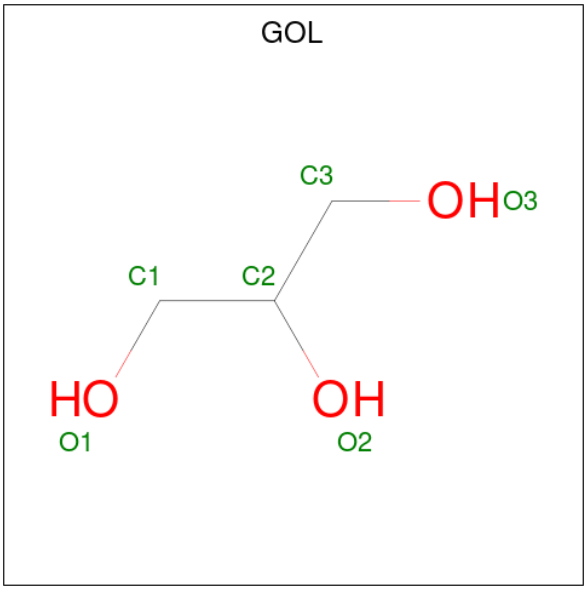
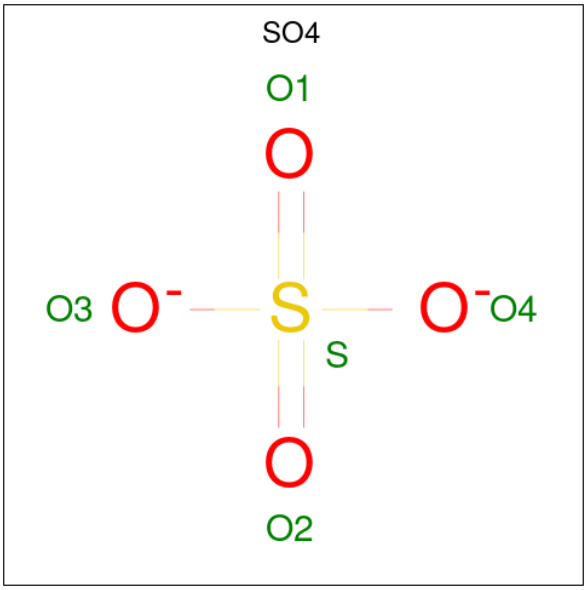
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	HIS	-	expression tag	UNP A8B8N3
B	-18	HIS	-	expression tag	UNP A8B8N3
B	-17	HIS	-	expression tag	UNP A8B8N3
B	-16	HIS	-	expression tag	UNP A8B8N3
B	-15	HIS	-	expression tag	UNP A8B8N3
B	-14	HIS	-	expression tag	UNP A8B8N3
B	-13	MET	-	expression tag	UNP A8B8N3
B	-12	GLY	-	expression tag	UNP A8B8N3
B	-11	THR	-	expression tag	UNP A8B8N3
B	-10	LEU	-	expression tag	UNP A8B8N3
B	-9	GLU	-	expression tag	UNP A8B8N3
B	-8	ALA	-	expression tag	UNP A8B8N3
B	-7	GLN	-	expression tag	UNP A8B8N3
B	-6	THR	-	expression tag	UNP A8B8N3
B	-5	GLN	-	expression tag	UNP A8B8N3
B	-4	GLY	-	expression tag	UNP A8B8N3
B	-3	PRO	-	expression tag	UNP A8B8N3
B	-2	GLY	-	expression tag	UNP A8B8N3
B	-1	SER	-	expression tag	UNP A8B8N3
B	0	MET	-	expression tag	UNP A8B8N3
B	384	THR	ALA	SEE REMARK 999	UNP A8B8N3

- 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 6 3 3	0	0

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



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

- Molecule 4 is water.

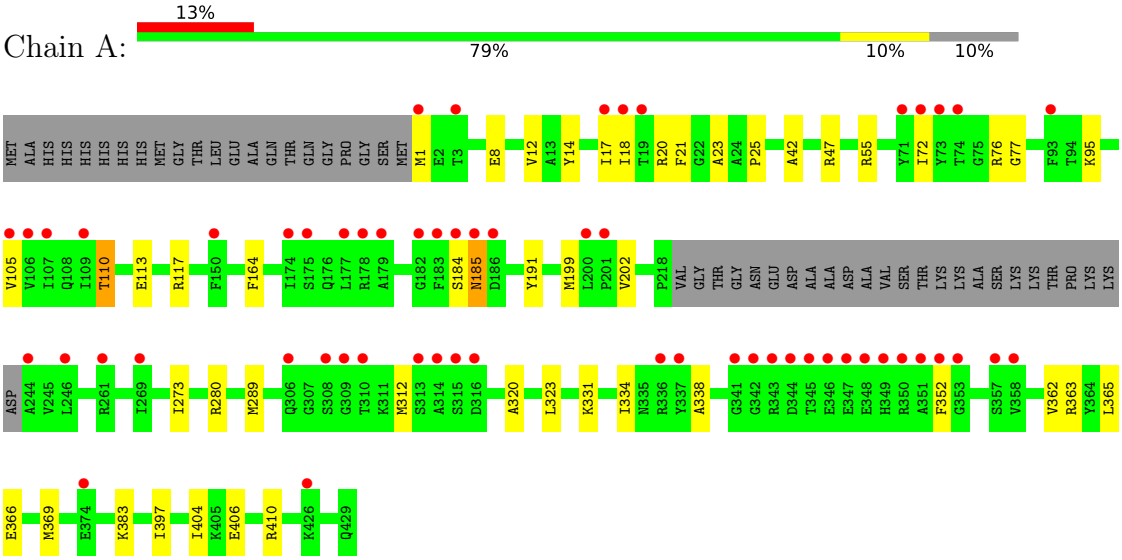
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	177	Total O 177 177	0	0
4	B	188	Total O 188 188	0	0

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.

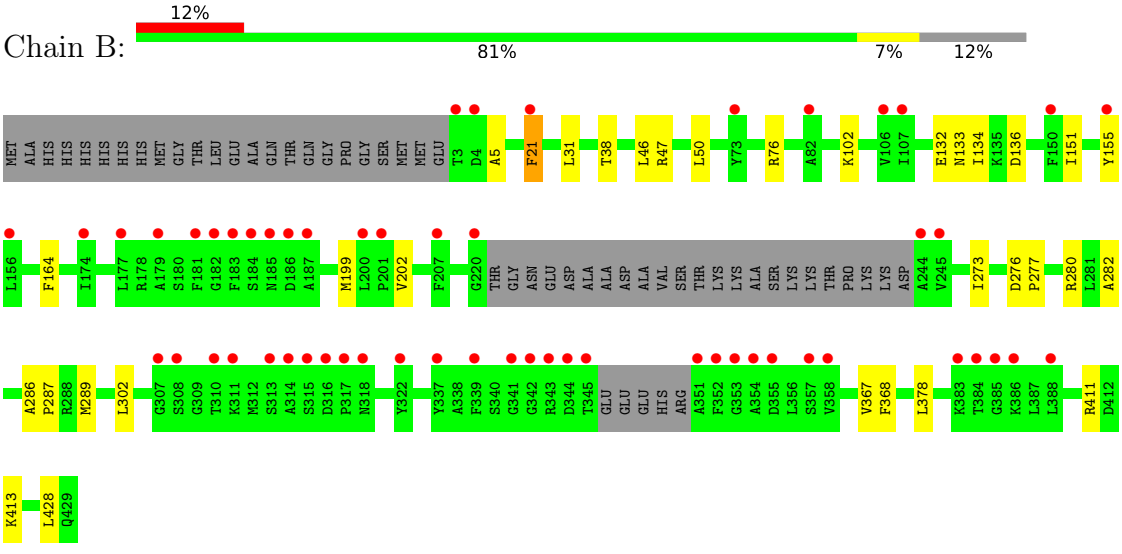
• Molecule 1: Tryptophanyl-tRNA synthetase

Chain A:



• Molecule 1: Tryptophanyl-tRNA synthetase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	106.71Å 140.15Å 90.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.09 39.88 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.7 (40.00-2.09) 89.0 (39.88-2.09)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.234 0.212 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	35.2	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6885	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.37	0/3360	0.53	0/4540
1	B	0.37	0/3354	0.52	0/4529
All	All	0.37	0/6714	0.53	0/9069

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3260	0	3243	37	0
1	B	3244	0	3271	25	0
2	A	6	0	8	0	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	177	0	0	1	0
4	B	188	0	0	2	0
All	All	6885	0	6522	60	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 5.

All (60) 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:17:ILE:HG22	1:A:18:ILE:HD13	1.45	0.96
1:A:365:LEU:HD22	1:A:369:MET:HE3	1.48	0.96
1:A:365:LEU:HD22	1:A:369:MET:CE	2.09	0.83
1:A:17:ILE:CG2	1:A:18:ILE:HD13	2.19	0.72
1:B:47[A]:ARG:NH2	4:B:496:HOH:O	2.23	0.68
1:A:110:THR:HG23	1:A:113:GLU:HB3	1.75	0.67
1:B:21[A]:PHE:CD1	1:B:21[A]:PHE:O	2.50	0.65
1:B:21[A]:PHE:HD1	1:B:21[A]:PHE:C	2.01	0.64
1:B:21[A]:PHE:O	1:B:21[A]:PHE:HD1	1.80	0.63
1:A:21:PHE:CE1	1:A:273:ILE:HD11	2.34	0.62
1:B:132:GLU:OE1	1:B:411[B]:ARG:NH2	2.34	0.60
1:A:18:ILE:HG23	1:A:23:ALA:HB3	1.84	0.60
1:B:21[A]:PHE:CD1	1:B:21[A]:PHE:C	2.74	0.59
1:A:77:GLY:CA	1:A:110:THR:HG22	2.34	0.58
1:A:77:GLY:HA2	1:A:110:THR:HG22	1.85	0.57
1:A:20:ARG:CD	1:B:273:ILE:HG21	2.36	0.55
1:B:50:LEU:HD23	1:B:367:VAL:HG22	1.87	0.55
1:B:413:LYS:NZ	4:B:594:HOH:O	2.40	0.54
1:A:110:THR:HG23	1:A:110:THR:O	2.07	0.54
1:A:406:GLU:OE2	1:A:410:ARG:NH2	2.40	0.54
1:A:110:THR:O	1:A:110:THR:CG2	2.56	0.53
1:B:199:MET:O	1:B:202:VAL:HG22	2.09	0.52
1:A:184:SER:O	1:A:185:ASN:CB	2.58	0.51
1:A:365:LEU:CD2	1:A:369:MET:HE3	2.33	0.50
1:A:14:TYR:CZ	1:A:18:ILE:HG13	2.46	0.50
1:B:134:ILE:HD11	1:B:151:ILE:HD11	1.93	0.50
1:B:202:VAL:HG21	1:B:282:ALA:HB1	1.94	0.50
1:A:1:MET:HE2	1:A:383:LYS:HD2	1.94	0.49
1:A:14:TYR:OH	1:A:25:PRO:HA	2.13	0.49
1:A:18:ILE:CG2	1:A:23:ALA:HB3	2.43	0.49
1:A:21:PHE:HE1	1:A:273:ILE:HD11	1.77	0.48
1:B:280:ARG:NH2	3:B:501:SO4:O1	2.46	0.48
1:B:136:ASP:OD2	1:B:411[B]:ARG:NH1	2.47	0.47
1:A:72:ILE:HB	1:A:105:VAL:HG22	1.97	0.47
1:A:312:MET:HB3	1:A:320:ALA:HB2	1.96	0.46
1:B:164:PHE:CZ	1:B:289:MET:HE1	2.51	0.46
1:B:302:LEU:HD11	1:B:368:PHE:CE2	2.50	0.46
1:B:31:LEU:HD21	1:B:46:LEU:HB3	1.97	0.46
1:B:76:ARG:NH1	1:B:133:ASN:OD1	2.49	0.45
1:A:362:VAL:O	1:A:366:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:MET:HE3	1:B:282:ALA:HA	2.01	0.43
1:B:276:ASP:HB3	1:B:277:PRO:HD3	1.99	0.43
1:A:42:ALA:HB3	1:A:47[B]:ARG:HG2	1.98	0.43
1:A:334:ILE:O	1:A:338:ALA:HB3	2.19	0.43
1:A:14:TYR:CE2	1:B:5:ALA:HB2	2.52	0.43
1:B:286:ALA:HB3	1:B:287:PRO:HD3	2.01	0.43
1:A:117:ARG:HG3	1:A:191:TYR:CE1	2.54	0.43
1:A:164:PHE:CZ	1:A:289:MET:HE1	2.54	0.42
1:A:323:LEU:HA	1:A:404:ILE:HD12	2.01	0.42
1:A:18:ILE:HD13	1:A:18:ILE:N	2.34	0.42
1:B:378:LEU:C	1:B:378:LEU:HD23	2.40	0.42
1:A:76:ARG:NH1	1:A:77:GLY:O	2.53	0.42
1:A:199:MET:O	1:A:202:VAL:HG22	2.19	0.42
1:A:95:LYS:NZ	4:A:493:HOH:O	2.51	0.41
1:A:55:ARG:NH2	1:A:280:ARG:HD2	2.35	0.41
1:A:365:LEU:HD22	1:A:369:MET:HE2	1.99	0.41
1:A:8:GLU:O	1:A:12:VAL:HG23	2.20	0.41
1:B:38:THR:O	1:B:102:LYS:NZ	2.54	0.41
1:A:331:LYS:HG3	1:A:397:ILE:HD13	2.03	0.41
1:B:155:TYR:HE1	1:B:428[A]:LEU:HD21	1.86	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	408/451 (90%)	396 (97%)	10 (2%)	2 (0%)	29 26
1	B	406/451 (90%)	399 (98%)	7 (2%)	0	100 100
All	All	814/902 (90%)	795 (98%)	17 (2%)	2 (0%)	41 49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
1	A	352	PHE

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	348/381 (91%)	346 (99%)	2 (1%)	86	90
1	B	349/381 (92%)	347 (99%)	2 (1%)	86	90
All	All	697/762 (92%)	693 (99%)	4 (1%)	91	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	THR
1	A	363	ARG
1	B	21[A]	PHE
1	B	21[B]	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

3 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	$\#\|Z\| > 2$
3	SO4	A	503	-	4,4,4	0.15	0	6,6,6	0.15	0
3	SO4	B	501	-	4,4,4	0.12	0	6,6,6	0.11	0
2	GOL	A	502	-	5,5,5	0.43	0	5,5,5	0.16	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	502	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	GOL	O1-C1-C2-O2
2	A	502	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	SO4	1	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^{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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	404/451 (89%)	0.80	58 (14%) 2 3	17, 26, 48, 55	3 (0%)
1	B	399/451 (88%)	0.70	56 (14%) 2 3	16, 26, 44, 51	7 (1%)
All	All	803/902 (89%)	0.75	114 (14%) 2 3	16, 26, 46, 55	10 (1%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	PHE	10.6
1	A	352	PHE	9.5
1	B	352	PHE	9.3
1	B	3	THR	7.6
1	A	345	THR	7.3
1	A	183	PHE	7.1
1	A	186	ASP	7.1
1	A	344	ASP	6.9
1	A	343	ARG	6.8
1	A	185	ASN	6.5
1	B	184	SER	6.0
1	A	351	ALA	5.8
1	B	186	ASP	5.7
1	A	349	HIS	5.7
1	A	184	SER	5.6
1	A	347	GLU	5.6
1	B	353	GLY	5.2
1	A	348	GLU	5.1
1	B	182	GLY	5.0
1	A	350	ARG	4.6
1	B	358	VAL	4.5
1	A	353	GLY	4.5
1	A	315	SER	4.5
1	B	344	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	384	THR	4.2
1	B	177	LEU	4.2
1	A	182	GLY	4.2
1	A	341	GLY	4.2
1	B	354	ALA	4.1
1	B	244	ALA	4.1
1	A	358	VAL	4.1
1	B	339	PHE	4.0
1	B	345	THR	4.0
1	A	310	THR	3.9
1	B	181	PHE	3.8
1	B	315	SER	3.8
1	B	351	ALA	3.7
1	B	4	ASP	3.4
1	A	261	ARG	3.4
1	A	346	GLU	3.3
1	A	314	ALA	3.3
1	A	178	ARG	3.1
1	A	306	GLN	3.1
1	A	174	ILE	3.1
1	B	314	ALA	3.0
1	A	308	SER	3.0
1	A	19	THR	3.0
1	A	316	ASP	3.0
1	A	1	MET	3.0
1	B	106	VAL	2.8
1	B	343	ARG	2.8
1	A	73	TYR	2.8
1	A	309	GLY	2.8
1	A	106	VAL	2.8
1	B	342	GLY	2.7
1	B	21[A]	PHE	2.7
1	B	385	GLY	2.7
1	B	185	ASN	2.7
1	B	337	TYR	2.6
1	A	72	ILE	2.6
1	A	201	PRO	2.6
1	B	317	PRO	2.6
1	B	308	SER	2.6
1	B	156	LEU	2.6
1	A	107	ILE	2.6
1	A	313	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	342	GLY	2.5
1	B	341	GLY	2.5
1	B	245	VAL	2.5
1	A	150	PHE	2.5
1	B	357	SER	2.5
1	A	244	ALA	2.5
1	B	187	ALA	2.5
1	A	179	ALA	2.4
1	A	357	SER	2.4
1	B	73	TYR	2.4
1	B	179	ALA	2.4
1	B	316	ASP	2.4
1	A	337	TYR	2.4
1	A	175	SER	2.4
1	B	355	ASP	2.4
1	A	71	TYR	2.4
1	B	311	LYS	2.3
1	B	313	SER	2.3
1	A	74	THR	2.3
1	B	318	ASN	2.3
1	A	269	ILE	2.3
1	B	82	ALA	2.3
1	B	386	LYS	2.3
1	B	307	GLY	2.3
1	A	17	ILE	2.3
1	A	105	VAL	2.2
1	B	310	THR	2.2
1	A	246	LEU	2.2
1	B	201	PRO	2.2
1	B	150	PHE	2.2
1	A	109	ILE	2.1
1	B	107	ILE	2.1
1	B	174	ILE	2.1
1	B	220	GLY	2.1
1	A	177	LEU	2.1
1	A	336	ARG	2.1
1	A	18	ILE	2.1
1	B	200	LEU	2.1
1	B	388	LEU	2.1
1	B	383	LYS	2.1
1	B	207	PHE	2.1
1	A	3	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	93	PHE	2.0
1	B	155	TYR	2.0
1	A	200	LEU	2.0
1	A	426[A]	LYS	2.0
1	B	322	TYR	2.0
1	A	374[A]	GLU	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	A	502	6/6	0.79	0.23	77,77,77,78	0
3	SO4	A	503	5/5	0.81	0.15	65,65,66,67	5
3	SO4	B	501	5/5	0.82	0.18	90,90,90,90	0

6.5 Other polymers (i)

There are no such residues in this entry.