Full wwPDB X-ray Structure Validation Report (i)

Mar 1, 2026 – 09:30 PM UTC

PDB ID	:	4Q41 / pdb_00004q41
Title	:	Crystal structure of Schistosoma mansoni arginase in complex with L-lysine
Authors	:	Hai, Y.; Edwards, J.E.; Van Zandt, M.C.; Hoffmann, K.F.; Christianson, D.W.
Deposited on	:	2014-04-12
Resolution	:	2.20 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 (i)) were used in the production of this report:

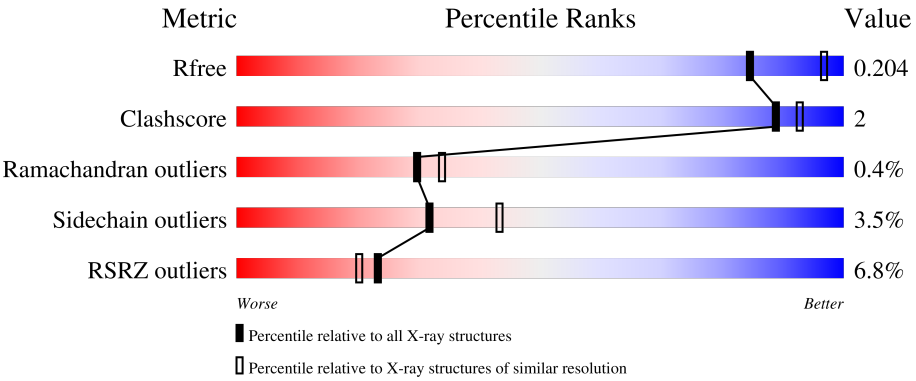
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

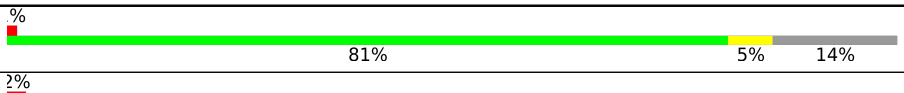
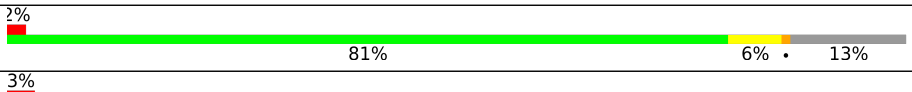
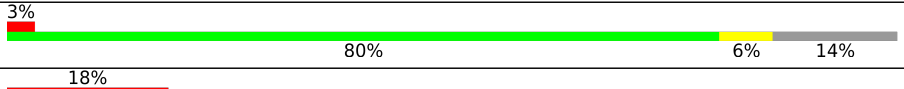
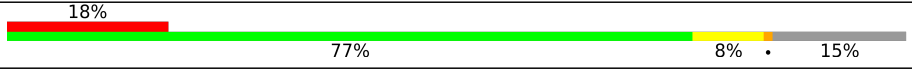
The reported resolution of this entry is 2.20 Å.

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 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	385	
1	B	385	
1	C	385	
1	D	385	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10684 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 Arginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2557	1612	447	483	15			
1	B	336	Total	C	N	O	S	0	1	0
			2586	1627	452	492	15			
1	C	333	Total	C	N	O	S	0	1	0
			2558	1612	446	484	16			
1	D	329	Total	C	N	O	S	0	0	0
			2522	1590	440	478	14			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q6WVP6
A	-19	GLY	-	expression tag	UNP Q6WVP6
A	-18	SER	-	expression tag	UNP Q6WVP6
A	-17	SER	-	expression tag	UNP Q6WVP6
A	-16	HIS	-	expression tag	UNP Q6WVP6
A	-15	HIS	-	expression tag	UNP Q6WVP6
A	-14	HIS	-	expression tag	UNP Q6WVP6
A	-13	HIS	-	expression tag	UNP Q6WVP6
A	-12	HIS	-	expression tag	UNP Q6WVP6
A	-11	HIS	-	expression tag	UNP Q6WVP6
A	-10	SER	-	expression tag	UNP Q6WVP6
A	-9	SER	-	expression tag	UNP Q6WVP6
A	-8	GLY	-	expression tag	UNP Q6WVP6
A	-7	LEU	-	expression tag	UNP Q6WVP6
A	-6	VAL	-	expression tag	UNP Q6WVP6
A	-5	PRO	-	expression tag	UNP Q6WVP6
A	-4	ARG	-	expression tag	UNP Q6WVP6
A	-3	GLY	-	expression tag	UNP Q6WVP6
A	-2	SER	-	expression tag	UNP Q6WVP6
A	-1	HIS	-	expression tag	UNP Q6WVP6
A	0	MET	-	expression tag	UNP Q6WVP6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP Q6WVP6
B	-19	GLY	-	expression tag	UNP Q6WVP6
B	-18	SER	-	expression tag	UNP Q6WVP6
B	-17	SER	-	expression tag	UNP Q6WVP6
B	-16	HIS	-	expression tag	UNP Q6WVP6
B	-15	HIS	-	expression tag	UNP Q6WVP6
B	-14	HIS	-	expression tag	UNP Q6WVP6
B	-13	HIS	-	expression tag	UNP Q6WVP6
B	-12	HIS	-	expression tag	UNP Q6WVP6
B	-11	HIS	-	expression tag	UNP Q6WVP6
B	-10	SER	-	expression tag	UNP Q6WVP6
B	-9	SER	-	expression tag	UNP Q6WVP6
B	-8	GLY	-	expression tag	UNP Q6WVP6
B	-7	LEU	-	expression tag	UNP Q6WVP6
B	-6	VAL	-	expression tag	UNP Q6WVP6
B	-5	PRO	-	expression tag	UNP Q6WVP6
B	-4	ARG	-	expression tag	UNP Q6WVP6
B	-3	GLY	-	expression tag	UNP Q6WVP6
B	-2	SER	-	expression tag	UNP Q6WVP6
B	-1	HIS	-	expression tag	UNP Q6WVP6
B	0	MET	-	expression tag	UNP Q6WVP6
C	-20	MET	-	expression tag	UNP Q6WVP6
C	-19	GLY	-	expression tag	UNP Q6WVP6
C	-18	SER	-	expression tag	UNP Q6WVP6
C	-17	SER	-	expression tag	UNP Q6WVP6
C	-16	HIS	-	expression tag	UNP Q6WVP6
C	-15	HIS	-	expression tag	UNP Q6WVP6
C	-14	HIS	-	expression tag	UNP Q6WVP6
C	-13	HIS	-	expression tag	UNP Q6WVP6
C	-12	HIS	-	expression tag	UNP Q6WVP6
C	-11	HIS	-	expression tag	UNP Q6WVP6
C	-10	SER	-	expression tag	UNP Q6WVP6
C	-9	SER	-	expression tag	UNP Q6WVP6
C	-8	GLY	-	expression tag	UNP Q6WVP6
C	-7	LEU	-	expression tag	UNP Q6WVP6
C	-6	VAL	-	expression tag	UNP Q6WVP6
C	-5	PRO	-	expression tag	UNP Q6WVP6
C	-4	ARG	-	expression tag	UNP Q6WVP6
C	-3	GLY	-	expression tag	UNP Q6WVP6
C	-2	SER	-	expression tag	UNP Q6WVP6
C	-1	HIS	-	expression tag	UNP Q6WVP6
C	0	MET	-	expression tag	UNP Q6WVP6

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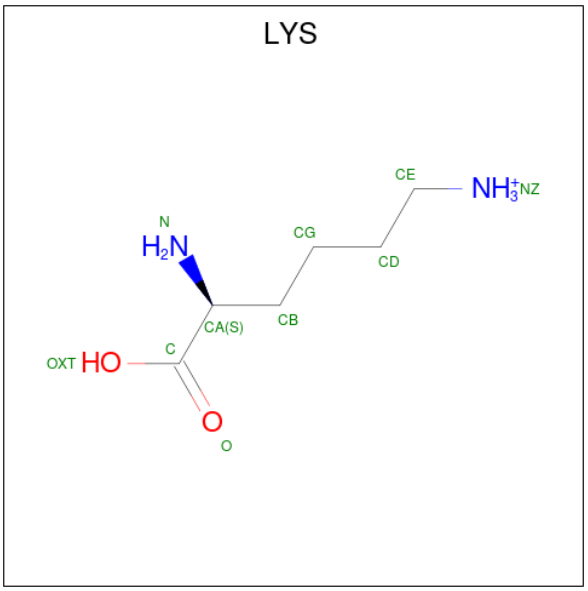
Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	expression tag	UNP Q6WVP6
D	-19	GLY	-	expression tag	UNP Q6WVP6
D	-18	SER	-	expression tag	UNP Q6WVP6
D	-17	SER	-	expression tag	UNP Q6WVP6
D	-16	HIS	-	expression tag	UNP Q6WVP6
D	-15	HIS	-	expression tag	UNP Q6WVP6
D	-14	HIS	-	expression tag	UNP Q6WVP6
D	-13	HIS	-	expression tag	UNP Q6WVP6
D	-12	HIS	-	expression tag	UNP Q6WVP6
D	-11	HIS	-	expression tag	UNP Q6WVP6
D	-10	SER	-	expression tag	UNP Q6WVP6
D	-9	SER	-	expression tag	UNP Q6WVP6
D	-8	GLY	-	expression tag	UNP Q6WVP6
D	-7	LEU	-	expression tag	UNP Q6WVP6
D	-6	VAL	-	expression tag	UNP Q6WVP6
D	-5	PRO	-	expression tag	UNP Q6WVP6
D	-4	ARG	-	expression tag	UNP Q6WVP6
D	-3	GLY	-	expression tag	UNP Q6WVP6
D	-2	SER	-	expression tag	UNP Q6WVP6
D	-1	HIS	-	expression tag	UNP Q6WVP6
D	0	MET	-	expression tag	UNP Q6WVP6

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

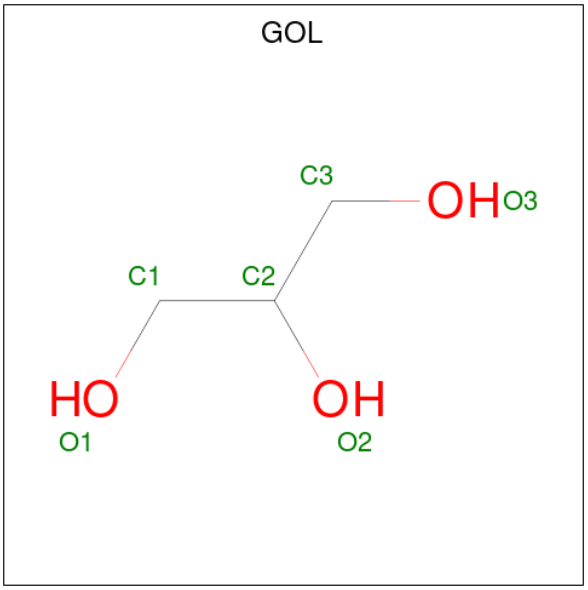
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0
2	B	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0

- Molecule 3 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 10 6 2 2	0	0
3	B	1	Total C N O 10 6 2 2	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 5 is water.

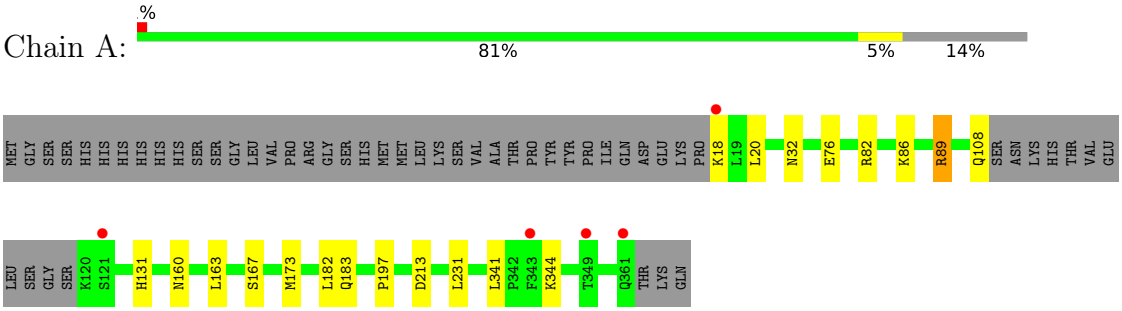
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	155	Total O 155 155	0	0
5	B	138	Total O 138 138	0	0
5	C	82	Total O 82 82	0	0
5	D	22	Total O 22 22	0	0

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.

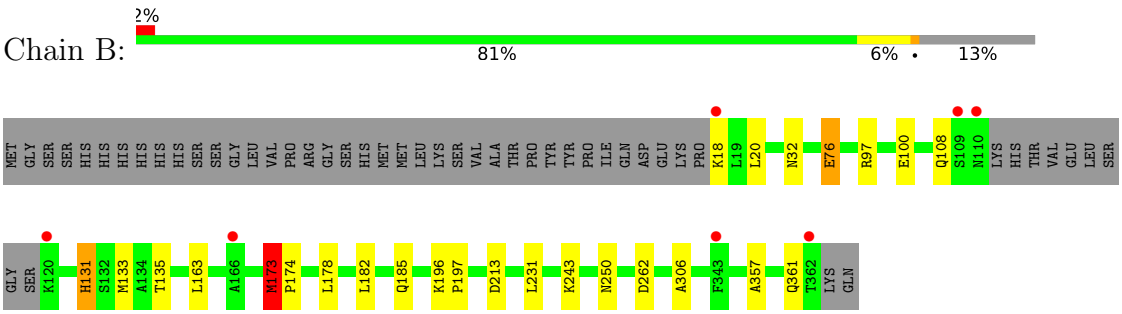
• Molecule 1: Arginase

Chain A:



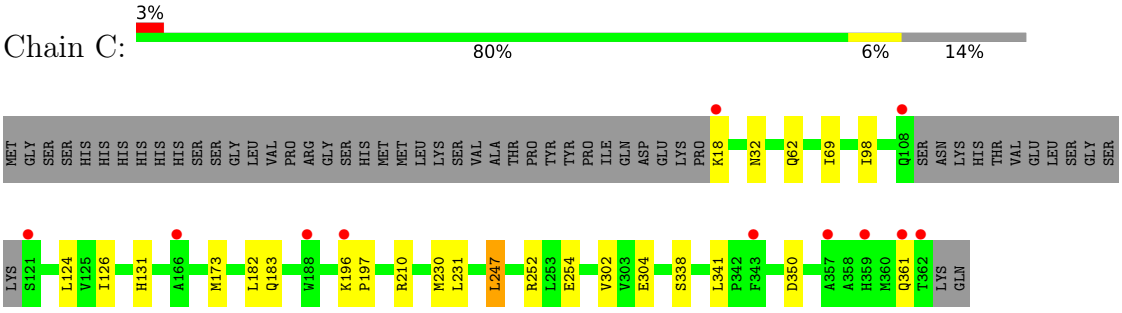
• Molecule 1: Arginase

Chain B:



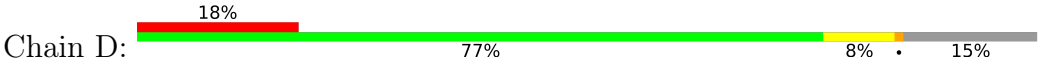
• Molecule 1: Arginase

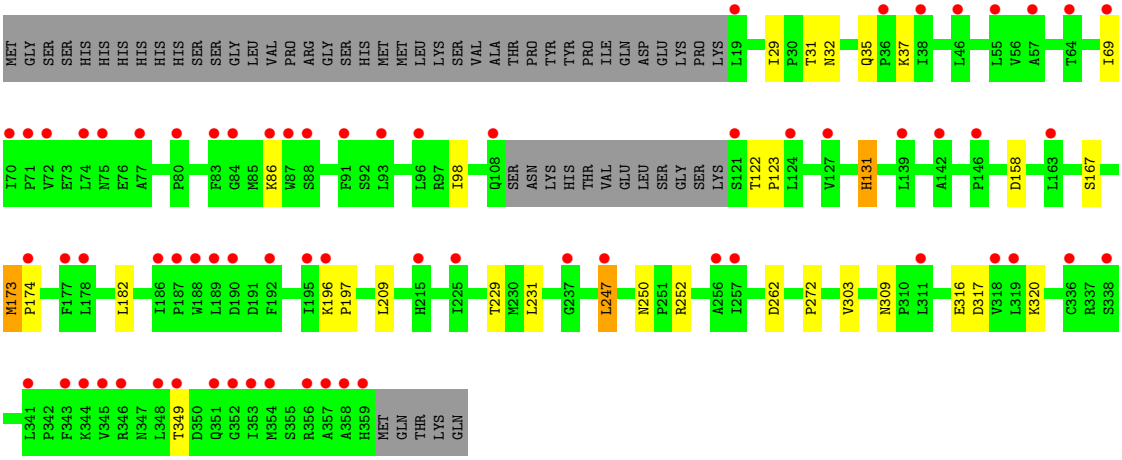
Chain C:



• Molecule 1: Arginase

Chain D:




MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET MET LEU LYS SER VAL ALA THR PRO TYR TYR PRO ILE GLN ASP GLU LYS PRO LYS L19 I29 P30 T31 N32 Q35 P36 K37 I38 L46 L55 V56 A57 T64 I69
I70 P71 V72 E73 L74 N75 E76 A77 P80 F83 G84 M85 K86 W87 S88 F91 S92 L93 L96 R97 I98 Q108 SER ASN LYS HIS THR VAL GLU LEU SER GLY SER LYS S121 T122 P123 L124 V127 H131 L139 A142 P146 D158 L163 S167
M173 P174 F177 L178 L182 I186 P187 W188 L189 D190 D191 F192 I195 K196 P197 L209 H215 I225 T229 M230 L231 G237 L247 N250 P251 R252 A256 I257 D262 P272 V303 M309 P310 L311 E316 D317 V318 L319 K320 C336 R337 S338
L341 P342 F343 K344 V345 R346 N347 L348 T349 D350 Q351 G352 I353 M354 S355 R356 A357 A358 H359 MET GLN THR LYS GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	177.45Å 177.45Å 177.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.22 – 2.20 49.22 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.22-2.20) 100.0 (49.22-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	3.21 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.172 , 0.201 0.177 , 0.204	Depositor DCC
R_{free} test set	4730 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10684	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: MN, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.60	0/2604	0.81	0/3528
1	B	0.57	0/2633	0.83	4/3568 (0.1%)
1	C	0.47	0/2608	0.79	0/3535
1	D	0.42	0/2569	0.78	6/3484 (0.2%)
All	All	0.52	0/10414	0.80	10/14115 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	250	ASN	CA-C-N	5.77	125.90	119.32
1	B	250	ASN	C-N-CA	5.77	125.90	119.32
1	B	173	MET	CA-C-N	-5.52	113.21	119.28
1	B	173	MET	C-N-CA	-5.52	113.21	119.28
1	D	35	GLN	CA-C-N	5.43	125.08	119.05
1	D	35	GLN	C-N-CA	5.43	125.08	119.05
1	D	250	ASN	CA-C-N	5.43	125.51	119.32
1	D	250	ASN	C-N-CA	5.43	125.51	119.32
1	D	309	ASN	CA-C-N	5.11	125.18	119.87
1	D	309	ASN	C-N-CA	5.11	125.18	119.87

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	2557	0	2574	8	0
1	B	2586	0	2595	9	0
1	C	2558	0	2573	9	0
1	D	2522	0	2531	13	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	10	0	12	2	0
3	B	10	0	12	1	0
4	A	12	0	16	0	0
4	B	12	0	16	0	0
4	C	12	0	16	0	0
5	A	155	0	0	2	0
5	B	138	0	0	0	0
5	C	82	0	0	0	0
5	D	22	0	0	0	0
All	All	10684	0	10345	39	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 2.

All (39) 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:D:131:HIS:CE1	1:D:262:ASP:HB2	2.37	0.59
1:B:213[A]:ASP:OD2	3:B:403:LYS:N	2.35	0.59
1:D:158:ASP:HB3	1:D:174:PRO:HD2	1.90	0.53
1:C:69:ILE:HD13	1:C:98:ILE:HA	1.91	0.53
1:B:76:GLU:H	1:B:76:GLU:CD	2.20	0.50
1:C:210:ARG:HD3	1:C:230:MET:HG3	1.92	0.50
1:A:160:ASN:ND2	3:A:403:LYS:OXT	2.45	0.49
1:D:173:MET:N	1:D:174:PRO:HD3	2.27	0.49
1:D:69:ILE:HD13	1:D:98:ILE:HA	1.95	0.49
1:D:316:GLU:HG2	1:D:320:LYS:HE3	1.95	0.48
1:D:29:ILE:HG22	1:D:31:THR:HG23	1.95	0.47
1:C:252:ARG:NH1	1:C:254:GLU:OE1	2.48	0.47
1:B:357:ALA:O	1:B:361:GLN:HG2	2.15	0.46
1:A:183:GLN:HG3	1:A:197:PRO:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:403:LYS:NZ	5:A:655:HOH:O	2.46	0.45
1:A:86:LYS:NZ	1:A:167:SER:O	2.49	0.45
1:D:86:LYS:HE2	1:D:167:SER:O	2.16	0.45
1:D:209:LEU:HB2	1:D:229:THR:HG22	1.99	0.45
1:A:82:ARG:NH2	1:A:89:ARG:HG3	2.32	0.44
1:A:213:ASP:HB3	5:A:625:HOH:O	2.18	0.44
1:A:18:LYS:HB2	1:A:18:LYS:HE3	1.84	0.44
1:B:133:MET:HE2	1:B:306:ALA:HB2	2.01	0.43
1:D:196:LYS:HA	1:D:197:PRO:HD3	1.92	0.42
1:B:131:HIS:CE1	1:B:262:ASP:HB2	2.54	0.42
1:C:196:LYS:HA	1:C:197:PRO:HD3	1.79	0.42
1:D:122:THR:HA	1:D:123:PRO:HD3	1.91	0.42
1:A:20:LEU:HD12	1:A:20:LEU:HA	1.87	0.41
1:C:247:LEU:HD12	1:C:247:LEU:HA	1.89	0.41
1:A:163:LEU:HA	1:A:163:LEU:HD13	1.86	0.41
1:B:196:LYS:HA	1:B:197:PRO:HD3	1.92	0.41
1:B:97:ARG:NE	1:C:350:ASP:O	2.53	0.41
1:D:158:ASP:O	1:D:174:PRO:HD2	2.21	0.41
1:D:247:LEU:HD12	1:D:247:LEU:HA	1.84	0.41
1:C:126:ILE:O	1:C:304:GLU:HA	2.21	0.40
1:B:173:MET:N	1:B:174:PRO:CD	2.85	0.40
1:C:124:LEU:HB3	1:C:302:VAL:HG22	2.02	0.40
1:B:135:THR:HA	1:B:178:LEU:HD11	2.03	0.40
1:D:272:PRO:HB2	1:D:317:ASP:HB3	2.04	0.40
1:C:183:GLN:HG3	1:C:197:PRO:HG2	2.04	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	329/385 (86%)	322 (98%)	6 (2%)	1 (0%)	36 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	333/385 (86%)	327 (98%)	5 (2%)	1 (0%)	36 42
1	C	330/385 (86%)	323 (98%)	5 (2%)	2 (1%)	21 23
1	D	325/385 (84%)	315 (97%)	9 (3%)	1 (0%)	36 42
All	All	1317/1540 (86%)	1287 (98%)	25 (2%)	5 (0%)	30 34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	361	GLN
1	A	173	MET
1	B	173	MET
1	C	173	MET
1	D	173	MET

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	280/327 (86%)	271 (97%)	9 (3%)	34 47
1	B	284/327 (87%)	272 (96%)	12 (4%)	26 36
1	C	281/327 (86%)	272 (97%)	9 (3%)	34 47
1	D	276/327 (84%)	267 (97%)	9 (3%)	33 45
All	All	1121/1308 (86%)	1082 (96%)	39 (4%)	32 43

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

Mol	Chain	Res	Type
1	A	32	ASN
1	A	76	GLU
1	A	89	ARG
1	A	108	GLN
1	A	131	HIS
1	A	182	LEU

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Mol	Chain	Res	Type
1	A	231	LEU
1	A	341	LEU
1	A	344	LYS
1	B	18	LYS
1	B	20	LEU
1	B	32	ASN
1	B	76	GLU
1	B	100	GLU
1	B	108	GLN
1	B	131	HIS
1	B	163	LEU
1	B	182	LEU
1	B	185	GLN
1	B	231	LEU
1	B	243	LYS
1	C	18	LYS
1	C	32	ASN
1	C	62	GLN
1	C	131	HIS
1	C	182	LEU
1	C	231	LEU
1	C	247	LEU
1	C	338	SER
1	C	341	LEU
1	D	32	ASN
1	D	37	LYS
1	D	131	HIS
1	D	182	LEU
1	D	231	LEU
1	D	247	LEU
1	D	252	ARG
1	D	303	VAL
1	D	349	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	GLN
1	B	25	ASN
1	C	160	ASN
1	C	200	ASN
1	D	335	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	A	405	-	5,5,5	0.23	0	5,5,5	1.12	1 (20%)
4	GOL	A	404	-	5,5,5	0.47	0	5,5,5	0.50	0
4	GOL	B	405	-	5,5,5	0.32	0	5,5,5	0.60	0
4	GOL	C	403	-	5,5,5	0.39	0	5,5,5	0.38	0
4	GOL	B	404	-	5,5,5	0.37	0	5,5,5	0.73	0
3	LYS	B	403	-	8,9,9	0.81	1 (12%)	7,10,10	1.19	1 (14%)
3	LYS	A	403	-	8,9,9	0.80	0	7,10,10	1.17	1 (14%)
4	GOL	C	404	-	5,5,5	0.36	0	5,5,5	0.26	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
4	GOL	A	405	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	404	-	-	2/4/4/4	-
4	GOL	B	405	-	-	0/4/4/4	-
4	GOL	C	403	-	-	1/4/4/4	-
4	GOL	B	404	-	-	2/4/4/4	-
3	LYS	B	403	-	-	0/9/9/9	-
3	LYS	A	403	-	-	2/9/9/9	-
4	GOL	C	404	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	LYS	OXT-C	-2.16	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	403	LYS	OXT-C-O	-3.07	117.13	124.08
3	A	403	LYS	OXT-C-O	-2.79	117.75	124.08
4	A	405	GOL	C3-C2-C1	-2.09	104.14	111.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	GOL	O1-C1-C2-C3
4	A	405	GOL	O1-C1-C2-O2
4	A	405	GOL	O1-C1-C2-C3
4	B	404	GOL	O1-C1-C2-C3
4	A	404	GOL	O1-C1-C2-O2
4	B	404	GOL	O1-C1-C2-O2
4	C	403	GOL	O1-C1-C2-O2
4	A	405	GOL	C1-C2-C3-O3
4	A	405	GOL	O2-C2-C3-O3
3	A	403	LYS	OXT-C-CA-CB
3	A	403	LYS	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	LYS	1	0
3	A	403	LYS	2	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	333/385 (86%)	-0.34	5 (1%) 72 69	20, 31, 59, 88	0
1	B	336/385 (87%)	-0.21	7 (2%) 63 60	19, 34, 57, 84	1 (0%)
1	C	333/385 (86%)	0.24	11 (3%) 49 46	37, 48, 70, 84	2 (0%)
1	D	329/385 (85%)	1.33	68 (20%) 2 2	46, 70, 90, 102	13 (3%)
All	All	1331/1540 (86%)	0.25	91 (6%) 23 20	19, 44, 82, 102	16 (1%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	343	PHE	6.3
1	C	362	THR	6.1
1	D	163	LEU	5.2
1	D	353	ILE	4.7
1	A	343	PHE	4.7
1	D	345	VAL	4.6
1	D	358	ALA	4.5
1	B	18	LYS	4.1
1	D	354	MET	4.0
1	D	188	TRP	4.0
1	D	357	ALA	3.9
1	D	349	THR	3.9
1	B	343	PHE	3.9
1	D	19	LEU	3.8
1	C	18	LYS	3.8
1	A	18	LYS	3.7
1	D	359	HIS	3.7
1	D	352	GLY	3.6
1	D	38	ILE	3.5
1	D	70	ILE	3.4
1	D	348	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	110	ASN	3.3
1	D	77	ALA	3.3
1	D	108	GLN	3.3
1	D	83	PHE	3.3
1	D	351	GLN	3.3
1	D	344	LYS	3.2
1	A	121	SER	3.2
1	D	74	LEU	3.1
1	C	343	PHE	3.0
1	C	361	GLN	2.9
1	D	356	ARG	2.9
1	D	195	ILE	2.9
1	A	349	THR	2.8
1	D	96	LEU	2.8
1	D	192	PHE	2.8
1	D	346	ARG	2.7
1	D	196	LYS	2.7
1	D	247	LEU	2.7
1	D	87	TRP	2.6
1	D	64	THR	2.6
1	D	318	VAL	2.6
1	D	341	LEU	2.6
1	A	361	GLN	2.6
1	D	311	LEU	2.6
1	D	215	HIS	2.5
1	D	146	PRO	2.5
1	D	319	LEU	2.5
1	D	139	LEU	2.5
1	B	109	SER	2.5
1	D	93	LEU	2.5
1	B	120	LYS	2.5
1	C	359	HIS	2.5
1	D	69	ILE	2.5
1	B	166	ALA	2.4
1	C	196	LYS	2.4
1	D	187	PRO	2.4
1	D	88	SER	2.4
1	C	357	ALA	2.3
1	D	189	LEU	2.3
1	D	121	SER	2.3
1	D	127	VAL	2.3
1	D	190	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	142	ALA	2.3
1	D	46	LEU	2.3
1	B	362	THR	2.3
1	D	174	PRO	2.3
1	D	36	PRO	2.2
1	D	71	PRO	2.2
1	D	256	ALA	2.2
1	D	336	CYS	2.2
1	D	55	LEU	2.2
1	C	108	GLN	2.2
1	C	188	TRP	2.2
1	D	72	VAL	2.2
1	D	86	LYS	2.2
1	D	186	ILE	2.1
1	D	237	GLY	2.1
1	D	178	LEU	2.1
1	D	84	GLY	2.1
1	D	91	PHE	2.1
1	D	177	PHE	2.1
1	C	166	ALA	2.1
1	D	57	ALA	2.1
1	D	338	SER	2.1
1	D	75	ASN	2.1
1	C	121	SER	2.1
1	D	80	PRO	2.0
1	D	225	ILE	2.0
1	D	257	ILE	2.0
1	D	124	LEU	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 oligosaccharides 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
3	LYS	A	403	10/10	0.84	0.16	36,44,49,54	0
4	GOL	C	403	6/6	0.86	0.13	58,60,64,70	0
3	LYS	B	403	10/10	0.87	0.14	41,49,58,58	0
4	GOL	A	405	6/6	0.88	0.16	36,50,57,61	0
4	GOL	C	404	6/6	0.88	0.15	57,65,69,69	0
4	GOL	B	404	6/6	0.89	0.12	45,51,58,63	0
4	GOL	A	404	6/6	0.90	0.11	42,45,53,55	0
4	GOL	B	405	6/6	0.92	0.12	41,51,58,65	0
2	MN	D	400	1/1	0.97	0.05	48,48,48,48	1
2	MN	D	401	1/1	0.98	0.03	53,53,53,53	0
2	MN	C	401	1/1	1.00	0.02	41,41,41,41	0
2	MN	C	402	1/1	1.00	0.03	40,40,40,40	0
2	MN	A	401	1/1	1.00	0.01	26,26,26,26	0
2	MN	A	402	1/1	1.00	0.05	25,25,25,25	0
2	MN	B	401	1/1	1.00	0.03	28,28,28,28	0
2	MN	B	402	1/1	1.00	0.02	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.