



Full wwPDB X-ray Structure Validation Report

Jul 29, 2014 – 02:18 PM EDT

PDB ID : 4Q3P
Title : Crystal structure of Schistosoma mansoni arginase
Authors : Hai, Y.; Edwards, J.E.; Van Zandt, M.C.; Hoffmann, K.F.; Christianson, D.W.
Deposited on : 2014-04-12
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

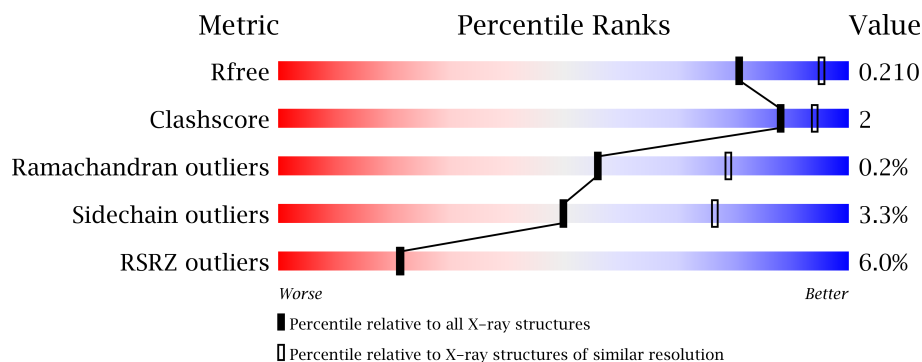
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	385	
1	B	385	
1	C	385	
1	D	385	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	A	403	-	X
3	GOL	A	404	-	X
3	GOL	B	403	-	X
3	GOL	C	404	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10810 atoms, of which 0 are hydrogen and 0 are deuterium.

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	336	Total	C	N	O	S	0	1	0
			2581	1625	451	489	16			
1	B	335	Total	C	N	O	S	0	1	0
			2573	1621	449	487	16			
1	C	335	Total	C	N	O	S	0	1	0
			2571	1620	448	487	16			
1	D	332	Total	C	N	O	S	0	0	0
			2546	1605	444	482	15			

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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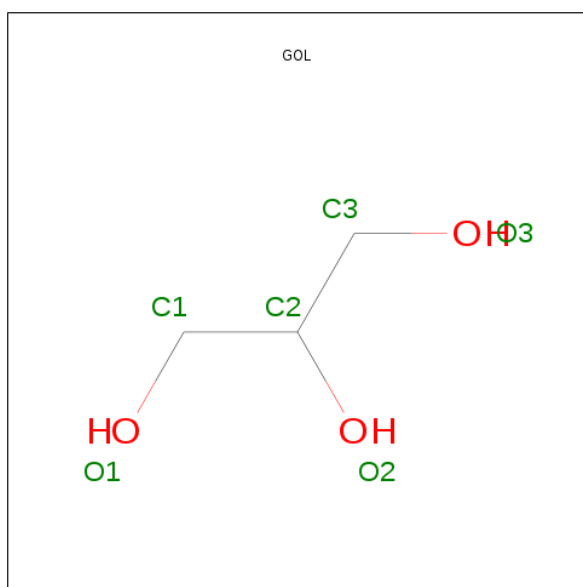
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	EXPRESSION TAG	UNP Q6WVP6
D	-19	GLY	-	EXPRESSION TAG	UNP Q6WVP6
D	-18	SER	-	EXPRESSION TAG	UNP Q6WVP6
D	-17	SER	-	EXPRESSION TAG	UNP Q6WVP6
D	-16	HIS	-	EXPRESSION TAG	UNP Q6WVP6
D	-15	HIS	-	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 (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is water.

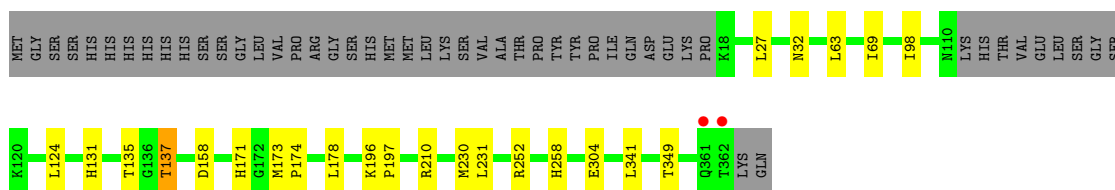
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	195	Total	O	0	0
			195	195		
4	B	172	Total	O	0	0
			172	172		
4	C	118	Total	O	0	0
			118	118		
4	D	10	Total	O	0	0
			10	10		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

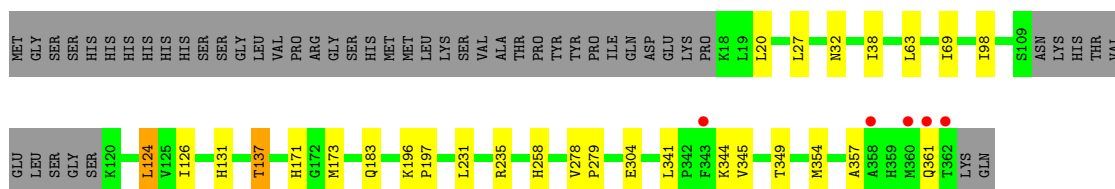
- Molecule 1: Arginase

Chain A: 



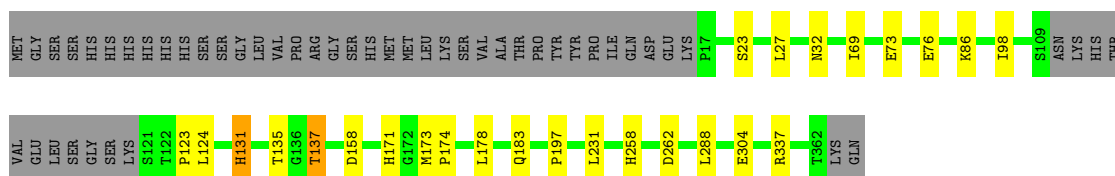
- Molecule 1: Arginase

Chain B: 



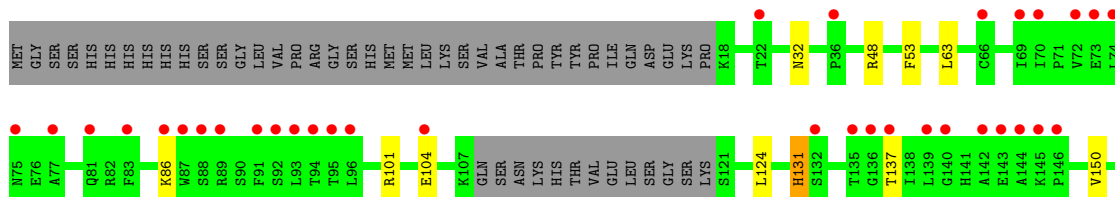
- Molecule 1: Arginase

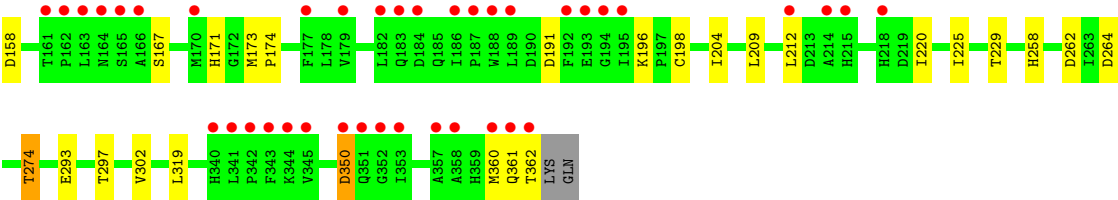
Chain C: 



- Molecule 1: Arginase

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	178.38Å 178.38Å 178.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.48 – 2.50 49.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.48-2.50) 99.7 (49.47-2.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.177 , 0.213 0.172 , 0.210	Depositor DCC
R_{free} test set	3295 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 21.9	EDS
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 65285 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10810	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.23	0/2631	0.43	0/3565
1	B	0.23	0/2623	0.43	0/3554
1	C	0.22	0/2622	0.43	0/3554
1	D	0.21	0/2593	0.40	0/3515
All	All	0.22	0/10469	0.42	0/14188

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2581	0	2597	8	0
1	B	2573	0	2591	12	0
1	C	2571	0	2586	11	0
1	D	2546	0	2560	19	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	16	0	0
3	B	12	0	16	0	0
3	C	12	0	16	2	0
4	A	195	0	0	1	0
4	B	172	0	0	1	0
4	C	118	0	0	0	0
4	D	10	0	0	0	0
All	All	10810	0	10382	50	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (50) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:344:LYS:NZ	1:B:345:VAL:O	2.32	0.62
1:D:264:ASP:HB3	1:D:274:THR:HG21	1.83	0.61
1:D:158:ASP:HB3	1:D:174:PRO:HD2	1.83	0.60
1:B:137:THR:HG23	1:B:258:HIS:HE1	1.70	0.57
1:D:137:THR:HG22	1:D:258:HIS:HE1	1.71	0.56
1:C:86:LYS:HG2	3:C:403:GOL:H31	1.91	0.53
1:A:137:THR:HG23	1:A:258:HIS:HE1	1.75	0.52
1:D:209:LEU:HB2	1:D:229:THR:HG22	1.92	0.52
1:B:137:THR:HG21	1:B:304:GLU:OE2	2.09	0.52
1:C:69:ILE:HD13	1:C:98:ILE:HA	1.91	0.51
1:A:69:ILE:HD13	1:A:98:ILE:HA	1.93	0.51
1:D:101:ARG:NH1	1:D:104:GLU:OE2	2.42	0.50
1:D:361:GLN:HG3	1:D:362:THR:H	1.77	0.50
1:C:137:THR:HG21	1:C:304:GLU:OE2	2.12	0.49
1:A:137:THR:HG21	1:A:304:GLU:OE2	2.13	0.49
1:D:220:ILE:HG23	1:D:225:ILE:HG23	1.95	0.48
1:B:235:ARG:NH1	4:B:664:HOH:O	2.46	0.48
1:D:124:LEU:HB3	1:D:302:VAL:HG22	1.96	0.48
1:D:173:MET:N	1:D:174:PRO:HD3	2.28	0.48
1:B:137:THR:HG23	1:B:258:HIS:CE1	2.49	0.47
1:C:183:GLN:HG3	1:C:197:PRO:HG3	1.96	0.47
1:D:131:HIS:CE1	1:D:262:ASP:HB2	2.49	0.47
1:B:69:ILE:HD13	1:B:98:ILE:HA	1.96	0.47
1:C:137:THR:HG23	1:C:258:HIS:HE1	1.81	0.45
1:D:293:GLU:O	1:D:297:THR:HG23	2.17	0.45
1:C:135:THR:HA	1:C:178:LEU:HD11	1.98	0.45
1:A:135:THR:HA	1:A:178:LEU:HD11	1.99	0.44
1:B:124:LEU:HD13	1:B:126:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:131:HIS:CE1	1:C:262:ASP:HB2	2.53	0.44
1:A:252:ARG:NH2	4:A:651:HOH:O	2.51	0.44
1:B:196:LYS:HA	1:B:197:PRO:HD3	1.90	0.44
1:A:158:ASP:HB3	1:A:174:PRO:HD2	1.99	0.43
1:B:20:LEU:HA	1:B:20:LEU:HD23	1.84	0.43
1:C:288:LEU:HD13	1:C:337:ARG:HD3	2.00	0.43
1:C:23:SER:O	1:C:123:PRO:HD2	2.19	0.43
1:D:191:ASP:N	1:D:191:ASP:OD2	2.51	0.42
1:A:196:LYS:HA	1:A:197:PRO:HD3	1.91	0.42
1:D:150:VAL:HB	1:D:204:ILE:HG23	2.00	0.42
1:D:319:LEU:HD23	1:D:319:LEU:HA	1.91	0.42
1:D:48:ARG:HA	1:D:53:PHE:HE2	1.85	0.41
1:D:209:LEU:HD13	1:D:212:LEU:HD21	2.02	0.41
1:A:210:ARG:HD3	1:A:230:MET:HG3	2.02	0.41
1:B:278:VAL:HA	1:B:279:PRO:HD3	1.93	0.41
1:B:183:GLN:HG3	1:B:197:PRO:HG2	2.02	0.41
1:D:350:ASP:N	1:D:350:ASP:OD2	2.52	0.41
1:B:357:ALA:O	1:B:361:GLN:HG2	2.21	0.41
1:C:73:GLU:OE1	3:C:404:GOL:O2	2.36	0.41
1:D:86:LYS:HE2	1:D:167:SER:O	2.21	0.41
1:D:196:LYS:HE2	1:D:198:CYS:HB3	2.03	0.40
1:C:158:ASP:HB3	1:C:174:PRO:HD2	2.03	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	333/385 (86%)	324 (97%)	8 (2%)	1 (0%)	50	73
1	B	332/385 (86%)	324 (98%)	7 (2%)	1 (0%)	50	73
1	C	332/385 (86%)	324 (98%)	7 (2%)	1 (0%)	50	73
1	D	328/385 (85%)	317 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1325/1540 (86%)	1289 (97%)	33 (2%)	3 (0%)	56 79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	MET
1	B	173	MET
1	C	173	MET

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	284/327 (87%)	274 (96%)	10 (4%)	48 74
1	B	283/327 (86%)	271 (96%)	12 (4%)	40 66
1	C	283/327 (86%)	275 (97%)	8 (3%)	56 82
1	D	279/327 (85%)	272 (98%)	7 (2%)	60 85
All	All	1129/1308 (86%)	1092 (97%)	37 (3%)	50 76

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	32	ASN
1	A	63	LEU
1	A	124	LEU
1	A	131	HIS
1	A	137	THR
1	A	171	HIS
1	A	231	LEU
1	A	341	LEU
1	A	349	THR
1	B	27	LEU
1	B	32	ASN
1	B	38	ILE

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Mol	Chain	Res	Type
1	B	63	LEU
1	B	124	LEU
1	B	131	HIS
1	B	137	THR
1	B	171	HIS
1	B	231	LEU
1	B	341	LEU
1	B	349	THR
1	B	354	MET
1	C	27	LEU
1	C	32	ASN
1	C	76	GLU
1	C	124	LEU
1	C	131	HIS
1	C	137	THR
1	C	171	HIS
1	C	231	LEU
1	D	32	ASN
1	D	63	LEU
1	D	131	HIS
1	D	171	HIS
1	D	274	THR
1	D	350	ASP
1	D	360	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	359	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	$\# Z > 2$
3	GOL	A	403	-	5,5,5	0.38	0	5,5,5	0.25	0
3	GOL	A	404	-	5,5,5	0.35	0	5,5,5	0.21	0
3	GOL	B	403	-	5,5,5	0.36	0	5,5,5	0.29	0
3	GOL	B	404	-	5,5,5	0.32	0	5,5,5	0.34	0
3	GOL	C	403	-	5,5,5	0.34	0	5,5,5	0.26	0
3	GOL	C	404	-	5,5,5	0.36	0	5,5,5	0.25	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
3	GOL	A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	A	404	-	-	0/4/4/4	0/0/0/0
3	GOL	B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	C	403	-	-	0/4/4/4	0/0/0/0
3	GOL	C	404	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	336/385 (87%)	-0.51	2 (0%) 86 88	12, 20, 47, 75	0
1	B	335/385 (87%)	-0.33	5 (1%) 70 72	13, 21, 50, 73	5 (1%)
1	C	335/385 (87%)	-0.37	0 100 100	19, 28, 48, 66	4 (1%)
1	D	332/385 (86%)	1.06	73 (21%) 1 1	50, 65, 81, 98	109 (32%)
All	All	1338/1540 (86%)	-0.04	80 (5%) 21 21	12, 28, 73, 98	118 (8%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	96	LEU	6.1
1	D	144	ALA	6.0
1	D	360	MET	5.1
1	D	357	ALA	5.0
1	B	361	GLN	4.9
1	B	362	THR	4.3
1	D	192	PHE	4.2
1	D	350	ASP	4.2
1	D	177	PHE	4.1
1	D	351	GLN	4.0
1	D	195	ILE	4.0
1	D	361	GLN	4.0
1	D	93	LEU	4.0
1	D	92	SER	3.9
1	D	72	VAL	3.9
1	D	139	LEU	3.7
1	D	166	ALA	3.6
1	D	344	LYS	3.6
1	D	146	PRO	3.6
1	D	343	PHE	3.6
1	D	183	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	162	PRO	3.6
1	D	189	LEU	3.5
1	D	194	GLY	3.4
1	D	88	SER	3.4
1	D	161	THR	3.3
1	D	70	ILE	3.3
1	D	81	GLN	3.3
1	D	164	ASN	3.2
1	D	95	THR	3.2
1	D	193	GLU	3.1
1	D	182	LEU	3.1
1	D	132	SER	3.1
1	D	22	THR	3.1
1	D	358	ALA	3.1
1	D	188	TRP	3.0
1	D	91	PHE	3.0
1	D	104	GLU	3.0
1	D	362	THR	3.0
1	D	186	ILE	3.0
1	D	165	SER	2.9
1	D	136	GLY	2.9
1	D	184	ASP	2.9
1	D	352	GLY	2.8
1	D	187	PRO	2.8
1	D	140	GLY	2.7
1	D	163	LEU	2.7
1	D	143	GLU	2.7
1	D	342	PRO	2.7
1	D	137	THR	2.6
1	D	345	VAL	2.6
1	D	94	THR	2.6
1	A	361	GLN	2.6
1	D	83	PHE	2.6
1	D	69	ILE	2.5
1	D	142	ALA	2.5
1	D	87	TRP	2.4
1	D	353	ILE	2.4
1	D	135	THR	2.4
1	D	74	LEU	2.4
1	D	212	LEU	2.3
1	B	360	MET	2.3
1	D	77	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	179	VAL	2.2
1	D	218	HIS	2.2
1	D	214	ALA	2.2
1	D	170	MET	2.2
1	B	343	PHE	2.2
1	D	66	CYS	2.2
1	D	145	LYS	2.2
1	D	73	GLU	2.2
1	D	86	LYS	2.1
1	B	358	ALA	2.1
1	D	215	HIS	2.1
1	D	36	PRO	2.0
1	D	340	HIS	2.0
1	A	362	THR	2.0
1	D	75	ASN	2.0
1	D	89	ARG	2.0
1	D	341	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	B	403	6/6	0.19	6.34	29,35,41,48	0
3	GOL	A	403	6/6	0.17	2.44	29,33,35,39	1
3	GOL	C	404	6/6	0.21	2.29	35,38,48,48	0
3	GOL	A	404	6/6	0.13	2.08	28,31,36,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	C	403	6/6	0.17	1.81	32,41,46,49	1
2	MN	B	401	1/1	0.15	1.77	17,17,17,17	0
2	MN	A	401	1/1	0.11	0.76	17,17,17,17	0
3	GOL	B	404	6/6	0.13	0.41	25,29,40,51	0
2	MN	C	401	1/1	0.10	-0.20	23,23,23,23	0
2	MN	C	402	1/1	0.11	-0.29	25,25,25,25	0
2	MN	B	402	1/1	0.12	-1.53	16,16,16,16	0
2	MN	A	402	1/1	0.10	-1.75	15,15,15,15	0
2	MN	D	401	1/1	0.05	-3.87	59,59,59,59	0
2	MN	D	400	1/1	0.04	-5.75	57,57,57,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.