



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 05:52 am BST

PDB ID : 4Q3U
Title : Crystal structure of Schistosoma mansoni arginase in complex with inhibitor nor-NOHA
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 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 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 : 2.11
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) : 2.11

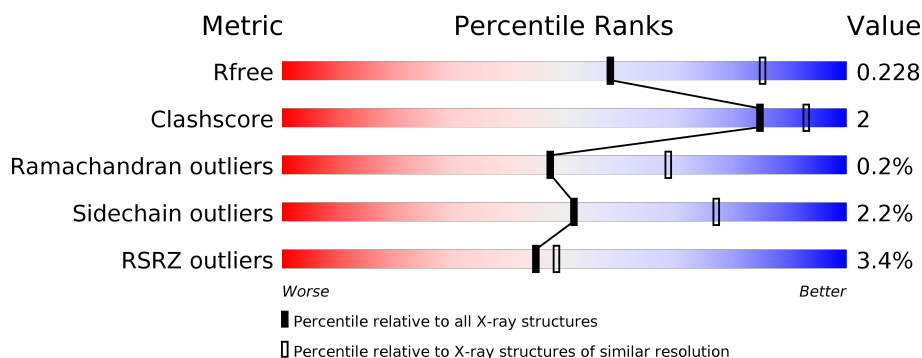
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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 $\leq 5\%$. 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>83%</div> <div>13%</div> </div>
1	B	385	<div>2%</div> <div>82%</div> <div>13%</div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10664 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	336	Total	C	N	O	S	0	1	0
			2586	1629	454	488	15			
1	B	335	Total	C	N	O	S	0	1	0
			2576	1623	451	487	15			
1	C	334	Total	C	N	O	S	0	2	0
			2573	1622	450	485	16			
1	D	318	Total	C	N	O	S	0	1	0
			2447	1547	425	462	13			

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 (three-letter code: MN) (formula: Mn).

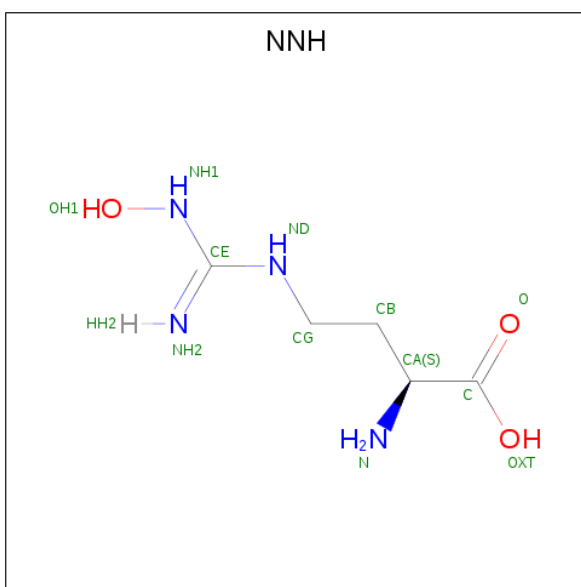
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mn 2 2	0	0
2	A	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0

- 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 NOR-N-OMEGA-HYDROXY-L-ARGININE (three-letter code: NNH) (formula: $C_5H_{12}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	5	4	3		
4	B	1	Total	C	N	O	0	0
			12	5	4	3		
4	C	1	Total	C	N	O	0	0
			12	5	4	3		
4	D	1	Total	C	N	O	0	0
			12	5	4	3		


- Molecule 5 is water.

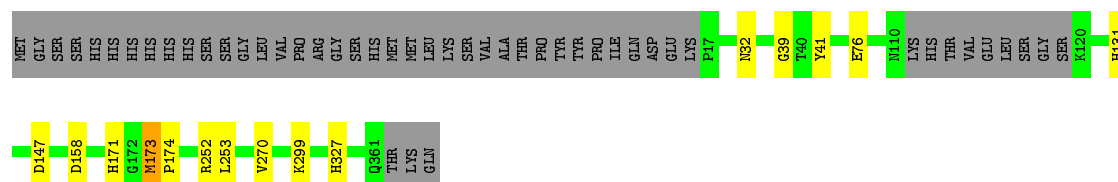
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	152	Total	O	0	0
			152	152		
5	B	151	Total	O	0	0
			151	151		
5	C	77	Total	O	0	0
			77	77		
5	D	10	Total	O	0	0
			10	10		

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.

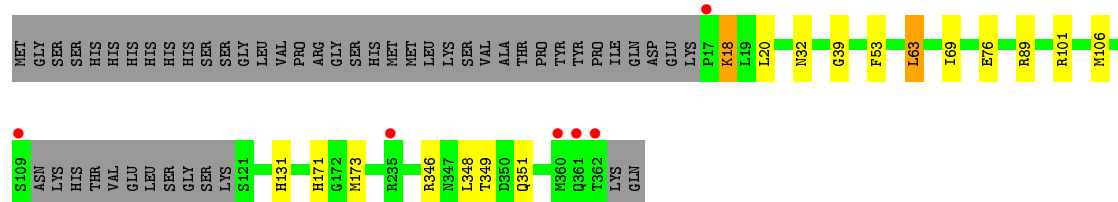
• Molecule 1: Arginase

Chain A: 




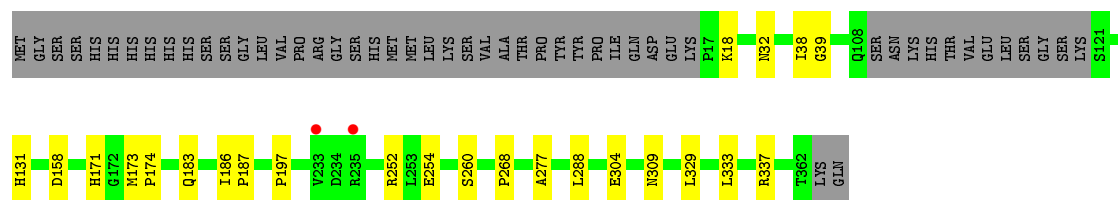
• Molecule 1: Arginase

Chain B: 



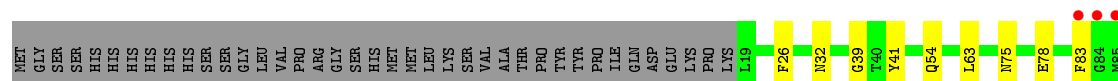
• Molecule 1: Arginase

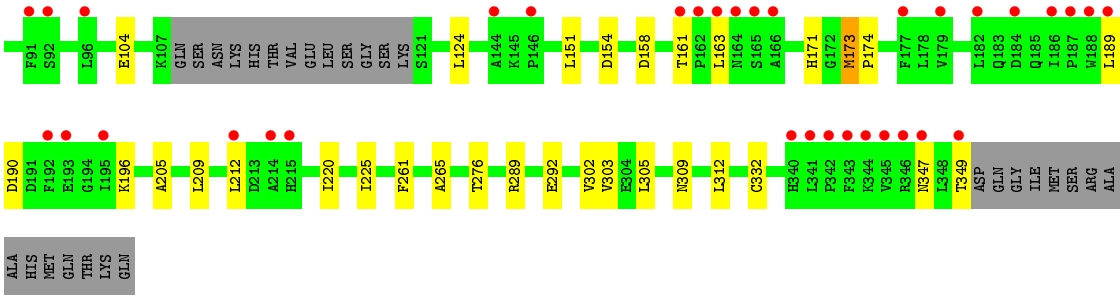
Chain C: 



• 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	178.32Å 178.32Å 178.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.46 – 2.50 49.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.8 (49.46-2.50) 93.8 (49.46-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.174 , 0.225 0.181 , 0.228	Depositor DCC
R_{free} test set	3101 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10664	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.42	0/2637	0.56	0/3572
1	B	0.42	0/2627	0.56	0/3560
1	C	0.37	0/2627	0.55	0/3560
1	D	0.36	0/2496	0.49	0/3386
All	All	0.39	0/10387	0.54	0/14078

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2586	0	2606	8	0
1	B	2576	0	2594	9	0
1	C	2573	0	2594	13	0
1	D	2447	0	2466	18	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	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	16	0	0
3	C	12	0	16	0	0
4	A	12	0	9	0	0
4	B	12	0	10	0	0
4	C	12	0	9	1	0
4	D	12	0	9	0	0
5	A	152	0	0	1	0
5	B	151	0	0	0	0
5	C	77	0	0	1	0
5	D	10	0	0	0	0
All	All	10664	0	10345	48	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 (48) 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:C:32:ASN:HD21	1:C:39:GLY:H	1.16	0.93
1:A:32:ASN:HD21	1:A:39:GLY:H	1.27	0.82
1:B:32:ASN:HD21	1:B:39:GLY:H	1.32	0.77
1:D:32:ASN:HD21	1:D:39:GLY:H	1.35	0.72
1:B:346:ARG:HH12	1:B:351:GLN:HE22	1.43	0.65
1:D:347:ASN:HD21	1:D:349:THR:HB	1.68	0.58
1:D:83:PHE:HE2	1:D:189:LEU:HD21	1.71	0.55
1:B:69:ILE:HD11	1:B:101:ARG:HB3	1.88	0.55
1:B:18:LYS:HD2	1:B:18:LYS:N	2.23	0.52
1:D:124:LEU:HB3	1:D:302:VAL:HG22	1.93	0.51
1:A:76:GLU:N	1:A:76:GLU:OE1	2.41	0.50
1:D:158:ASP:HB3	1:D:174:PRO:HD2	1.94	0.50
1:D:32:ASN:ND2	1:D:41:TYR:HD1	2.10	0.49
1:C:252:ARG:NH1	1:C:254:GLU:OE1	2.40	0.49
1:D:209:LEU:HD13	1:D:212:LEU:HD21	1.94	0.49
1:D:220:ILE:HA	1:D:225:ILE:HD12	1.96	0.47
1:A:158:ASP:HB3	1:A:174:PRO:HD2	1.97	0.47
1:D:173:MET:N	1:D:174:PRO:HD3	2.29	0.47
1:B:20:LEU:HA	1:B:20:LEU:HD23	1.77	0.46
1:B:53:PHE:CE2	1:B:63:LEU:HD13	2.50	0.46
1:B:346:ARG:NH1	1:B:351:GLN:HE22	2.11	0.46
1:D:75:ASN:ND2	1:D:78:GLU:OE1	2.48	0.46
1:C:158:ASP:OD1	4:C:405:NNH:NH1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:ARG:HD2	1:D:292:GLU:OE1	2.16	0.45
1:D:32:ASN:HD22	1:D:41:TYR:HD1	1.65	0.44
1:B:106:MET:HE2	1:B:106:MET:HB3	1.78	0.44
1:C:183:GLN:HG3	1:C:197:PRO:HG3	1.99	0.44
1:D:151:LEU:HD23	1:D:205:ALA:HB3	2.00	0.44
1:A:299:LYS:HA	1:A:299:LYS:HD2	1.78	0.44
1:D:261:PHE:O	1:D:305:LEU:HD12	2.17	0.44
1:D:26:PHE:HB2	1:D:63:LEU:HD11	2.00	0.43
1:A:32:ASN:ND2	1:A:41:TYR:H	2.16	0.43
1:C:39:GLY:HA3	1:C:309:ASN:OD1	2.18	0.43
1:A:173:MET:N	1:A:174:PRO:CD	2.82	0.43
1:D:154:ASP:HA	1:D:265:ALA:HB2	1.99	0.43
1:C:260:SER:HA	1:C:304:GLU:HG2	2.00	0.43
1:A:253:LEU:O	1:A:299:LYS:HE2	2.19	0.42
1:D:309:ASN:HB3	1:D:312:LEU:HD12	2.00	0.42
1:A:327:HIS:HD2	5:A:591:HOH:O	2.02	0.42
1:C:288:LEU:HD13	1:C:337:ARG:HD3	2.02	0.42
1:C:38:ILE:HG22	5:C:550:HOH:O	2.19	0.42
1:D:303:VAL:HG21	1:D:332:CYS:SG	2.60	0.41
1:C:158:ASP:HB3	1:C:174:PRO:HD2	2.03	0.41
1:C:186:ILE:HA	1:C:187:PRO:HD3	1.92	0.41
1:C:268:PRO:HG3	1:C:277:ALA:HB1	2.02	0.41
1:C:333:LEU:HD23	1:C:333:LEU:HA	1.90	0.41
1:B:348:LEU:HD12	1:B:348:LEU:HA	1.89	0.40
1:C:329:LEU:HD23	1:C:329:LEU:HA	1.96	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%)	323 (97%)	9 (3%)	1 (0%)	41 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	332/385 (86%)	324 (98%)	7 (2%)	1 (0%)	41	61
1	C	332/385 (86%)	322 (97%)	9 (3%)	1 (0%)	41	61
1	D	315/385 (82%)	308 (98%)	7 (2%)	0	100	100
All	All	1312/1540 (85%)	1277 (97%)	32 (2%)	3 (0%)	47	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	MET
1	C	173	MET
1	B	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%)	279 (98%)	5 (2%)	59	81
1	B	283/327 (86%)	276 (98%)	7 (2%)	47	73
1	C	283/327 (86%)	280 (99%)	3 (1%)	73	89
1	D	269/327 (82%)	260 (97%)	9 (3%)	38	64
All	All	1119/1308 (86%)	1095 (98%)	24 (2%)	52	78

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	147	ASP
1	A	171	HIS
1	A	252	ARG
1	A	270	VAL
1	B	18	LYS
1	B	63	LEU
1	B	76	GLU

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Mol	Chain	Res	Type
1	B	89	ARG
1	B	131	HIS
1	B	171	HIS
1	B	349	THR
1	C	18	LYS
1	C	131	HIS
1	C	171	HIS
1	D	54	GLN
1	D	104	GLU
1	D	161	THR
1	D	163	LEU
1	D	171	HIS
1	D	173	MET
1	D	190	ASP
1	D	196	LYS
1	D	276	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	110	ASN
1	B	32	ASN
1	B	351	GLN
1	C	32	ASN
1	D	32	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	NNH	D	403	2	6,11,11	2.83	2 (33%)	4,13,13	0.97	0
3	GOL	C	404	-	5,5,5	0.32	0	5,5,5	0.47	0
3	GOL	A	404	-	5,5,5	0.40	0	5,5,5	1.08	0
3	GOL	A	403	-	5,5,5	0.50	0	5,5,5	0.39	0
4	NNH	A	405	2	6,11,11	2.70	2 (33%)	4,13,13	1.54	1 (25%)
4	NNH	B	405	2	6,11,11	2.58	2 (33%)	4,13,13	2.29	2 (50%)
3	GOL	C	403	-	5,5,5	0.28	0	5,5,5	0.34	0
3	GOL	B	404	-	5,5,5	0.38	0	5,5,5	0.30	0
3	GOL	B	403	-	5,5,5	0.25	0	5,5,5	0.70	0
4	NNH	C	405	2	6,11,11	2.68	2 (33%)	4,13,13	1.83	1 (25%)

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	NNH	D	403	2	-	0/6/12/12	-
3	GOL	C	404	-	-	4/4/4/4	-
3	GOL	A	404	-	-	1/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
4	NNH	A	405	2	-	0/6/12/12	-
4	NNH	B	405	2	-	0/6/12/12	-
3	GOL	C	403	-	-	0/4/4/4	-
3	GOL	B	404	-	-	4/4/4/4	-
3	GOL	B	403	-	-	4/4/4/4	-
4	NNH	C	405	2	-	0/6/12/12	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	403	NNH	CE-NH1	6.48	1.49	1.34
4	A	405	NNH	CE-NH1	6.16	1.48	1.34
4	C	405	NNH	CE-NH1	6.12	1.48	1.34
4	B	405	NNH	CE-NH1	5.88	1.48	1.34
4	D	403	NNH	OH1-NH1	-2.24	1.34	1.40
4	A	405	NNH	OH1-NH1	-2.16	1.34	1.40
4	B	405	NNH	OH1-NH1	-2.14	1.34	1.40
4	C	405	NNH	OH1-NH1	-2.00	1.35	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	405	NNH	CG-ND-CE	4.03	130.86	123.50
4	C	405	NNH	CG-ND-CE	3.38	129.67	123.50
4	A	405	NNH	CG-ND-CE	2.38	127.84	123.50
4	B	405	NNH	CB-CG-ND	-2.14	105.68	111.87

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	404	GOL	O1-C1-C2-C3
3	A	403	GOL	O1-C1-C2-C3
3	B	404	GOL	O1-C1-C2-C3
3	B	403	GOL	O1-C1-C2-O2
3	B	403	GOL	O1-C1-C2-C3
3	B	403	GOL	C1-C2-C3-O3
3	B	403	GOL	O2-C2-C3-O3
3	B	404	GOL	C1-C2-C3-O3
3	A	403	GOL	O1-C1-C2-O2
3	B	404	GOL	O1-C1-C2-O2
3	B	404	GOL	O2-C2-C3-O3
3	C	404	GOL	O1-C1-C2-O2
3	C	404	GOL	C1-C2-C3-O3
3	C	404	GOL	O2-C2-C3-O3
3	A	404	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	405	NNH	1	0

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%)	-0.49	0 100 100	23, 32, 55, 75	4 (1%)
1	B	335/385 (87%)	-0.22	6 (1%) 68 71	24, 33, 58, 83	7 (2%)
1	C	334/385 (86%)	-0.34	2 (0%) 89 90	31, 41, 60, 87	1 (0%)
1	D	318/385 (82%)	0.52	37 (11%) 4 4	48, 65, 79, 86	15 (4%)
All	All	1323/1540 (85%)	-0.14	45 (3%) 45 48	23, 39, 74, 87	27 (2%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	343	PHE	4.2
1	D	345	VAL	4.0
1	B	361	GLN	4.0
1	D	346	ARG	3.8
1	D	83	PHE	3.6
1	D	212	LEU	3.6
1	D	186	ILE	3.6
1	D	195	ILE	3.5
1	D	161	THR	3.5
1	D	344	LYS	3.5
1	D	163	LEU	3.4
1	D	342	PRO	3.2
1	D	164	ASN	3.0
1	D	184	ASP	2.9
1	C	235[A]	ARG	2.9
1	D	177	PHE	2.8
1	D	162	PRO	2.8
1	D	166	ALA	2.8
1	D	187	PRO	2.7
1	D	215	HIS	2.7
1	D	214	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	92	SER	2.7
1	D	340	HIS	2.7
1	D	144	ALA	2.6
1	D	85	MET	2.6
1	B	362	THR	2.6
1	D	146	PRO	2.6
1	D	84	GLY	2.6
1	D	349	THR	2.5
1	D	347	ASN	2.5
1	D	192	PHE	2.5
1	B	360	MET	2.4
1	D	188	TRP	2.4
1	D	341	LEU	2.3
1	D	91	PHE	2.3
1	D	165	SER	2.2
1	B	17	PRO	2.2
1	B	235[A]	ARG	2.2
1	D	189	LEU	2.1
1	C	233	VAL	2.1
1	D	179	VAL	2.1
1	B	109	SER	2.1
1	D	96	LEU	2.0
1	D	182	LEU	2.0
1	D	193	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 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. 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	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	403	6/6	0.92	0.18	38,39,42,42	1
3	GOL	A	404	6/6	0.93	0.14	40,43,48,48	0
3	GOL	C	404	6/6	0.93	0.17	45,49,53,55	1
3	GOL	B	404	6/6	0.94	0.14	37,44,51,54	1
4	NNH	D	403	12/12	0.95	0.13	53,59,67,68	0
3	GOL	C	403	6/6	0.95	0.12	45,48,52,53	1
3	GOL	B	403	6/6	0.96	0.19	39,43,44,46	1
2	MN	D	402	1/1	0.98	0.08	60,60,60,60	0
4	NNH	C	405	12/12	0.98	0.12	32,36,40,41	0
4	NNH	A	405	12/12	0.98	0.13	29,30,34,37	0
4	NNH	B	405	12/12	0.98	0.16	27,31,34,37	0
2	MN	C	402	1/1	0.99	0.14	37,37,37,37	0
2	MN	B	401	1/1	0.99	0.17	28,28,28,28	0
2	MN	C	401	1/1	0.99	0.12	35,35,35,35	0
2	MN	D	401	1/1	0.99	0.07	51,51,51,51	0
2	MN	A	402	1/1	1.00	0.13	27,27,27,27	0
2	MN	B	402	1/1	1.00	0.18	26,26,26,26	0
2	MN	A	401	1/1	1.00	0.16	29,29,29,29	0

6.5 Other polymers

There are no such residues in this entry.