



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:25 pm BST

PDB ID : 4RHM
Title : Crystal structure of T. brucei arginase-like protein quadruple mutant S149D/R151H/S153D/S226D
Authors : Hai, Y.; Barrett, M.P.; Christianson, D.W.
Deposited on : 2014-10-02
Resolution : 1.95 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

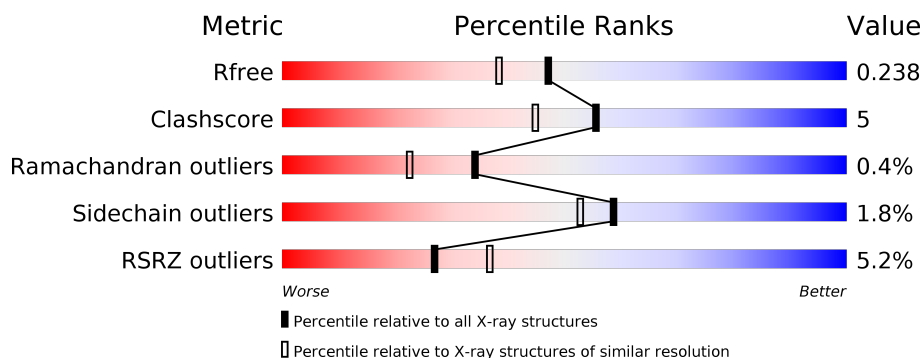
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	351	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>12%</div> </div> </div>
1	B	351	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>13%</div> </div> </div>
1	C	351	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>14%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7261 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	308	Total	C	N	O	S	0	1	0
			2381	1520	402	444	15			
1	B	306	Total	C	N	O	S	0	0	0
			2363	1508	401	439	15			
1	C	302	Total	C	N	O	S	0	0	0
			2337	1492	395	435	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q581Y0
A	-18	GLY	-	EXPRESSION TAG	UNP Q581Y0
A	-17	SER	-	EXPRESSION TAG	UNP Q581Y0
A	-16	SER	-	EXPRESSION TAG	UNP Q581Y0
A	-15	HIS	-	EXPRESSION TAG	UNP Q581Y0
A	-14	HIS	-	EXPRESSION TAG	UNP Q581Y0
A	-13	HIS	-	EXPRESSION TAG	UNP Q581Y0
A	-12	HIS	-	EXPRESSION TAG	UNP Q581Y0
A	-11	HIS	-	EXPRESSION TAG	UNP Q581Y0
A	-10	HIS	-	EXPRESSION TAG	UNP Q581Y0
A	-9	SER	-	EXPRESSION TAG	UNP Q581Y0
A	-8	SER	-	EXPRESSION TAG	UNP Q581Y0
A	-7	GLY	-	EXPRESSION TAG	UNP Q581Y0
A	-6	LEU	-	EXPRESSION TAG	UNP Q581Y0
A	-5	VAL	-	EXPRESSION TAG	UNP Q581Y0
A	-4	PRO	-	EXPRESSION TAG	UNP Q581Y0
A	-3	ARG	-	EXPRESSION TAG	UNP Q581Y0
A	-2	GLY	-	EXPRESSION TAG	UNP Q581Y0
A	-1	SER	-	EXPRESSION TAG	UNP Q581Y0
A	0	HIS	-	EXPRESSION TAG	UNP Q581Y0
A	149	ASP	SER	ENGINEERED MUTATION	UNP Q581Y0
A	151	HIS	ARG	ENGINEERED MUTATION	UNP Q581Y0
A	153	ASP	SER	ENGINEERED MUTATION	UNP Q581Y0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	226	ASP	SER	ENGINEERED MUTATION	UNP Q581Y0
B	-19	MET	-	EXPRESSION TAG	UNP Q581Y0
B	-18	GLY	-	EXPRESSION TAG	UNP Q581Y0
B	-17	SER	-	EXPRESSION TAG	UNP Q581Y0
B	-16	SER	-	EXPRESSION TAG	UNP Q581Y0
B	-15	HIS	-	EXPRESSION TAG	UNP Q581Y0
B	-14	HIS	-	EXPRESSION TAG	UNP Q581Y0
B	-13	HIS	-	EXPRESSION TAG	UNP Q581Y0
B	-12	HIS	-	EXPRESSION TAG	UNP Q581Y0
B	-11	HIS	-	EXPRESSION TAG	UNP Q581Y0
B	-10	HIS	-	EXPRESSION TAG	UNP Q581Y0
B	-9	SER	-	EXPRESSION TAG	UNP Q581Y0
B	-8	SER	-	EXPRESSION TAG	UNP Q581Y0
B	-7	GLY	-	EXPRESSION TAG	UNP Q581Y0
B	-6	LEU	-	EXPRESSION TAG	UNP Q581Y0
B	-5	VAL	-	EXPRESSION TAG	UNP Q581Y0
B	-4	PRO	-	EXPRESSION TAG	UNP Q581Y0
B	-3	ARG	-	EXPRESSION TAG	UNP Q581Y0
B	-2	GLY	-	EXPRESSION TAG	UNP Q581Y0
B	-1	SER	-	EXPRESSION TAG	UNP Q581Y0
B	0	HIS	-	EXPRESSION TAG	UNP Q581Y0
B	149	ASP	SER	ENGINEERED MUTATION	UNP Q581Y0
B	151	HIS	ARG	ENGINEERED MUTATION	UNP Q581Y0
B	153	ASP	SER	ENGINEERED MUTATION	UNP Q581Y0
B	226	ASP	SER	ENGINEERED MUTATION	UNP Q581Y0
C	-19	MET	-	EXPRESSION TAG	UNP Q581Y0
C	-18	GLY	-	EXPRESSION TAG	UNP Q581Y0
C	-17	SER	-	EXPRESSION TAG	UNP Q581Y0
C	-16	SER	-	EXPRESSION TAG	UNP Q581Y0
C	-15	HIS	-	EXPRESSION TAG	UNP Q581Y0
C	-14	HIS	-	EXPRESSION TAG	UNP Q581Y0
C	-13	HIS	-	EXPRESSION TAG	UNP Q581Y0
C	-12	HIS	-	EXPRESSION TAG	UNP Q581Y0
C	-11	HIS	-	EXPRESSION TAG	UNP Q581Y0
C	-10	HIS	-	EXPRESSION TAG	UNP Q581Y0
C	-9	SER	-	EXPRESSION TAG	UNP Q581Y0
C	-8	SER	-	EXPRESSION TAG	UNP Q581Y0
C	-7	GLY	-	EXPRESSION TAG	UNP Q581Y0
C	-6	LEU	-	EXPRESSION TAG	UNP Q581Y0
C	-5	VAL	-	EXPRESSION TAG	UNP Q581Y0
C	-4	PRO	-	EXPRESSION TAG	UNP Q581Y0
C	-3	ARG	-	EXPRESSION TAG	UNP Q581Y0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	EXPRESSION TAG	UNP Q581Y0
C	-1	SER	-	EXPRESSION TAG	UNP Q581Y0
C	0	HIS	-	EXPRESSION TAG	UNP Q581Y0
C	149	ASP	SER	ENGINEERED MUTATION	UNP Q581Y0
C	151	HIS	ARG	ENGINEERED MUTATION	UNP Q581Y0
C	153	ASP	SER	ENGINEERED MUTATION	UNP Q581Y0
C	226	ASP	SER	ENGINEERED MUTATION	UNP Q581Y0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

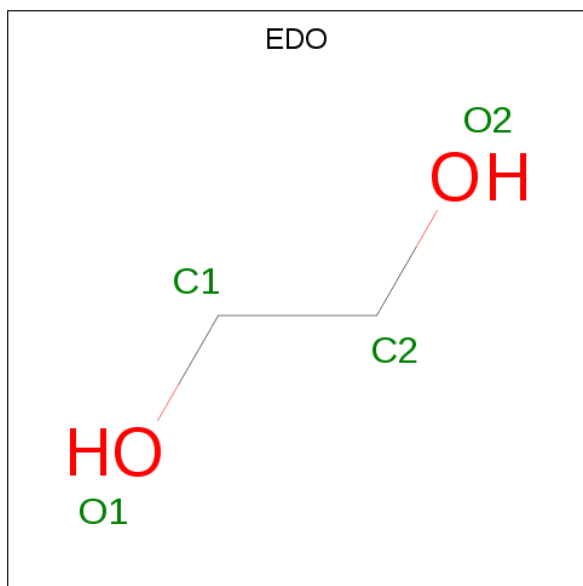


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

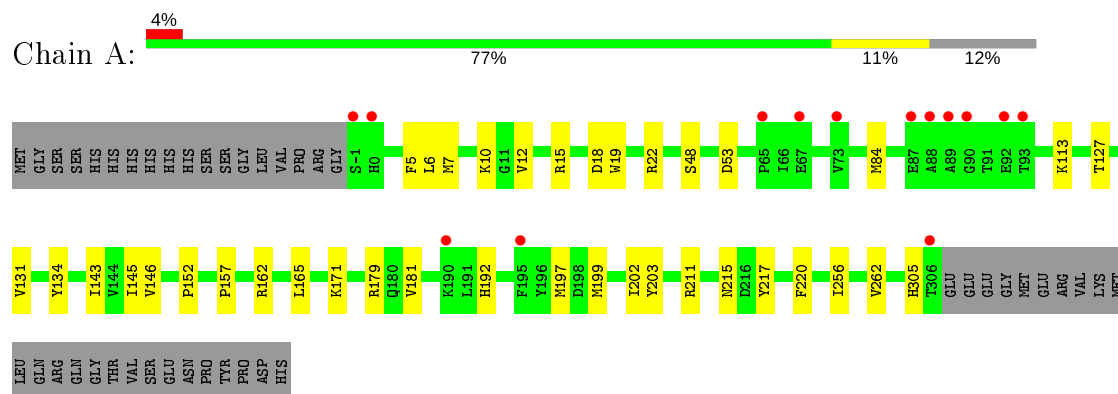
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	44	Total	O	0	0
			44	44		
5	B	46	Total	O	0	0
			46	46		
5	C	39	Total	O	0	0
			39	39		

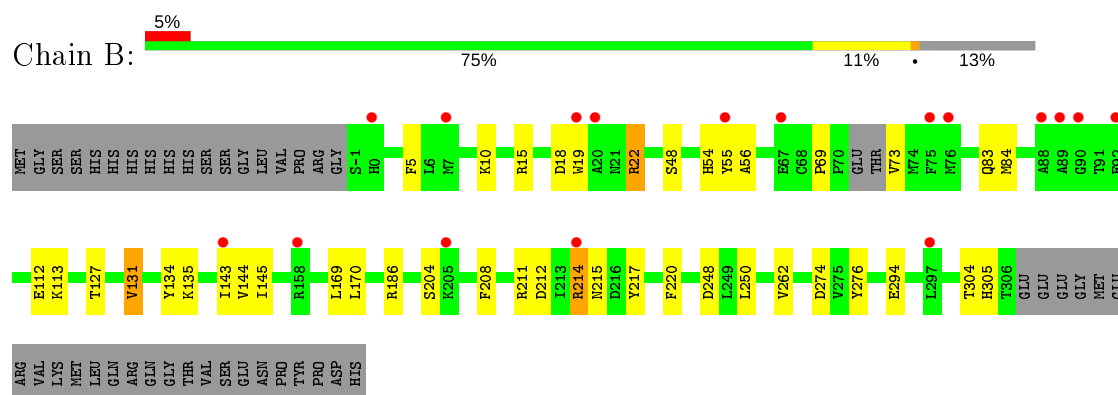
3 Residue-property plots [i](#)

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.

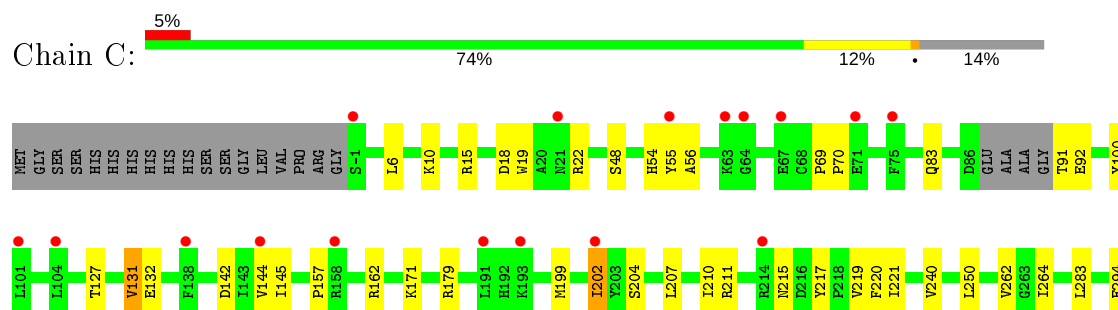
• Molecule 1: Arginase



• Molecule 1: Arginase



• Molecule 1: Arginase



T304
HIS
THR
GLU
GLU
GLU
GLY
MET
GLU
ARG
VAL
LYS
MET
LEU
GLN
ARG
GLN
GLY
THR
VAL
SER
GLU
ASN
PRO
TYR
PRO
ASP
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	82.12Å 137.35Å 87.78Å 90.00° 102.28° 90.00°	Depositor
Resolution (Å)	42.88 – 1.95 42.88 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.0 (42.88-1.95) 94.0 (42.88-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.201 , 0.237 0.201 , 0.238	Depositor DCC
R_{free} test set	3250 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	1.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7261	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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, EDO

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	0.25	0/2441	0.44	0/3314
1	B	0.24	0/2419	0.44	0/3281
1	C	0.25	0/2392	0.43	0/3244
All	All	0.25	0/7252	0.44	0/9839

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	2381	0	2374	25	0
1	B	2363	0	2358	23	0
1	C	2337	0	2331	29	0
2	A	12	0	16	1	0
2	B	6	0	8	0	0
2	C	18	0	24	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	6	0	0
4	C	4	0	6	0	0
5	A	44	0	0	0	0
5	B	46	0	0	1	0
5	C	39	0	0	1	0
All	All	7261	0	7129	72	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 (72) 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:157:PRO:HA	1:A:162:ARG:HG2	1.66	0.76
1:C:215:ASN:ND2	1:C:217:TYR:O	2.21	0.72
1:A:211:ARG:NH2	1:C:204:SER:O	2.24	0.69
1:C:48:SER:HB3	2:C:405:GOL:H31	1.75	0.69
1:B:15:ARG:NH2	1:B:22:ARG:O	2.26	0.68
1:A:145[B]:ILE:HG12	1:A:220:PHE:HB3	1.77	0.67
1:C:202:ILE:HG12	1:C:210:ILE:HD11	1.78	0.64
1:A:48:SER:HB3	2:C:401:GOL:H31	1.80	0.63
2:A:403:GOL:H31	1:B:48:SER:HB3	1.82	0.61
1:C:157:PRO:HA	1:C:162:ARG:HG2	1.83	0.61
1:C:92:GLU:N	1:C:92:GLU:OE1	2.33	0.61
1:B:204:SER:O	1:C:211:ARG:NH2	2.33	0.61
1:B:15:ARG:HE	1:B:19:TRP:HB3	1.66	0.60
1:C:83:GLN:NE2	5:C:527:HOH:O	2.35	0.59
1:B:214:ARG:H	1:B:214:ARG:HD2	1.68	0.59
1:C:15:ARG:HE	1:C:19:TRP:HB3	1.71	0.56
1:A:15:ARG:HE	1:A:19:TRP:HB3	1.71	0.55
1:C:179:ARG:HD3	1:C:199:MET:HG3	1.90	0.53
1:B:22:ARG:NH2	1:B:69:PRO:O	2.40	0.53
1:C:220:PHE:HD2	1:C:262:VAL:HG22	1.74	0.53
1:A:6:LEU:O	1:A:10:LYS:HG2	2.08	0.53
1:B:54:HIS:O	1:B:56:ALA:N	2.42	0.53
1:C:144:VAL:HG11	1:C:215:ASN:OD1	2.10	0.52
1:A:179:ARG:HD3	1:A:199:MET:HG3	1.90	0.52
1:B:144:VAL:HG11	1:B:215:ASN:OD1	2.10	0.52
1:B:215:ASN:ND2	1:B:217:TYR:O	2.35	0.51
1:C:15:ARG:NH2	1:C:22:ARG:O	2.44	0.51
1:A:12:VAL:O	1:A:113:LYS:NZ	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:TYR:OH	1:C:132:GLU:OE2	2.20	0.50
1:C:145:ILE:HG12	1:C:220:PHE:HB3	1.94	0.49
1:C:142:ASP:HB3	1:C:171:LYS:HB2	1.94	0.49
1:A:215:ASN:ND2	1:A:217:TYR:O	2.44	0.49
1:A:146:VAL:HG21	1:A:256:ILE:HD12	1.96	0.48
1:C:127:THR:O	1:C:131:VAL:HG13	2.14	0.48
1:A:220:PHE:HD1	1:A:262:VAL:HG22	1.79	0.47
1:B:18:ASP:OD1	1:B:18:ASP:N	2.47	0.47
1:A:18:ASP:N	1:A:18:ASP:OD1	2.45	0.47
1:A:127:THR:O	1:A:131:VAL:HG13	2.15	0.47
1:B:135:LYS:HG2	1:B:169:LEU:HD22	1.95	0.47
1:A:211:ARG:HH12	1:C:204:SER:HB2	1.80	0.47
1:C:221:ILE:HB	1:C:264:ILE:HG12	1.97	0.47
1:C:54:HIS:O	1:C:56:ALA:N	2.48	0.47
1:A:134:TYR:HD1	1:A:143:ILE:HD11	1.80	0.46
1:B:145:ILE:HG12	1:B:220:PHE:HB3	1.98	0.46
1:A:152:PRO:HG2	1:A:181:VAL:HG13	1.98	0.46
1:B:274:ASP:HB3	1:B:276:TYR:CE2	2.51	0.46
1:C:6:LEU:O	1:C:10:LYS:HG2	2.15	0.46
1:C:202:ILE:HG23	1:C:207:LEU:HD21	1.98	0.46
1:C:211:ARG:HA	1:C:211:ARG:HD3	1.67	0.46
1:B:10:LYS:O	1:B:113:LYS:NZ	2.48	0.45
1:B:208:PHE:O	1:B:211:ARG:NH2	2.47	0.45
1:C:18:ASP:OD1	1:C:18:ASP:N	2.50	0.44
1:A:134:TYR:CD1	1:A:143:ILE:HD11	2.53	0.44
1:A:165:LEU:HB3	1:A:192:HIS:CD2	2.53	0.44
1:B:83:GLN:NE2	5:B:510:HOH:O	2.49	0.44
1:A:5:PHE:CG	1:A:84:MET:HA	2.52	0.44
1:B:250:LEU:HD22	1:B:294:GLU:HG3	2.00	0.44
1:B:134:TYR:HD1	1:B:143:ILE:HD11	1.82	0.43
1:B:127:THR:O	1:B:131:VAL:HG13	2.19	0.42
1:A:203:TYR:OH	1:B:248:ASP:OD1	2.30	0.42
1:C:179:ARG:HG3	1:C:240:VAL:HG11	2.00	0.42
1:A:211:ARG:HA	1:A:211:ARG:HD3	1.88	0.42
1:A:10:LYS:HE2	1:A:10:LYS:HB3	1.74	0.42
1:B:220:PHE:HD1	1:B:262:VAL:HG22	1.85	0.42
1:A:171:LYS:HE2	1:A:217:TYR:CZ	2.54	0.42
1:B:5:PHE:CG	1:B:84:MET:HA	2.54	0.42
1:C:144:VAL:HG13	1:C:219:VAL:HG12	2.02	0.41
1:C:250:LEU:HD22	1:C:294:GLU:HG3	2.03	0.41
1:A:197:MET:HB3	1:A:202:ILE:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ARG:HD2	1:C:55:TYR:CG	2.56	0.41
1:A:131:VAL:HG11	1:A:145[B]:ILE:HD11	2.02	0.40
1:C:69:PRO:HA	1:C:70:PRO:HD3	2.00	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	307/351 (88%)	301 (98%)	4 (1%)	2 (1%)	22	11
1	B	302/351 (86%)	295 (98%)	5 (2%)	2 (1%)	22	11
1	C	298/351 (85%)	291 (98%)	7 (2%)	0	100	100
All	All	907/1053 (86%)	887 (98%)	16 (2%)	4 (0%)	34	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	305	HIS
1	B	55	TYR
1	A	53	ASP
1	A	305	HIS

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	262/300 (87%)	260 (99%)	2 (1%)	81	80
1	B	260/300 (87%)	252 (97%)	8 (3%)	40	28
1	C	258/300 (86%)	254 (98%)	4 (2%)	62	58
All	All	780/900 (87%)	766 (98%)	14 (2%)	59	53

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	MET
1	A	22	ARG
1	B	22	ARG
1	B	73	VAL
1	B	112	GLU
1	B	131	VAL
1	B	170	LEU
1	B	212	ASP
1	B	214	ARG
1	B	304	THR
1	C	91	THR
1	C	131	VAL
1	C	202	ILE
1	C	283	LEU

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

Mol	Chain	Res	Type
1	A	192	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	EDO	B	403	-	3,3,3	0.45	0	2,2,2	0.44	0
2	GOL	C	405	-	5,5,5	0.38	0	5,5,5	0.36	0
2	GOL	A	401	-	5,5,5	0.36	0	5,5,5	0.35	0
2	GOL	C	401	-	5,5,5	0.39	0	5,5,5	0.34	0
4	EDO	A	404	-	3,3,3	0.47	0	2,2,2	0.46	0
2	GOL	B	401	-	5,5,5	0.35	0	5,5,5	0.38	0
4	EDO	C	402	-	3,3,3	0.45	0	2,2,2	0.38	0
2	GOL	C	403	-	5,5,5	0.35	0	5,5,5	0.19	0
2	GOL	A	403	-	5,5,5	0.38	0	5,5,5	0.33	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	EDO	B	403	-	-	0/1/1/1	-
2	GOL	C	405	-	-	4/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-
2	GOL	C	401	-	-	4/4/4/4	-
4	EDO	A	404	-	-	0/1/1/1	-
2	GOL	B	401	-	-	2/4/4/4	-
4	EDO	C	402	-	-	0/1/1/1	-
2	GOL	C	403	-	-	3/4/4/4	-
2	GOL	A	403	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	405	GOL	C1-C2-C3-O3
2	A	401	GOL	C1-C2-C3-O3
2	C	401	GOL	C1-C2-C3-O3
2	B	401	GOL	O1-C1-C2-C3
2	A	403	GOL	C1-C2-C3-O3
2	C	405	GOL	O1-C1-C2-C3
2	C	401	GOL	O1-C1-C2-C3
2	C	403	GOL	O1-C1-C2-C3
2	C	403	GOL	C1-C2-C3-O3
2	A	403	GOL	O1-C1-C2-C3
2	C	405	GOL	O2-C2-C3-O3
2	A	401	GOL	O2-C2-C3-O3
2	C	401	GOL	O2-C2-C3-O3
2	B	401	GOL	O1-C1-C2-O2
2	C	403	GOL	O2-C2-C3-O3
2	A	403	GOL	O2-C2-C3-O3
2	C	405	GOL	O1-C1-C2-O2
2	A	403	GOL	O1-C1-C2-O2
2	C	401	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	405	GOL	1	0
2	C	401	GOL	1	0
2	A	403	GOL	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, 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	308/351 (87%)	0.49	14 (4%)	33 43	25, 47, 74, 99	0
1	B	306/351 (87%)	0.51	17 (5%)	24 33	27, 49, 77, 103	0
1	C	302/351 (86%)	0.56	17 (5%)	24 33	26, 53, 81, 91	0
All	All	916/1053 (86%)	0.52	48 (5%)	27 37	25, 50, 78, 103	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	HIS	5.1
1	A	88	ALA	4.8
1	A	306	THR	4.5
1	B	88	ALA	4.5
1	C	21	ASN	3.7
1	A	-1	SER	3.5
1	B	55	TYR	3.5
1	C	214	ARG	3.4
1	B	89	ALA	3.4
1	C	101	LEU	3.4
1	A	87	GLU	3.2
1	B	90	GLY	3.2
1	B	214	ARG	3.2
1	C	55	TYR	3.2
1	C	202	ILE	3.2
1	C	67	GLU	3.1
1	A	89	ALA	3.0
1	C	63	LYS	3.0
1	A	90	GLY	2.9
1	A	93	THR	2.9
1	C	64	GLY	2.9
1	C	-1	SER	2.9
1	C	138	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	158	ARG	2.7
1	B	75	PHE	2.6
1	A	195	PHE	2.6
1	A	67	GLU	2.6
1	A	65	PRO	2.6
1	B	76	MET	2.5
1	C	158	ARG	2.5
1	B	297	LEU	2.5
1	B	143	ILE	2.5
1	A	190	LYS	2.5
1	C	191	LEU	2.5
1	B	67	GLU	2.4
1	B	0	HIS	2.4
1	B	205	LYS	2.3
1	C	193	LYS	2.3
1	B	20	ALA	2.2
1	A	92	GLU	2.2
1	C	104	LEU	2.2
1	C	75	PHE	2.2
1	B	7	MET	2.2
1	C	144	VAL	2.2
1	B	92	GLU	2.1
1	C	71	GLU	2.1
1	B	19	TRP	2.1
1	A	73	VAL	2.1

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. 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
2	GOL	A	403	6/6	0.76	0.29	56,68,74,77	0
2	GOL	A	401	6/6	0.83	0.28	62,68,74,77	0
4	EDO	A	404	4/4	0.83	0.30	41,54,55,62	0
4	EDO	C	402	4/4	0.83	0.36	54,55,55,61	0
2	GOL	C	403	6/6	0.83	0.23	59,68,75,77	0
2	GOL	C	405	6/6	0.83	0.22	56,68,74,77	0
4	EDO	B	403	4/4	0.87	0.28	58,60,61,63	0
2	GOL	C	401	6/6	0.91	0.18	56,68,74,77	0
2	GOL	B	401	6/6	0.93	0.19	57,72,74,77	0
3	MN	C	404	1/1	0.98	0.09	29,29,29,29	0
3	MN	A	402	1/1	0.99	0.17	35,35,35,35	0
3	MN	B	402	1/1	0.99	0.15	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.