



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:15 PM UTC

PDB ID : 3WQG / pdb_00003wqg
Title : D-threo-3-hydroxyaspartate dehydratase C353A mutant in the metal-free form
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Deposited on : 2014-01-25
Resolution : 1.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 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

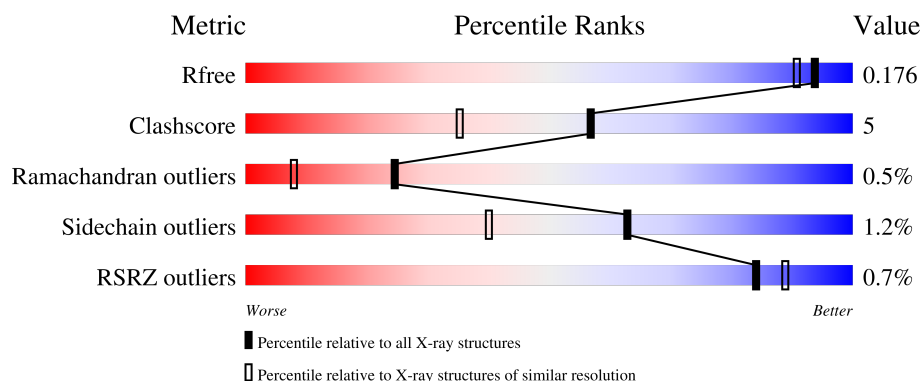
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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 $\leq 5\%$. 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	390	 88% 8% . .
1	B	390	 86% 13% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6415 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 D-threo-3-hydroxyaspartate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	6	0
			2861	1778	535	534	14			
1	B	389	Total	C	N	O	S	0	6	0
			2944	1829	554	544	17			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP B2DFG5
A	-8	HIS	-	expression tag	UNP B2DFG5
A	-7	HIS	-	expression tag	UNP B2DFG5
A	-6	HIS	-	expression tag	UNP B2DFG5
A	-5	HIS	-	expression tag	UNP B2DFG5
A	-4	HIS	-	expression tag	UNP B2DFG5
A	-3	HIS	-	expression tag	UNP B2DFG5
A	-2	ALA	-	expression tag	UNP B2DFG5
A	-1	MET	-	expression tag	UNP B2DFG5
A	0	SER	-	expression tag	UNP B2DFG5
A	353	ALA	CYS	engineered mutation	UNP B2DFG5
B	-9	GLY	-	expression tag	UNP B2DFG5
B	-8	HIS	-	expression tag	UNP B2DFG5
B	-7	HIS	-	expression tag	UNP B2DFG5
B	-6	HIS	-	expression tag	UNP B2DFG5
B	-5	HIS	-	expression tag	UNP B2DFG5
B	-4	HIS	-	expression tag	UNP B2DFG5
B	-3	HIS	-	expression tag	UNP B2DFG5
B	-2	ALA	-	expression tag	UNP B2DFG5
B	-1	MET	-	expression tag	UNP B2DFG5
B	0	SER	-	expression tag	UNP B2DFG5
B	353	ALA	CYS	engineered mutation	UNP B2DFG5

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

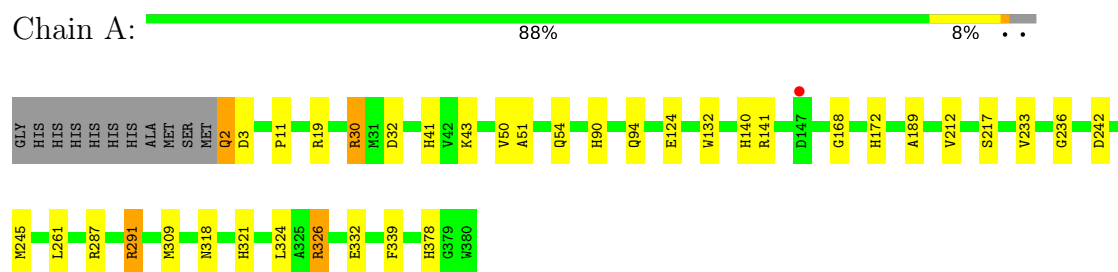
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	295	Total	O	0	0
			295	295		
4	B	267	Total	O	0	0
			267	267		

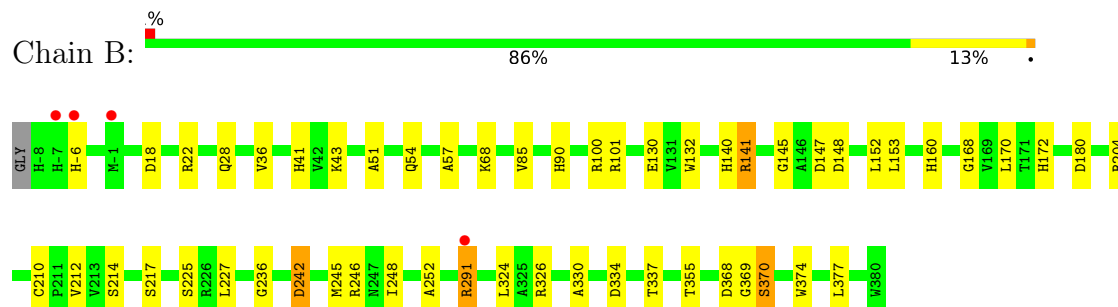
3 Residue-property plots [i](#)

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: D-threo-3-hydroxyaspartate dehydratase



- Molecule 1: D-threo-3-hydroxyaspartate dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	158.04Å 158.04Å 159.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.34 – 1.55 35.34 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (35.34-1.55) 99.7 (35.34-1.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.48 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.143 , 0.179 0.140 , 0.176	Depositor DCC
R_{free} test set	7208 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h 0.004 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6415	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: PLP, 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	1.60	18/2926 (0.6%)	1.23	9/3969 (0.2%)
1	B	1.65	26/3015 (0.9%)	1.28	8/4087 (0.2%)
All	All	1.63	44/5941 (0.7%)	1.25	17/8056 (0.2%)

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	318	ASN	CG-OD1	-10.22	1.04	1.23
1	A	172	HIS	ND1-CE1	9.14	1.41	1.32
1	A	378	HIS	ND1-CE1	8.86	1.41	1.32
1	A	19	ARG	CZ-NH1	7.43	1.43	1.32
1	A	212	VAL	C-O	7.39	1.32	1.24
1	B	140	HIS	CG-CD2	7.20	1.43	1.35
1	B	172	HIS	C-O	7.12	1.32	1.24
1	B	-6	HIS	CE1-NE2	6.80	1.39	1.32
1	B	90	HIS	ND1-CE1	6.75	1.39	1.32
1	B	141	ARG	CA-C	6.54	1.61	1.52
1	A	287	ARG	CZ-NH2	6.35	1.41	1.33
1	B	140	HIS	ND1-CE1	6.34	1.38	1.32
1	B	41	HIS	CG-CD2	6.30	1.42	1.35
1	A	140	HIS	ND1-CE1	6.20	1.38	1.32
1	A	172	HIS	CG-CD2	6.18	1.42	1.35
1	B	36	VAL	C-O	6.07	1.30	1.24
1	B	152	LEU	CB-CG	-6.03	1.41	1.53
1	A	168	GLY	N-CA	5.91	1.50	1.45
1	A	189	ALA	N-CA	5.79	1.53	1.46
1	A	90	HIS	ND1-CE1	5.61	1.38	1.32
1	A	41	HIS	CE1-NE2	5.55	1.38	1.32
1	A	321	HIS	CE1-NE2	5.55	1.38	1.32
1	B	140	HIS	CE1-NE2	5.52	1.38	1.32
1	A	326	ARG	CD-NE	5.51	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	ASP	CB-CG	-5.48	1.38	1.52
1	B	141	ARG	C-O	-5.37	1.17	1.24
1	B	242	ASP	C-O	5.36	1.29	1.24
1	B	148	ASP	CG-OD1	5.31	1.35	1.25
1	A	132	TRP	CD2-CE2	5.30	1.50	1.41
1	B	-6	HIS	CG-CD2	5.30	1.41	1.35
1	B	252	ALA	N-CA	5.25	1.51	1.45
1	A	233	VAL	C-O	5.23	1.29	1.24
1	B	130	GLU	C-O	5.19	1.30	1.24
1	B	101	ARG	CA-CB	5.15	1.62	1.53
1	A	242	ASP	C-O	5.14	1.29	1.24
1	B	225	SER	N-CA	5.13	1.52	1.46
1	A	32	ASP	CA-C	5.13	1.59	1.52
1	B	90	HIS	CE1-NE2	5.09	1.37	1.32
1	B	145	GLY	C-O	5.09	1.28	1.23
1	B	374	TRP	CD2-CE2	5.09	1.50	1.41
1	B	180	ASP	CA-C	5.06	1.57	1.52
1	B	355	THR	N-CA	5.06	1.52	1.46
1	B	160	HIS	ND1-CE1	5.03	1.37	1.32
1	B	168	GLY	N-CA	-5.00	1.40	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	MET	CG-SD-CE	-7.76	83.82	100.90
1	B	370	SER	N-CA-CB	-6.94	99.76	109.97
1	A	3	ASP	N-CA-CB	6.46	119.47	109.97
1	B	217	SER	N-CA-C	-6.29	99.75	109.24
1	B	369	GLY	CA-C-N	6.20	129.68	120.87
1	B	369	GLY	C-N-CA	6.20	129.68	120.87
1	A	217	SER	N-CA-C	-6.02	99.99	108.96
1	A	19	ARG	NE-CZ-NH2	-5.90	113.89	119.20
1	B	204	ARG	CB-CG-CD	-5.83	97.90	111.30
1	B	210	CYS	CA-C-N	-5.69	113.90	119.64
1	B	210	CYS	C-N-CA	-5.69	113.90	119.64
1	A	287	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	A	50	VAL	N-CA-C	-5.34	105.51	110.53
1	A	321	HIS	CB-CA-C	-5.29	100.12	109.70
1	A	19	ARG	NE-CZ-NH1	5.26	126.76	121.50
1	B	41	HIS	CA-CB-CG	-5.23	108.57	113.80
1	A	124	GLU	CB-CA-C	5.19	119.41	110.79

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	2861	0	2868	18	0
1	B	2944	0	2940	36	0
2	A	15	0	6	1	0
2	B	15	0	6	1	0
3	A	6	0	8	0	0
3	B	12	0	15	0	0
4	A	295	0	0	1	0
4	B	267	0	0	7	0
All	All	6415	0	5843	54	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 (54) 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:B:100[B]:ARG:HH11	1:B:100[B]:ARG:CG	1.26	1.40
1:B:245[B]:MET:HE3	1:B:245[B]:MET:HA	1.30	1.06
1:B:100[B]:ARG:CG	1:B:100[B]:ARG:NH1	2.02	1.05
1:A:30:ARG:HH11	1:A:30:ARG:HG3	1.15	1.05
1:B:100[B]:ARG:HH11	1:B:100[B]:ARG:HG2	0.84	0.99
1:B:100[B]:ARG:NH1	1:B:100[B]:ARG:HG2	1.69	0.93
1:B:100[B]:ARG:NH1	1:B:100[B]:ARG:HG3	1.87	0.90
1:A:2:GLN:HE21	1:A:2:GLN:HA	1.36	0.89
1:B:368:ASP:OD1	1:B:370:SER:HB2	1.78	0.82
1:B:18:ASP:HB3	1:B:22:ARG:NH2	1.97	0.80
1:A:2:GLN:HA	1:A:2:GLN:NE2	1.97	0.79
1:B:245[B]:MET:HE3	1:B:245[B]:MET:CA	2.09	0.78
1:B:245[B]:MET:HA	1:B:245[B]:MET:CE	2.13	0.78
1:B:68[A]:LYS:CE	4:B:703:HOH:O	2.35	0.75
1:B:368:ASP:OD1	1:B:370:SER:CB	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ARG:HH11	1:A:30:ARG:CG	1.99	0.74
1:B:68[A]:LYS:CE	1:B:377:LEU:HD11	2.21	0.71
1:A:291:ARG:HG3	1:A:291:ARG:HH11	1.55	0.70
1:B:51:ALA:HA	1:B:54:GLN:HE21	1.64	0.62
1:A:51:ALA:HA	1:A:54:GLN:HE21	1.65	0.61
1:A:30:ARG:HG3	1:A:30:ARG:NH1	1.95	0.61
1:B:68[A]:LYS:CD	4:B:703:HOH:O	2.54	0.55
1:B:68[A]:LYS:HG2	1:B:377:LEU:HD21	1.88	0.54
1:A:326:ARG:HD2	1:A:332:GLU:OE1	2.08	0.53
1:A:2:GLN:HE21	1:A:2:GLN:CA	2.16	0.53
1:B:227:LEU:HD11	4:B:653:HOH:O	2.08	0.53
1:B:368:ASP:OD1	1:B:370:SER:HB3	2.09	0.52
1:A:2:GLN:NE2	1:A:2:GLN:CA	2.72	0.52
1:B:100[A]:ARG:HD2	4:B:745:HOH:O	2.09	0.52
1:B:18:ASP:HB3	1:B:22:ARG:HH21	1.72	0.51
1:B:68[A]:LYS:NZ	4:B:703:HOH:O	2.39	0.51
1:B:43:LYS:NZ	2:B:401:PLP:O3	2.42	0.51
1:B:291:ARG:HD2	1:B:291:ARG:H	1.75	0.51
1:A:291:ARG:HH11	1:A:291:ARG:CG	2.22	0.50
1:B:68[A]:LYS:CD	1:B:377:LEU:HD11	2.43	0.49
1:A:309:MET:HE1	1:A:339:PHE:CZ	2.48	0.49
1:B:43:LYS:NZ	4:B:701:HOH:O	2.35	0.47
1:A:30:ARG:CG	1:A:30:ARG:NH1	2.67	0.45
1:B:132:TRP:CH2	1:B:212:VAL:HG11	2.52	0.45
1:B:28:GLN:HG2	1:B:57:ALA:O	2.17	0.44
1:A:11:PRO:HA	1:A:261:LEU:O	2.18	0.44
1:B:245[B]:MET:HE1	1:B:248:ILE:HD12	2.00	0.44
1:B:100[A]:ARG:CD	4:B:745:HOH:O	2.65	0.44
1:B:242:ASP:OD1	1:B:245[B]:MET:HG2	2.19	0.43
1:A:324:LEU:HD23	1:A:324:LEU:C	2.43	0.43
1:B:245[B]:MET:CE	1:B:248:ILE:HD12	2.49	0.43
1:B:324:LEU:C	1:B:324:LEU:HD23	2.44	0.42
1:A:94[A]:GLN:HG3	4:A:638:HOH:O	2.19	0.42
1:B:170:LEU:HA	1:B:214:SER:O	2.20	0.42
1:B:246:ARG:HD3	1:B:246:ARG:C	2.45	0.41
1:B:326:ARG:HD3	1:B:330:ALA:HB3	2.02	0.41
1:A:43:LYS:NZ	2:A:401:PLP:O3	2.54	0.41
1:A:291:ARG:CG	1:A:291:ARG:NH1	2.83	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	383/390 (98%)	374 (98%)	7 (2%)	2 (0%)	24	8
1	B	393/390 (101%)	384 (98%)	7 (2%)	2 (0%)	24	8
All	All	776/780 (100%)	758 (98%)	14 (2%)	4 (0%)	24	8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ARG
1	B	141	ARG
1	A	236	GLY
1	B	236	GLY

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	285/288 (99%)	282 (99%)	3 (1%)	65	43
1	B	294/288 (102%)	290 (99%)	4 (1%)	59	33
All	All	579/576 (100%)	572 (99%)	7 (1%)	63	40

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	30	ARG

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Mol	Chain	Res	Type
1	A	291	ARG
1	B	153	LEU
1	B	291	ARG
1	B	334	ASP
1	B	337	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	28	GLN
1	A	54	GLN
1	A	116	GLN
1	B	28	GLN
1	B	54	GLN
1	B	94	GLN
1	B	363	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	B	402	-	5,5,5	0.66	0	5,5,5	1.58	1 (20%)
3	GOL	A	402	-	5,5,5	0.92	0	5,5,5	0.56	0
3	GOL	B	403	-	5,5,5	0.96	0	5,5,5	2.36	4 (80%)
2	PLP	A	401	1	15,15,16	2.75	6 (40%)	21,22,23	2.00	6 (28%)
2	PLP	B	401	1	15,15,16	1.99	5 (33%)	21,22,23	1.69	4 (19%)

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	B	402	-	-	0/4/4/4	-
3	GOL	A	402	-	-	0/4/4/4	-
3	GOL	B	403	-	-	0/4/4/4	-
2	PLP	A	401	1	-	0/6/6/8	0/1/1/1
2	PLP	B	401	1	-	0/6/6/8	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PLP	C3-C2	6.48	1.47	1.41
2	A	401	PLP	C5-C4	6.19	1.47	1.40
2	B	401	PLP	C3-C2	3.68	1.44	1.41
2	B	401	PLP	C5-C4	3.28	1.44	1.40
2	A	401	PLP	C4A-C4	-3.17	1.45	1.51
2	B	401	PLP	C3-C4	2.93	1.45	1.40
2	A	401	PLP	O3-C3	-2.84	1.30	1.36
2	B	401	PLP	C4A-C4	-2.80	1.46	1.51
2	A	401	PLP	C3-C4	2.23	1.44	1.40
2	B	401	PLP	O3-C3	-2.18	1.31	1.36
2	A	401	PLP	C6-C5	2.04	1.41	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	PLP	O3P-P-O4P	-3.82	96.71	106.67
2	A	401	PLP	C2A-C2-N1	3.79	124.78	117.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PLP	C6-N1-C2	3.69	125.89	119.20
2	A	401	PLP	O4P-C5A-C5	-3.60	102.61	109.36
2	A	401	PLP	O3P-P-O2P	3.19	119.75	107.80
3	B	403	GOL	C3-C2-C1	-3.14	100.28	111.80
2	A	401	PLP	C2A-C2-C3	-3.10	117.17	120.80
2	B	401	PLP	C6-C5-C4	2.91	120.48	118.10
3	B	403	GOL	O2-C2-C3	2.80	120.78	109.18
2	B	401	PLP	C6-N1-C2	2.38	123.52	119.20
2	A	401	PLP	C3-C2-N1	-2.38	117.96	120.96
3	B	402	GOL	O1-C1-C2	-2.30	100.03	110.38
2	B	401	PLP	O4P-P-O1P	-2.19	100.52	106.44
3	B	403	GOL	O2-C2-C1	-2.10	100.48	109.18
3	B	403	GOL	O3-C3-C2	2.02	119.46	110.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PLP	1	0
2	B	401	PLP	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	379/390 (97%)	-0.56	1 (0%)	90 93	6, 19, 39, 81	6 (1%)
1	B	389/390 (99%)	-0.41	4 (1%)	79 85	8, 21, 45, 75	6 (1%)
All	All	768/780 (98%)	-0.48	5 (0%)	84 89	6, 20, 42, 81	12 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-6	HIS	2.9
1	B	-1	MET	2.5
1	A	147	ASP	2.3
1	B	291	ARG	2.3
1	B	-7	HIS	2.2

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, 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($\text{\AA}^2$)	Q<0.9
3	GOL	B	403	6/6	0.93	0.13	21,24,25,29	6
3	GOL	B	402	6/6	0.95	0.11	29,31,40,44	0
3	GOL	A	402	6/6	0.96	0.07	24,28,32,36	0
2	PLP	B	401	15/16	0.99	0.04	13,15,21,30	0
2	PLP	A	401	15/16	0.99	0.04	14,16,19,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.