Full wwPDB X-ray Structure Validation Report (i)

Dec 23, 2024 – 02:06 PM EST

PDB ID	:	9AZH
Title	:	Native nnhA in P1
Authors	:	Peat, T.S.; Newman, J.
Deposited on	:	2024-03-11
Resolution	:	2.04 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

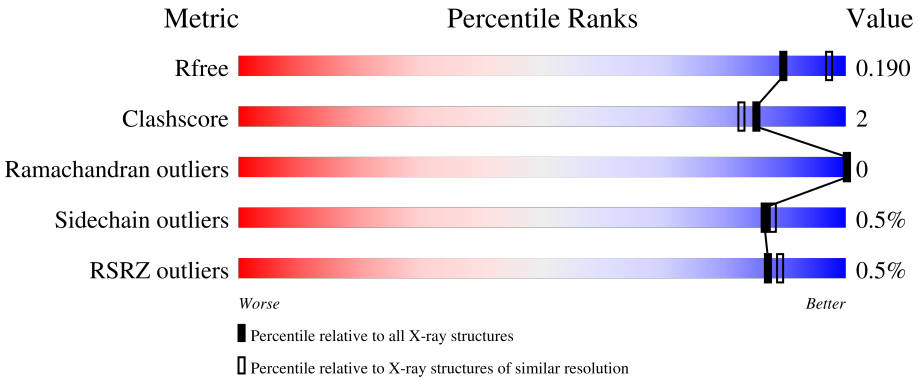
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.04 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}	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	386	89% 6%
1	B	386	2% 90% 5%
1	C	386	90% 5%
1	D	386	90% 5%
1	E	386	90% 6%

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Mol	Chain	Length	Quality of chain
1	F	386	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19372 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 2-nitroimidazole nitrohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	6	0
			2932	1852	511	555	14			
1	B	369	Total	C	N	O	S	0	3	0
			2917	1841	511	551	14			
1	C	369	Total	C	N	O	S	0	8	0
			2960	1865	517	564	14			
1	D	369	Total	C	N	O	S	0	6	0
			2944	1856	514	559	15			
1	E	369	Total	C	N	O	S	0	3	0
			2915	1841	510	549	15			
1	F	369	Total	C	N	O	S	0	6	0
			2942	1854	515	559	14			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP F4ZCI3
A	-5	HIS	-	expression tag	UNP F4ZCI3
A	-4	HIS	-	expression tag	UNP F4ZCI3
A	-3	HIS	-	expression tag	UNP F4ZCI3
A	-2	HIS	-	expression tag	UNP F4ZCI3
A	-1	HIS	-	expression tag	UNP F4ZCI3
A	0	HIS	-	expression tag	UNP F4ZCI3
A	2	ILE	THR	engineered mutation	UNP F4ZCI3
A	14	ASP	GLY	engineered mutation	UNP F4ZCI3
A	73	ARG	LYS	engineered mutation	UNP F4ZCI3
B	-6	MET	-	initiating methionine	UNP F4ZCI3
B	-5	HIS	-	expression tag	UNP F4ZCI3
B	-4	HIS	-	expression tag	UNP F4ZCI3
B	-3	HIS	-	expression tag	UNP F4ZCI3
B	-2	HIS	-	expression tag	UNP F4ZCI3
B	-1	HIS	-	expression tag	UNP F4ZCI3
B	0	HIS	-	expression tag	UNP F4ZCI3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	ILE	THR	engineered mutation	UNP F4ZCI3
B	14	ASP	GLY	engineered mutation	UNP F4ZCI3
B	73	ARG	LYS	engineered mutation	UNP F4ZCI3
C	-6	MET	-	initiating methionine	UNP F4ZCI3
C	-5	HIS	-	expression tag	UNP F4ZCI3
C	-4	HIS	-	expression tag	UNP F4ZCI3
C	-3	HIS	-	expression tag	UNP F4ZCI3
C	-2	HIS	-	expression tag	UNP F4ZCI3
C	-1	HIS	-	expression tag	UNP F4ZCI3
C	0	HIS	-	expression tag	UNP F4ZCI3
C	2	ILE	THR	engineered mutation	UNP F4ZCI3
C	14	ASP	GLY	engineered mutation	UNP F4ZCI3
C	73	ARG	LYS	engineered mutation	UNP F4ZCI3
D	-6	MET	-	initiating methionine	UNP F4ZCI3
D	-5	HIS	-	expression tag	UNP F4ZCI3
D	-4	HIS	-	expression tag	UNP F4ZCI3
D	-3	HIS	-	expression tag	UNP F4ZCI3
D	-2	HIS	-	expression tag	UNP F4ZCI3
D	-1	HIS	-	expression tag	UNP F4ZCI3
D	0	HIS	-	expression tag	UNP F4ZCI3
D	2	ILE	THR	engineered mutation	UNP F4ZCI3
D	14	ASP	GLY	engineered mutation	UNP F4ZCI3
D	73	ARG	LYS	engineered mutation	UNP F4ZCI3
E	-6	MET	-	initiating methionine	UNP F4ZCI3
E	-5	HIS	-	expression tag	UNP F4ZCI3
E	-4	HIS	-	expression tag	UNP F4ZCI3
E	-3	HIS	-	expression tag	UNP F4ZCI3
E	-2	HIS	-	expression tag	UNP F4ZCI3
E	-1	HIS	-	expression tag	UNP F4ZCI3
E	0	HIS	-	expression tag	UNP F4ZCI3
E	2	ILE	THR	engineered mutation	UNP F4ZCI3
E	14	ASP	GLY	engineered mutation	UNP F4ZCI3
E	73	ARG	LYS	engineered mutation	UNP F4ZCI3
F	-6	MET	-	initiating methionine	UNP F4ZCI3
F	-5	HIS	-	expression tag	UNP F4ZCI3
F	-4	HIS	-	expression tag	UNP F4ZCI3
F	-3	HIS	-	expression tag	UNP F4ZCI3
F	-2	HIS	-	expression tag	UNP F4ZCI3
F	-1	HIS	-	expression tag	UNP F4ZCI3
F	0	HIS	-	expression tag	UNP F4ZCI3
F	2	ILE	THR	engineered mutation	UNP F4ZCI3
F	14	ASP	GLY	engineered mutation	UNP F4ZCI3

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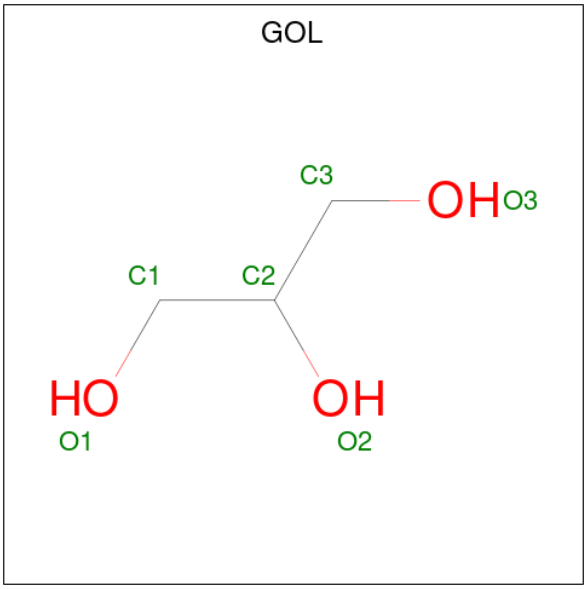
Chain	Residue	Modelled	Actual	Comment	Reference
F	73	ARG	LYS	engineered mutation	UNP F4ZCI3

- 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 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is water.

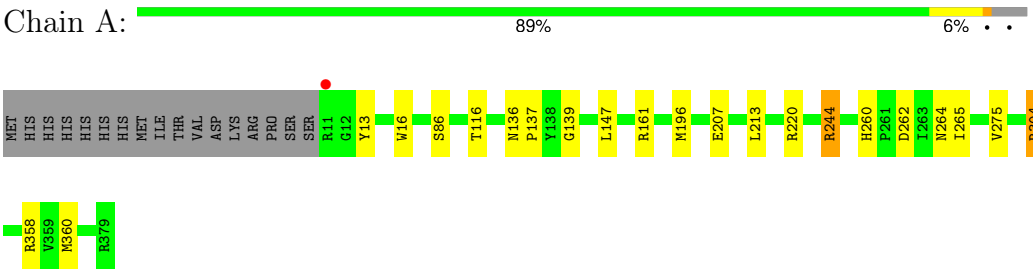
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	323	Total O 323 323	0	0
5	B	270	Total O 270 270	0	0
5	C	292	Total O 292 292	0	0
5	D	303	Total O 303 303	0	0
5	E	242	Total O 242 242	0	0
5	F	303	Total O 303 303	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

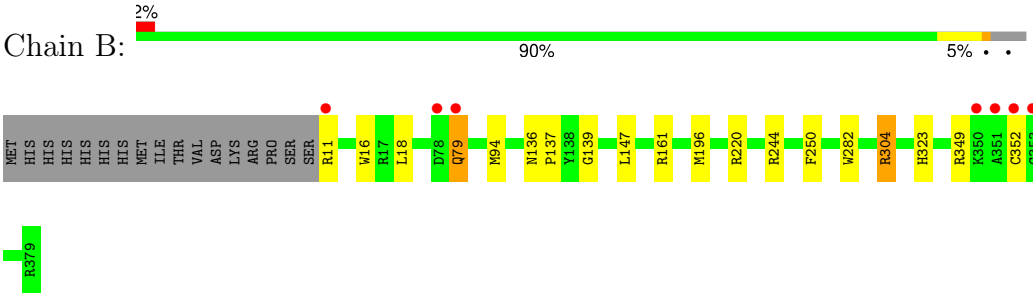
• Molecule 1: 2-nitroimidazole nitrohydrolase

Chain A:



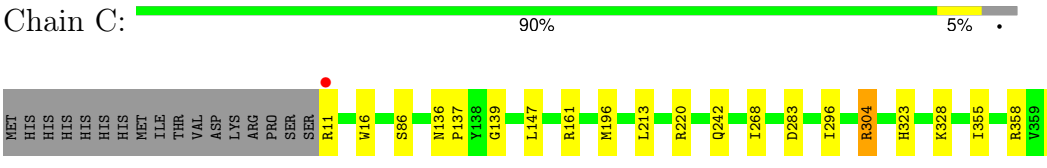
• Molecule 1: 2-nitroimidazole nitrohydrolase

Chain B:



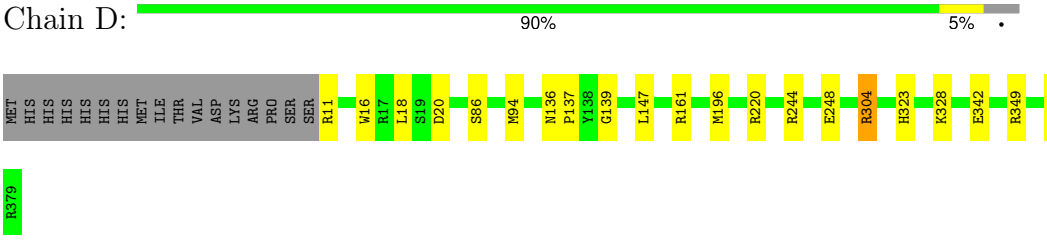
• Molecule 1: 2-nitroimidazole nitrohydrolase

Chain C:



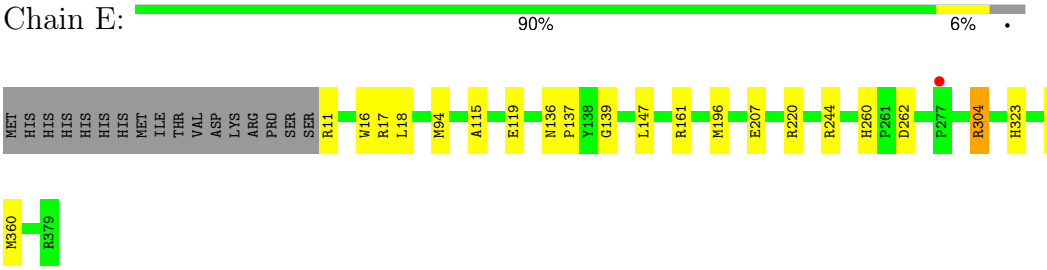
• Molecule 1: 2-nitroimidazole nitrohydrolase

Chain D:



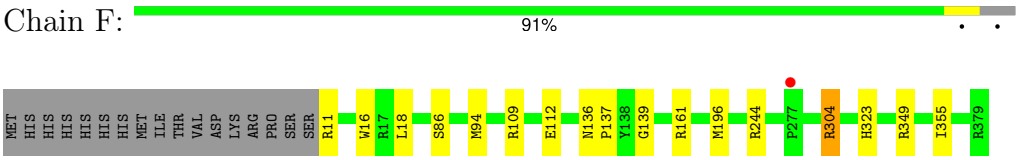
• Molecule 1: 2-nitroimidazole nitrohydrolase

Chain E:



• Molecule 1: 2-nitroimidazole nitrohydrolase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.73Å 117.38Å 121.12Å 117.14° 91.30° 101.38°	Depositor
Resolution (Å)	54.09 – 2.04 54.09 – 2.04	Depositor EDS
% Data completeness (in resolution range)	98.0 (54.09-2.04) 98.0 (54.09-2.04)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.156 , 0.178 0.168 , 0.190	Depositor DCC
R_{free} test set	8787 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	13.9	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19372	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.51	0/3010	0.77	2/4098 (0.0%)
1	B	0.49	0/2992	0.79	2/4071 (0.0%)
1	C	0.47	0/3034	0.76	2/4126 (0.0%)
1	D	0.47	0/3018	0.77	2/4103 (0.0%)
1	E	0.46	0/2993	0.76	5/4072 (0.1%)
1	F	0.49	0/3017	0.78	2/4106 (0.0%)
All	All	0.48	0/18064	0.77	15/24576 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	3
All	All	0	23

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	94	MET	CG-SD-CE	8.29	113.46	100.20
1	A	304	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	F	304	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	D	304	ARG	NE-CZ-NH1	6.37	123.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	304	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	304	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	304	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	E	94[A]	MET	CG-SD-CE	-5.99	90.62	100.20
1	E	94[B]	MET	CG-SD-CE	-5.99	90.62	100.20
1	B	304	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	D	304	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	E	17	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	304	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	E	304	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	304	ARG	NE-CZ-NH1	5.38	122.99	120.30

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ARG	Sidechain
1	A	220	ARG	Sidechain
1	A	244	ARG	Sidechain
1	A	304	ARG	Sidechain
1	B	161	ARG	Sidechain
1	B	220	ARG	Sidechain
1	B	304	ARG	Sidechain
1	B	349	ARG	Sidechain
1	C	161	ARG	Sidechain
1	C	220	ARG	Sidechain
1	C	304	ARG	Sidechain
1	C	379[A]	ARG	Sidechain
1	D	161	ARG	Sidechain
1	D	220	ARG	Sidechain
1	D	304	ARG	Sidechain
1	D	349	ARG	Sidechain
1	E	161	ARG	Sidechain
1	E	220	ARG	Sidechain
1	E	304	ARG	Sidechain
1	E	349	ARG	Sidechain
1	F	161	ARG	Sidechain
1	F	304	ARG	Sidechain
1	F	349	ARG	Sidechain

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	2932	0	2822	15	0
1	B	2917	0	2806	21	0
1	C	2960	0	2836	14	0
1	D	2944	0	2826	15	0
1	E	2915	0	2809	12	0
1	F	2942	0	2820	14	0
2	A	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
2	F	6	0	8	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	323	0	0	3	0
5	B	270	0	0	1	0
5	C	292	0	0	1	0
5	D	303	0	0	3	0
5	E	242	0	0	0	0
5	F	303	0	0	1	0
All	All	19372	0	16951	74	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 (74) 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:262[A]:ASP:OD2	5:A:501:HOH:O	1.70	1.07
1:D:328:LYS:HE3	5:D:697:HOH:O	1.70	0.89
1:F:109[B]:ARG:NH2	1:F:112:GLU:OE2	2.05	0.89
1:B:94:MET:CE	1:B:352:CYS:HB3	2.09	0.83
1:B:94:MET:HE2	1:B:352:CYS:HB3	1.64	0.79
1:B:244:ARG:HD3	1:D:244:ARG:HD3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:ARG:HD3	1:F:244:ARG:HD3	1.64	0.76
1:A:116[B]:THR:HG21	5:A:522:HOH:O	1.89	0.71
1:E:260:HIS:HB3	1:E:262[B]:ASP:OD1	1.92	0.69
1:B:94:MET:HE1	1:B:352:CYS:HB3	1.80	0.64
1:A:260:HIS:HB3	1:A:262[A]:ASP:OD1	1.98	0.64
1:B:11:ARG:NH1	5:B:503:HOH:O	2.30	0.63
1:B:94:MET:CE	1:B:94:MET:HA	2.28	0.63
1:A:265:ILE:HG13	1:A:275[B]:VAL:HG12	1.80	0.62
1:D:20:ASP:OD1	5:D:501:HOH:O	2.17	0.58
1:C:268:ILE:HD11	1:C:296:ILE:HD13	1.85	0.57
1:F:11:ARG:NH1	5:F:504:HOH:O	2.36	0.57
1:B:94:MET:HE3	1:B:250:PHE:CB	2.37	0.55
1:B:94:MET:HE1	1:B:352:CYS:CB	2.36	0.54
1:B:94:MET:HA	1:B:94:MET:HE3	1.92	0.52
1:A:213[A]:LEU:HD21	1:C:283:ASP:OD1	2.10	0.52
1:C:11:ARG:HD2	1:C:16:TRP:CZ2	2.45	0.52
1:D:16:TRP:CD2	1:F:139:GLY:HA2	2.45	0.52
1:D:139:GLY:HA2	1:F:16:TRP:CD2	2.46	0.51
1:C:328:LYS:HE2	5:C:622:HOH:O	2.10	0.51
1:D:11:ARG:HD2	1:D:16:TRP:CZ2	2.45	0.51
1:F:11:ARG:HD2	1:F:16:TRP:CZ2	2.45	0.51
1:E:11:ARG:HD2	1:E:16:TRP:CZ2	2.47	0.50
1:B:11:ARG:HD2	1:B:16:TRP:CZ2	2.47	0.49
1:C:139:GLY:HA2	1:E:16:TRP:CD2	2.47	0.49
1:C:16:TRP:CD2	1:E:139:GLY:HA2	2.48	0.49
1:F:109[B]:ARG:CZ	1:F:112:GLU:OE2	2.62	0.48
1:A:16:TRP:CD2	1:B:139:GLY:HA2	2.49	0.48
1:A:86:SER:HB3	1:B:18:LEU:HD11	1.96	0.47
1:F:136:ASN:HB2	1:F:137:PRO:CD	2.44	0.47
1:E:115:ALA:O	1:E:119:GLU:HG2	2.14	0.47
1:D:18:LEU:HD11	1:F:86:SER:HB3	1.96	0.47
1:F:323:HIS:CE1	1:F:355:ILE:H	2.32	0.47
1:B:323:HIS:CE1	1:B:355:ILE:H	2.33	0.47
1:C:323:HIS:CE1	1:C:355:ILE:H	2.32	0.47
1:F:11:ARG:HD2	1:F:16:TRP:CE2	2.49	0.47
1:D:136:ASN:HB2	1:D:137:PRO:CD	2.46	0.46
1:A:136:ASN:HB2	1:A:137:PRO:CD	2.46	0.46
1:F:109[B]:ARG:NH1	1:F:109[B]:ARG:HG2	2.31	0.46
1:D:86:SER:HB3	1:F:18:LEU:HD11	1.97	0.45
1:E:323:HIS:CE1	1:E:355:ILE:H	2.34	0.45
1:C:136:ASN:HB2	1:C:137:PRO:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:ARG:HD2	1:D:16:TRP:CE2	2.51	0.45
1:D:323:HIS:CE1	1:D:355:ILE:H	2.34	0.45
1:A:139:GLY:HA2	1:B:16:TRP:CD2	2.51	0.45
1:A:323:HIS:CE1	1:A:355:ILE:H	2.34	0.45
1:B:147:LEU:HB3	1:B:360:MET:HB2	1.99	0.45
1:E:136:ASN:HB2	1:E:137:PRO:CD	2.46	0.45
1:A:264[A]:ASN:OD1	5:A:502:HOH:O	2.21	0.44
1:B:136:ASN:HB2	1:B:137:PRO:CD	2.47	0.44
1:C:86:SER:HB3	1:E:18:LEU:HD11	1.99	0.44
1:B:94:MET:HE3	1:B:250:PHE:HB3	1.99	0.44
1:B:11:ARG:HD2	1:B:16:TRP:CE2	2.52	0.44
1:E:11:ARG:HD2	1:E:16:TRP:CE2	2.53	0.44
1:C:11:ARG:HD2	1:C:16:TRP:CE2	2.52	0.44
1:D:342:GLU:OE2	5:D:502:HOH:O	2.21	0.44
1:A:13:TYR:HE2	1:B:79:GLN:OE1	2.01	0.43
1:C:213[B]:LEU:HD11	1:C:242:GLN:OE1	2.18	0.43
1:A:244:ARG:NH1	1:C:283:ASP:OD2	2.53	0.42
1:C:147:LEU:HB3	1:C:360:MET:HB2	2.02	0.42
1:E:147:LEU:HB3	1:E:360:MET:HB2	2.02	0.42
1:E:260:HIS:CB	1:E:262[B]:ASP:OD1	2.65	0.41
1:A:355:ILE:O	1:A:358:ARG:HG2	2.21	0.41
1:B:282:TRP:HZ3	1:D:248:GLU:O	2.03	0.41
1:B:244:ARG:CD	1:D:244:ARG:HD3	2.43	0.41
1:F:109[B]:ARG:HG2	1:F:109[B]:ARG:HH11	1.85	0.41
1:C:355:ILE:O	1:C:358:ARG:HG2	2.21	0.40
1:A:147:LEU:HB3	1:A:360:MET:HB2	2.02	0.40
1:D:147:LEU:HB3	1:D:360:MET:HB2	2.02	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	373/386 (97%)	364 (98%)	9 (2%)	0	100	100
1	B	370/386 (96%)	361 (98%)	9 (2%)	0	100	100
1	C	374/386 (97%)	366 (98%)	8 (2%)	0	100	100
1	D	372/386 (96%)	364 (98%)	8 (2%)	0	100	100
1	E	370/386 (96%)	361 (98%)	9 (2%)	0	100	100
1	F	373/386 (97%)	365 (98%)	8 (2%)	0	100	100
All	All	2232/2316 (96%)	2181 (98%)	51 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	310/321 (97%)	308 (99%)	2 (1%)	84	86
1	B	307/321 (96%)	305 (99%)	2 (1%)	81	83
1	C	312/321 (97%)	311 (100%)	1 (0%)	91	92
1	D	310/321 (97%)	307 (99%)	3 (1%)	73	74
1	E	307/321 (96%)	305 (99%)	2 (1%)	81	83
1	F	310/321 (97%)	309 (100%)	1 (0%)	91	92
All	All	1856/1926 (96%)	1845 (99%)	11 (1%)	86	86

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	MET
1	A	207	GLU
1	B	79	GLN
1	B	196	MET
1	C	196	MET
1	D	94[A]	MET
1	D	94[B]	MET

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Mol	Chain	Res	Type
1	D	196	MET
1	E	196	MET
1	E	207	GLU
1	F	196	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	D	120	ASN

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)

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	GOL	D	401	-	5,5,5	0.19	0	5,5,5	0.43	0
2	GOL	C	401	-	5,5,5	0.15	0	5,5,5	0.29	0
2	GOL	A	401	-	5,5,5	0.16	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	F	401	-	5,5,5	0.15	0	5,5,5	0.27	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
2	GOL	D	401	-	-	2/4/4/4	-
2	GOL	C	401	-	-	2/4/4/4	-
2	GOL	A	401	-	-	4/4/4/4	-
2	GOL	F	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	O1-C1-C2-C3
2	D	401	GOL	O1-C1-C2-C3
2	C	401	GOL	O1-C1-C2-O2
2	A	401	GOL	C1-C2-C3-O3
2	C	401	GOL	O1-C1-C2-C3
2	F	401	GOL	C1-C2-C3-O3
2	A	401	GOL	O2-C2-C3-O3
2	A	401	GOL	O1-C1-C2-O2
2	D	401	GOL	O1-C1-C2-O2
2	F	401	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	369/386 (95%)	-0.64	1 (0%) 90 92	5, 11, 21, 51	6 (1%)
1	B	369/386 (95%)	-0.45	7 (1%) 66 69	5, 14, 31, 47	3 (0%)
1	C	369/386 (95%)	-0.58	1 (0%) 90 92	5, 13, 25, 51	8 (2%)
1	D	369/386 (95%)	-0.55	0 100 100	5, 13, 23, 43	6 (1%)
1	E	369/386 (95%)	-0.35	1 (0%) 90 92	8, 16, 32, 43	3 (0%)
1	F	369/386 (95%)	-0.59	1 (0%) 90 92	6, 12, 23, 43	6 (1%)
All	All	2214/2316 (95%)	-0.52	11 (0%) 87 89	5, 13, 27, 51	32 (1%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	277	PRO	4.8
1	B	352	CYS	4.3
1	B	79	GLN	2.6
1	B	353	GLY	2.5
1	F	277	PRO	2.5
1	B	351	ALA	2.3
1	B	350	LYS	2.1
1	A	11	ARG	2.1
1	B	78	ASP	2.1
1	C	11	ARG	2.1
1	B	11	ARG	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	C	401	6/6	0.79	0.19	45,47,48,48	0
2	GOL	A	401	6/6	0.80	0.16	45,46,47,48	0
2	GOL	F	401	6/6	0.82	0.17	37,39,40,40	0
2	GOL	D	401	6/6	0.83	0.16	40,42,46,46	0
3	NA	B	401	1/1	0.91	0.15	44,44,44,44	0
3	NA	A	402	1/1	0.98	0.08	26,26,26,26	0
3	NA	C	402	1/1	0.99	0.09	23,23,23,23	0
4	CL	C	403	1/1	0.99	0.04	19,19,19,19	0
4	CL	D	402	1/1	0.99	0.03	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.