



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 07:05 AM GMT

PDB ID : 2O7E
Title : Tyrosine ammonia-lyase from Rhodobacter sphaeroides (His89Phe variant),
bound to 2-aminoindan-2-phosphonicacid
Authors : Louie, G.V.; Bowman, M.E.; Moffitt, M.C.; Baiga, T.J.; Moore, B.S.; Noel,
J.P.
Deposited on : 2006-12-11
Resolution : 1.75 Å(reported)

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

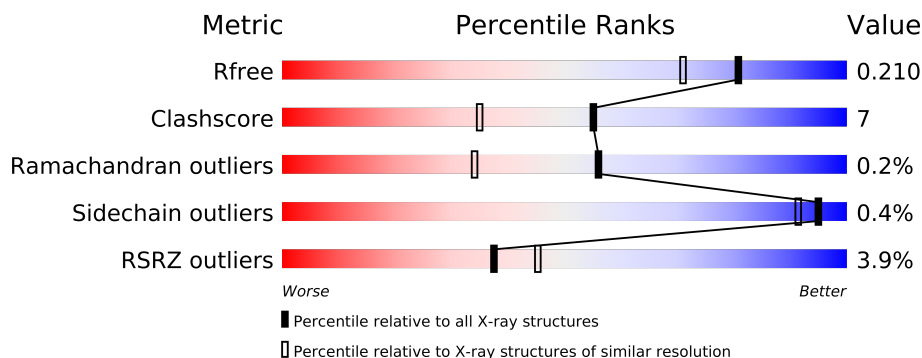
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1134 (1.76-1.76)
Clashscore	79885	1304 (1.76-1.76)
Ramachandran outliers	78287	1288 (1.76-1.76)
Sidechain outliers	78261	1288 (1.76-1.76)
RSRZ outliers	66119	1135 (1.76-1.76)

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

Mol	Chain	Length	Quality of chain
1	A	521	
1	B	521	
1	C	521	
1	D	521	
1	E	521	
1	F	521	
1	G	521	
1	H	521	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33671 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative histidine ammonia-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			3814	2366	729	705	14			
1	B	515	Total	C	N	O	S	0	0	0
			3814	2366	729	705	14			
1	C	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			
1	D	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			
1	E	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			
1	F	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			
1	G	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			
1	H	514	Total	C	N	O	S	0	0	0
			3807	2361	728	704	14			

There are 32 discrepancies between the modelled and reference sequences:

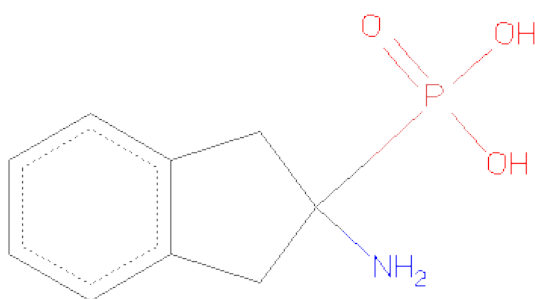
Chain	Residue	Modelled	Actual	Comment	Reference
A	89	PHE	HIS	ENGINEERED	UNP Q3IWB0
A	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
A	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
A	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
B	89	PHE	HIS	ENGINEERED	UNP Q3IWB0
B	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
B	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
B	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
C	89	PHE	HIS	ENGINEERED	UNP Q3IWB0
C	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
C	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
C	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
D	89	PHE	HIS	ENGINEERED	UNP Q3IWB0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
D	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
D	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
E	89	PHE	HIS	ENGINEERED	UNP Q3IWB0
E	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
E	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
E	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
F	89	PHE	HIS	ENGINEERED	UNP Q3IWB0
F	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
F	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
F	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
G	89	PHE	HIS	ENGINEERED	UNP Q3IWB0
G	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
G	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
G	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
H	89	PHE	HIS	ENGINEERED	UNP Q3IWB0
H	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
H	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
H	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0

- Molecule 2 is (2-AMINO-2,3-DIHYDRO-1H-INDEN-2-YL)PHOSPHONICACID (three-letter code: PMI) (formula: C₉H₁₂NO₃P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			14	9	1	3	1		

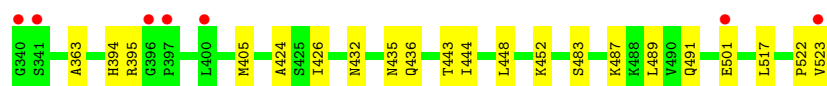
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			14	9	1	3	1		
2	C	1	Total	C	N	O	P	0	0
			14	9	1	3	1		
2	D	1	Total	C	N	O	P	0	0
			14	9	1	3	1		
2	E	1	Total	C	N	O	P	0	0
			14	9	1	3	1		
2	F	1	Total	C	N	O	P	0	0
			14	9	1	3	1		
2	G	1	Total	C	N	O	P	0	0
			14	9	1	3	1		
2	H	1	Total	C	N	O	P	0	0
			14	9	1	3	1		

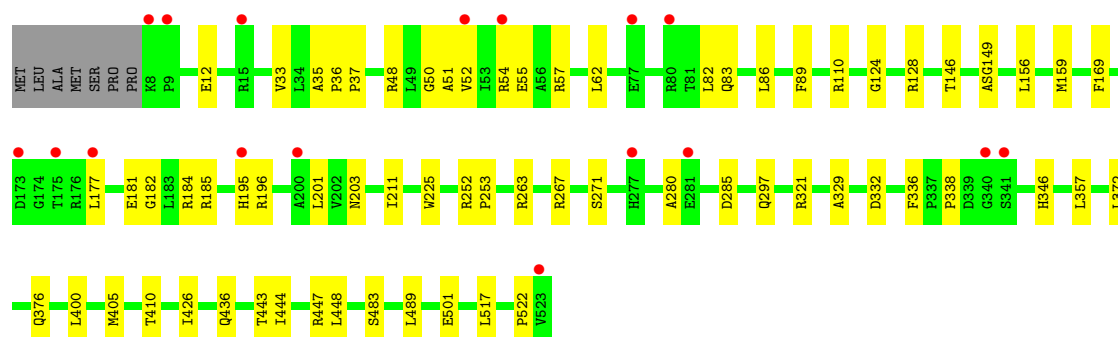
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	325	Total	O	0	0
			325	325		
3	B	373	Total	O	0	0
			373	373		
3	C	414	Total	O	0	0
			414	414		
3	D	355	Total	O	0	0
			355	355		
3	E	380	Total	O	0	0
			380	380		
3	F	479	Total	O	0	0
			479	479		
3	G	413	Total	O	0	0
			413	413		
3	H	350	Total	O	0	0
			350	350		



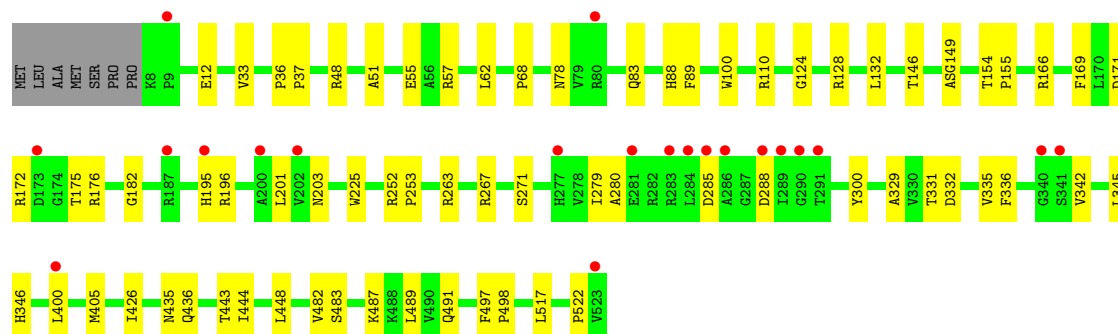
● Molecule 1: Putative histidine ammonia-lyase

Chain D:



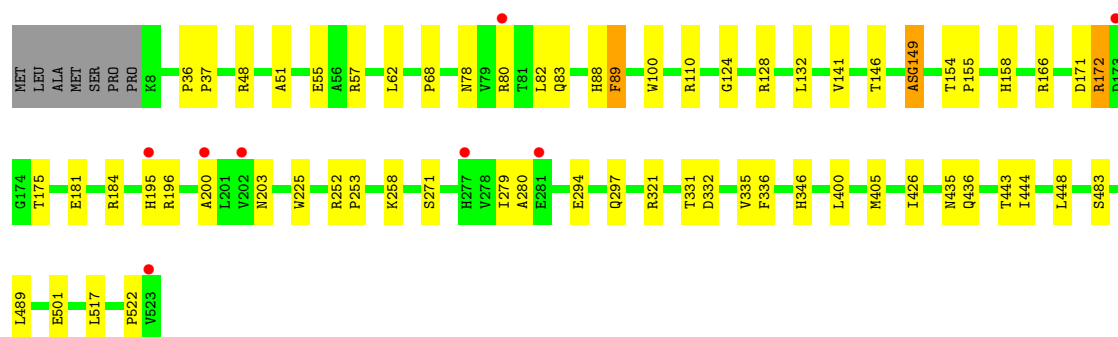
● Molecule 1: Putative histidine ammonia-lyase

Chain E:



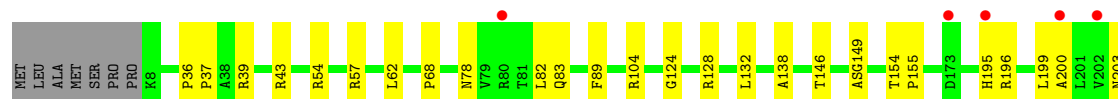
● Molecule 1: Putative histidine ammonia-lyase

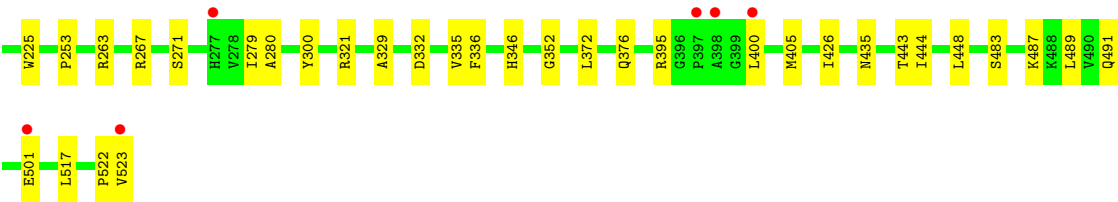
Chain F:



● Molecule 1: Putative histidine ammonia-lyase

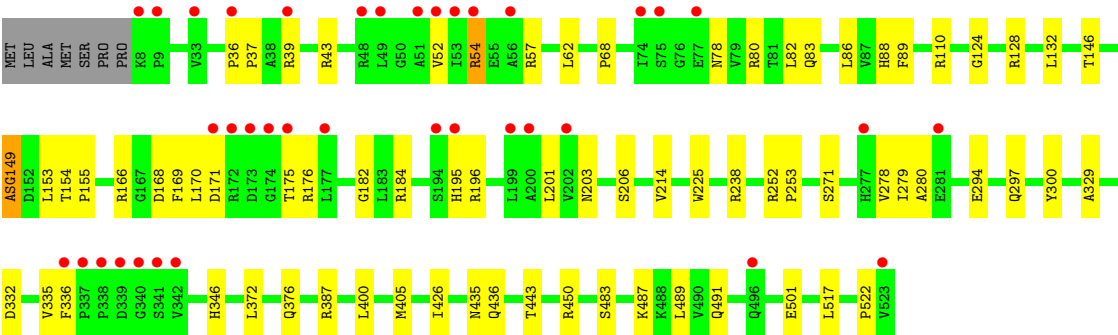
Chain G:





● Molecule 1: Putative histidine ammonia-lyase

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.57Å 154.84Å 164.53Å 90.00° 94.16° 90.00°	Depositor
Resolution (Å)	500.00 – 1.75 37.68 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.4 (500.00-1.75) 96.3 (37.68-1.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.75Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.189 , 0.210 0.189 , 0.210	Depositor DCC
R_{free} test set	21241 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 422368 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33671	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.31	0/3863	0.58	0/5254
1	B	0.31	0/3863	0.58	0/5254
1	C	0.31	0/3855	0.59	0/5243
1	D	0.31	0/3855	0.58	0/5243
1	E	0.31	0/3855	0.58	0/5243
1	F	0.34	0/3855	0.60	0/5243
1	G	0.33	0/3855	0.60	0/5243
1	H	0.30	0/3855	0.57	0/5243
All	All	0.31	0/30856	0.58	0/41966

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	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
All	All	0	16

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	MDO	Mainchain,Peptide
1	B	149	MDO	Mainchain,Peptide
1	C	149	MDO	Mainchain,Peptide
1	D	149	MDO	Mainchain,Peptide
1	E	149	MDO	Mainchain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3814	0	3864	59	0
1	B	3814	0	3865	56	0
1	C	3807	0	3857	64	0
1	D	3807	0	3856	54	0
1	E	3807	0	3857	51	0
1	F	3807	0	3857	57	0
1	G	3807	0	3856	50	0
1	H	3807	0	3857	69	0
2	A	14	0	9	2	0
2	B	14	0	9	3	0
2	C	14	0	9	3	0
2	D	14	0	9	0	0
2	E	14	0	9	2	0
2	F	14	0	9	2	0
2	G	14	0	9	2	0
2	H	14	0	9	3	0
3	A	325	0	0	9	0
3	B	373	0	0	7	0
3	C	414	0	0	12	0
3	D	355	0	0	4	0
3	E	380	0	0	5	0
3	F	479	0	0	11	0
3	G	413	0	0	8	0
3	H	350	0	0	9	0
All	All	33671	0	30941	412	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 412 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:83:GLN:HE22	1:H:196:ARG:HA	1.17	1.08
1:A:83:GLN:HE22	1:A:196:ARG:HA	1.21	1.02
1:B:83:GLN:HE22	1:B:196:ARG:HA	1.25	0.97
1:F:200:ALA:HB2	3:F:3012:HOH:O	1.64	0.97
1:G:83:GLN:HE22	1:G:196:ARG:HA	1.28	0.96

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	512/521 (98%)	499 (98%)	11 (2%)	2 (0%)	43	21
1	B	512/521 (98%)	504 (98%)	7 (1%)	1 (0%)	56	34
1	C	511/521 (98%)	504 (99%)	6 (1%)	1 (0%)	56	34
1	D	511/521 (98%)	503 (98%)	7 (1%)	1 (0%)	56	34
1	E	511/521 (98%)	502 (98%)	8 (2%)	1 (0%)	56	34
1	F	511/521 (98%)	503 (98%)	7 (1%)	1 (0%)	56	34
1	G	511/521 (98%)	505 (99%)	5 (1%)	1 (0%)	56	34
1	H	511/521 (98%)	499 (98%)	11 (2%)	1 (0%)	56	34
All	All	4090/4168 (98%)	4019 (98%)	62 (2%)	9 (0%)	56	34

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	253	PRO
1	E	253	PRO
1	A	8	LYS
1	A	253	PRO
1	H	253	PRO

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	384/389 (99%)	383 (100%)	1 (0%)	96	93
1	B	384/389 (99%)	383 (100%)	1 (0%)	96	93
1	C	383/389 (98%)	381 (100%)	2 (0%)	94	88
1	D	383/389 (98%)	382 (100%)	1 (0%)	96	93
1	E	383/389 (98%)	382 (100%)	1 (0%)	96	93
1	F	383/389 (98%)	380 (99%)	3 (1%)	89	80
1	G	383/389 (98%)	382 (100%)	1 (0%)	96	93
1	H	383/389 (98%)	381 (100%)	2 (0%)	94	88
All	All	3066/3112 (98%)	3054 (100%)	12 (0%)	95	91

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	443	THR
1	F	89	PHE
1	G	443	THR
1	D	443	THR
1	F	443	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	491	GLN
1	E	394	HIS
1	H	394	HIS
1	E	83	GLN
1	E	189	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

8 non-standard protein/DNA/RNA residues 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$
1	MDO	A	149	1,2	13,13,14	5.67	7 (53%)	16,18,20	2.13	7 (43%)
1	MDO	B	149	1,2	13,13,14	5.74	8 (61%)	16,18,20	2.11	7 (43%)
1	MDO	C	149	1,2	13,13,14	5.94	8 (61%)	16,18,20	1.96	7 (43%)
1	MDO	D	149	1,2	13,13,14	5.62	7 (53%)	16,18,20	2.01	7 (43%)
1	MDO	E	149	1,2	13,13,14	5.56	7 (53%)	16,18,20	2.06	7 (43%)
1	MDO	F	149	1,2	13,13,14	5.60	8 (61%)	16,18,20	2.05	7 (43%)
1	MDO	G	149	1,2	13,13,14	5.78	8 (61%)	16,18,20	2.10	7 (43%)
1	MDO	H	149	1,2	13,13,14	5.82	8 (61%)	16,18,20	2.02	7 (43%)

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
1	MDO	A	149	1,2	-	0/4/23/24	0/1/1/1
1	MDO	B	149	1,2	-	0/4/23/24	0/1/1/1
1	MDO	C	149	1,2	-	0/4/23/24	0/1/1/1
1	MDO	D	149	1,2	-	0/4/23/24	0/1/1/1
1	MDO	E	149	1,2	-	0/4/23/24	0/1/1/1
1	MDO	F	149	1,2	-	0/4/23/24	0/1/1/1
1	MDO	G	149	1,2	-	0/4/23/24	0/1/1/1
1	MDO	H	149	1,2	-	0/4/23/24	0/1/1/1

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	149	MDO	O-C	17.79	1.23	1.11
1	H	149	MDO	O-C	17.51	1.23	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	149	MDO	O-C	17.15	1.23	1.11
1	G	149	MDO	O-C	17.13	1.23	1.11
1	B	149	MDO	O-C	17.03	1.23	1.11

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	MDO	O2-C2-CA2	-4.70	128.24	130.96
1	F	149	MDO	O2-C2-CA2	-4.68	128.25	130.96
1	B	149	MDO	O2-C2-CA2	-4.16	128.55	130.96
1	G	149	MDO	O2-C2-CA2	-4.11	128.58	130.96
1	H	149	MDO	O2-C2-CA2	-3.92	128.69	130.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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	$\# Z > 2$
2	PMI	A	701	1	15,15,15	1.88	2 (13%)	24,24,24	1.55	4 (16%)
2	PMI	B	701	1	15,15,15	1.87	2 (13%)	24,24,24	1.56	3 (12%)
2	PMI	C	701	1	15,15,15	1.85	1 (6%)	24,24,24	1.53	4 (16%)
2	PMI	D	701	1	15,15,15	1.87	1 (6%)	24,24,24	1.48	2 (8%)
2	PMI	E	701	1	15,15,15	1.82	1 (6%)	24,24,24	1.57	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PMI	F	701	1	15,15,15	1.90	2 (13%)	24,24,24	1.53	4 (16%)
2	PMI	G	701	1	15,15,15	1.83	1 (6%)	24,24,24	1.53	3 (12%)
2	PMI	H	701	1	15,15,15	1.84	1 (6%)	24,24,24	1.46	3 (12%)

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	PMI	A	701	1	-	0/9/19/19	0/0/2/2
2	PMI	B	701	1	-	0/9/19/19	0/0/2/2
2	PMI	C	701	1	-	0/9/19/19	0/0/2/2
2	PMI	D	701	1	-	0/9/19/19	0/0/2/2
2	PMI	E	701	1	-	0/9/19/19	0/0/2/2
2	PMI	F	701	1	-	0/9/19/19	0/0/2/2
2	PMI	G	701	1	-	0/9/19/19	0/0/2/2
2	PMI	H	701	1	-	0/9/19/19	0/0/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	PMI	C1'-C2'	5.95	1.49	1.39
2	B	701	PMI	C1'-C2'	5.91	1.49	1.39
2	F	701	PMI	C1'-C2'	5.86	1.49	1.39
2	C	701	PMI	C1'-C2'	5.76	1.49	1.39
2	E	701	PMI	C1'-C2'	5.75	1.49	1.39

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	PMI	C7'-C8'-C9'	4.58	110.52	104.22
2	B	701	PMI	C7'-C8'-C9'	4.54	110.47	104.22
2	E	701	PMI	C7'-C8'-C9'	4.53	110.45	104.22
2	F	701	PMI	C7'-C8'-C9'	4.46	110.35	104.22
2	G	701	PMI	C7'-C8'-C9'	4.44	110.33	104.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	515/521 (98%)	0.35	32 (6%)	20	26	12, 21, 41, 56	0
1	B	515/521 (98%)	0.21	20 (3%)	37	45	9, 18, 37, 52	0
1	C	514/521 (98%)	0.08	13 (2%)	54	65	9, 17, 33, 46	0
1	D	514/521 (98%)	0.19	17 (3%)	44	53	8, 19, 39, 52	0
1	E	514/521 (98%)	0.12	21 (4%)	35	43	9, 17, 36, 62	0
1	F	514/521 (98%)	-0.02	8 (1%)	68	79	7, 14, 29, 41	0
1	G	514/521 (98%)	0.03	11 (2%)	60	72	7, 16, 31, 46	0
1	H	514/521 (98%)	0.30	37 (7%)	15	21	8, 19, 40, 55	0
All	All	4114/4168 (98%)	0.16	159 (3%)	37	45	7, 18, 37, 62	0

The worst 5 of 159 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	523	VAL	9.2
1	E	523	VAL	8.8
1	D	523	VAL	8.6
1	G	523	VAL	8.5
1	H	523	VAL	8.3

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	MDO	B	149	13/14	0.15	0.68	16,19,23,26	0
1	MDO	H	149	13/14	0.14	0.44	16,19,26,26	0
1	MDO	C	149	13/14	0.12	0.09	13,14,18,19	0
1	MDO	A	149	13/14	0.14	-0.08	15,18,21,21	0
1	MDO	G	149	13/14	0.12	-0.17	13,14,17,19	0
1	MDO	F	149	13/14	0.11	-0.18	12,15,20,21	0
1	MDO	E	149	13/14	0.11	-0.20	12,14,18,18	0
1	MDO	D	149	13/14	0.10	-0.66	18,20,22,24	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	PMI	F	701	14/14	0.14	0.99	21,25,27,28	0
2	PMI	E	701	14/14	0.12	0.80	20,24,26,27	0
2	PMI	H	701	14/14	0.14	0.62	25,31,32,33	0
2	PMI	B	701	14/14	0.13	0.58	26,29,31,31	0
2	PMI	C	701	14/14	0.12	0.33	19,22,23,23	0
2	PMI	A	701	14/14	0.12	0.02	23,26,28,29	0
2	PMI	G	701	14/14	0.10	-0.21	21,22,23,24	0
2	PMI	D	701	14/14	0.10	-0.49	26,27,29,32	0

6.5 Other polymers

There are no such residues in this entry.