



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 10:13 PM GMT

PDB ID : 2O6Y
Title : Tyrosine ammonia-lyase from Rhodobacter sphaeroides
Authors : Louie, G.V.; Bowman, M.E.; Moffitt, M.C.; Baiga, T.J.; Moore, B.S.; Noel, J.P.
Deposited on : 2006-12-09
Resolution : 1.50 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>

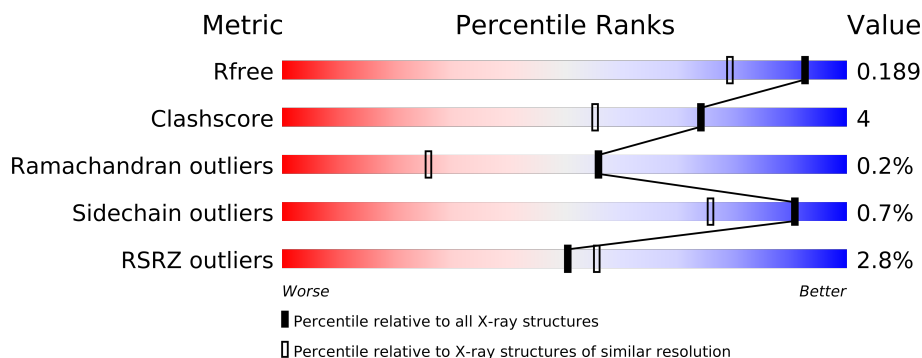
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1513 (1.50-1.50)
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)
RSRZ outliers	66119	1514 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 2 unique types of molecules in this entry. The entry contains 34467 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
			3813	2363	731	705	14			
1	B	515	Total	C	N	O	S	0	0	0
			3813	2363	731	705	14			
1	C	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			
1	D	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			
1	E	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			
1	F	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			
1	G	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			
1	H	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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	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	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
E	149	MDO	GLY	SEE REMARK 999	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	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	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 water.

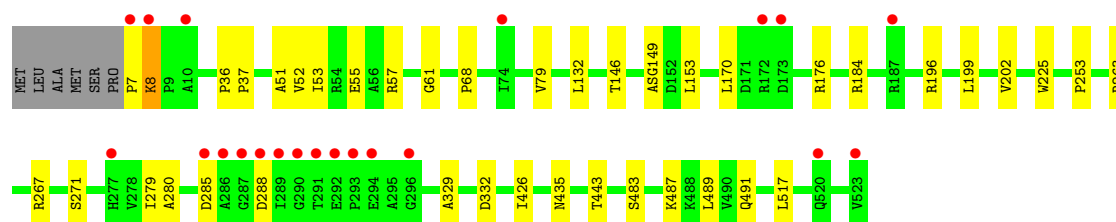
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	458	Total O 458 458	0	0
2	B	487	Total O 487 487	0	0
2	C	496	Total O 496 496	0	0
2	D	494	Total O 494 494	0	0
2	E	498	Total O 498 498	0	0
2	F	586	Total O 586 586	0	0
2	G	523	Total O 523 523	0	0
2	H	463	Total O 463 463	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

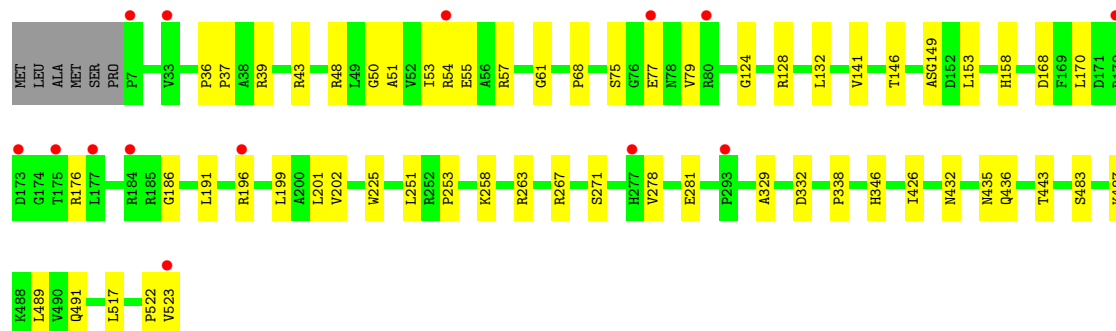
- Molecule 1: Putative histidine ammonia-lyase

Chain A: 



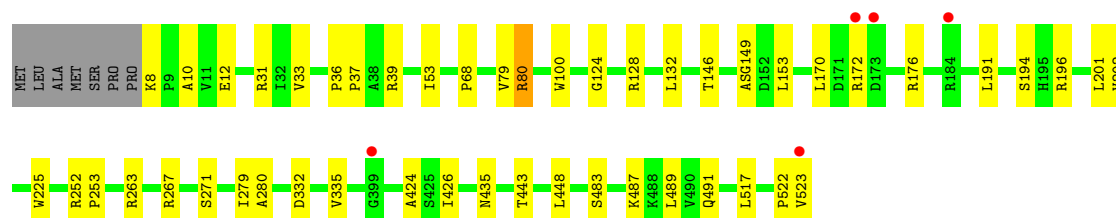
- Molecule 1: Putative histidine ammonia-lyase

Chain B: 



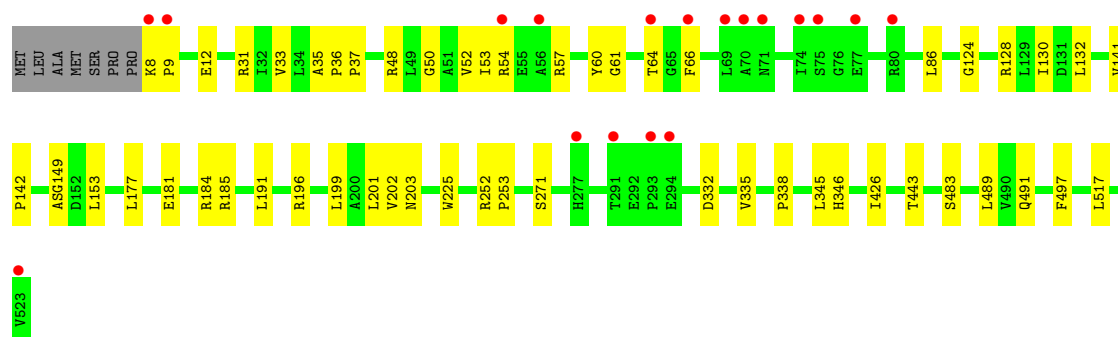
- Molecule 1: Putative histidine ammonia-lyase

Chain C: 



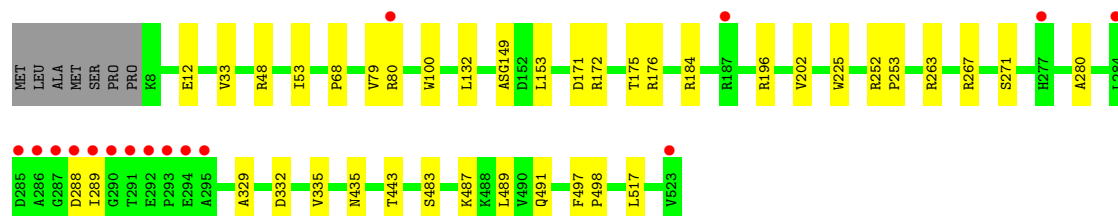
- Molecule 1: Putative histidine ammonia-lyase

Chain D: 



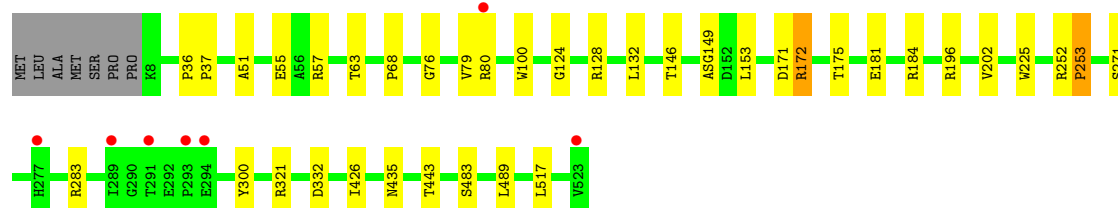
- Molecule 1: Putative histidine ammonia-lyase

Chain E:



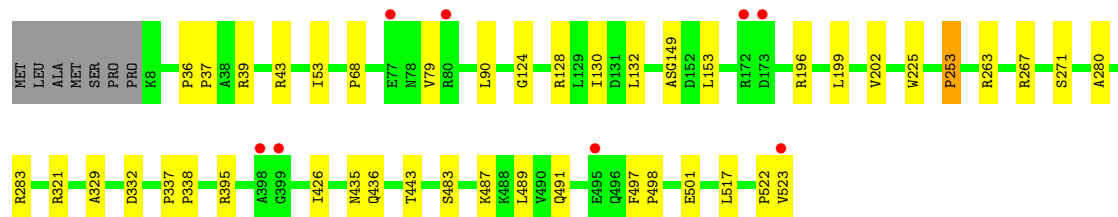
- Molecule 1: Putative histidine ammonia-lyase

Chain F:



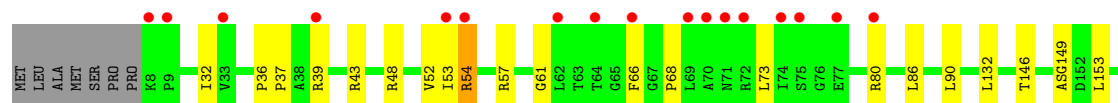
- Molecule 1: Putative histidine ammonia-lyase

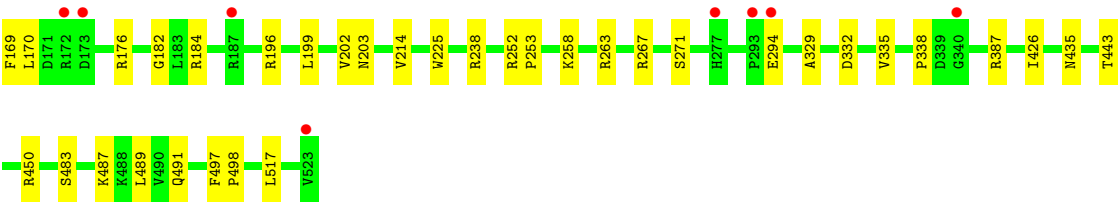
Chain G:



- 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	87.92Å 155.63Å 164.35Å 90.00° 94.13° 90.00°	Depositor
Resolution (Å)	500.00 – 1.50 25.78 – 1.50	Depositor EDS
% Data completeness (in resolution range)	0.9 (500.00-1.50) 93.2 (25.78-1.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.174 , 0.189 0.174 , 0.189	Depositor DCC
R_{free} test set	32530 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 652351 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	34467	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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

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	0/3862	0.54	0/5253
1	B	0.25	0/3862	0.54	0/5253
1	C	0.26	0/3854	0.55	0/5242
1	D	0.25	0/3854	0.55	0/5242
1	E	0.25	0/3854	0.55	0/5242
1	F	0.26	0/3854	0.57	1/5242 (0.0%)
1	G	0.26	0/3854	0.57	1/5242 (0.0%)
1	H	0.24	0/3854	0.54	0/5242
All	All	0.25	0/30848	0.55	2/41958 (0.0%)

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.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	253	PRO	N-CA-C	5.20	125.62	112.10
1	G	253	PRO	N-CA-C	5.02	125.15	112.10

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	3813	0	3864	25	0
1	B	3813	0	3864	39	0
1	C	3806	0	3856	35	0
1	D	3806	0	3856	34	0
1	E	3806	0	3856	29	0
1	F	3806	0	3856	27	0
1	G	3806	0	3856	28	0
1	H	3806	0	3856	48	0
2	A	458	0	0	3	0
2	B	487	0	0	5	0
2	C	496	0	0	4	0
2	D	494	0	0	4	0
2	E	498	0	0	7	0
2	F	586	0	0	6	0
2	G	523	0	0	4	0
2	H	463	0	0	5	0
All	All	34467	0	30864	250	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 4.

The worst 5 of 250 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:153:LEU:HD22	1:D:202:VAL:HG12	1.63	0.80
1:B:53:ILE:HG21	1:B:196:ARG:HH11	1.44	0.80
1:H:53:ILE:HG21	1:H:196:ARG:HH11	1.47	0.79
1:H:153:LEU:HD22	1:H:202:VAL:HG12	1.65	0.78
1:E:153:LEU:HD22	1:E:202:VAL:HG12	1.70	0.73

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%)	504 (98%)	6 (1%)	2 (0%)	43	15
1	B	512/521 (98%)	507 (99%)	4 (1%)	1 (0%)	56	26
1	C	511/521 (98%)	506 (99%)	4 (1%)	1 (0%)	56	26
1	D	511/521 (98%)	504 (99%)	6 (1%)	1 (0%)	56	26
1	E	511/521 (98%)	504 (99%)	6 (1%)	1 (0%)	56	26
1	F	511/521 (98%)	504 (99%)	6 (1%)	1 (0%)	56	26
1	G	511/521 (98%)	506 (99%)	4 (1%)	1 (0%)	56	26
1	H	511/521 (98%)	504 (99%)	6 (1%)	1 (0%)	56	26
All	All	4090/4168 (98%)	4039 (99%)	42 (1%)	9 (0%)	56	26

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	253	PRO
1	E	253	PRO
1	B	253	PRO
1	C	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%)	382 (100%)	2 (0%)	94	83
1	B	384/389 (99%)	382 (100%)	2 (0%)	94	83
1	C	383/389 (98%)	380 (99%)	3 (1%)	89	73
1	D	383/389 (98%)	381 (100%)	2 (0%)	94	83
1	E	383/389 (98%)	381 (100%)	2 (0%)	94	83
1	F	383/389 (98%)	380 (99%)	3 (1%)	89	73
1	G	383/389 (98%)	381 (100%)	2 (0%)	94	83
1	H	383/389 (98%)	379 (99%)	4 (1%)	85	65
All	All	3066/3112 (98%)	3046 (99%)	20 (1%)	91	76

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	332	ASP
1	E	443	THR
1	H	32	ILE
1	D	332	ASP
1	D	443	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	496	GLN
1	E	189	GLN
1	G	394	HIS
1	D	394	HIS
1	D	491	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	13,13,14	6.01	8 (61%)	16,18,20	2.36	6 (37%)
1	MDO	B	149	1	13,13,14	6.05	8 (61%)	16,18,20	2.32	6 (37%)
1	MDO	C	149	1	13,13,14	6.05	8 (61%)	16,18,20	2.38	6 (37%)
1	MDO	D	149	1	13,13,14	5.98	8 (61%)	16,18,20	2.35	6 (37%)
1	MDO	E	149	1	13,13,14	6.07	8 (61%)	16,18,20	2.40	6 (37%)
1	MDO	F	149	1	13,13,14	5.90	8 (61%)	16,18,20	2.41	7 (43%)
1	MDO	G	149	1	13,13,14	6.04	8 (61%)	16,18,20	2.42	7 (43%)
1	MDO	H	149	1	13,13,14	6.08	8 (61%)	16,18,20	2.31	6 (37%)

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

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	149	MDO	O-C	18.02	1.23	1.11
1	H	149	MDO	O-C	18.02	1.23	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	149	MDO	O-C	17.94	1.23	1.11
1	B	149	MDO	O-C	17.85	1.23	1.11
1	A	149	MDO	O-C	17.75	1.23	1.11

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	149	MDO	O2-C2-CA2	-5.04	128.04	130.96
1	E	149	MDO	O2-C2-CA2	-5.00	128.07	130.96
1	F	149	MDO	O2-C2-CA2	-4.96	128.09	130.96
1	A	149	MDO	O2-C2-CA2	-4.78	128.19	130.96
1	C	149	MDO	O2-C2-CA2	-4.68	128.25	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

There are no ligands in this entry.

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%)	0.11	21 (4%) 35 39	8, 16, 34, 53	0
1	B	515/521 (98%)	-0.01	14 (2%) 52 58	7, 15, 31, 48	0
1	C	514/521 (98%)	-0.15	5 (0%) 79 86	7, 13, 28, 41	0
1	D	514/521 (98%)	0.01	18 (3%) 42 45	6, 14, 34, 48	0
1	E	514/521 (98%)	-0.02	16 (3%) 47 51	7, 14, 31, 59	0
1	F	514/521 (98%)	-0.27	7 (1%) 72 79	6, 11, 25, 37	0
1	G	514/521 (98%)	-0.18	8 (1%) 68 75	6, 12, 26, 39	0
1	H	514/521 (98%)	0.14	25 (4%) 28 32	7, 16, 36, 52	0
All	All	4114/4168 (98%)	-0.04	114 (2%) 50 56	6, 14, 31, 59	0

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	74	ILE	8.6
1	A	7	PRO	8.5
1	H	523	VAL	7.6
1	H	74	ILE	7.6
1	A	286	ALA	7.4

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	E	149	13/14	0.11	4.37	11,12,16,22	0
1	MDO	G	149	13/14	0.09	4.33	9,11,15,21	0
1	MDO	F	149	13/14	0.10	2.73	9,11,17,23	0
1	MDO	C	149	13/14	0.09	2.56	10,11,18,21	0
1	MDO	A	149	13/14	0.09	2.24	11,13,20,21	0
1	MDO	H	149	13/14	0.10	1.69	12,15,21,23	0
1	MDO	D	149	13/14	0.10	1.47	14,16,20,21	0
1	MDO	B	149	13/14	0.09	1.36	12,14,20,24	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.