



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2024 – 07:37 PM EDT

PDB ID : 4R5Z
Title : Crystal structure of Rv3772 encoded aminotransferase
Authors : Nasir, N.; Anant, A.; Vyas, R.; Biswal, B.K.
Deposited on : 2014-08-22
Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

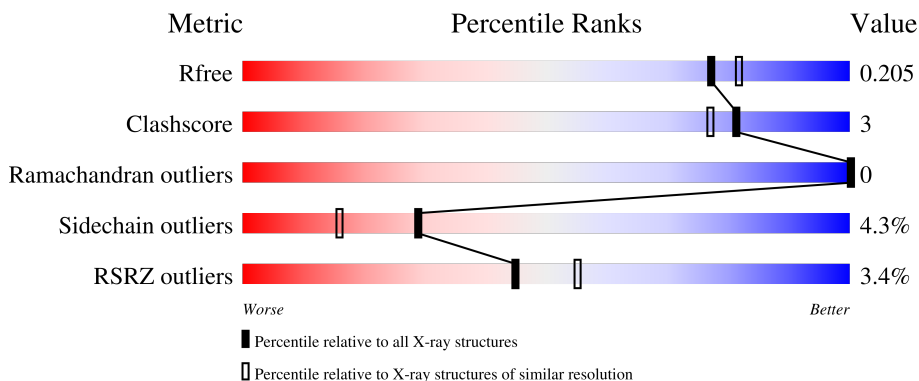
1 Overall quality at a glance

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 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	367	 2% 88% 8% .
1	B	367	 3% 87% 8% . .
1	C	367	 4% 89% 7% .
1	D	367	 4% 87% 8% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PMP	C	402	-	-	X	-

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 12296 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 Putative phenylalanine aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	353	2706	1722	483	495	6	0	4	0
1	B	353	2691	1710	481	494	6	0	1	0
1	C	353	2691	1710	481	494	6	0	1	0
1	D	353	2689	1709	479	495	6	0	1	0

There are 60 discrepancies between the modelled and reference sequences:

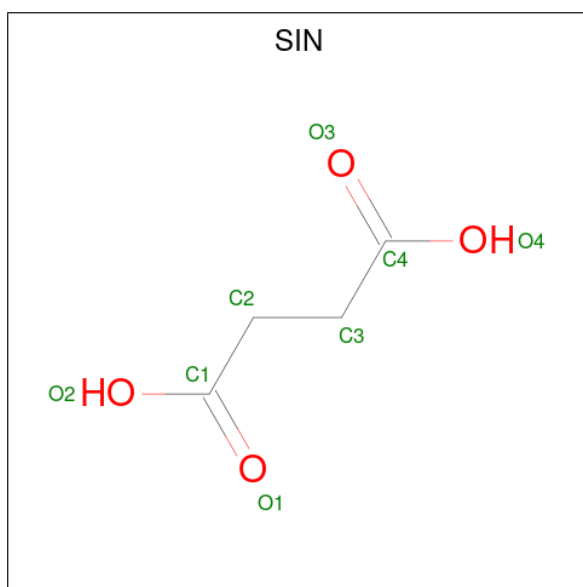
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP I6Y4H4
A	1	VAL	-	expression tag	UNP I6Y4H4
A	354	LYS	-	expression tag	UNP I6Y4H4
A	355	LEU	-	expression tag	UNP I6Y4H4
A	356	ALA	-	expression tag	UNP I6Y4H4
A	357	ALA	-	expression tag	UNP I6Y4H4
A	358	ALA	-	expression tag	UNP I6Y4H4
A	359	LEU	-	expression tag	UNP I6Y4H4
A	360	GLU	-	expression tag	UNP I6Y4H4
A	361	HIS	-	expression tag	UNP I6Y4H4
A	362	HIS	-	expression tag	UNP I6Y4H4
A	363	HIS	-	expression tag	UNP I6Y4H4
A	364	HIS	-	expression tag	UNP I6Y4H4
A	365	HIS	-	expression tag	UNP I6Y4H4
A	366	HIS	-	expression tag	UNP I6Y4H4
B	0	MET	-	expression tag	UNP I6Y4H4
B	1	VAL	-	expression tag	UNP I6Y4H4
B	354	LYS	-	expression tag	UNP I6Y4H4
B	355	LEU	-	expression tag	UNP I6Y4H4
B	356	ALA	-	expression tag	UNP I6Y4H4
B	357	ALA	-	expression tag	UNP I6Y4H4

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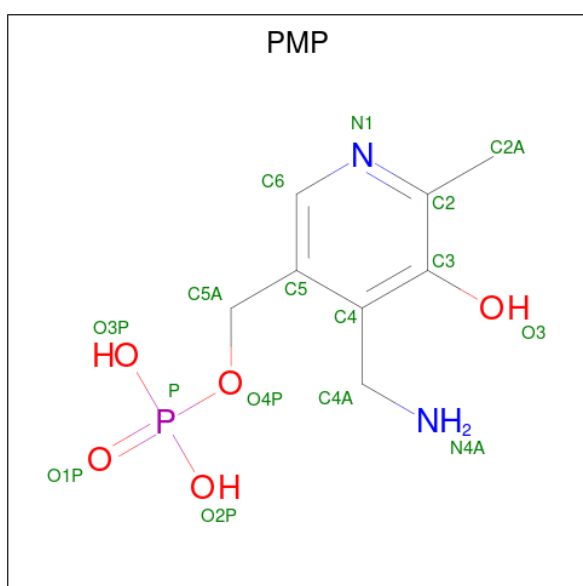
Chain	Residue	Modelled	Actual	Comment	Reference
B	358	ALA	-	expression tag	UNP I6Y4H4
B	359	LEU	-	expression tag	UNP I6Y4H4
B	360	GLU	-	expression tag	UNP I6Y4H4
B	361	HIS	-	expression tag	UNP I6Y4H4
B	362	HIS	-	expression tag	UNP I6Y4H4
B	363	HIS	-	expression tag	UNP I6Y4H4
B	364	HIS	-	expression tag	UNP I6Y4H4
B	365	HIS	-	expression tag	UNP I6Y4H4
B	366	HIS	-	expression tag	UNP I6Y4H4
C	0	MET	-	expression tag	UNP I6Y4H4
C	1	VAL	-	expression tag	UNP I6Y4H4
C	354	LYS	-	expression tag	UNP I6Y4H4
C	355	LEU	-	expression tag	UNP I6Y4H4
C	356	ALA	-	expression tag	UNP I6Y4H4
C	357	ALA	-	expression tag	UNP I6Y4H4
C	358	ALA	-	expression tag	UNP I6Y4H4
C	359	LEU	-	expression tag	UNP I6Y4H4
C	360	GLU	-	expression tag	UNP I6Y4H4
C	361	HIS	-	expression tag	UNP I6Y4H4
C	362	HIS	-	expression tag	UNP I6Y4H4
C	363	HIS	-	expression tag	UNP I6Y4H4
C	364	HIS	-	expression tag	UNP I6Y4H4
C	365	HIS	-	expression tag	UNP I6Y4H4
C	366	HIS	-	expression tag	UNP I6Y4H4
D	0	MET	-	expression tag	UNP I6Y4H4
D	1	VAL	-	expression tag	UNP I6Y4H4
D	354	LYS	-	expression tag	UNP I6Y4H4
D	355	LEU	-	expression tag	UNP I6Y4H4
D	356	ALA	-	expression tag	UNP I6Y4H4
D	357	ALA	-	expression tag	UNP I6Y4H4
D	358	ALA	-	expression tag	UNP I6Y4H4
D	359	LEU	-	expression tag	UNP I6Y4H4
D	360	GLU	-	expression tag	UNP I6Y4H4
D	361	HIS	-	expression tag	UNP I6Y4H4
D	362	HIS	-	expression tag	UNP I6Y4H4
D	363	HIS	-	expression tag	UNP I6Y4H4
D	364	HIS	-	expression tag	UNP I6Y4H4
D	365	HIS	-	expression tag	UNP I6Y4H4
D	366	HIS	-	expression tag	UNP I6Y4H4

- Molecule 2 is SUCCINIC ACID (three-letter code: SIN) (formula: C₄H₆O₄).



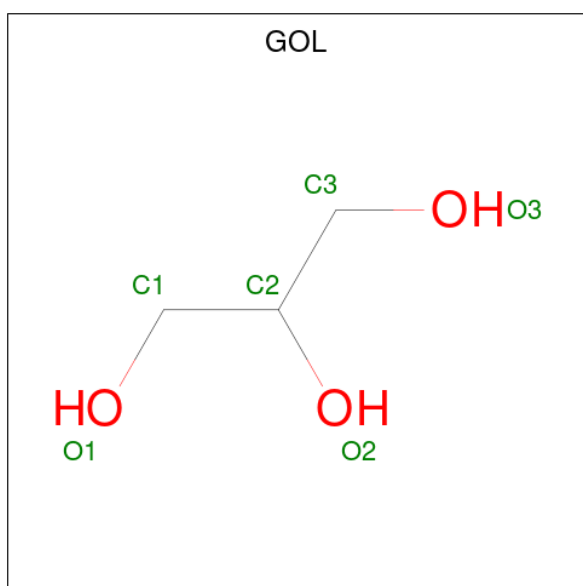
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 8 4 4	0	0
2	B	1	Total C O 8 4 4	0	0
2	C	1	Total C O 8 4 4	0	0
2	D	1	Total C O 8 4 4	0	0

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: C₈H₁₃N₂O₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	C	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



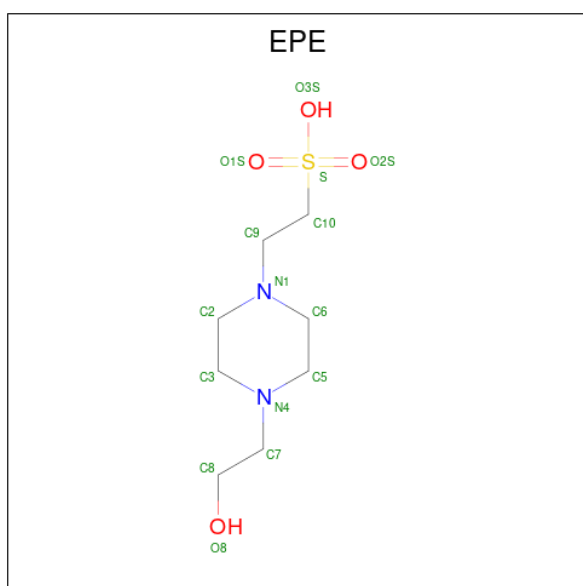
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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

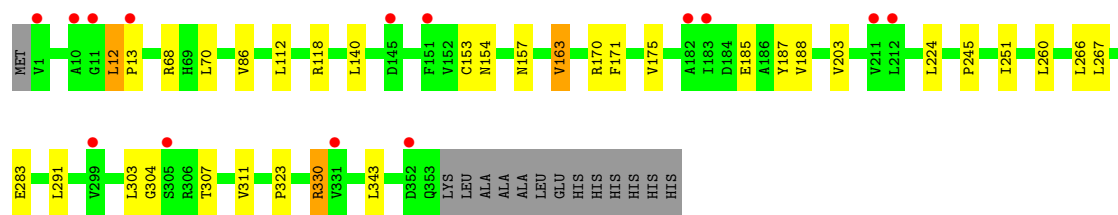
- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	354	Total	O	0	0
			354	354		
6	B	302	Total	O	0	0
			302	302		
6	C	281	Total	O	0	0
			281	281		
6	D	306	Total	O	0	0
			306	306		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	256.92Å 77.56Å 117.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.41 – 1.95 27.41 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.6 (27.41-1.95) 96.6 (27.41-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.179 , 0.203 0.184 , 0.205	Depositor DCC
R_{free} test set	8361 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtrriage
Anisotropy	0.048	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12296	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: EPE, SIN, GOL, PMP

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	0.33	0/2779	0.59	0/3805
1	B	0.32	0/2754	0.58	0/3770
1	C	0.31	0/2754	0.56	0/3770
1	D	0.31	0/2752	0.59	1/3768 (0.0%)
All	All	0.32	0/11039	0.58	1/15113 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	330	ARG	NE-CZ-NH2	-5.09	117.75	120.30

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	2706	0	2733	15	0
1	B	2691	0	2710	15	0
1	C	2691	0	2710	14	0
1	D	2689	0	2705	14	0
2	A	8	0	4	0	0
2	B	8	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	8	0	4	1	0
2	D	8	0	4	1	0
3	A	16	0	10	4	0
3	B	16	0	10	3	0
3	C	16	0	10	7	0
3	D	16	0	10	5	0
4	A	36	0	48	1	0
4	B	36	0	48	1	0
4	C	24	0	32	1	0
4	D	24	0	32	0	0
5	A	15	0	18	0	0
5	B	15	0	18	0	0
5	C	15	0	18	0	0
5	D	15	0	18	0	0
6	A	354	0	0	0	0
6	B	302	0	0	0	0
6	C	281	0	0	1	0
6	D	306	0	0	1	0
All	All	12296	0	11146	58	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 3.

The worst 5 of 58 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:304:GLY:O	1:B:307:THR:HG23	1.81	0.79
1:A:304:GLY:O	1:A:307:THR:HG23	1.83	0.79
1:C:187:TYR:OH	3:C:402:PMP:N4A	2.20	0.73
1:B:92:LEU:HD13	1:B:239:LEU:HD21	1.70	0.71
1:D:154:ASN:HD21	1:D:163:VAL:H	1.41	0.67

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	355/367 (97%)	347 (98%)	8 (2%)	0	100	100
1	B	352/367 (96%)	345 (98%)	7 (2%)	0	100	100
1	C	352/367 (96%)	343 (97%)	9 (3%)	0	100	100
1	D	352/367 (96%)	342 (97%)	10 (3%)	0	100	100
All	All	1411/1468 (96%)	1377 (98%)	34 (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	286/293 (98%)	277 (97%)	9 (3%)	40	28
1	B	283/293 (97%)	269 (95%)	14 (5%)	25	12
1	C	283/293 (97%)	274 (97%)	9 (3%)	39	27
1	D	283/293 (97%)	267 (94%)	16 (6%)	20	9
All	All	1135/1172 (97%)	1087 (96%)	48 (4%)	29	17

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	283	GLU
1	D	118	ARG
1	C	291	LEU
1	D	12	LEU
1	D	163	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	232	HIS
1	D	154	ASN
1	D	232	HIS
1	D	156	ASN
1	B	116	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

32 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
4	GOL	A	407	-	5,5,5	0.25	0	5,5,5	0.25	0
3	PMP	D	402	-	16,16,16	2.81	3 (18%)	21,23,23	1.40	4 (19%)
4	GOL	A	403	-	5,5,5	0.48	0	5,5,5	0.39	0
4	GOL	D	405	-	5,5,5	0.31	0	5,5,5	0.26	0
4	GOL	A	406	-	5,5,5	0.28	0	5,5,5	0.18	0
4	GOL	C	405	-	5,5,5	0.21	0	5,5,5	0.28	0
5	EPE	B	409	-	15,15,15	1.92	1 (6%)	18,20,20	2.80	10 (55%)
4	GOL	B	408	-	5,5,5	0.32	0	5,5,5	0.36	0
4	GOL	B	406	-	5,5,5	0.34	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	403	-	5,5,5	0.41	0	5,5,5	0.35	0
4	GOL	C	406	-	5,5,5	0.19	0	5,5,5	0.25	0
4	GOL	C	403	-	5,5,5	0.27	0	5,5,5	0.20	0
2	SIN	A	401	-	7,7,7	1.08	0	8,8,8	1.21	0
5	EPE	D	407	-	15,15,15	1.94	1 (6%)	18,20,20	2.70	9 (50%)
4	GOL	A	404	-	5,5,5	0.20	0	5,5,5	0.39	0
2	SIN	B	401	-	7,7,7	1.04	0	8,8,8	1.06	0
4	GOL	D	406	-	5,5,5	0.31	0	5,5,5	0.35	0
3	PMP	B	402	-	16,16,16	2.79	3 (18%)	21,23,23	1.44	4 (19%)
4	GOL	B	407	-	5,5,5	0.26	0	5,5,5	0.26	0
5	EPE	A	409	-	15,15,15	1.89	1 (6%)	18,20,20	2.69	9 (50%)
4	GOL	B	405	-	5,5,5	0.22	0	5,5,5	0.26	0
4	GOL	C	404	-	5,5,5	0.34	0	5,5,5	0.55	0
2	SIN	C	401	-	7,7,7	1.10	0	8,8,8	1.24	0
2	SIN	D	401	-	7,7,7	1.08	0	8,8,8	1.37	1 (12%)
3	PMP	A	402	-	16,16,16	2.65	3 (18%)	21,23,23	1.41	5 (23%)
4	GOL	A	405	-	5,5,5	0.22	0	5,5,5	0.30	0
4	GOL	B	403	-	5,5,5	0.34	0	5,5,5	0.38	0
4	GOL	B	404	-	5,5,5	0.28	0	5,5,5	0.25	0
4	GOL	A	408	-	5,5,5	0.32	0	5,5,5	0.25	0
5	EPE	C	407	-	15,15,15	1.97	1 (6%)	18,20,20	2.68	9 (50%)
3	PMP	C	402	-	16,16,16	2.68	3 (18%)	21,23,23	1.40	3 (14%)
4	GOL	D	404	-	5,5,5	0.27	0	5,5,5	0.31	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	GOL	A	407	-	-	2/4/4/4	-
3	PMP	D	402	-	-	7/8/8/8	0/1/1/1
4	GOL	A	403	-	-	2/4/4/4	-
4	GOL	D	405	-	-	0/4/4/4	-
4	GOL	A	406	-	-	1/4/4/4	-
4	GOL	C	405	-	-	1/4/4/4	-
5	EPE	B	409	-	-	2/9/19/19	0/1/1/1
4	GOL	B	408	-	-	4/4/4/4	-
4	GOL	B	406	-	-	1/4/4/4	-
4	GOL	D	403	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	406	-	-	2/4/4/4	-
4	GOL	C	403	-	-	0/4/4/4	-
2	SIN	A	401	-	-	4/5/5/5	-
5	EPE	D	407	-	-	6/9/19/19	0/1/1/1
4	GOL	A	404	-	-	0/4/4/4	-
2	SIN	B	401	-	-	1/5/5/5	-
4	GOL	D	406	-	-	2/4/4/4	-
3	PMP	B	402	-	-	5/8/8/8	0/1/1/1
4	GOL	B	407	-	-	2/4/4/4	-
5	EPE	A	409	-	-	5/9/19/19	0/1/1/1
4	GOL	B	405	-	-	0/4/4/4	-
4	GOL	C	404	-	-	2/4/4/4	-
2	SIN	C	401	-	-	1/5/5/5	-
2	SIN	D	401	-	-	2/5/5/5	-
3	PMP	A	402	-	-	7/8/8/8	0/1/1/1
4	GOL	A	405	-	-	0/4/4/4	-
4	GOL	B	403	-	-	2/4/4/4	-
4	GOL	B	404	-	-	2/4/4/4	-
4	GOL	A	408	-	-	2/4/4/4	-
5	EPE	C	407	-	-	2/9/19/19	0/1/1/1
3	PMP	C	402	-	-	2/8/8/8	0/1/1/1
4	GOL	D	404	-	-	3/4/4/4	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	PMP	C3-C2	7.54	1.48	1.40
3	B	402	PMP	C3-C2	7.44	1.48	1.40
5	C	407	EPE	C10-S	-7.32	1.67	1.77
3	C	402	PMP	C3-C2	7.31	1.48	1.40
5	D	407	EPE	C10-S	-7.24	1.67	1.77

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	407	EPE	C5-N4-C3	5.40	120.99	108.83
5	D	407	EPE	C5-N4-C3	5.39	120.95	108.83
5	C	407	EPE	C6-N1-C2	5.31	120.77	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	407	EPE	C6-N1-C2	5.12	120.35	108.83
5	B	409	EPE	C6-N1-C2	5.07	120.24	108.83

There are no chirality outliers.

5 of 74 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	PMP	C3-C4-C4A-N4A
3	A	402	PMP	C5-C4-C4A-N4A
3	A	402	PMP	C5A-O4P-P-O1P
3	A	402	PMP	C5A-O4P-P-O2P
3	A	402	PMP	C5A-O4P-P-O3P

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	PMP	5	0
4	B	408	GOL	1	0
3	B	402	PMP	3	0
4	C	404	GOL	1	0
2	C	401	SIN	1	0
2	D	401	SIN	1	0
3	A	402	PMP	4	0
4	A	408	GOL	1	0
3	C	402	PMP	7	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	353/367 (96%)	-0.06	8 (2%) 60 69	18, 25, 36, 57	0
1	B	353/367 (96%)	0.02	12 (3%) 45 55	20, 27, 38, 57	0
1	C	353/367 (96%)	0.06	14 (3%) 38 48	21, 29, 46, 67	0
1	D	353/367 (96%)	0.11	14 (3%) 38 48	23, 30, 42, 59	0
All	All	1412/1468 (96%)	0.03	48 (3%) 45 55	18, 28, 42, 67	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	137	TYR	5.2
1	C	22	PRO	4.0
1	C	1	VAL	4.0
1	D	1	VAL	3.8
1	C	318	ARG	3.4

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 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, 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
4	GOL	B	408	6/6	0.65	0.31	48,50,51,53	0
4	GOL	A	406	6/6	0.76	0.39	50,59,62,65	0
4	GOL	B	406	6/6	0.80	0.30	59,59,60,61	0
4	GOL	D	406	6/6	0.80	0.33	48,52,53,53	0
4	GOL	A	407	6/6	0.82	0.26	60,61,61,62	0
4	GOL	C	406	6/6	0.83	0.29	73,74,75,76	0
4	GOL	A	408	6/6	0.85	0.26	52,53,54,56	0
4	GOL	B	405	6/6	0.87	0.21	49,51,51,51	0
4	GOL	B	404	6/6	0.88	0.16	46,48,49,50	0
4	GOL	C	403	6/6	0.88	0.23	46,48,48,49	0
4	GOL	A	404	6/6	0.90	0.17	37,40,41,42	0
4	GOL	D	405	6/6	0.90	0.20	55,56,57,57	0
4	GOL	B	407	6/6	0.90	0.16	62,62,63,63	0
5	EPE	D	407	15/15	0.90	0.26	56,66,68,68	0
4	GOL	D	403	6/6	0.91	0.14	33,35,36,36	0
3	PMP	A	402	16/16	0.91	0.19	29,36,38,38	16
4	GOL	A	405	6/6	0.91	0.15	41,41,42,42	0
4	GOL	A	403	6/6	0.91	0.12	29,31,32,32	0
3	PMP	D	402	16/16	0.92	0.20	34,41,43,44	16
5	EPE	C	407	15/15	0.92	0.30	51,62,66,66	0
3	PMP	B	402	16/16	0.92	0.21	30,39,41,41	16
4	GOL	C	405	6/6	0.93	0.18	42,45,46,46	0
5	EPE	A	409	15/15	0.93	0.27	47,54,57,57	0
5	EPE	B	409	15/15	0.93	0.29	52,61,64,64	0
4	GOL	D	404	6/6	0.93	0.13	43,48,48,49	0
3	PMP	C	402	16/16	0.93	0.18	34,38,41,43	16
4	GOL	B	403	6/6	0.94	0.12	27,30,30,30	0
4	GOL	C	404	6/6	0.94	0.13	35,36,37,37	0
2	SIN	D	401	8/8	0.95	0.11	26,28,32,34	0
2	SIN	C	401	8/8	0.96	0.09	30,32,34,37	0
2	SIN	A	401	8/8	0.98	0.07	25,27,30,32	0
2	SIN	B	401	8/8	0.98	0.09	24,27,30,32	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.