



wwPDB X-ray Structure Validation Summary Report i

May 28, 2014 – 12:18 AM EDT

PDB ID : 4NH2
Title : Crystal structure of AmtB from E. coli bound to phosphatidylglycerol
Authors : Laganowsky, A.; Reading, E.; Allison, T.M.; Robinson, C.V.
Deposited on : 2013-11-04
Resolution : 2.30 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>

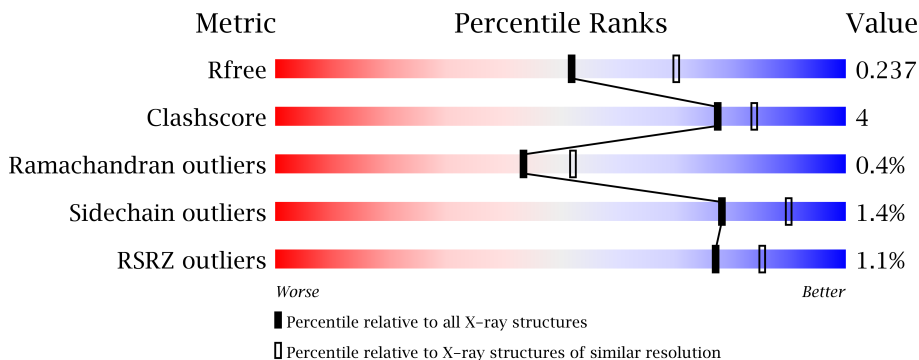
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	FAILED
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23161
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)	:	stable23161

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	406	
1	B	406	
1	C	406	
1	D	406	
1	E	406	
1	F	406	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	P6L	A	501	-	X
2	P6L	C	501	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	P6L	C	502	-	X
2	P6L	E	501	-	X
2	P6L	F	501	-	X
2	P6L	F	502	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16260 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 Ammonia channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2614	1728	418	449	19			
1	B	367	Total	C	N	O	S	0	0	0
			2645	1751	420	455	19			
1	C	368	Total	C	N	O	S	0	0	0
			2657	1757	423	458	19			
1	D	366	Total	C	N	O	S	0	0	0
			2645	1751	421	454	19			
1	E	371	Total	C	N	O	S	0	0	0
			2665	1762	425	459	19			
1	F	364	Total	C	N	O	S	0	0	0
			2630	1742	419	450	19			

There are 18 discrepancies between the modelled and reference sequences:

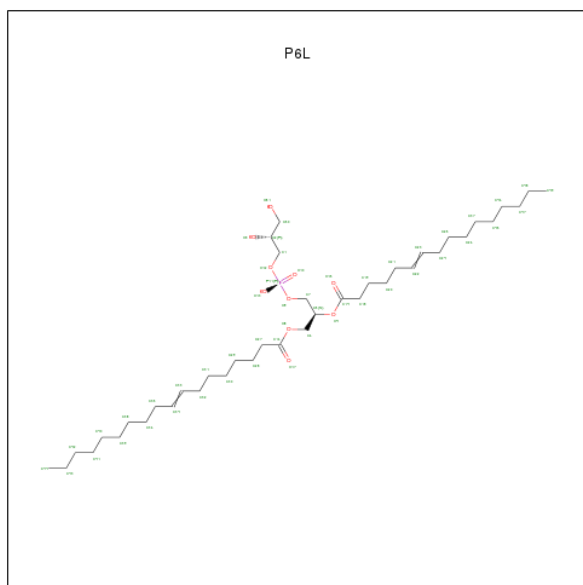
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP P69680
A	2	ALA	-	EXPRESSION TAG	UNP P69680
A	3	SER	-	EXPRESSION TAG	UNP P69680
B	1	GLY	-	EXPRESSION TAG	UNP P69680
B	2	ALA	-	EXPRESSION TAG	UNP P69680
B	3	SER	-	EXPRESSION TAG	UNP P69680
C	1	GLY	-	EXPRESSION TAG	UNP P69680
C	2	ALA	-	EXPRESSION TAG	UNP P69680
C	3	SER	-	EXPRESSION TAG	UNP P69680
D	1	GLY	-	EXPRESSION TAG	UNP P69680
D	2	ALA	-	EXPRESSION TAG	UNP P69680
D	3	SER	-	EXPRESSION TAG	UNP P69680
E	1	GLY	-	EXPRESSION TAG	UNP P69680
E	2	ALA	-	EXPRESSION TAG	UNP P69680
E	3	SER	-	EXPRESSION TAG	UNP P69680
F	1	GLY	-	EXPRESSION TAG	UNP P69680
F	2	ALA	-	EXPRESSION TAG	UNP P69680

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Chain	Residue	Modelled	Actual	Comment	Reference
F	3	SER	-	EXPRESSION TAG	UNP P69680

- Molecule 2 is (2S)-3-[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-2-[(6E)-HEXADEC-6-ENOYLOXY]PROPYL(8E)-OCTADEC-8-ENOATE (three-letter code: P6L) (formula: C₄₀H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			25	14	10	1		
2	B	1	Total	C	O	P	0	0
			23	12	10	1		
2	C	1	Total	C	O	P	0	0
			39	28	10	1		
2	C	1	Total	C	O	P	0	0
			51	40	10	1		
2	D	1	Total	C	O	P	0	0
			34	23	10	1		
2	E	1	Total	C	O	P	0	0
			35	24	10	1		
2	F	1	Total	C	O	P	0	0
			35	24	10	1		
2	F	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 3 is water.

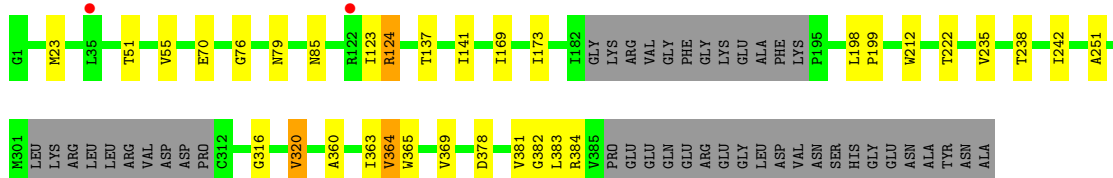
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total 19	O 19	0	0
3	B	19	Total 19	O 19	0	0
3	C	17	Total 17	O 17	0	0
3	D	17	Total 17	O 17	0	0
3	E	19	Total 19	O 19	0	0
3	F	20	Total 20	O 20	0	0

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.

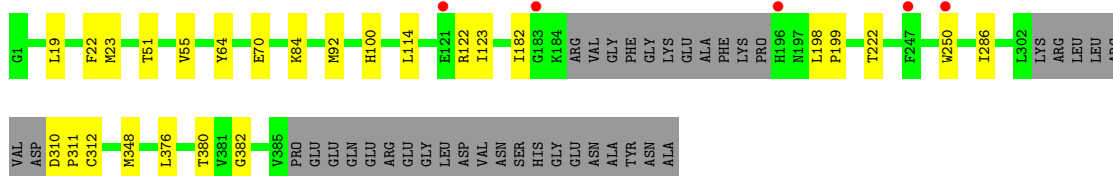
- Molecule 1: Ammonia channel

Chain A: 



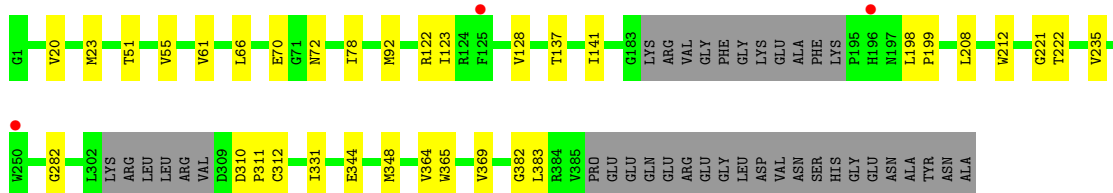
- Molecule 1: Ammonia channel

Chain B: 



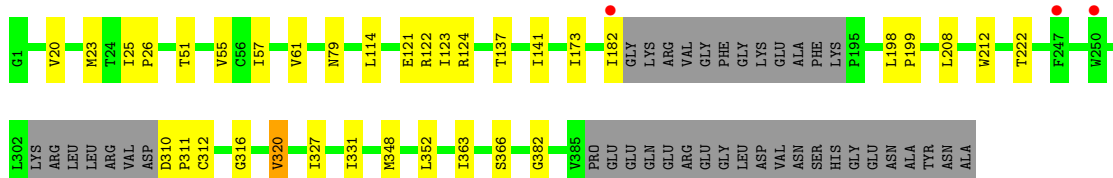
- Molecule 1: Ammonia channel

Chain C: 



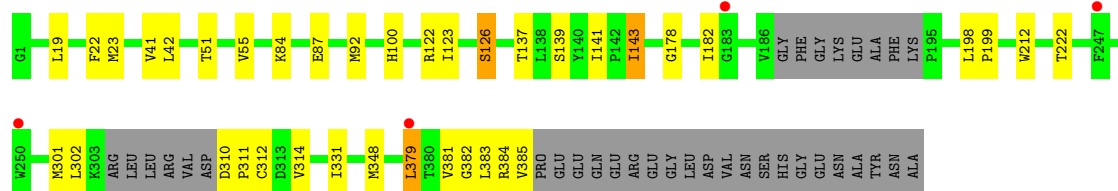
- Molecule 1: Ammonia channel

Chain D: 



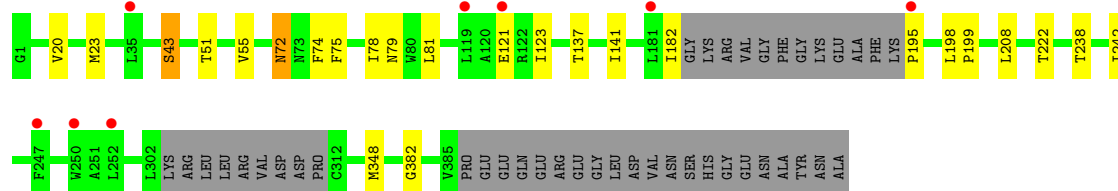
- Molecule 1: Ammonia channel

Chain E:



- Molecule 1: Ammonia channel

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	116.19Å 201.19Å 232.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.74 – 2.30 38.74 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.74-2.30) 99.3 (38.74-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.202 , 0.234 0.206 , 0.237	Depositor DCC
R_{free} test set	5989 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	1.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 25.9	EDS
Estimated twinning fraction	0.432 for H, K, L 0.287 for -1/2H+1/2K, 3/2H+1/2K, -L 0.281 for -1/2H-1/2K, -3/2H+1/2K, -L 0.419 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.435 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
Reported twinning fraction	0.432 for H, K, L 0.287 for -1/2H+1/2K, 3/2H+1/2K, -L 0.281 for -1/2H-1/2K, -3/2H+1/2K, -L	Depositor
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 119767 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16260	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.84 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.9231e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: P6L

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	0.79	1/2672 (0.0%)	0.79	3/3646 (0.1%)
1	B	0.78	0/2704	0.79	3/3690 (0.1%)
1	C	0.81	0/2717	0.79	3/3708 (0.1%)
1	D	0.74	0/2705	0.78	4/3692 (0.1%)
1	E	0.82	3/2725 (0.1%)	0.80	4/3721 (0.1%)
1	F	0.78	1/2689 (0.0%)	0.79	2/3669 (0.1%)
All	All	0.79	5/16212 (0.0%)	0.79	19/22126 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	87	GLU	CD-OE1	5.84	1.32	1.25
1	F	72	ASN	CB-CG	-5.77	1.37	1.51
1	E	87	GLU	CG-CD	5.71	1.60	1.51
1	E	126	SER	CB-OG	-5.35	1.35	1.42
1	A	382	GLY	N-CA	5.09	1.53	1.46

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	122	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	C	92	MET	CG-SD-CE	7.03	111.45	100.20
1	B	122	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	F	348	MET	CG-SD-CE	6.59	110.74	100.20
1	F	72	ASN	CB-CA-C	-6.55	97.29	110.40

There are no chirality outliers.

There are no planarity outliers.

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	2614	0	2661	18	0
1	B	2645	0	2694	13	0
1	C	2657	0	2704	21	0
1	D	2645	0	2697	23	0
1	E	2665	0	2697	17	0
1	F	2630	0	2686	20	0
2	A	25	0	20	1	0
2	B	23	0	16	2	0
2	C	90	0	123	9	0
2	D	34	0	36	2	0
2	E	35	0	38	1	0
2	F	86	0	112	8	0
3	A	19	0	0	3	0
3	B	19	0	0	0	0
3	C	17	0	0	2	0
3	D	17	0	0	1	0
3	E	19	0	0	0	0
3	F	20	0	0	1	0
All	All	16260	0	16484	120	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 120 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:501:P6L:H2	2:B:501:P6L:O10	1.77	0.85
1:F:79:ASN:ND2	3:F:615:HOH:O	2.09	0.84
1:D:331:ILE:HG23	1:D:348:MET:HE1	1.66	0.78
1:A:124:ARG:HG3	1:A:384:ARG:O	1.84	0.78
1:F:78:ILE:HD13	2:F:501:P6L:C30	2.14	0.78

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	357/406 (88%)	343 (96%)	14 (4%)	0	100	100
1	B	361/406 (89%)	346 (96%)	13 (4%)	2 (1%)	33	39
1	C	362/406 (89%)	346 (96%)	14 (4%)	2 (1%)	33	39
1	D	360/406 (89%)	343 (95%)	15 (4%)	2 (1%)	33	39
1	E	365/406 (90%)	346 (95%)	17 (5%)	2 (0%)	38	45
1	F	358/406 (88%)	344 (96%)	13 (4%)	1 (0%)	50	60
All	All	2163/2436 (89%)	2068 (96%)	86 (4%)	9 (0%)	43	52

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	311	PRO
1	C	311	PRO
1	D	311	PRO
1	E	311	PRO
1	E	382	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/297 (86%)	253 (98%)	4 (2%)	75	88
1	B	261/297 (88%)	258 (99%)	3 (1%)	84	93
1	C	263/297 (89%)	260 (99%)	3 (1%)	84	93
1	D	262/297 (88%)	258 (98%)	4 (2%)	76	89
1	E	261/297 (88%)	256 (98%)	5 (2%)	69	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	260/297 (88%)	257 (99%)	3 (1%)	82	92
All	All	1564/1782 (88%)	1542 (99%)	22 (1%)	78	90

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	222	THR
1	D	212	TRP
1	F	195	PRO
1	D	114	LEU
1	D	121	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	40	ASN
1	F	79	ASN
1	D	79	ASN
1	B	79	ASN
1	C	79	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

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	363/406 (89%)	-0.10	2 (0%) 86 92	21, 40, 72, 91	0
1	B	367/406 (90%)	-0.02	5 (1%) 72 80	23, 42, 74, 99	0
1	C	368/406 (90%)	-0.06	3 (0%) 83 90	21, 41, 77, 96	0
1	D	366/406 (90%)	-0.10	3 (0%) 83 90	25, 43, 77, 103	0
1	E	371/406 (91%)	-0.03	4 (1%) 77 85	21, 41, 72, 92	0
1	F	364/406 (89%)	-0.04	8 (2%) 59 69	22, 40, 77, 93	0
All	All	2199/2436 (90%)	-0.06	25 (1%) 77 85	21, 41, 76, 103	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	250	TRP	4.4
1	B	250	TRP	4.1
1	D	247	PHE	3.6
1	B	121	GLU	3.4
1	E	250	TRP	3.1

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 ⓘ

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(Å ²)	Q<0.9
2	P6L	F	501	35/51	0.24	4.60	44,57,71,73	0
2	P6L	F	502	51/51	0.25	3.34	47,66,127,139	0
2	P6L	E	501	35/51	0.24	3.32	43,68,80,81	0
2	P6L	C	501	39/51	0.20	2.89	38,62,77,77	0
2	P6L	C	502	51/51	0.19	2.41	44,63,108,123	0
2	P6L	A	501	25/51	0.16	2.32	32,53,65,79	0
2	P6L	B	501	23/51	0.17	1.83	43,58,68,71	0
2	P6L	D	501	34/51	0.14	1.00	40,61,73,75	0

6.5 Other polymers ⓘ

There are no such residues in this entry.