



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 6, 2017 – 04:28 AM EST

PDB ID : 1B7Y
Title : PHENYLALANYL TRNA SYNTHETASE COMPLEXED WITH PHENYL
ALANINYL-ADENYLATE
Authors : Reshetnikova, L.; Moor, N.; Lavrik, O.; Vassilyev, D.G.
Deposited on : 1999-01-26
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

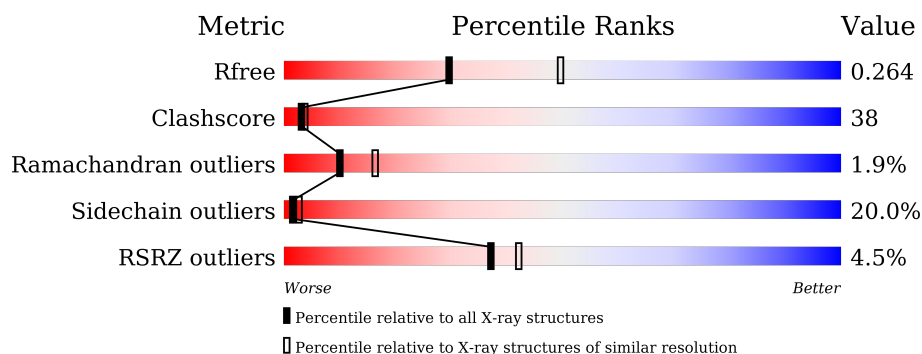
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	350	<div> <div>2%</div> <div>33%</div> <div>34%</div> <div>9%</div> <div>24%</div> </div>
2	B	785	<div> <div>5%</div> <div>43%</div> <div>43%</div> <div>12%</div> <div>..</div> </div>

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	MG	A	1001	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8439 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 PROTEIN (PHENYLALANYL-TRNA SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2112	1382	359	364	7			

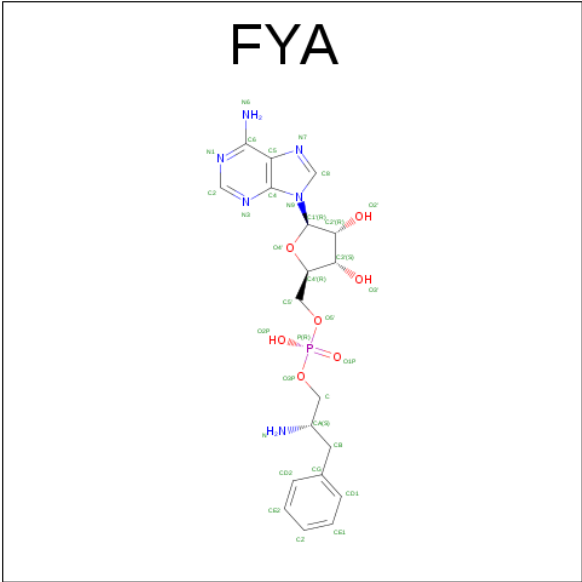
- Molecule 2 is a protein called PROTEIN (PHENYLALANYL-TRNA SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	775	Total	C	N	O	S	0	0	0
			6054	3879	1078	1087	10			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-[PHENYLALANINOL-PHOSPHATE] (three-letter code: FYA) (formula: C₁₉H₂₅N₆O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			33	19	6	7	1		

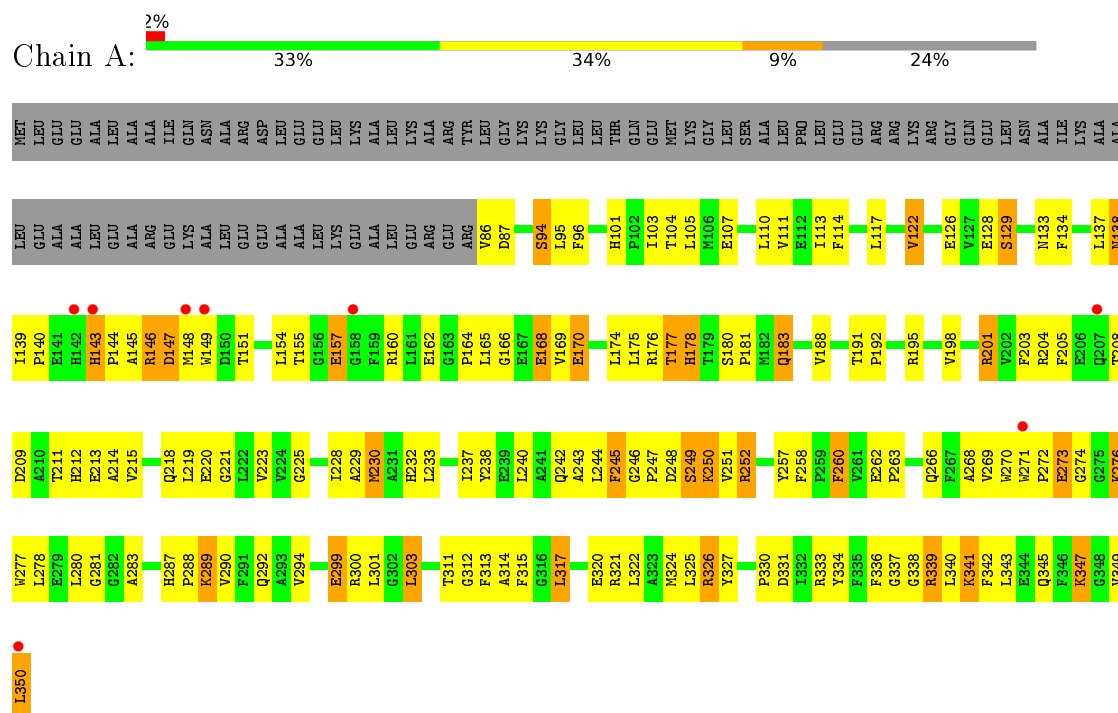
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	48	Total	O	0	0
			48	48		
5	B	191	Total	O	0	0
			191	191		

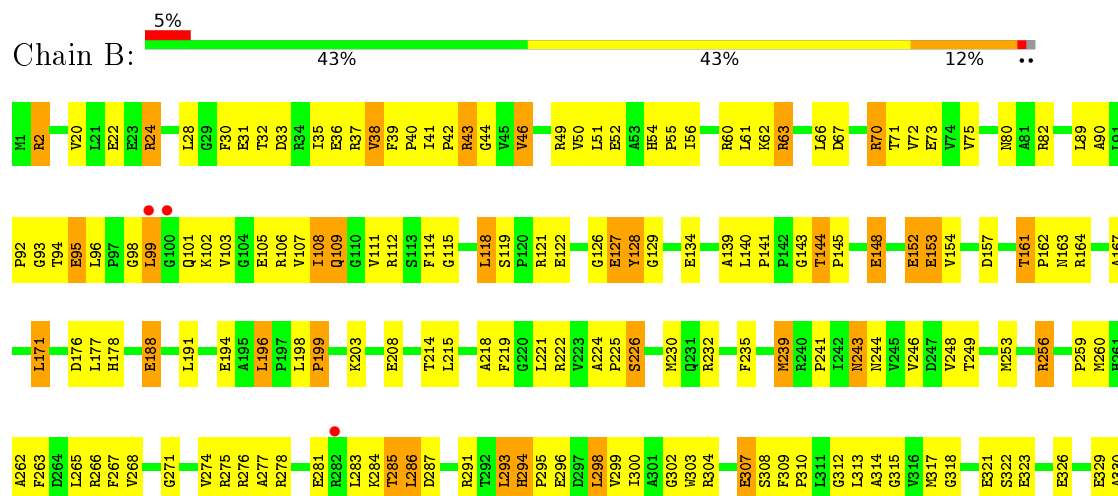
3 Residue-property plots

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: PROTEIN (PHENYLALANYL-TRNA SYNTHETASE)



• Molecule 2: PROTEIN (PHENYLALANYL-TRNA SYNTHETASE)



LEU ARG GLY LEU ASP THR PRO	A717	●	A718	G650	E581	D517	T417	I331
	●	F651	●	F652	E582	P519	●	A332
	Y721	L652	●	●	T583	E519	I427	C337
	E723	●	●	●	H584	D520	I428	F338
	S724	●	●	●	●	A521	R430	D339
L727	●	●	●	●	G587	R522	●	●
	F728	●	●	●	L588	R523	E438	R344
	D729	●	●	●	L589	F524	●	R345
	L730	●	●	●	F590	R525	T441	●
	Y731	●	●	●	G591	L526	●	E355
Q732	●	●	●	●	E592	D527	●	A356
	●	●	●	●	G593	P528	P446	S357
	●	●	●	●	V594	P529	P447	S358
	●	●	●	●	E595	R530	S448	H556
	●	●	●	●	L596	L531	R449	R359
P733	●	●	●	●	P597	L532	R450	F360
	●	●	●	●	V598	L533	L451	E361
	●	●	●	●	A599	L534	D452	●
	●	●	●	●	K600	N535	●	V364
	●	●	●	●	L670	P536	D458	S365
E738	●	●	●	●	E601	L537	L459	P366
	●	●	●	●	L602	A538	V460	L367
	G739	●	●	●	L603	P539	E461	G368
	H740	●	●	●	S604	E540	E462	G369
	K741	●	●	●	●	X541	V370	V370
S742	●	●	●	●	L608	A542	R465	●
	●	●	●	●	L609	A543	I466	P371
	●	●	●	●	K610	L544	Q467	●
	●	●	●	●	L613	R545	●	R374
	●	●	●	●	E614	T546	P473	L377
R748	●	●	●	●	A615	H547	●	S378
	●	●	●	●	L616	L548	D484	L379
	●	●	●	●	F617	P549	I485	L380
	●	●	●	●	A618	P550	R486	G381
	●	●	●	●	●	G551	G487	●
R750	●	●	●	●	G621	L552	V488	G385
	●	●	●	●	L622	V553	E489	A386
	●	●	●	●	A623	R554	A490	R387
	●	●	●	●	F624	V555	P491	V388
	●	●	●	●	●	L556	●	A389
D758	●	●	●	●	Q629	K557	K494	E390
	●	●	●	●	A630	E558	●	●
	●	●	●	●	F631	L562	R497	L393
	●	●	●	●	P632	D563	L498	E394
	●	●	●	●	F633	R564	R499	●
A764	●	●	●	●	L634	P565	E500	S397
	●	●	●	●	P635	E566	V501	P398
	●	●	●	●	P636	R567	●	K399
	●	●	●	●	G637	L570	L505	P400
	●	●	●	●	V638	F571	G506	P401
R767	●	●	●	●	S639	E572	F507	E402
	●	●	●	●	●	E573	Q508	A403
	●	●	●	●	V642	V570	E509	L404
	●	●	●	●	L643	V510	V510	●
	●	●	●	●	V644	G574	Y511	E409
A774	●	●	●	●	E645	R575	T512	●
	●	●	●	●	G646	R576	Y513	R413
	●	●	●	●	E647	E579	S514	L414
	●	●	●	●	V649	R580	F515	L415
	●	●	●	●	●	●	M516	G416

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.50Å 174.50Å 140.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 47.41 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-2.50) 95.7 (47.41-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	15112.19 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.230 , 0.267 0.229 , 0.264	Depositor DCC
R_{free} test set	4107 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 82.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.056 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8439	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: MG, FYA

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	0.54	0/2180	0.76	0/2957
2	B	0.53	0/6205	0.79	4/8436 (0.0%)
All	All	0.53	0/8385	0.78	4/11393 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	115	GLY	N-CA-C	-5.83	98.54	113.10
2	B	601	GLU	CB-CA-C	-5.59	99.22	110.40
2	B	128	TYR	N-CA-C	5.35	125.44	111.00
2	B	570	LEU	CA-CB-CG	5.28	127.44	115.30

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	2112	0	2062	164	0
2	B	6054	0	6109	495	0
3	A	1	0	0	0	0
4	A	33	0	24	4	0
5	A	48	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	191	0	0	6	0
All	All	8439	0	8195	626	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 38.

The worst 5 of 626 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:GLU:HG2	5:A:1015:HOH:O	1.45	1.16
2:B:600:LYS:HG2	2:B:601:GLU:H	1.04	1.14
2:B:75:VAL:HG11	2:B:108:ILE:HG21	1.31	1.12
2:B:285:THR:HG21	2:B:291:ARG:HE	1.20	1.02
2:B:294:HIS:CD2	2:B:296:GLU:H	1.79	1.00

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	263/350 (75%)	244 (93%)	14 (5%)	5 (2%)	10	16
2	B	773/785 (98%)	695 (90%)	63 (8%)	15 (2%)	10	16
All	All	1036/1135 (91%)	939 (91%)	77 (7%)	20 (2%)	10	16

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
2	B	488	VAL
2	B	664	GLU

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Mol	Chain	Res	Type
1	A	338	GLY
2	B	708	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	213/277 (77%)	176 (83%)	37 (17%)	2	4
2	B	623/630 (99%)	493 (79%)	130 (21%)	1	2
All	All	836/907 (92%)	669 (80%)	167 (20%)	1	3

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	243	ASN
2	B	361	GLU
2	B	716	GLU
2	B	283	LEU
2	B	307	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	54	HIS
2	B	212	HIS
2	B	656	HIS
2	B	109	GLN
2	B	178	HIS

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
4	FYA	A	1002	-	33,36,36	1.19	2 (6%)	30,52,52	0.59	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	FYA	A	1002	-	-	0/16/36/36	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	FYA	O3P-C	-4.31	1.27	1.44
4	A	1002	FYA	O4'-C1'	2.46	1.44	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	FYA	4	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	265/350 (75%)	0.07	8 (3%) 54 59	27, 54, 103, 129	0
2	B	775/785 (98%)	0.08	39 (5%) 32 37	21, 59, 108, 128	0
All	All	1040/1135 (91%)	0.08	47 (4%) 37 42	21, 58, 107, 129	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	TRP	5.6
2	B	718	ALA	5.1
1	A	350	LEU	4.9
2	B	753	LYS	4.8
2	B	739	GLY	4.7

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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	A	1001	1/1	0.84	0.26	9.05	42,42,42,42	0
4	FYA	A	1002	33/33	0.97	0.15	-0.01	40,65,73,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.