



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2016 – 10:49 PM EDT

PDB ID : 5T3D
Title : Crystal structure of holo-EntF a nonribosomal peptide synthetase in the thioester-forming conformation
Authors : Miller, B.R.; Drake, E.J.; Sundlov, J.A.; Gulick, A.M.
Deposited on : 2016-08-25
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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-20027939
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-20027939

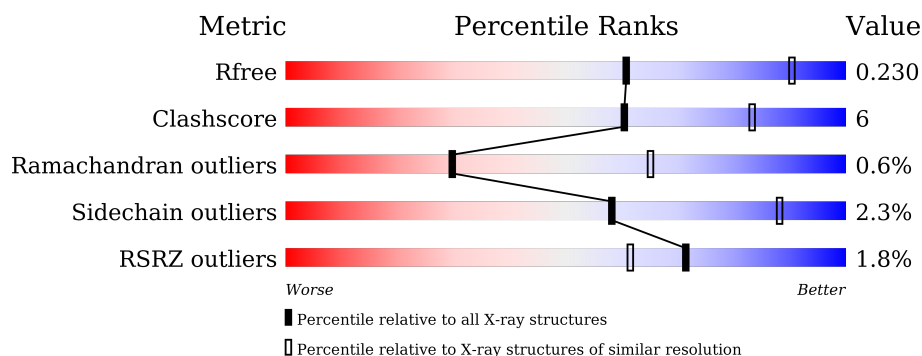
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	1295	<div> <div></div> <div>69%</div> <div>11%</div> <div>20%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7865 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.

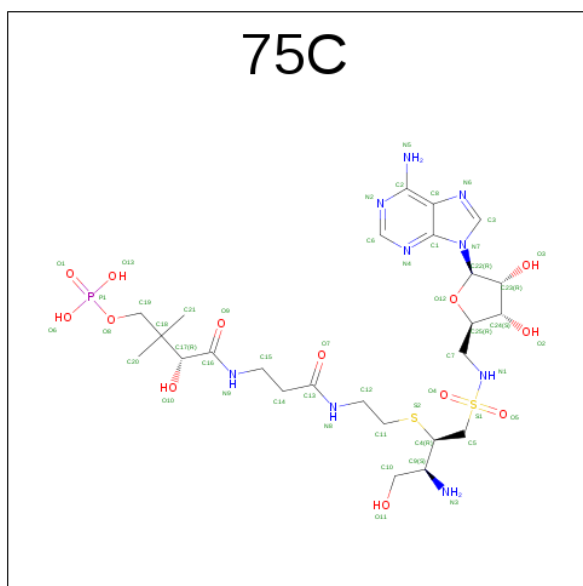
- Molecule 1 is a protein called Enterobactin synthase component F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1042	Total	C	N	O	S	0	0	0
			7803	4981	1339	1450	33			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P11454
A	0	HIS	-	expression tag	UNP P11454

- Molecule 2 is 5'-($\{[(2R,3S)$ -3-amino-4-hydroxy-2- $\{[2-(\{N-[(2R)$ -2-hydroxy-3,3-dimethyl-4-(p
hosphonoxy)butanoyl]-beta-alanyl}amino)ethyl]sulfanyl}butyl]sulfonyl}amino)-5'-deoxyad
enosine (three-letter code: 75C) (formula: C₂₅H₄₄N₉O₁₃PS₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			49	25	9	12	1	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	0
			13	13		

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	127.71Å 127.71Å 186.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.43 – 2.80 81.31 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (60.43-2.80) 100.0 (81.31-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.185 , 0.232 0.181 , 0.230	Depositor DCC
R_{free} test set	1944 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7865	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: 75C

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	0.56	2/7994 (0.0%)	0.72	4/10958 (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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	721	CYS	CB-SG	-7.54	1.69	1.82
1	A	929	THR	C-N	5.54	1.46	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	787	LEU	CB-CG-CD1	-5.90	100.96	111.00
1	A	543	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	291	LEU	CB-CG-CD1	-5.55	101.57	111.00
1	A	80	GLU	C-N-CA	-5.09	108.96	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	635	GLY	Peptide

5.2 Too-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 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	7803	0	7566	87	0
2	A	49	0	0	1	0
3	A	13	0	0	1	0
All	All	7865	0	7566	87	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 6.

All (87) 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:88:ARG:HB3	1:A:125:VAL:H	1.28	0.98
1:A:93:PRO:HG2	1:A:96:THR:HG23	1.55	0.86
1:A:861:LYS:HE2	2:A:1301:75C:O12	1.83	0.79
1:A:862:ILE:O	1:A:865:GLN:HG2	1.86	0.74
1:A:141:VAL:HG11	1:A:146:PHE:HB3	1.71	0.73
1:A:456:THR:HG22	1:A:458:SER:H	1.53	0.73
1:A:635:GLY:HA2	1:A:662:ALA:HA	1.71	0.71
1:A:456:THR:HG21	1:A:592:SER:HB3	1.73	0.70
1:A:224:ILE:HG21	1:A:375:VAL:HG13	1.73	0.70
1:A:91:ILE:HG22	1:A:93:PRO:HD2	1.74	0.69
1:A:204:LEU:HD12	1:A:205:PRO:HD2	1.79	0.65
1:A:633:LEU:HD22	1:A:656:TRP:CE2	2.31	0.64
1:A:48:VAL:O	1:A:52:LEU:HG	1.99	0.62
1:A:277:ARG:HD2	1:A:292:ASN:HB2	1.82	0.61
1:A:88:ARG:CZ	1:A:126:ALA:HB3	2.34	0.58
1:A:124:GLN:N	1:A:125:VAL:HA	2.20	0.57
1:A:473:ALA:HB2	1:A:483:TYR:CD2	2.40	0.57
1:A:1034:THR:HG23	1:A:1037:LYS:H	1.71	0.56
1:A:142:ASP:HB3	1:A:144:PHE:H	1.70	0.56
1:A:998:ASP:HB3	1:A:1001:ALA:HB3	1.88	0.54
1:A:416:LEU:HD11	1:A:433:ILE:HG22	1.90	0.54
1:A:247:GLN:O	1:A:249:THR:N	2.41	0.54
1:A:181:TYR:HA	1:A:184:TYR:HB3	1.89	0.54
1:A:639:VAL:O	1:A:664:LEU:HD12	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ASP:OD1	3:A:1401:HOH:O	2.18	0.53
1:A:458:SER:OG	1:A:526:VAL:HG12	2.09	0.53
1:A:642:LYS:HE2	1:A:691:HIS:O	2.09	0.53
1:A:226:ARG:HH21	1:A:372:THR:HG23	1.74	0.52
1:A:86:ASP:O	1:A:88:ARG:HG2	2.10	0.51
1:A:514:ARG:HD2	1:A:667:ALA:O	2.11	0.51
1:A:299:HIS:O	1:A:312:ARG:NH2	2.45	0.51
1:A:970:ARG:HG2	1:A:971:ALA:O	2.11	0.50
1:A:506:ASP:HB3	1:A:554:SER:OG	2.11	0.50
1:A:532:TRP:CD1	1:A:534:PRO:HD3	2.47	0.49
1:A:141:VAL:CG1	1:A:146:PHE:HB3	2.40	0.49
1:A:277:ARG:NH2	1:A:327:ASP:OD1	2.41	0.49
1:A:225:LEU:HD22	1:A:403:GLU:HG3	1.93	0.49
1:A:200:GLN:O	1:A:204:LEU:HB2	2.14	0.48
1:A:124:GLN:CB	1:A:130:TRP:HA	2.45	0.47
1:A:35:LEU:O	1:A:130:TRP:N	2.46	0.47
1:A:265:ASN:O	1:A:266:ARG:NH1	2.42	0.47
1:A:347:PRO:HA	1:A:378:LEU:O	2.14	0.47
1:A:412:ARG:HD3	1:A:433:ILE:HB	1.95	0.47
1:A:184:TYR:OH	1:A:193:ASP:OD2	2.23	0.47
1:A:497:LEU:HD21	1:A:557:ILE:HD11	1.97	0.46
1:A:456:THR:HG22	1:A:458:SER:N	2.24	0.46
1:A:563:LEU:HA	1:A:566:PHE:HD2	1.80	0.46
1:A:756:SER:HA	1:A:777:TYR:O	2.16	0.46
1:A:224:ILE:HD12	1:A:395:LEU:HB3	1.97	0.46
1:A:532:TRP:HZ2	1:A:651:VAL:HG22	1.79	0.46
1:A:676:LEU:HD23	1:A:676:LEU:HA	1.72	0.46
1:A:142:ASP:HB2	1:A:278:ARG:HH21	1.80	0.45
1:A:525:ILE:HG23	1:A:530:ALA:HB3	1.97	0.45
1:A:226:ARG:NH2	1:A:372:THR:HG23	2.32	0.45
1:A:258:LEU:HD23	1:A:300:ILE:HD12	1.99	0.44
1:A:457:LEU:HG	1:A:617:GLN:OE1	2.17	0.44
1:A:409:HIS:O	1:A:412:ARG:HB2	2.17	0.44
1:A:607:THR:O	1:A:874:ARG:NE	2.50	0.44
1:A:593:GLN:HB2	1:A:596:HIS:CE1	2.53	0.43
1:A:752:ALA:HB3	1:A:808:GLN:HG2	2.00	0.43
1:A:539:TYR:CE1	1:A:931:PRO:HB3	2.53	0.43
1:A:514:ARG:NH1	1:A:668:GLU:O	2.51	0.43
1:A:950:ASN:ND2	1:A:952:LYS:HD3	2.33	0.43
1:A:49:VAL:HG22	1:A:80:GLU:O	2.18	0.43
1:A:1034:THR:HG22	1:A:1037:LYS:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ARG:HG3	1:A:89:THR:H	1.82	0.42
1:A:304:GLU:OE2	1:A:312:ARG:NH1	2.52	0.42
1:A:146:PHE:N	1:A:147:PRO:HD2	2.34	0.42
1:A:785:ARG:HB2	1:A:803:TYR:HB2	2.00	0.42
1:A:863:ARG:NH2	1:A:904:GLN:OE1	2.52	0.42
1:A:664:LEU:HG	1:A:666:MET:HE1	2.01	0.41
1:A:86:ASP:O	1:A:88:ARG:N	2.53	0.41
1:A:146:PHE:N	1:A:147:PRO:CD	2.83	0.41
1:A:143:GLY:HA2	1:A:146:PHE:CE2	2.55	0.41
1:A:991:ASP:N	1:A:991:ASP:OD1	2.54	0.41
1:A:512:LEU:HB2	1:A:518:LEU:HD13	2.03	0.41
1:A:600:ILE:HD13	1:A:814:LEU:HD12	2.02	0.41
1:A:474:LEU:HD11	1:A:666:MET:HE3	2.03	0.41
1:A:998:ASP:OD2	1:A:1001:ALA:N	2.42	0.41
1:A:867:ILE:HD13	1:A:905:LEU:HD11	2.02	0.41
1:A:132:TRP:CZ2	1:A:134:GLN:NE2	2.89	0.41
1:A:561:ASP:OD1	1:A:561:ASP:N	2.52	0.41
1:A:10:ALA:O	1:A:14:ILE:HG13	2.20	0.40
1:A:26:ALA:O	1:A:374:PRO:HD3	2.21	0.40
1:A:419:GLN:OE1	1:A:431:VAL:HG23	2.21	0.40
1:A:124:GLN:H	1:A:125:VAL:HA	1.85	0.40
1:A:1027:GLY:O	1:A:1031:VAL:HG23	2.22	0.40

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	1040/1295 (80%)	998 (96%)	36 (4%)	6 (1%)	30 65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	LEU
1	A	126	ALA
1	A	124	GLN
1	A	127	ASP
1	A	339	ALA
1	A	353	VAL

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	783/1050 (75%)	765 (98%)	18 (2%)	58 88

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	33	VAL
1	A	57	THR
1	A	73	VAL
1	A	111	VAL
1	A	118	VAL
1	A	353	VAL
1	A	507	SER
1	A	569	VAL
1	A	606	SER
1	A	630	HIS
1	A	633	LEU
1	A	642	LYS
1	A	693	VAL
1	A	715	THR
1	A	721	CYS
1	A	748	PRO
1	A	1024	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	630	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	75C	A	1301	1	38,51,52	1.48	6 (15%)	39,73,76	3.12	14 (35%)

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	75C	A	1301	1	-	0/42/66/67	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	75C	C11-S2	-4.83	1.74	1.81
2	A	1301	75C	C4-S2	-3.17	1.76	1.82
2	A	1301	75C	C16-N9	-3.00	1.27	1.33
2	A	1301	75C	C5-S1	-2.62	1.67	1.77
2	A	1301	75C	C13-N8	-2.60	1.27	1.33
2	A	1301	75C	O5-S1	-2.45	1.39	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	75C	O5-S1-O4	-8.08	105.24	119.31
2	A	1301	75C	N4-C6-N2	-7.08	123.31	128.87
2	A	1301	75C	C21-C18-C20	-3.99	100.48	109.22
2	A	1301	75C	C22-N7-C1	-3.78	122.59	126.81
2	A	1301	75C	O11-C10-C9	-3.03	105.09	111.44
2	A	1301	75C	C25-C7-N1	-2.46	107.25	112.58
2	A	1301	75C	O3-C23-C22	-2.40	104.12	111.61
2	A	1301	75C	C21-C18-C17	-2.35	104.89	109.17
2	A	1301	75C	C4-C5-S1	2.39	119.42	113.83
2	A	1301	75C	O5-S1-C5	2.71	112.58	107.86
2	A	1301	75C	C20-C18-C17	5.15	118.57	109.17
2	A	1301	75C	C12-N8-C13	5.40	133.50	122.79
2	A	1301	75C	C21-C18-C19	7.14	117.76	108.50
2	A	1301	75C	O4-S1-C5	7.75	121.31	107.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	75C	1	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 ⓘ

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	1042/1295 (80%)	-0.14	19 (1%) 71 61	32, 70, 127, 197	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	GLY	4.6
1	A	130	TRP	3.3
1	A	122	LEU	3.3
1	A	1045	GLU	3.2
1	A	1038	LEU	2.7
1	A	365	ALA	2.6
1	A	62	PHE	2.6
1	A	70	TRP	2.5
1	A	69	VAL	2.5
1	A	966	GLN	2.4
1	A	39	VAL	2.4
1	A	363	VAL	2.3
1	A	1041	ILE	2.2
1	A	1042	ILE	2.2
1	A	35	LEU	2.2
1	A	185	ARG	2.2
1	A	128	ASN	2.2
1	A	6	PRO	2.1
1	A	105	LEU	2.0

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 [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
2	75C	A	1301	49/50	0.98	0.20	1.01	15,38,55,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.