Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 07:28 AM JST

PDB ID	:	6L78
Title	:	Quinolone synthase (QNS) from Aegle marmelos
Authors	:	Mallika, V.; Abhinav, K.V.; Soniya, E.V.
Deposited on	:	2019-10-31
Resolution	:	1.55 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
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:

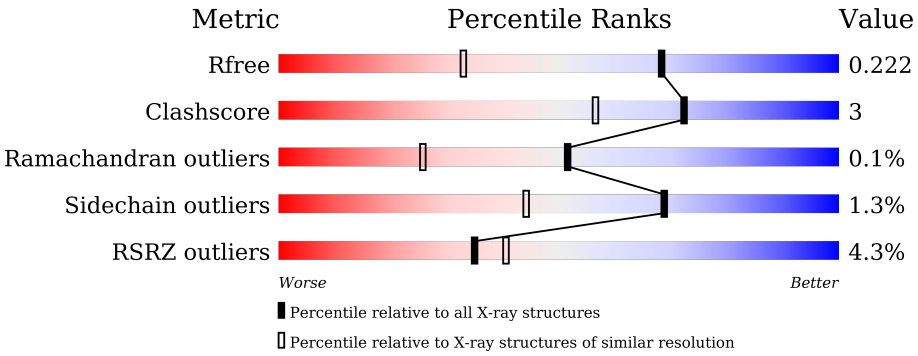
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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 <=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	391	89% 7%
1	B	391	91%
1	C	391	4% 87% 8%
1	D	391	10% 84% 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12785 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 Type III polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2850	1805	486	539	20			
1	B	375	Total	C	N	O	S	0	0	0
			2850	1805	486	539	20			
1	C	375	Total	C	N	O	S	0	0	0
			2850	1805	486	539	20			
1	D	375	Total	C	N	O	S	0	0	0
			2850	1805	486	539	20			

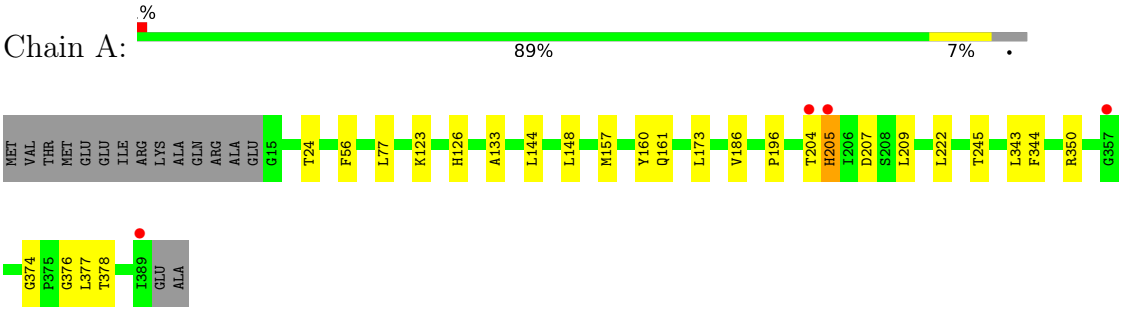
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	387	Total	O	0	0
			387	387		
2	B	400	Total	O	0	0
			400	400		
2	C	309	Total	O	0	0
			309	309		
2	D	289	Total	O	0	0
			289	289		

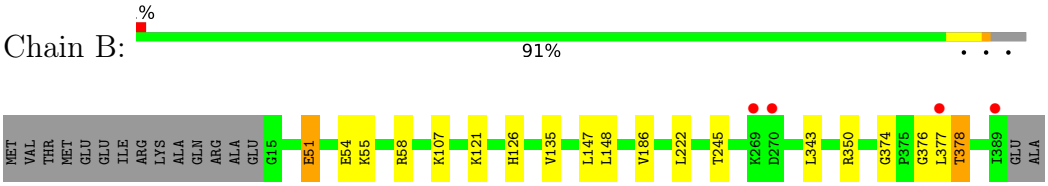
3 Residue-property plots (i)

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

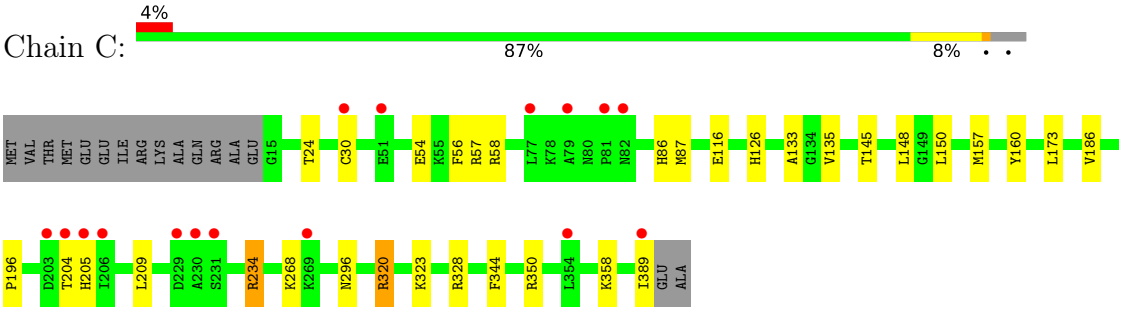
• Molecule 1: Type III polyketide synthase



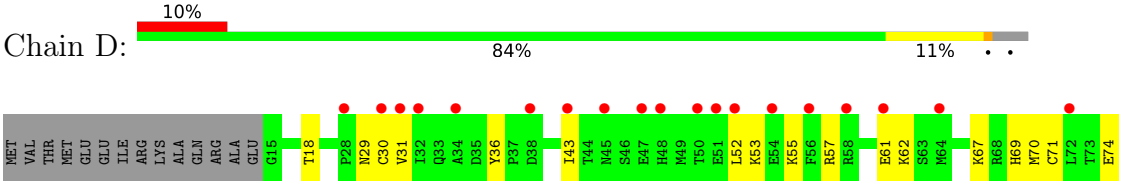
• Molecule 1: Type III polyketide synthase

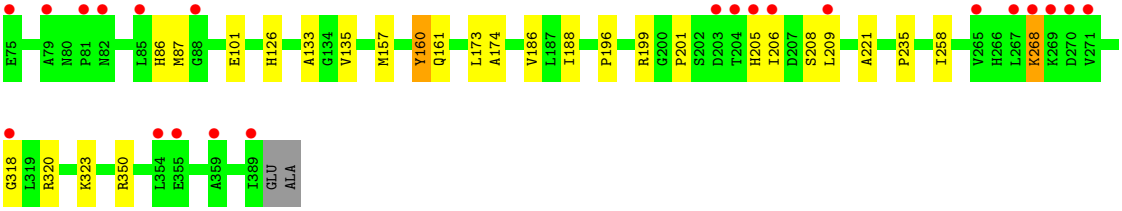


• Molecule 1: Type III polyketide synthase



• Molecule 1: Type III polyketide synthase




E75
A79
N80
P81
N82
L85
H86
M87
G88
E101
H126
A133
G134
V135
M157
Y160
Q161
L173
A174
V186
L187
I188
P196
R199
G200
P201
S202
D203
T204
H205
I206
D207
S208
L209
A221
P235
I258
V265
H266
L267
K268
K269
D270
V271
G318
L319
R320
K323
R350
L354
E355
A359
I389
GLU
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.77Å 115.77Å 85.89Å 90.00° 105.79° 90.00°	Depositor
Resolution (Å)	24.88 – 1.55 24.88 – 1.55	Depositor EDS
% Data completeness (in resolution range)	90.2 (24.88-1.55) 90.2 (24.88-1.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 1.55Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.184 , 0.222 0.184 , 0.222	Depositor DCC
R_{free} test set	8967 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	14.0	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12785	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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 40.03 % 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 2.9078e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.37	0/2906	0.59	0/3942
1	B	0.38	0/2906	0.61	0/3942
1	C	0.36	1/2906 (0.0%)	0.57	0/3942
1	D	0.34	0/2906	0.54	0/3942
All	All	0.36	1/11624 (0.0%)	0.58	0/15768

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	320	ARG	CZ-NH1	-6.13	1.25	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2850	0	2855	20	0
1	B	2850	0	2855	15	0
1	C	2850	0	2855	18	0
1	D	2850	0	2855	28	0
2	A	387	0	0	0	0
2	B	400	0	0	0	0
2	C	309	0	0	3	1
2	D	289	0	0	1	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12785	0	11420	78	1

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.

All (78) 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:161:GLN:HG3	1:B:135:VAL:HG11	1.58	0.85
1:D:206:ILE:HA	1:D:209:LEU:HD12	1.56	0.84
1:C:126:HIS:HB2	1:C:186:VAL:HG22	1.67	0.76
1:C:116:GLU:OE2	1:C:234:ARG:NH2	2.14	0.75
1:A:374:GLY:O	1:A:377:LEU:O	2.07	0.72
1:D:126:HIS:HB2	1:D:186:VAL:HG22	1.72	0.70
1:B:374:GLY:O	1:B:377:LEU:O	2.11	0.69
1:D:31:VAL:HG21	1:D:36:TYR:CD1	2.27	0.69
1:C:54:GLU:OE1	1:C:57:ARG:NH1	2.28	0.66
1:D:43:ILE:HD12	1:D:74:GLU:HG3	1.79	0.64
1:B:126:HIS:HB2	1:B:186:VAL:HG22	1.79	0.63
1:C:204:THR:OG1	1:C:205:HIS:ND1	2.31	0.63
1:A:126:HIS:HB2	1:A:186:VAL:HG22	1.82	0.61
1:D:52:LEU:HD21	1:D:201:PRO:HB2	1.82	0.60
1:D:206:ILE:HA	1:D:209:LEU:CD1	2.32	0.57
1:D:31:VAL:HG21	1:D:36:TYR:HD1	1.65	0.57
1:D:30:CYS:SG	1:D:67:LYS:HD2	2.46	0.56
1:B:54:GLU:HG3	1:B:58:ARG:NH1	2.20	0.56
1:B:55:LYS:HD3	1:B:58:ARG:HH21	1.71	0.56
1:A:245:THR:O	1:A:378:THR:HA	2.06	0.56
1:B:245:THR:O	1:B:378:THR:HA	2.06	0.56
1:C:54:GLU:O	1:C:58:ARG:HG2	2.05	0.55
1:D:53:LYS:NZ	1:D:57:ARG:HH21	2.06	0.54
1:A:144:LEU:C	1:A:144:LEU:HD13	2.28	0.54
1:D:174:ALA:HB2	1:D:188:ILE:HD11	1.90	0.54
1:A:207:ASP:N	1:A:207:ASP:OD1	2.44	0.51
1:B:107:LYS:HD2	1:B:147:LEU:HB3	1.93	0.51
1:A:204:THR:C	1:A:205:HIS:HD1	2.15	0.50
1:C:320:ARG:NH1	2:C:410:HOH:O	2.44	0.50
1:D:133:ALA:HA	1:D:196:PRO:HG3	1.93	0.50
1:A:222:LEU:HD11	1:A:343:LEU:HD13	1.94	0.50
1:D:67:LYS:NZ	1:D:69:HIS:HE1	2.10	0.49
1:C:24:THR:HB	1:C:344:PHE:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LYS:HE3	1:B:148:LEU:O	2.13	0.49
1:C:133:ALA:HA	1:C:196:PRO:HG3	1.94	0.49
1:D:53:LYS:HZ3	1:D:57:ARG:HH21	1.59	0.49
1:C:135:VAL:CG1	1:D:161:GLN:HG2	2.42	0.48
1:D:57:ARG:HG2	1:D:61:GLU:OE1	2.14	0.48
1:C:56:PHE:CD1	1:C:209:LEU:HD22	2.48	0.47
1:D:268:LYS:HB3	1:D:268:LYS:HE2	1.57	0.47
1:A:133:ALA:HA	1:A:196:PRO:HG2	1.96	0.47
1:C:145:THR:HG23	1:C:150:LEU:HB2	1.96	0.47
1:A:56:PHE:CD1	1:A:209:LEU:HD22	2.49	0.47
1:D:188:ILE:O	1:D:221:ALA:HA	2.16	0.46
1:D:29:ASN:HB3	1:D:70:MET:O	2.15	0.46
1:D:86:HIS:ND1	1:D:87:MET:HG2	2.31	0.46
1:D:86:HIS:O	1:D:199:ARG:HD3	2.16	0.46
1:D:55:LYS:HG3	2:D:519:HOH:O	2.16	0.45
1:A:157:MET:HG2	1:A:173:LEU:HD21	1.99	0.45
1:D:71:CYS:SG	1:D:101:GLU:HG2	2.56	0.45
1:C:157:MET:HG2	1:C:173:LEU:HD21	1.97	0.45
1:B:51:GLU:H	1:B:51:GLU:CD	2.20	0.45
1:D:135:VAL:HG12	1:D:160:TYR:CG	2.52	0.44
1:D:205:HIS:ND1	1:D:208:SER:HB2	2.33	0.44
1:A:376:GLY:N	1:A:377:LEU:HA	2.32	0.44
1:C:296:ASN:HA	1:C:323:LYS:HE3	1.99	0.43
1:D:258:ILE:HD12	1:D:258:ILE:N	2.34	0.43
1:D:18:THR:HG21	1:D:235:PRO:HB3	2.00	0.43
1:A:377:LEU:O	1:A:378:THR:CB	2.66	0.42
1:D:157:MET:HG2	1:D:173:LEU:HD21	2.00	0.42
1:B:377:LEU:O	1:B:378:THR:CB	2.66	0.42
1:C:204:THR:HG1	1:C:205:HIS:CE1	2.34	0.42
1:A:24:THR:HB	1:A:344:PHE:CZ	2.55	0.42
1:A:377:LEU:O	1:A:378:THR:HB	2.20	0.42
1:C:328:ARG:HD3	2:C:587:HOH:O	2.20	0.41
1:A:144:LEU:HD13	1:A:144:LEU:O	2.20	0.41
1:B:376:GLY:N	1:B:377:LEU:HA	2.36	0.41
1:B:121:LYS:HB2	1:B:121:LYS:HE2	1.72	0.41
1:C:204:THR:OG1	1:C:205:HIS:CE1	2.73	0.41
1:B:222:LEU:HD11	1:B:343:LEU:HD13	2.01	0.40
1:C:86:HIS:ND1	1:C:87:MET:HG2	2.36	0.40
1:B:377:LEU:HA	1:B:377:LEU:HD23	1.82	0.40
1:A:123:LYS:HA	1:A:123:LYS:HD3	1.83	0.40
1:C:389:ILE:HA	2:C:646:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:HD23	1:A:77:LEU:HA	1.97	0.40
1:A:161:GLN:CG	1:B:135:VAL:HG11	2.40	0.40
1:A:144:LEU:HD11	1:A:148:LEU:HD12	2.03	0.40
1:D:320:ARG:HB2	1:D:323:LYS:HG2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:410:HOH:O	2:D:544:HOH:O[1_455]	2.15	0.05

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	373/391 (95%)	363 (97%)	10 (3%)	0	100	100
1	B	373/391 (95%)	361 (97%)	11 (3%)	1 (0%)	41	19
1	C	373/391 (95%)	364 (98%)	9 (2%)	0	100	100
1	D	373/391 (95%)	363 (97%)	9 (2%)	1 (0%)	41	19
All	All	1492/1564 (95%)	1451 (97%)	39 (3%)	2 (0%)	51	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	318	GLY
1	B	378	THR

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	309/327 (94%)	306 (99%)	3 (1%)	76	57
1	B	309/327 (94%)	307 (99%)	2 (1%)	86	73
1	C	309/327 (94%)	302 (98%)	7 (2%)	50	21
1	D	309/327 (94%)	305 (99%)	4 (1%)	69	44
All	All	1236/1308 (94%)	1220 (99%)	16 (1%)	69	44

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	TYR
1	A	205	HIS
1	A	350	ARG
1	B	51	GLU
1	B	350	ARG
1	C	30	CYS
1	C	148	LEU
1	C	160	TYR
1	C	234	ARG
1	C	268	LYS
1	C	350	ARG
1	C	358	LYS
1	D	62	LYS
1	D	160	TYR
1	D	268	LYS
1	D	350	ARG

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

Mol	Chain	Res	Type
1	C	86	HIS
1	D	69	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 monosaccharides 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, 95^{th} 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	375/391 (95%)	-0.11	4 (1%) 80 84	7, 14, 24, 41	0
1	B	375/391 (95%)	-0.13	4 (1%) 80 84	7, 13, 23, 33	0
1	C	375/391 (95%)	0.30	16 (4%) 35 40	9, 18, 33, 45	0
1	D	375/391 (95%)	0.58	41 (10%) 5 5	10, 20, 37, 53	0
All	All	1500/1564 (95%)	0.16	65 (4%) 35 40	7, 16, 30, 53	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	389	ILE	12.7
1	D	50	THR	7.7
1	D	269	LYS	6.9
1	D	206	ILE	5.0
1	C	269	LYS	4.9
1	A	389	ILE	4.9
1	D	204	THR	4.9
1	C	204	THR	4.9
1	B	389	ILE	4.6
1	D	205	HIS	4.3
1	D	203	ASP	4.2
1	C	206	ILE	4.0
1	D	354	LEU	3.7
1	D	79	ALA	3.6
1	A	204	THR	3.5
1	D	30	CYS	3.4
1	D	209	LEU	3.4
1	D	355	GLU	3.3
1	D	318	GLY	3.3
1	D	389	ILE	3.3
1	D	31	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	269	LYS	3.2
1	D	28	PRO	3.2
1	C	203	ASP	3.1
1	D	267	LEU	3.1
1	D	61	GLU	3.1
1	D	45	ASN	2.9
1	C	205	HIS	2.9
1	D	52	LEU	2.9
1	D	88	GLY	2.9
1	D	265	VAL	2.9
1	D	75	GLU	2.8
1	D	81	PRO	2.8
1	D	270	ASP	2.8
1	C	354	LEU	2.7
1	D	47	GLU	2.7
1	D	54	GLU	2.7
1	D	72	LEU	2.7
1	D	56	PHE	2.6
1	C	231	SER	2.6
1	D	64	MET	2.6
1	D	51	GLU	2.6
1	C	79	ALA	2.5
1	C	82	ASN	2.5
1	D	38	ASP	2.5
1	D	85	LEU	2.5
1	D	32	ILE	2.5
1	A	205	HIS	2.4
1	A	357	GLY	2.4
1	D	268	LYS	2.3
1	D	48	HIS	2.3
1	D	43	ILE	2.3
1	C	51	GLU	2.3
1	D	82	ASN	2.3
1	D	58	ARG	2.3
1	D	271	VAL	2.2
1	C	229	ASP	2.2
1	C	81	PRO	2.2
1	D	359	ALA	2.1
1	B	377	LEU	2.1
1	C	77	LEU	2.1
1	D	34	ALA	2.1
1	C	30	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	270	ASP	2.1
1	C	230	ALA	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.