Full wwPDB X-ray Structure Validation Report (i)

Jun 1, 2021 – 08:08 PM JST

PDB ID	:	6LE0
Title	:	A nonspecific heme-binding cyclase catalyzes [4 + 2] cycloaddition during neoabyssomicin biosynthesis
Authors	:	Ju, J.J.
Deposited on	:	2019-11-23
Resolution	:	2.51 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 (i) symbol.

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

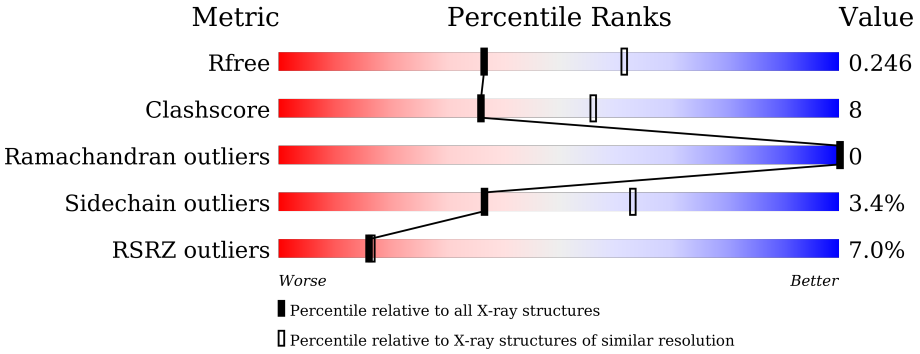
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.19
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.19

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 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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	219	5%, 79%, 16%, • 5%
1	B	219	.%, 75%, 16%, • 8%
1	C	219	11%, 70%, 23%, 6%
1	D	219	8%, 72%, 18%, • 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6419 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 AbmU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	209	1602	1013	279	305	5	0	0	0
1	B	201	1540	976	267	292	5	0	0	0
1	C	206	1572	998	273	296	5	0	0	0
1	D	200	1531	971	266	289	5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MSE	-	initiating methionine	UNP A0A2P1BT29
B	2	MSE	-	initiating methionine	UNP A0A2P1BT29
C	2	MSE	-	initiating methionine	UNP A0A2P1BT29
D	2	MSE	-	initiating methionine	UNP A0A2P1BT29

- Molecule 2 is water.

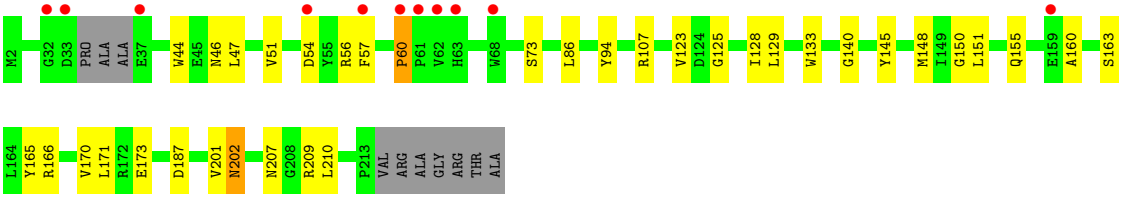
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	81	81	81	0	0
2	B	66	66	66	0	0
2	C	16	16	16	0	0
2	D	11	11	11	0	0

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.

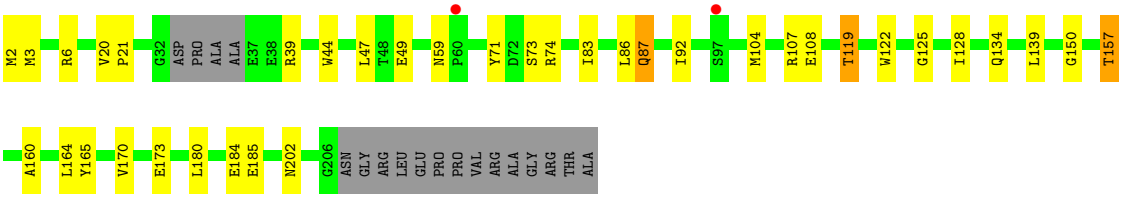
• Molecule 1: AbmU

Chain A:



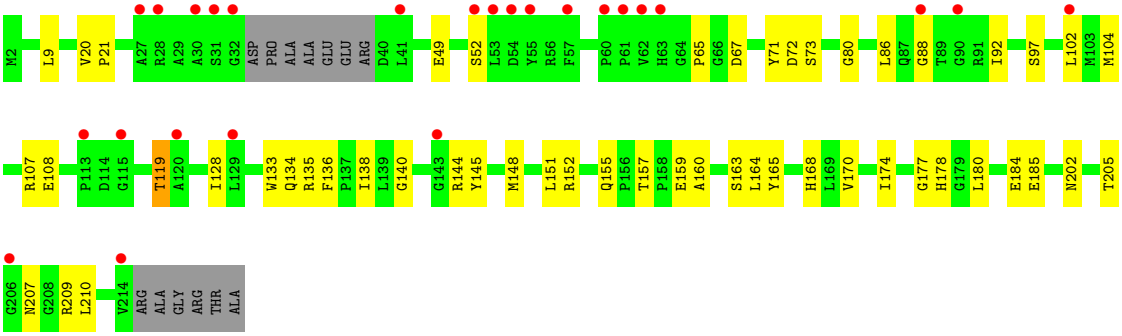
• Molecule 1: AbmU

Chain B:



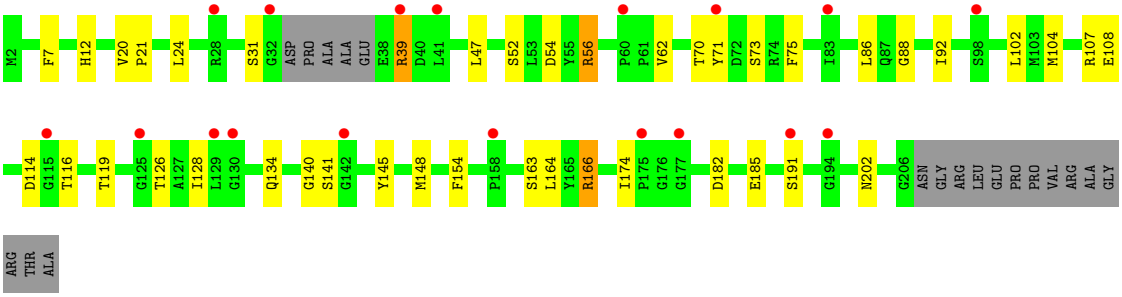
• Molecule 1: AbmU

Chain C:



• Molecule 1: AbmU

Chain D:


M2
F7
H12
V20
P21
L24
R28
S31
G32
ASP
PRO
ALA
ALA
GLU
E38
R39
D40
L41
L47
S52
L53
D54
Y55
R56
P60
P61
V62
T70
Y71
D72
S73
R74
F75
I83
L86
Q87
G88
I92
S98
L102
M103
M104
R107
E108
D114
G115
T116
T119
G125
T126
A127
I128
L129
G130
Q134
G140
S141
G142
Y145
M148
F154
P158
S163
L164
Y165
R166
I174
P175
G176
G177
D182
E185
S191
G194
N202
G206
ASN
GLY
ARG
LEU
GLU
PRO
PRO
VAL
ARG
ALA
GLY
ARG
THR
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	66.61Å 65.35Å 101.40Å 90.00° 90.19° 90.00°	Depositor
Resolution (Å)	27.88 – 2.51 34.37 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.3 (27.88-2.51) 98.3 (34.37-2.51)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.200 , 0.245 0.200 , 0.246	Depositor DCC
R_{free} test set	1458 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	41.7	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.006 for -k,-h,-l 0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6419	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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	0.59	1/1644 (0.1%)	0.79	0/2237
1	B	0.54	0/1580	0.74	0/2149
1	C	0.45	0/1614	0.72	0/2198
1	D	0.44	0/1571	0.72	2/2137 (0.1%)
All	All	0.51	1/6409 (0.0%)	0.74	2/8721 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	VAL	CB-CG2	-5.04	1.42	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	166	ARG	CG-CD-NE	-8.37	94.23	111.80
1	D	166	ARG	NE-CZ-NH2	-5.69	117.45	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	59	ASN	Peptide

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	1602	0	1524	21	0
1	B	1540	0	1467	21	0
1	C	1572	0	1504	36	0
1	D	1531	0	1461	29	0
2	A	81	0	0	0	0
2	B	66	0	0	2	0
2	C	16	0	0	2	0
2	D	11	0	0	0	0
All	All	6419	0	5956	97	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 8.

All (97) 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:C:86:LEU:HD21	1:C:108:GLU:HB3	1.55	0.87
1:D:128:ILE:HD11	1:D:134:GLN:HG2	1.65	0.77
1:D:108:GLU:HB2	1:D:119:THR:HG22	1.69	0.75
1:D:182:ASP:HB3	1:D:185:GLU:HG2	1.70	0.73
1:C:128:ILE:HD11	1:C:134:GLN:HG3	1.70	0.72
1:B:44:TRP:HB3	1:B:47:LEU:HD21	1.74	0.70
1:B:157:THR:HG22	1:B:160:ALA:H	1.55	0.70
1:C:67:ASP:HB2	1:C:92:ILE:HD13	1.76	0.66
1:C:73:SER:HB2	1:C:86:LEU:HB3	1.80	0.64
1:A:107:ARG:NH2	1:A:187:ASP:OD1	2.26	0.63
1:A:140:GLY:HA3	1:A:145:TYR:O	2.00	0.61
1:B:92:ILE:HG12	1:B:104:MSE:HE3	1.81	0.60
1:D:73:SER:HB2	1:D:86:LEU:HB3	1.83	0.59
1:B:73:SER:HB2	1:B:86:LEU:HB3	1.83	0.59
1:C:160:ALA:HB1	1:C:163:SER:OG	2.04	0.58
1:D:182:ASP:HB3	1:D:185:GLU:CG	2.32	0.58
1:B:134:GLN:NE2	2:B:301:HOH:O	2.24	0.58
1:D:116:THR:OG1	1:D:141:SER:O	2.19	0.57
1:A:210:LEU:HD11	1:B:107:ARG:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ARG:HH21	1:D:174:ILE:HA	1.70	0.57
1:D:108:GLU:HB2	1:D:119:THR:CG2	2.35	0.57
1:C:107:ARG:NH1	1:D:202:ASN:O	2.39	0.56
1:A:46:ASN:OD1	1:A:166:ARG:NH1	2.39	0.55
1:D:54:ASP:CG	1:D:56:ARG:HH21	2.11	0.54
1:C:71:TYR:CE1	1:C:88:GLY:HA3	2.42	0.54
1:C:170:VAL:HG23	1:D:7:PHE:CZ	2.43	0.54
1:B:157:THR:HB	1:B:164:LEU:O	2.09	0.53
1:D:71:TYR:CZ	1:D:88:GLY:HA3	2.44	0.53
1:B:125:GLY:O	1:B:128:ILE:HG22	2.10	0.51
1:C:92:ILE:HG13	1:C:104:MSE:HG2	1.91	0.51
1:B:87:GLN:NE2	2:B:306:HOH:O	2.44	0.51
1:C:9:LEU:HD12	1:D:24:LEU:HG	1.92	0.51
1:A:44:TRP:HB3	1:A:47:LEU:HD21	1.93	0.51
1:D:128:ILE:HD11	1:D:134:GLN:CG	2.37	0.51
1:C:140:GLY:HA3	1:C:145:TYR:O	2.10	0.50
1:A:133:TRP:CD2	1:A:155:GLN:HB2	2.47	0.50
1:B:39:ARG:HB3	1:B:173:GLU:HB3	1.94	0.50
1:A:73:SER:HB2	1:A:86:LEU:HB3	1.92	0.49
1:C:207:ASN:HD22	1:C:209:ARG:HE	1.60	0.49
1:D:114:ASP:OD1	1:D:114:ASP:N	2.40	0.48
1:A:51:VAL:HG21	1:A:165:TYR:CE2	2.49	0.48
1:A:202:ASN:O	1:B:107:ARG:NH1	2.47	0.48
1:A:150:GLY:HA3	1:A:171:LEU:HD23	1.96	0.48
1:D:145:TYR:HA	1:D:148:MSE:HE3	1.96	0.48
1:C:157:THR:HG22	1:C:159:GLU:H	1.78	0.47
1:C:180:LEU:HD12	1:C:185:GLU:HB3	1.96	0.47
1:C:20:VAL:HG21	1:D:20:VAL:HG21	1.97	0.47
1:C:49:GLU:HB3	1:C:165:TYR:HB2	1.95	0.47
1:C:92:ILE:CD1	1:C:104:MSE:HE3	2.45	0.47
1:D:102:LEU:H	1:D:126:THR:HG23	1.80	0.46
1:A:133:TRP:CE2	1:B:6:ARG:HD2	2.51	0.46
1:B:71:TYR:OH	1:B:108:GLU:OE2	2.24	0.46
1:C:168:HIS:HB3	1:D:7:PHE:CZ	2.51	0.46
1:C:210:LEU:HD11	1:D:107:ARG:HG3	1.97	0.46
1:A:94:TYR:OH	1:A:201:VAL:HG13	2.16	0.46
1:C:160:ALA:HB3	1:C:164:LEU:HD12	1.97	0.46
1:D:12:HIS:HB3	1:D:185:GLU:OE2	2.16	0.46
1:B:44:TRP:CE2	1:B:83:ILE:HD13	2.51	0.45
1:C:119:THR:HG23	1:C:136:PHE:HB3	1.99	0.45
1:C:133:TRP:CD2	1:C:155:GLN:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:GLY:HA3	1:D:145:TYR:O	2.16	0.45
1:C:178:HIS:N	2:C:305:HOH:O	2.51	0.44
1:C:135:ARG:HB3	1:C:151:LEU:HD11	1.99	0.44
1:C:174:ILE:HD11	1:C:177:GLY:O	2.17	0.44
1:B:2:MSE:HG2	1:B:3:MSE:N	2.33	0.44
1:B:180:LEU:HD12	1:B:185:GLU:HB3	1.99	0.44
1:C:65:PRO:HA	1:C:92:ILE:HG22	2.00	0.43
1:A:148:MSE:HG2	1:A:173:GLU:HA	2.00	0.43
1:A:160:ALA:HB1	1:A:163:SER:OG	2.18	0.43
1:A:207:ASN:O	1:A:209:ARG:HG3	2.18	0.43
1:C:144:ARG:O	1:C:148:MSE:HE3	2.18	0.43
1:D:164:LEU:HD12	1:D:164:LEU:HA	1.79	0.43
1:B:49:GLU:HB3	1:B:165:TYR:HB2	2.00	0.43
1:D:154:PHE:HA	1:D:166:ARG:O	2.19	0.43
1:A:128:ILE:HG13	1:A:129:LEU:H	1.83	0.42
1:B:150:GLY:HA3	1:B:170:VAL:O	2.19	0.42
1:D:71:TYR:CE2	1:D:88:GLY:HA3	2.54	0.42
1:D:92:ILE:HG12	1:D:104:MSE:HE3	2.02	0.42
1:A:201:VAL:HG11	1:B:122:TRP:CZ2	2.55	0.42
1:B:108:GLU:OE1	1:B:119:THR:HG21	2.19	0.42
1:C:80:GLY:N	2:C:301:HOH:O	2.51	0.42
1:C:102:LEU:HD12	1:C:102:LEU:HA	1.86	0.42
1:C:97:SER:HB3	1:C:205:THR:HG21	2.02	0.42
1:A:54:ASP:HB3	1:A:56:ARG:NH1	2.35	0.41
1:C:174:ILE:HD11	1:C:178:HIS:HA	2.01	0.41
1:C:135:ARG:HD2	1:C:151:LEU:HD21	2.02	0.41
1:C:138:ILE:HD11	1:C:152:ARG:HB2	2.03	0.41
1:D:20:VAL:HB	1:D:21:PRO:HD3	2.03	0.41
1:D:47:LEU:HD22	1:D:75:PHE:HB3	2.03	0.41
1:A:57:PHE:HB3	1:A:60:PRO:HA	2.03	0.41
1:A:150:GLY:HA3	1:A:170:VAL:O	2.20	0.41
1:C:52:SER:O	1:C:71:TYR:HA	2.21	0.41
1:A:125:GLY:HA2	1:A:128:ILE:HG12	2.03	0.40
1:C:67:ASP:CB	1:C:92:ILE:HD13	2.49	0.40
1:B:20:VAL:HB	1:B:21:PRO:HD3	2.02	0.40
1:C:20:VAL:HB	1:C:21:PRO:HD3	2.03	0.40
1:D:71:TYR:OH	1:D:108:GLU:OE2	2.30	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	205/219 (94%)	200 (98%)	5 (2%)	0	100	100
1	B	197/219 (90%)	194 (98%)	3 (2%)	0	100	100
1	C	202/219 (92%)	199 (98%)	3 (2%)	0	100	100
1	D	196/219 (90%)	193 (98%)	3 (2%)	0	100	100
All	All	800/876 (91%)	786 (98%)	14 (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	165/165 (100%)	162 (98%)	3 (2%)	59	81
1	B	158/165 (96%)	151 (96%)	7 (4%)	28	52
1	C	162/165 (98%)	158 (98%)	4 (2%)	47	73
1	D	157/165 (95%)	149 (95%)	8 (5%)	24	45
All	All	642/660 (97%)	620 (97%)	22 (3%)	37	63

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	PRO
1	A	151	LEU

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Mol	Chain	Res	Type
1	A	202	ASN
1	B	74	ARG
1	B	87	GLN
1	B	119	THR
1	B	139	LEU
1	B	157	THR
1	B	184	GLU
1	B	202	ASN
1	C	72	ASP
1	C	119	THR
1	C	184	GLU
1	C	202	ASN
1	D	31	SER
1	D	39	ARG
1	D	52	SER
1	D	56	ARG
1	D	62	VAL
1	D	70	THR
1	D	163	SER
1	D	191	SER

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

Mol	Chain	Res	Type
1	B	87	GLN
1	D	59	ASN

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)

There are no ligands in this entry.

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	204/219 (93%)	0.20	11 (5%) 25 27	17, 31, 65, 97	0
1	B	196/219 (89%)	0.05	2 (1%) 82 84	18, 35, 61, 89	0
1	C	201/219 (91%)	0.95	25 (12%) 4 3	34, 65, 92, 110	0
1	D	195/219 (89%)	0.81	18 (9%) 9 9	33, 63, 92, 118	0
All	All	796/876 (90%)	0.50	56 (7%) 16 16	17, 47, 88, 118	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	129	LEU	8.5
1	C	55	TYR	6.0
1	D	142	GLY	5.6
1	C	54	ASP	4.6
1	C	61	PRO	4.5
1	A	37	GLU	4.5
1	C	62	VAL	4.4
1	D	177	GLY	4.3
1	A	54	ASP	4.3
1	C	57	PHE	3.9
1	C	53	LEU	3.8
1	D	39	ARG	3.7
1	C	143	GLY	3.7
1	C	63	HIS	3.4
1	A	62	VAL	3.4
1	C	115	GLY	3.3
1	D	175	PRO	3.3
1	C	31	SER	3.3
1	A	63	HIS	3.3
1	D	130	GLY	3.3
1	D	41	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	83	ILE	3.0
1	D	115	GLY	3.0
1	C	27	ALA	3.0
1	C	28	ARG	3.0
1	C	41	LEU	2.9
1	B	60	PRO	2.9
1	C	129	LEU	2.8
1	C	102	LEU	2.8
1	C	60	PRO	2.7
1	C	214	VAL	2.7
1	C	30	ALA	2.6
1	A	57	PHE	2.6
1	D	158	PRO	2.6
1	A	159	GLU	2.6
1	C	88	GLY	2.6
1	C	90	GLY	2.6
1	D	32	GLY	2.5
1	D	98	SER	2.5
1	A	33	ASP	2.5
1	C	32	GLY	2.5
1	D	60	PRO	2.5
1	D	191	SER	2.4
1	B	97	SER	2.4
1	D	125	GLY	2.3
1	A	61	PRO	2.3
1	A	32	GLY	2.3
1	C	206	GLY	2.3
1	D	71	TYR	2.3
1	D	194	GLY	2.3
1	C	113	PRO	2.3
1	A	68	TRP	2.3
1	C	120	ALA	2.2
1	D	28	ARG	2.2
1	A	60	PRO	2.2
1	C	52	SER	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.