



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:47 am GMT

PDB ID : 2OVL
Title : Crystal structure of a racemase from *Streptomyces coelicolor* A3(2)
Authors : Rao, K.N.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center
for Structural Genomics (NYSGXRC)
Deposited on : 2007-02-14
Resolution : 2.13 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

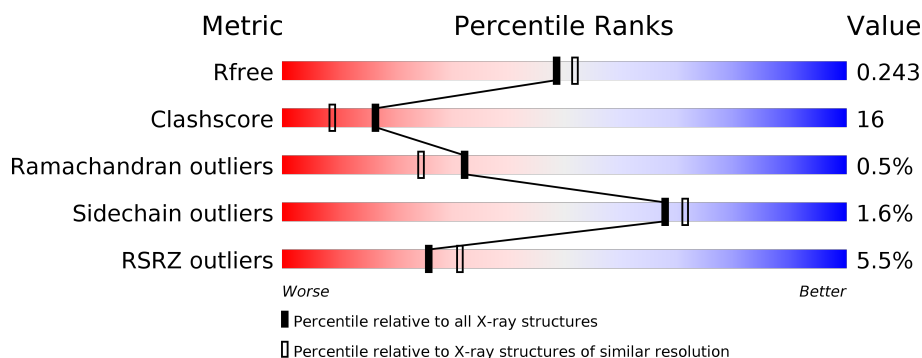
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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}	100719	1915 (2.16-2.12)
Clashscore	112137	2047 (2.16-2.12)
Ramachandran outliers	110173	2020 (2.16-2.12)
Sidechain outliers	110143	2019 (2.16-2.12)
RSRZ outliers	101464	1921 (2.16-2.12)

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	371	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>
1	B	371	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>• •</div> </div> </div>
1	C	371	<div> <div>7%</div> <div> <div></div> <div>69%</div> <div>27%</div> <div>• •</div> </div> </div>
1	D	371	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>20%</div> <div>• 10%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	B	400	-	-	-	X
2	NA	C	400	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11225 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 Putative racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	Se	0	0	0
			2749	1738	492	506	2	11			
1	B	357	Total	C	N	O	S	Se	0	0	0
			2749	1738	492	506	2	11			
1	C	357	Total	C	N	O	S	Se	0	0	0
			2749	1738	492	506	2	11			
1	D	334	Total	C	N	O	S	Se	0	0	0
			2577	1631	462	474	2	8			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	CLONING ARTIFACT	UNP Q9RKF7
A	2	SER	-	CLONING ARTIFACT	UNP Q9RKF7
A	3	LEU	-	CLONING ARTIFACT	UNP Q9RKF7
A	28	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
A	29	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
A	63	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
A	87	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
A	167	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
A	195	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
A	200	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
A	294	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
A	318	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
A	329	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
A	333	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
A	364	GLU	-	CLONING ARTIFACT	UNP Q9RKF7
A	365	GLY	-	CLONING ARTIFACT	UNP Q9RKF7
A	366	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
A	367	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
A	368	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
A	369	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
A	370	HIS	-	CLONING ARTIFACT	UNP Q9RKF7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	371	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
B	1	MSE	-	CLONING ARTIFACT	UNP Q9RKF7
B	2	SER	-	CLONING ARTIFACT	UNP Q9RKF7
B	3	LEU	-	CLONING ARTIFACT	UNP Q9RKF7
B	28	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
B	29	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
B	63	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
B	87	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
B	167	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
B	195	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
B	200	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
B	294	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
B	318	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
B	329	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
B	333	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
B	364	GLU	-	CLONING ARTIFACT	UNP Q9RKF7
B	365	GLY	-	CLONING ARTIFACT	UNP Q9RKF7
B	366	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
B	367	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
B	368	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
B	369	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
B	370	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
B	371	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
C	1	MSE	-	CLONING ARTIFACT	UNP Q9RKF7
C	2	SER	-	CLONING ARTIFACT	UNP Q9RKF7
C	3	LEU	-	CLONING ARTIFACT	UNP Q9RKF7
C	28	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
C	29	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
C	63	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
C	87	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
C	167	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
C	195	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
C	200	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
C	294	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
C	318	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
C	329	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
C	333	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
C	364	GLU	-	CLONING ARTIFACT	UNP Q9RKF7
C	365	GLY	-	CLONING ARTIFACT	UNP Q9RKF7
C	366	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
C	367	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
C	368	HIS	-	CLONING ARTIFACT	UNP Q9RKF7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	369	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
C	370	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
C	371	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
D	1	MSE	-	CLONING ARTIFACT	UNP Q9RKF7
D	2	SER	-	CLONING ARTIFACT	UNP Q9RKF7
D	3	LEU	-	CLONING ARTIFACT	UNP Q9RKF7
D	28	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
D	29	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
D	63	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
D	87	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
D	167	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
D	195	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
D	200	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
D	294	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
D	318	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
D	329	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
D	333	MSE	MET	MODIFIED RESIDUE	UNP Q9RKF7
D	364	GLU	-	CLONING ARTIFACT	UNP Q9RKF7
D	365	GLY	-	CLONING ARTIFACT	UNP Q9RKF7
D	366	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
D	367	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
D	368	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
D	369	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
D	370	HIS	-	CLONING ARTIFACT	UNP Q9RKF7
D	371	HIS	-	CLONING ARTIFACT	UNP Q9RKF7

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0

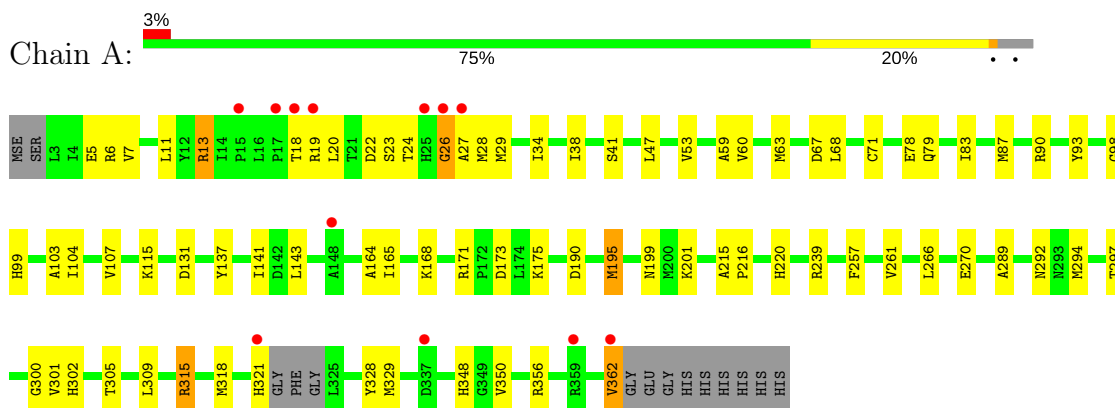
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total 130	O 130	0	0
3	B	107	Total 107	O 107	0	0
3	C	85	Total 85	O 85	0	0
3	D	75	Total 75	O 75	0	0

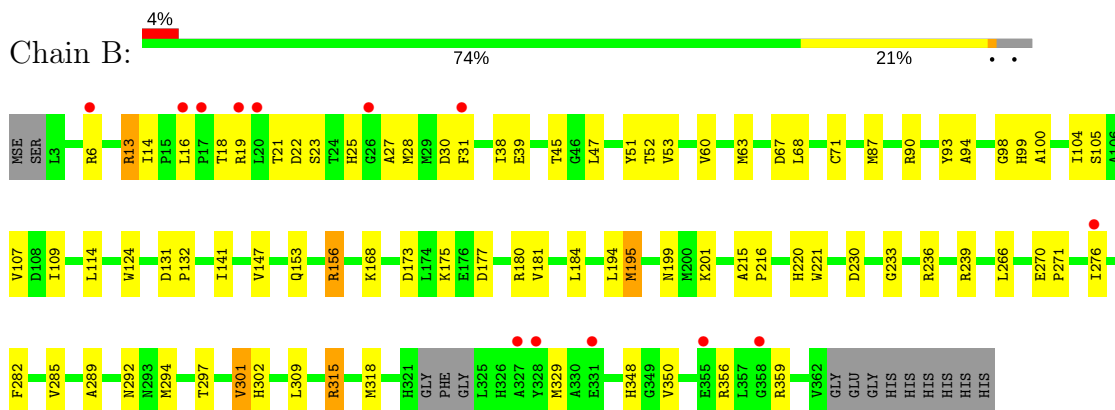
3 Residue-property plots

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

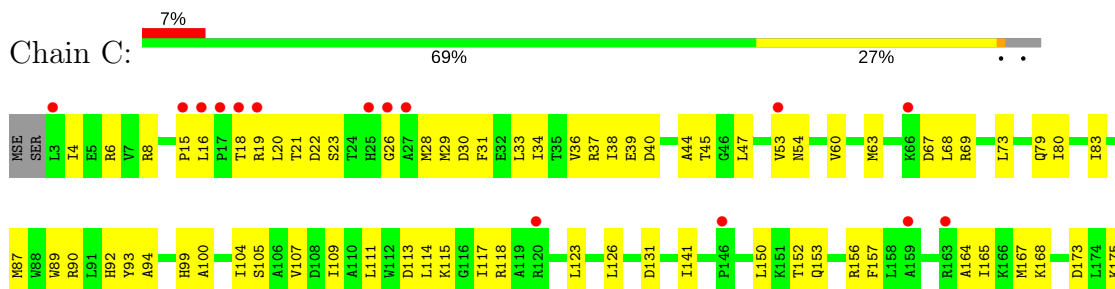
• Molecule 1: Putative racemase



• Molecule 1: Putative racemase

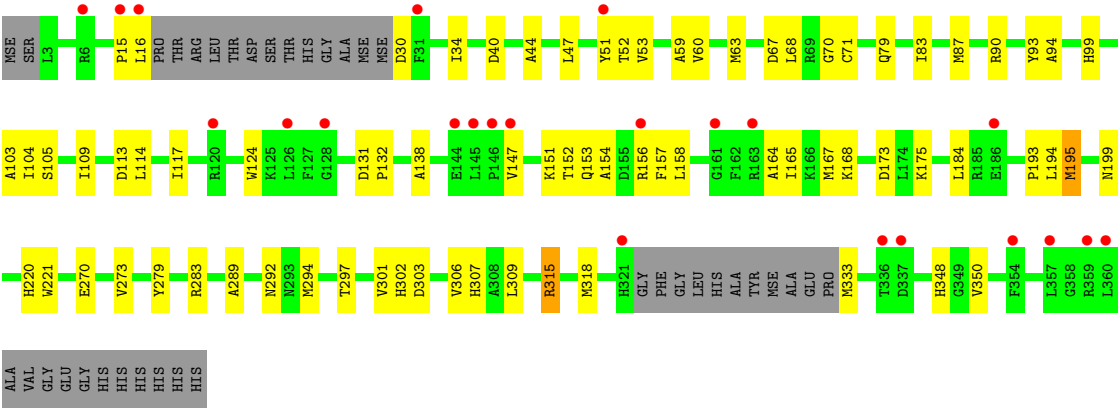


• Molecule 1: Putative racemase





● Molecule 1: Putative racemase



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	177.60Å 177.60Å 111.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.05 – 2.13 32.05 – 2.13	Depositor EDS
% Data completeness (in resolution range)	97.4 (32.05-2.13) 97.2 (32.05-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.243 0.215 , 0.243	Depositor DCC
R_{free} test set	2431 reflections (2.50%)	DCC
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11225	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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:
NA

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	0.35	0/2802	0.61	0/3794
1	B	0.33	0/2802	0.60	0/3794
1	C	0.31	0/2802	0.57	0/3794
1	D	0.31	0/2628	0.58	0/3561
All	All	0.32	0/11034	0.59	0/14943

There are no bond length outliers.

There are no bond angle outliers.

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	2749	0	2711	76	0
1	B	2749	0	2711	86	0
1	C	2749	0	2711	107	0
1	D	2577	0	2543	77	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	130	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	107	0	0	1	0
3	C	85	0	0	0	0
3	D	75	0	0	0	0
All	All	11225	0	10676	341	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 16.

The worst 5 of 341 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:68:LEU:HD13	1:C:87:MSE:HE3	1.30	1.13
1:B:68:LEU:HD13	1:B:87:MSE:HE3	1.27	1.13
1:D:60:VAL:HA	1:D:63:MSE:HE2	1.27	1.12
1:A:13:ARG:HH11	1:A:13:ARG:HB2	1.12	1.11
1:B:60:VAL:HA	1:B:63:MSE:HE3	1.30	1.10

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	353/371 (95%)	340 (96%)	10 (3%)	3 (1%)	22	13
1	B	353/371 (95%)	338 (96%)	14 (4%)	1 (0%)	44	39
1	C	353/371 (95%)	336 (95%)	15 (4%)	2 (1%)	28	20
1	D	328/371 (88%)	314 (96%)	13 (4%)	1 (0%)	44	39
All	All	1387/1484 (94%)	1328 (96%)	52 (4%)	7 (0%)	32	24

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	GLY
1	A	27	ALA
1	C	330	ALA
1	C	301	VAL
1	A	301	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	283/281 (101%)	277 (98%)	6 (2%)	59	61
1	B	283/281 (101%)	278 (98%)	5 (2%)	64	66
1	C	283/281 (101%)	279 (99%)	4 (1%)	71	75
1	D	265/281 (94%)	262 (99%)	3 (1%)	78	81
All	All	1114/1124 (99%)	1096 (98%)	18 (2%)	68	71

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	156	ARG
1	B	195	MSE
1	C	315	ARG
1	B	13	ARG
1	B	114	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	348	HIS
1	C	153	GLN
1	D	54	ASN
1	B	199	ASN
1	D	153	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	346/371 (93%)	0.01	12 (3%) 44 51	15, 25, 46, 64	0
1	B	346/371 (93%)	0.05	13 (3%) 41 47	16, 27, 46, 59	0
1	C	346/371 (93%)	0.42	27 (7%) 14 17	20, 35, 55, 65	0
1	D	326/371 (87%)	0.24	23 (7%) 17 21	19, 33, 52, 61	0
All	All	1364/1484 (91%)	0.18	75 (5%) 26 31	15, 30, 51, 65	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	25	HIS	9.6
1	C	26	GLY	7.1
1	A	26	GLY	6.9
1	A	25	HIS	6.3
1	C	27	ALA	6.1

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 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	NA	C	400	1/1	0.88	0.24	5.05	48,48,48,48	0
2	NA	B	400	1/1	0.89	0.17	2.40	37,37,37,37	0
2	NA	D	400	1/1	0.86	0.11	-	46,46,46,46	0
2	NA	A	400	1/1	0.92	0.22	-	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.