



wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 03:39 PM GMT

PDB ID : 2ONL
Title : Crystal Structure of the p38a-MAPKAP kinase 2 Heterodimer
Authors : Ter Haar, E.
Deposited on : 2007-01-24
Resolution : 4.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

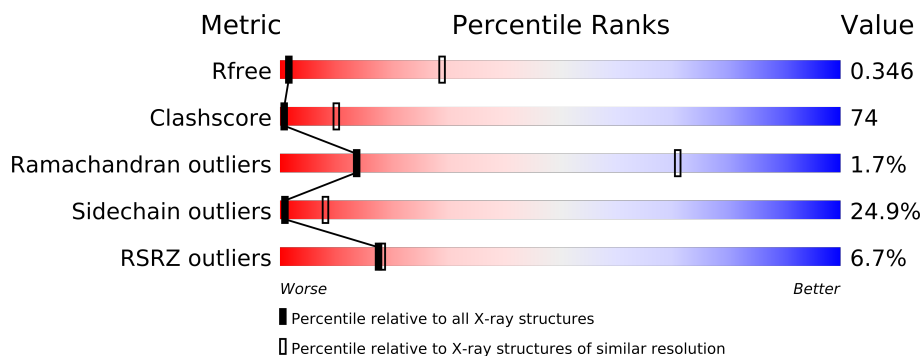
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 4.00 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}	66092	1035 (4.52-3.46)
Clashscore	79885	1235 (4.50-3.50)
Ramachandran outliers	78287	1170 (4.50-3.50)
Sidechain outliers	78261	1156 (4.50-3.50)
RSRZ outliers	66119	1035 (4.52-3.46)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	366	
1	B	366	
2	C	406	
2	D	406	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10466 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2709	1737	466	494	12			
1	B	339	Total	C	N	O	S	0	0	0
			2714	1740	467	495	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	CLONING ARTIFACT	UNP Q16539
A	-4	SER	-	CLONING ARTIFACT	UNP Q16539
A	-3	HIS	-	CLONING ARTIFACT	UNP Q16539
A	-2	MET	-	CLONING ARTIFACT	UNP Q16539
A	-1	LEU	-	CLONING ARTIFACT	UNP Q16539
A	0	GLU	-	CLONING ARTIFACT	UNP Q16539
A	1	MET	-	CLONING ARTIFACT	UNP Q16539
B	-5	GLY	-	CLONING ARTIFACT	UNP Q16539
B	-4	SER	-	CLONING ARTIFACT	UNP Q16539
B	-3	HIS	-	CLONING ARTIFACT	UNP Q16539
B	-2	MET	-	CLONING ARTIFACT	UNP Q16539
B	-1	LEU	-	CLONING ARTIFACT	UNP Q16539
B	0	GLU	-	CLONING ARTIFACT	UNP Q16539
B	1	MET	-	CLONING ARTIFACT	UNP Q16539

- Molecule 2 is a protein called MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	317	Total	C	N	O	S	0	0	0
			2531	1611	440	462	18			
2	D	313	Total	C	N	O	S	0	0	0
			2512	1597	437	460	18			

There are 12 discrepancies between the modelled and reference sequences:

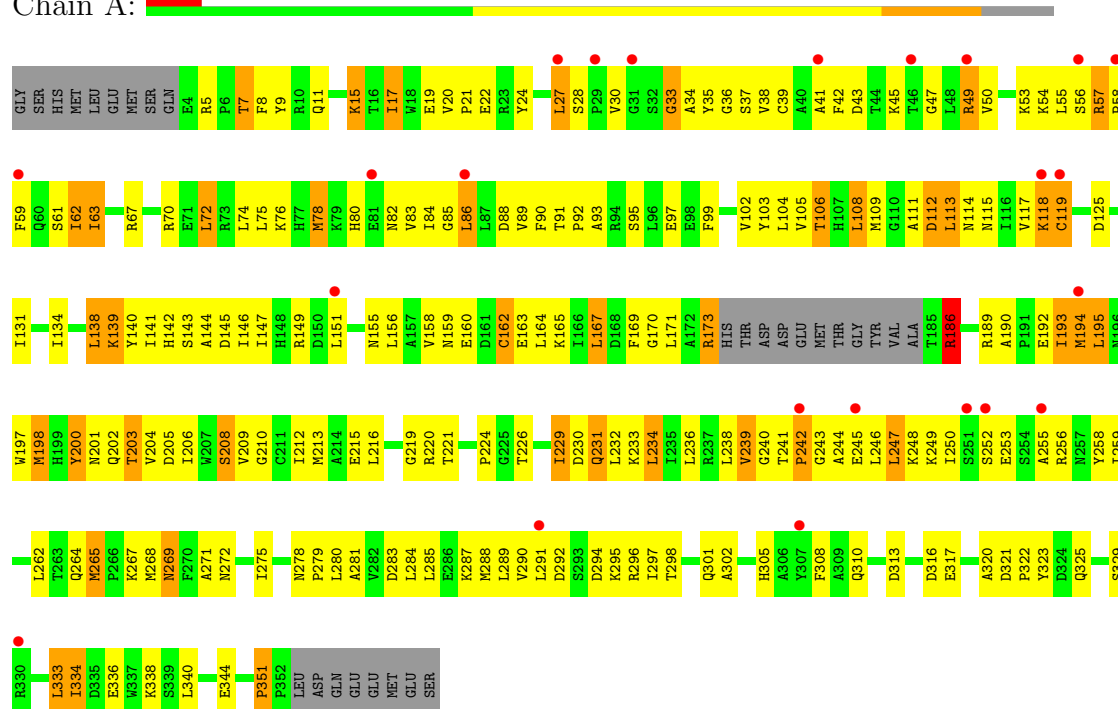
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	CLONING ARTIFACT	UNP P49137
C	-4	SER	-	CLONING ARTIFACT	UNP P49137
C	-3	HIS	-	CLONING ARTIFACT	UNP P49137
C	-2	MET	-	CLONING ARTIFACT	UNP P49137
C	-1	LEU	-	CLONING ARTIFACT	UNP P49137
C	0	GLU	-	CLONING ARTIFACT	UNP P49137
D	-5	GLY	-	CLONING ARTIFACT	UNP P49137
D	-4	SER	-	CLONING ARTIFACT	UNP P49137
D	-3	HIS	-	CLONING ARTIFACT	UNP P49137
D	-2	MET	-	CLONING ARTIFACT	UNP P49137
D	-1	LEU	-	CLONING ARTIFACT	UNP P49137
D	0	GLU	-	CLONING ARTIFACT	UNP P49137

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.

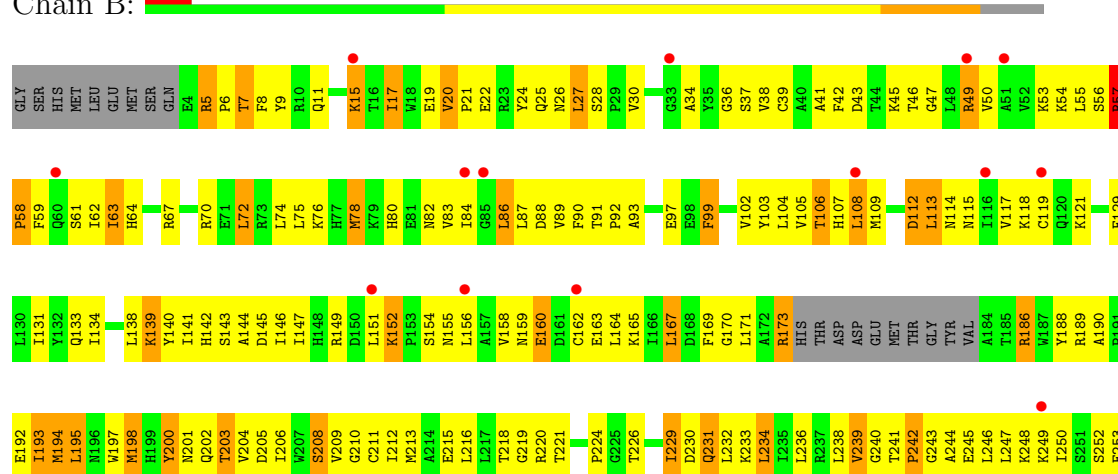
- Molecule 1: Mitogen-activated protein kinase 14

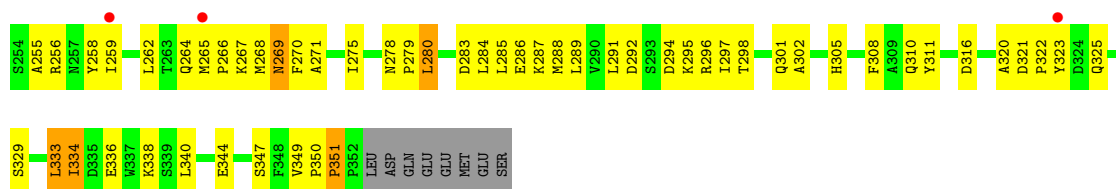
Chain A:



- Molecule 1: Mitogen-activated protein kinase 14

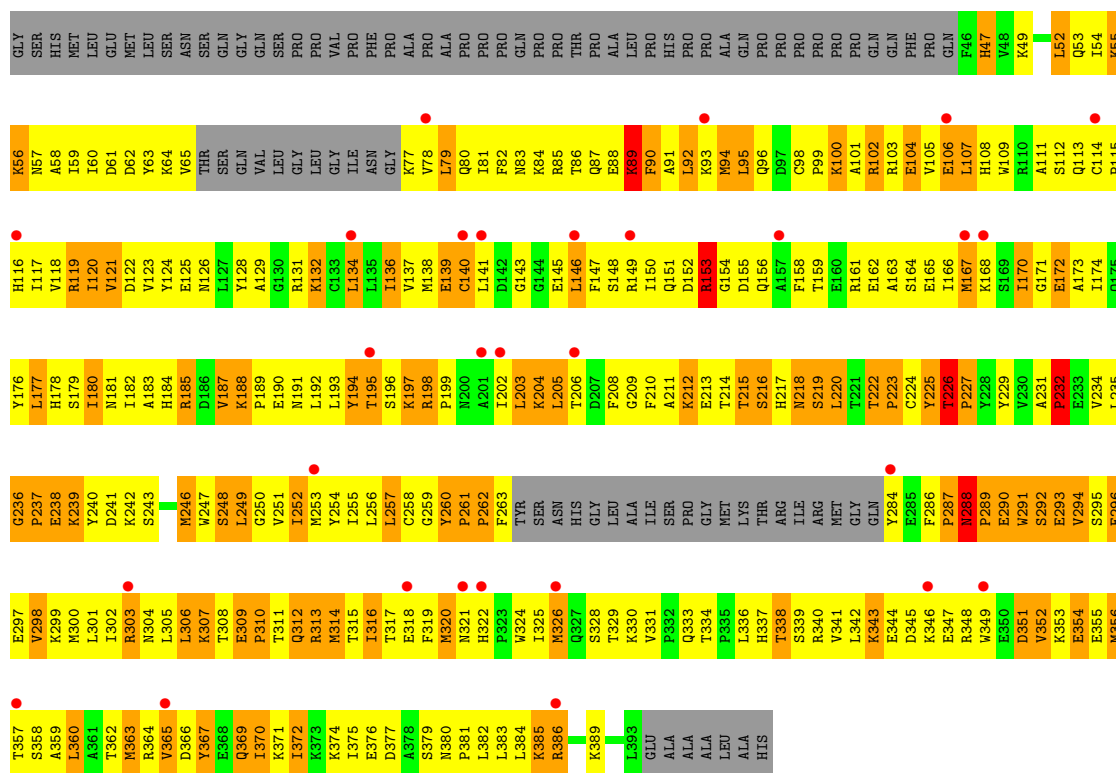
Chain B:





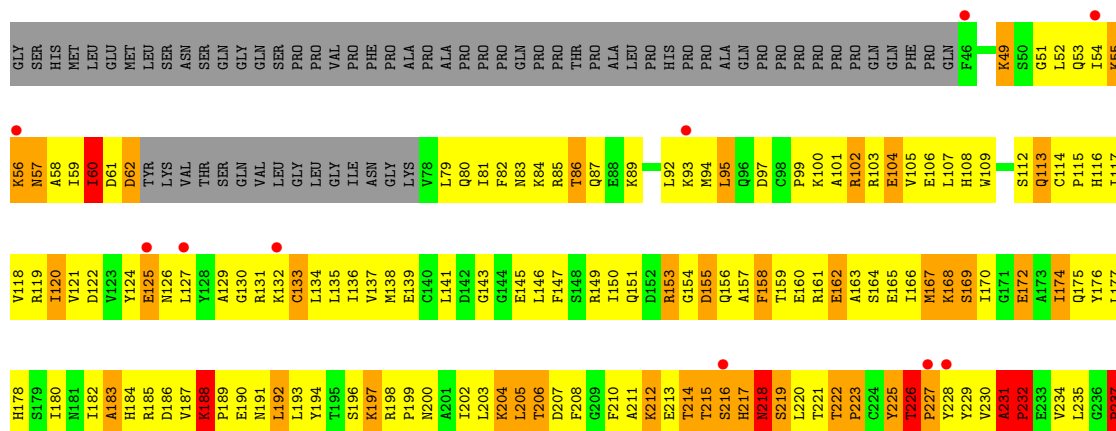
• Molecule 2: MAP kinase-activated protein kinase 2

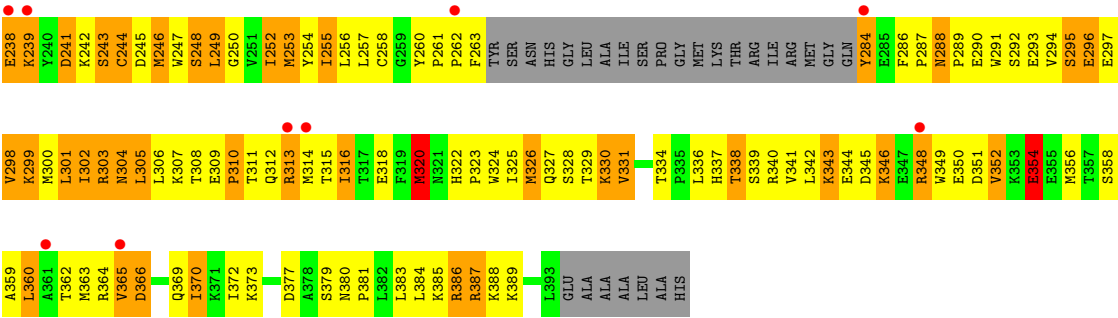
Chain C:



• Molecule 2: MAP kinase-activated protein kinase 2

Chain D:





4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	103.15Å 103.15Å 231.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.34 – 4.00 45.34 – 4.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (45.34-4.00) 95.9 (45.34-4.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 4.00Å)	Xtriage
Refinement program	BUSTER-TNT V. 1.1.0	Depositor
R, R_{free}	0.314 , 0.331 0.328 , 0.346	Depositor DCC
R_{free} test set	984 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	106.4	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 80.6	EDS
Estimated twinning fraction	0.219 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 19569 reflections	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	10466	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.27	0/2770	0.51	2/3758 (0.1%)
1	B	0.26	0/2775	0.48	2/3765 (0.1%)
2	C	0.25	0/2583	0.59	3/3480 (0.1%)
2	D	0.32	2/2563 (0.1%)	0.57	4/3453 (0.1%)
All	All	0.28	2/10691 (0.0%)	0.54	11/14456 (0.1%)

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	2
1	B	0	1
2	C	0	24
2	D	0	25
All	All	0	52

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	354	GLU	CD-OE2	6.41	1.32	1.25
2	D	354	GLU	CD-OE1	5.65	1.31	1.25

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	231	ALA	C-N-CD	-7.96	103.09	120.60
2	C	194	TYR	CB-CA-C	-7.67	95.06	110.40
1	A	265	MET	N-CA-C	7.67	131.71	111.00
2	C	234	VAL	N-CA-C	6.29	128.00	111.00
2	D	237	PRO	N-CA-CB	5.93	110.41	103.30

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ARG	Peptide
1	A	33	GLY	Peptide
2	C	153	ARG	Peptide
2	C	154	GLY	Peptide
2	C	89	LYS	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2709	0	2701	298	0
1	B	2714	0	2706	325	0
2	C	2531	0	2509	517	6
2	D	2512	0	2500	495	2
All	All	10466	0	10416	1540	8

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 74.

The worst 5 of 1540 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:159:ASN:C	2:D:370:ILE:HD13	1.35	1.42
2:D:214:THR:HG23	2:D:237:PRO:O	1.24	1.37
2:C:315:THR:CG2	2:C:318:GLU:CB	2.02	1.36
2:D:214:THR:CG2	2:D:238:GLU:HA	1.58	1.33
2:D:99:PRO:O	2:D:103:ARG:HG3	1.22	1.32

The worst 5 of 8 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	Distance(Å)	Clash(Å)
2:C:58:ALA:CB	2:C:226:THR:OG1[4_574]	1.62	0.58
2:C:58:ALA:CA	2:C:226:THR:OG1[4_574]	1.75	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:58:ALA:N	2:D:226:THR:O[3.745]	1.87	0.33
2:D:58:ALA:CA	2:D:226:THR:O[3.745]	1.87	0.33
2:C:58:ALA:N	2:C:226:THR:OG1[4.574]	1.90	0.30

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	334/366 (91%)	307 (92%)	25 (8%)	2 (1%)	33	86
1	B	335/366 (92%)	309 (92%)	23 (7%)	3 (1%)	25	81
2	C	311/406 (77%)	262 (84%)	40 (13%)	9 (3%)	7	59
2	D	307/406 (76%)	247 (80%)	52 (17%)	8 (3%)	8	61
All	All	1287/1544 (83%)	1125 (87%)	140 (11%)	22 (2%)	14	71

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	237	PRO
2	D	232	PRO
2	D	237	PRO
2	C	222	THR
2	C	232	PRO

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	294/325 (90%)	240 (82%)	54 (18%)	2	18
1	B	294/325 (90%)	243 (83%)	51 (17%)	3	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	272/362 (75%)	182 (67%)	90 (33%)	0	4
2	D	273/362 (75%)	186 (68%)	87 (32%)	0	4
All	All	1133/1374 (82%)	851 (75%)	282 (25%)	1	8

5 of 282 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	351	ASP
1	B	78	MET
2	D	313	ARG
2	C	360	LEU
2	C	389	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	64	HIS
1	B	202	GLN
2	D	288	ASN
1	B	114	ASN
1	B	228	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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, 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	338/366 (92%)	0.75	23 (6%) 17 17	100, 100, 100, 100	0
1	B	339/366 (92%)	0.63	17 (5%) 28 24	100, 100, 100, 100	0
2	C	317/406 (78%)	0.74	29 (9%) 9 12	20, 100, 100, 100	0
2	D	313/406 (77%)	0.65	19 (6%) 21 20	100, 100, 100, 100	0
All	All	1307/1544 (84%)	0.69	88 (6%) 17 18	20, 100, 100, 100	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	251	SER	5.1
2	C	202	ILE	5.1
1	A	27	LEU	3.8
1	B	162	CYS	3.8
1	B	249	LYS	3.7

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.