



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 06:41 pm GMT

PDB ID : 3M0C
Title : The X-ray Crystal Structure of PCSK9 in Complex with the LDL receptor
Authors : Spraggon, G.; Hampton, E.N.
Deposited on : 2010-03-02
Resolution : 7.01 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

<https://www.wwpdb.org/validation/2017/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) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

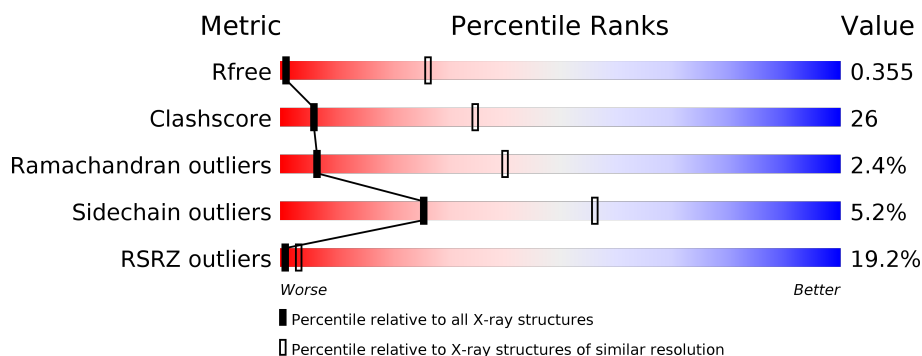
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.01 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}	111664	1067 (10.00-3.80)
Clashscore	122126	1146 (10.00-3.80)
Ramachandran outliers	120053	1071 (10.00-3.80)
Sidechain outliers	120020	1038 (10.00-3.80)
RSRZ outliers	108989	1012 (9.50-3.70)

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	124	<div> <div>10%</div> <div>69%</div> <div>5%</div> <div>26%</div> </div>
2	B	546	<div> <div>17%</div> <div>71%</div> <div>16%</div> <div>• 11%</div> </div>
3	C	791	<div> <div>11%</div> <div>35%</div> <div>14%</div> <div>5%</div> <div>• 46%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7705 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 Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	S	0	1	0
			748	479	136	131	2			

- Molecule 2 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	486	Total	C	N	O	S	0	1	0
			3618	2234	668	684	32			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	374	TYR	ASP	ENGINEERED	UNP Q8NBP7
B	693	HIS	-	EXPRESSION TAG	UNP Q8NBP7
B	694	HIS	-	EXPRESSION TAG	UNP Q8NBP7
B	695	HIS	-	EXPRESSION TAG	UNP Q8NBP7
B	696	HIS	-	EXPRESSION TAG	UNP Q8NBP7
B	697	HIS	-	EXPRESSION TAG	UNP Q8NBP7
B	698	HIS	-	EXPRESSION TAG	UNP Q8NBP7

- Molecule 3 is a protein called Low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	430	Total	C	N	O	S	0	0	0
			3336	2079	578	647	32			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	768	HIS	-	EXPRESSION TAG	UNP P01130
C	769	HIS	-	EXPRESSION TAG	UNP P01130
C	770	HIS	-	EXPRESSION TAG	UNP P01130

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Chain	Residue	Modelled	Actual	Comment	Reference
C	771	HIS	-	EXPRESSION TAG	UNP P01130
C	772	HIS	-	EXPRESSION TAG	UNP P01130
C	773	HIS	-	EXPRESSION TAG	UNP P01130

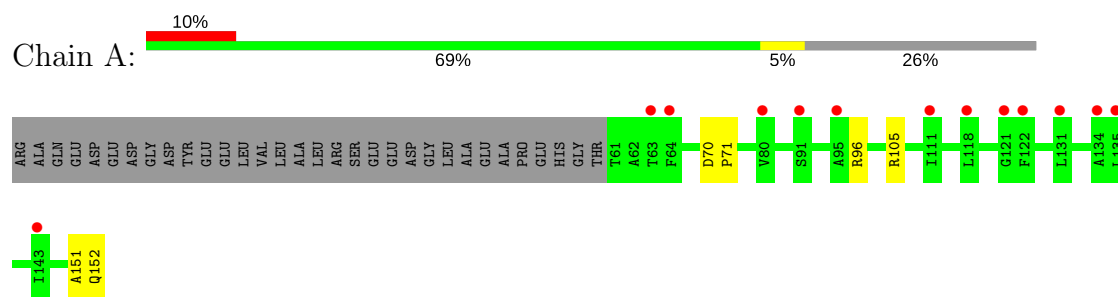
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total 3	Ca 3	0	0

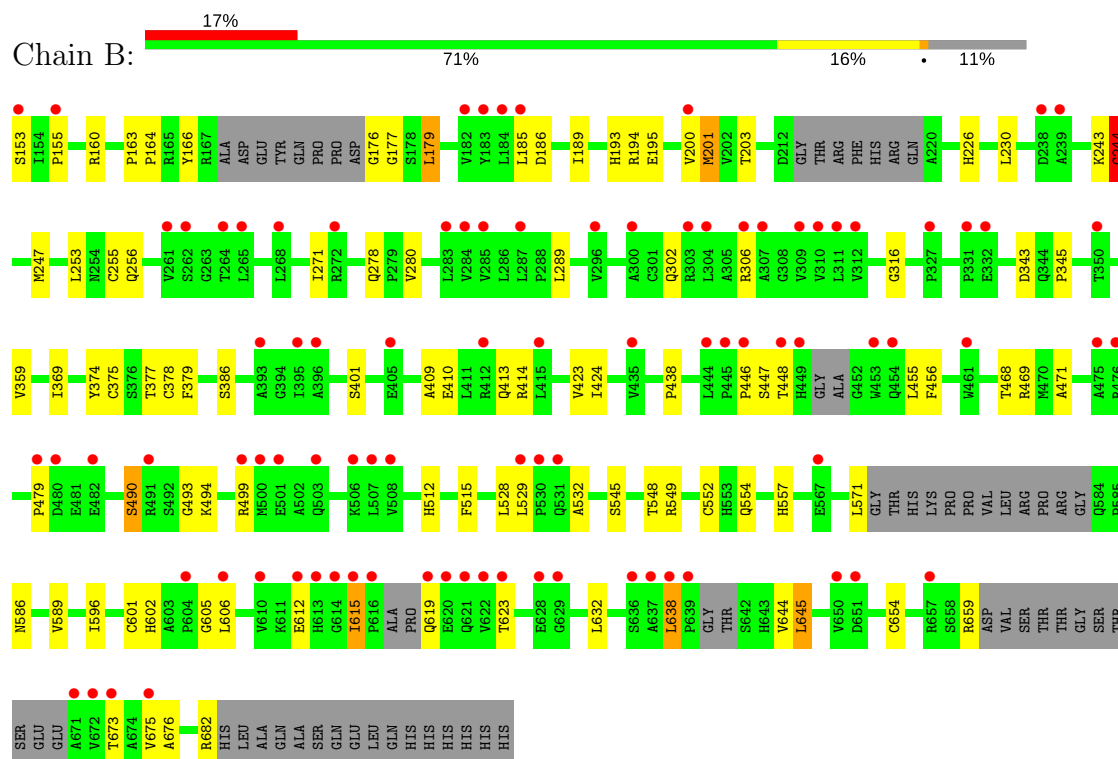
3 Residue-property plots

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.

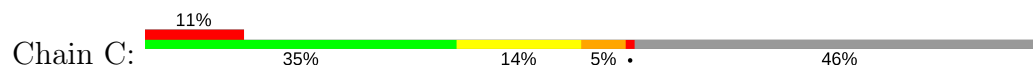
- Molecule 1: Proprotein convertase subtilisin/kexin type 9



- Molecule 2: Proprotein convertase subtilisin/kexin type 9



- Molecule 3: Low-density lipoprotein receptor



HIS	VAL	L633	K522	SER	K355	D283	SER	CYS	ARG	GLN	LEU	TRP
HIS	SER	F634	L526	Y444	C356	W284	ASP	ARG	GLN	PHE	SER	GLY
HIS	THR	H635	N527	V447	C357	D286	ASN	GLY	VAL	THR	VAL	LYS
	ALA	F640	G528	I452	F362	E287	ILE	TYR	ASP	ASP	CYS	ARG
	VAL	R641	V529	Q453	Q363	I289	HIS	PHE	VAL	THR	LYS	TRP
	ARG	G642	D530	A454	L364	K290	GLY	GLN	ASP	THR	SER	THR
	THR	G643	V535	P455	D365	E291	SER	GLY	ASP	VAL	GLY	VAL
	GLN	R644	N543	D456	R366	C292	ARG	ASP	ASP	PHE	ASP	ALA
	HIS	W645	G544	G457	R367	G293	GLN	SER	CYS	THR	SER	LEU
	THR	C646	N543	L458	T368	T294	CYS	PRO	LEU	CYS	CYS	LEU
	THR	E647	G544	A459	K369		ASP	ASP	ASP	GLY	GLY	LEU
	THR	R648	I545	V460	A370		ASP	GLY	GLY	ALA	ALA	ALA
	ARG	T649	T546			C297	ARG	CYS	SER	ARG	ALA	ALA
	PRO	T650	L550	I463	C371	L298	GLU	SER	VAL	VAL	ARG	ALA
	VAL	L651	L550	H464	K372	D299	TYR	ALA	ASP	GLU	ASP	ALA
	PRO	R652	Y555	S465	A373	N300	CYS	PHE	GLU	ASN	GLY	THR
	ASP	R653	W556	W466	V374	N301	ASP	GLY	ALA	ARG	ALA	THR
	THR	G654	W556	I467	G375		LYS	PHE	SER	CYS	ALA	ALA
	SER	G655		S376	S377	C304	ASP	CYS	ILE	VAL	VAL	VAL
	ARG		L584	Y468	I377		MET	CYS	PRO	PRO	GLY	GLY
	LEU	Y658	L578	W469	A378	V307	SER	LEU	VAL	GLN	ASP	ASP
	PRO	L659	E579	T470	Y379	C308	ASP	SER	LEU	PHE	ASP	ASP
	GLY	C680	D580	V473	L380	N309	GLU	THR	THR	TRP	CYS	ARG
	ALA	L681			F381		VAL	GLY	CYS	GLY	ARG	GLY
	THR	P682			F382	K312	GLY	CYS	GLY	PRO	CYS	ARG
	PRO	A683	R583	V477	V388	C317	CYS	ILE	ASN	ASN	ASP	ASN
	GLY	P684	L584	S478	I402	L318	VAL	HIS	ALA	GLY	GLY	GLN
	LEU		A585	V479	R406	C319	ASN	SER	SER	GLN	GLN	PHE
	THR	N687	H586		T489	P320	VAL	SER	PHE	VAL	VAL	GLN
	THR	P688	L590	G484	L411	R321	THR	TRP	GLN	ASP	ASP	CYS
	VAL		A591	W485	L401		LEU	ARG	CYS	CYS	CYS	GLN
	GLU	R672	V592	K486	I402	G322	C265	CYS	ASN	ASP	ASP	ASP
	ILE	F673	V592	R487	L402	F323	E256	SER	ASN	SER	ASN	GLY
	VAL	T674		K488	R406	Q324	G257	GLY	SER	GLY	GLY	LYS
	THR		V597	T489	L411	L325	THR	GLY	SER	THR	SER	CYS
	MET		F598	L490	D412		N259	PRO	CYS	ILE	ASP	ILE
	SER		W599	F491	T413	C331	K260	ASP	ASP	GLU	ASP	SER
	HIS					E332	F261	PRO	GLN	GLN	GLU	TYR
	GLN		I602	R499	A416	D333	K262	LYS	GLN	GLY	GLY	LYS
	ALA	C690	I603	A500	A416	I334	H264	LYS	TRP	PRO	PRO	VAL
	LEU	L691	S609	I501	V502	D335	S265	ALA	ALA	CYS	PRO	CYS
	GLY	T692		V503	Y421	C337	G266	CYS	CYS	LYS	LYS	ASP
	ASP			D504		Q338	E267	ASP	ASP	THR	THR	GLY
	VAL	ALA	R612	P505	L425	D339	C268	GLU	ASP	CYS	SER	SER
	GLU	ALA	L613	P506	S426	P340	I269	ASN	ASN	CYS	ALA	ALA
	ALA	T614	G615	W507	Q427	D341	CYS	PRO	PRO	GLN	SER	GLY
	ARG	G615		H507	R428	T342	ALA	ASP	ASP	ASP	GLY	CYS
	GLY	VAL	V618	G508	W429	C343	L271	VAL	CYS	GLY	GLN	GLN
	ASN	ALA		F509	I430	S344	D272	GLU	CYS	PHE	ASP	ASP
	GLU	THR	L621	W510		Q345	K273	ALA	GLU	THR	GLY	GLY
	LYS	GLN	A622	Y511	L435	L346	V274	THR	ASP	ARG	ARG	GLY
	LYS	GLU	E623	W512	T513	C347	C275	CYS	GLY	CYS	CYS	SER
	PRO	THR		T513		V348	N276	ARG	SER	SER	HIS	ASP
	SER	SER			ASP	N349	M277	PRO	ASP	ASP	GLY	GLY
	THR	THR	P628	T517	ARG		A278	ASP	GLY	GLY	ASP	SER
	VAL	VAL	E629	P518	ALA	L350	R279	GLU	TRP	TRP	LYS	GLN
	ARG	ARG	D630	A519	HIS	E351	D280	PHE	PRO	PRO	CYS	THR
	HIS	HIS	M631	K520	GLY	G352	C281	GLN	GLN	ILE	ILE	THR
	LEU	LYS	V632	I521	SER		R282	CYS	ARG	SER	SER	CYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	322.91Å 322.91Å 76.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	279.64 – 7.01 279.64 – 7.01	Depositor EDS
% Data completeness (in resolution range)	82.2 (279.64-7.01) 97.6 (279.64-7.01)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 6.74Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.341 , 0.362 0.339 , 0.355	Depositor DCC
R_{free} test set	339 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	247.1	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 199.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	0.189 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	7705	wwPDB-VP
Average B, all atoms (Å ²)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	0.80	0/768	0.77	0/1037
2	B	0.73	3/3687 (0.1%)	0.75	1/5003 (0.0%)
3	C	0.65	3/3405 (0.1%)	1.09	21/4628 (0.5%)
All	All	0.70	6/7860 (0.1%)	0.91	22/10668 (0.2%)

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
2	B	0	2
3	C	0	2
All	All	0	4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	487	ARG	CD-NE	-17.20	1.17	1.46
3	C	444	TYR	N-CA	-17.05	1.12	1.46
3	C	343	CYS	CB-SG	-8.72	1.67	1.82
2	B	654	CYS	CB-SG	-6.39	1.71	1.82
2	B	255	CYS	C-N	-5.59	1.21	1.34

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	428	ARG	NE-CZ-NH2	-9.01	115.80	120.30
3	C	518	PRO	N-CA-CB	8.64	113.67	103.30
3	C	517	THR	CA-C-O	-8.61	102.01	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	346	LEU	N-CA-C	7.29	130.68	111.00
3	C	444	TYR	N-CA-CB	6.68	122.63	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	244	GLY	Peptide
2	B	494	LYS	Peptide
3	C	517	THR	Mainchain,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	748	0	763	5	2
2	B	3618	0	3529	93	6
3	C	3336	0	3186	326	8
4	C	3	0	0	0	0
All	All	7705	0	7478	399	8

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 26.

The worst 5 of 399 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)
3:C:527:ASN:HA	3:C:661:LEU:CD1	1.32	1.52
3:C:340:PRO:O	3:C:342:THR:N	1.58	1.35
3:C:339:ASP:HA	3:C:340:PRO:O	1.35	1.25
3:C:323:PHE:CZ	3:C:351:GLU:OE2	1.94	1.21
3:C:339:ASP:OD1	3:C:342:THR:HG21	1.41	1.20

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	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:PRO:CA	3:C:284:TRP:CA[3_655]	1.95	0.25
2:B:164:PRO:CA	3:C:284:TRP:CB[3_655]	1.98	0.22
2:B:164:PRO:CB	3:C:286:ASP:O[3_655]	2.01	0.19
1:A:105[A]:ARG:CZ	3:C:530:ASP:OD1[4_545]	2.07	0.13
2:B:164:PRO:C	3:C:284:TRP:CB[3_655]	2.08	0.12

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	91/124 (73%)	90 (99%)	1 (1%)	0	100	100
2	B	471/546 (86%)	459 (98%)	9 (2%)	3 (1%)	27	70
3	C	426/791 (54%)	362 (85%)	43 (10%)	21 (5%)	2	26
All	All	988/1461 (68%)	911 (92%)	53 (5%)	24 (2%)	6	40

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	257	GLY
3	C	271	LEU
3	C	287	GLU
3	C	291	GLU
3	C	340	PRO

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	80/104 (77%)	79 (99%)	1 (1%)	71	86
2	B	389/437 (89%)	378 (97%)	11 (3%)	47	71
3	C	374/691 (54%)	342 (91%)	32 (9%)	11	39
All	All	843/1232 (68%)	799 (95%)	44 (5%)	25	56

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	317	CYS
3	C	339	ASP
3	C	612	ARG
3	C	318	LEU
3	C	336	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	264	HIS
3	C	309	ASN
3	C	543	ASN
2	B	619	GLN
3	C	453	GLN

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 ⓘ

Of 3 ligands modelled in this entry, 3 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	92/124 (74%)	0.85	13 (14%)	2 5	106, 181, 209, 231	0
2	B	486/546 (89%)	0.77	91 (18%)	1 3	81, 178, 253, 349	0
3	C	430/791 (54%)	1.06	90 (20%)	1 3	79, 170, 278, 322	1 (0%)
All	All	1008/1461 (68%)	0.90	194 (19%)	1 3	79, 176, 268, 349	1 (0%)

The worst 5 of 194 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	642	GLY	10.1
3	C	649	THR	8.7
3	C	648	ARG	8.0
3	C	412	ASP	7.9
3	C	641	ARG	7.7

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. 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	B-factors(\AA^2)	Q<0.9
4	CA	C	1002	1/1	0.74	0.34	153,153,153,153	0
4	CA	C	1001	1/1	0.87	0.32	136,136,136,136	0
4	CA	C	1003	1/1	0.94	0.25	170,170,170,170	0

6.5 Other polymers [i](#)

There are no such residues in this entry.