



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2016 – 02:21 PM EST

PDB ID : 5L2D
Title : Streptococcal surface adhesin - CshA NR2
Authors : Back, C.R.; Race, P.R.; Jenkinson, H.F.
Deposited on : 2016-08-01
Resolution : 2.66 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

<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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	rb-20028442

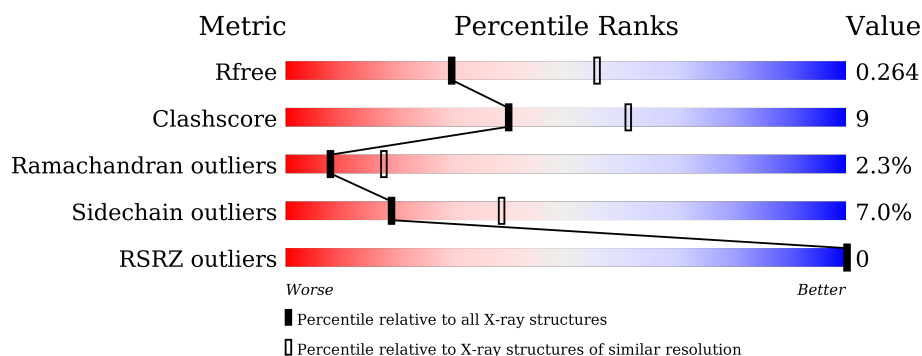
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	338	<div> <div style="width: 46%;"></div> <div style="width: 13%;"></div> <div style="width: 38%;"></div> </div>
1	B	338	<div> <div style="width: 51%;"></div> <div style="width: 10%;"></div> <div style="width: 38%;"></div> </div>
1	C	338	<div> <div style="width: 9%;"></div> <div style="width: 90%;"></div> </div>
1	D	338	<div> <div style="width: 7%;"></div> <div style="width: 90%;"></div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3649 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 Surface-associated protein CshA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1565	1005	243	312	5			
1	B	211	Total	C	N	O	S	0	0	0
			1616	1039	254	317	6			
1	C	33	Total	C	N	O	S	0	0	0
			233	151	38	41	3			
1	D	33	Total	C	N	O	S	0	0	0
			233	151	38	41	3			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A8AWJ3
A	-18	ALA	-	expression tag	UNP A8AWJ3
A	-17	HIS	-	expression tag	UNP A8AWJ3
A	-16	HIS	-	expression tag	UNP A8AWJ3
A	-15	HIS	-	expression tag	UNP A8AWJ3
A	-14	HIS	-	expression tag	UNP A8AWJ3
A	-13	HIS	-	expression tag	UNP A8AWJ3
A	-12	HIS	-	expression tag	UNP A8AWJ3
A	-11	SER	-	expression tag	UNP A8AWJ3
A	-10	SER	-	expression tag	UNP A8AWJ3
A	-9	GLY	-	expression tag	UNP A8AWJ3
A	-8	LEU	-	expression tag	UNP A8AWJ3
A	-7	GLU	-	expression tag	UNP A8AWJ3
A	-6	VAL	-	expression tag	UNP A8AWJ3
A	-5	LEU	-	expression tag	UNP A8AWJ3
A	-4	PHE	-	expression tag	UNP A8AWJ3
A	-3	GLN	-	expression tag	UNP A8AWJ3
A	-2	GLY	-	expression tag	UNP A8AWJ3
A	-1	PRO	-	expression tag	UNP A8AWJ3
A	0	MET	-	expression tag	UNP A8AWJ3
B	-19	MET	-	initiating methionine	UNP A8AWJ3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	ALA	-	expression tag	UNP A8AWJ3
B	-17	HIS	-	expression tag	UNP A8AWJ3
B	-16	HIS	-	expression tag	UNP A8AWJ3
B	-15	HIS	-	expression tag	UNP A8AWJ3
B	-14	HIS	-	expression tag	UNP A8AWJ3
B	-13	HIS	-	expression tag	UNP A8AWJ3
B	-12	HIS	-	expression tag	UNP A8AWJ3
B	-11	SER	-	expression tag	UNP A8AWJ3
B	-10	SER	-	expression tag	UNP A8AWJ3
B	-9	GLY	-	expression tag	UNP A8AWJ3
B	-8	LEU	-	expression tag	UNP A8AWJ3
B	-7	GLU	-	expression tag	UNP A8AWJ3
B	-6	VAL	-	expression tag	UNP A8AWJ3
B	-5	LEU	-	expression tag	UNP A8AWJ3
B	-4	PHE	-	expression tag	UNP A8AWJ3
B	-3	GLN	-	expression tag	UNP A8AWJ3
B	-2	GLY	-	expression tag	UNP A8AWJ3
B	-1	PRO	-	expression tag	UNP A8AWJ3
B	0	MET	-	expression tag	UNP A8AWJ3
C	-19	MET	-	initiating methionine	UNP A8AWJ3
C	-18	ALA	-	expression tag	UNP A8AWJ3
C	-17	HIS	-	expression tag	UNP A8AWJ3
C	-16	HIS	-	expression tag	UNP A8AWJ3
C	-15	HIS	-	expression tag	UNP A8AWJ3
C	-14	HIS	-	expression tag	UNP A8AWJ3
C	-13	HIS	-	expression tag	UNP A8AWJ3
C	-12	HIS	-	expression tag	UNP A8AWJ3
C	-11	SER	-	expression tag	UNP A8AWJ3
C	-10	SER	-	expression tag	UNP A8AWJ3
C	-9	GLY	-	expression tag	UNP A8AWJ3
C	-8	LEU	-	expression tag	UNP A8AWJ3
C	-7	GLU	-	expression tag	UNP A8AWJ3
C	-6	VAL	-	expression tag	UNP A8AWJ3
C	-5	LEU	-	expression tag	UNP A8AWJ3
C	-4	PHE	-	expression tag	UNP A8AWJ3
C	-3	GLN	-	expression tag	UNP A8AWJ3
C	-2	GLY	-	expression tag	UNP A8AWJ3
C	-1	PRO	-	expression tag	UNP A8AWJ3
C	0	MET	-	expression tag	UNP A8AWJ3
D	-19	MET	-	initiating methionine	UNP A8AWJ3
D	-18	ALA	-	expression tag	UNP A8AWJ3
D	-17	HIS	-	expression tag	UNP A8AWJ3

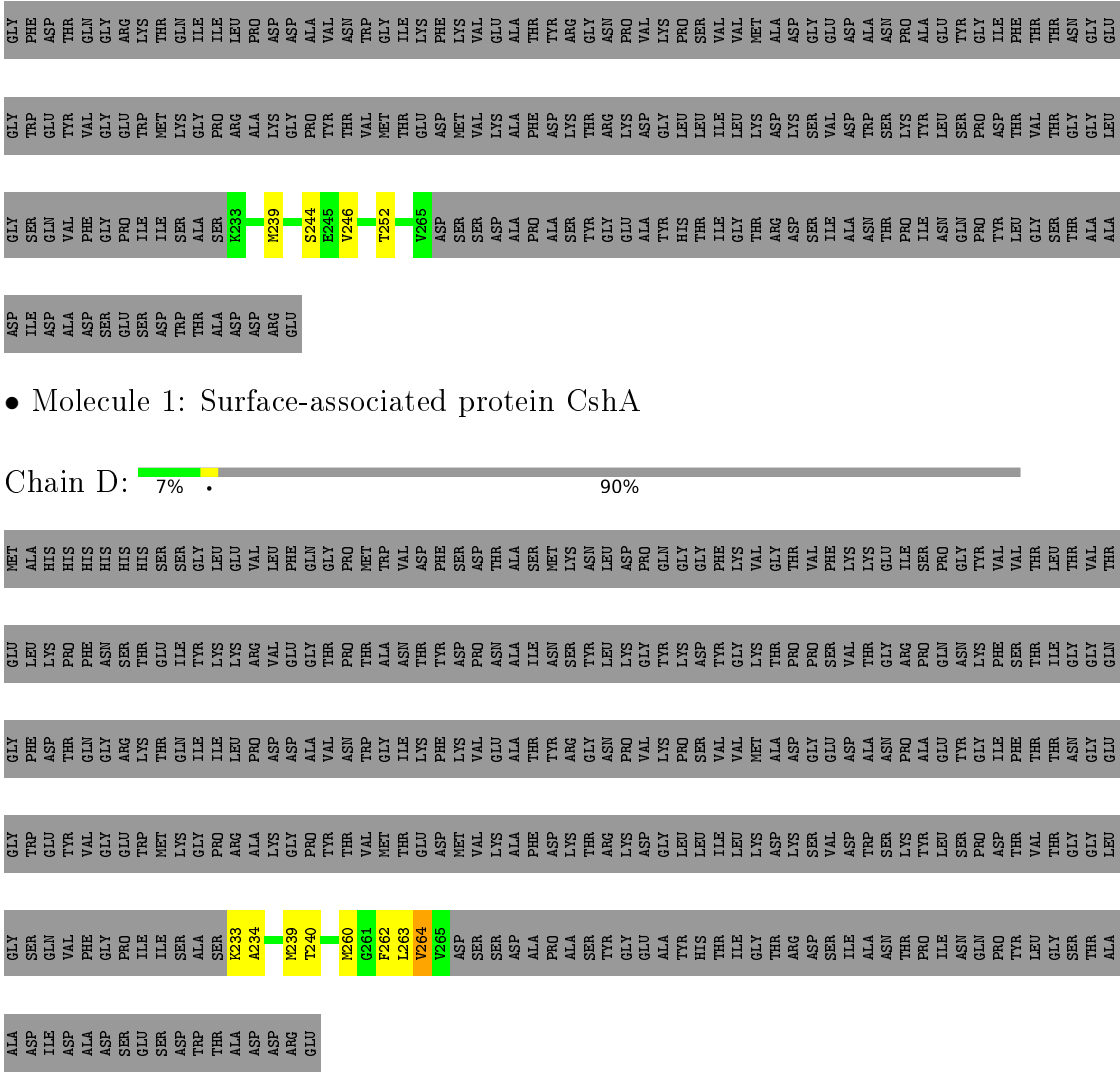
Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	HIS	-	expression tag	UNP A8AWJ3
D	-15	HIS	-	expression tag	UNP A8AWJ3
D	-14	HIS	-	expression tag	UNP A8AWJ3
D	-13	HIS	-	expression tag	UNP A8AWJ3
D	-12	HIS	-	expression tag	UNP A8AWJ3
D	-11	SER	-	expression tag	UNP A8AWJ3
D	-10	SER	-	expression tag	UNP A8AWJ3
D	-9	GLY	-	expression tag	UNP A8AWJ3
D	-8	LEU	-	expression tag	UNP A8AWJ3
D	-7	GLU	-	expression tag	UNP A8AWJ3
D	-6	VAL	-	expression tag	UNP A8AWJ3
D	-5	LEU	-	expression tag	UNP A8AWJ3
D	-4	PHE	-	expression tag	UNP A8AWJ3
D	-3	GLN	-	expression tag	UNP A8AWJ3
D	-2	GLY	-	expression tag	UNP A8AWJ3
D	-1	PRO	-	expression tag	UNP A8AWJ3
D	0	MET	-	expression tag	UNP A8AWJ3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total O 2 2	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	173.93Å 173.93Å 104.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.01 – 2.66 61.01 – 2.66	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.01-2.66) 100.0 (61.01-2.66)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.201 , 0.264 0.208 , 0.264	Depositor DCC
R_{free} test set	1363 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3649	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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](#)

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	0.77	0/1606	0.88	1/2198 (0.0%)
1	B	0.81	0/1658	0.91	1/2257 (0.0%)
1	C	0.79	0/236	0.84	0/319
1	D	0.82	0/236	0.91	0/319
All	All	0.79	0/3736	0.89	2/5093 (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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	226	GLY	N-CA-C	-6.73	96.27	113.10
1	A	226	GLY	N-CA-C	-6.64	96.49	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	GLY	Peptide
1	B	225	PHE	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	1565	0	1458	39	0
1	B	1616	0	1566	20	4
1	C	233	0	236	5	0
1	D	233	0	236	6	4
2	B	2	0	0	0	0
All	All	3649	0	3496	63	4

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 9.

All (63) 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:3:ASP:OD1	1:A:5:SER:OG	1.67	1.11
1:B:28:GLU:OE2	1:B:31:PRO:O	1.74	1.04
1:A:202:ASP:OD1	1:A:204:SER:OG	1.85	0.94
1:A:60:THR:O	1:A:63:THR:HG22	1.75	0.87
1:A:217:THR:HG22	1:A:218:GLY:H	1.46	0.81
1:A:217:THR:HG22	1:A:218:GLY:N	1.99	0.78
1:A:182:THR:O	1:A:186:VAL:HG23	1.87	0.75
1:B:179:THR:HB	1:B:229:ILE:HG22	1.73	0.71
1:A:63:THR:OG1	1:A:204:SER:O	2.09	0.70
1:A:212:SER:HB2	1:A:226:GLY:HA3	1.73	0.69
1:A:58:THR:HB	1:A:59:PRO:HD2	1.75	0.67
1:B:30:SER:OG	1:B:31:PRO:HD2	1.95	0.66
1:A:192:THR:C	1:A:194:LYS:H	1.99	0.65
1:A:193:ARG:O	1:A:195:ASP:N	2.30	0.64
1:A:158:ASN:HD21	1:C:244:SER:H	1.44	0.64
1:A:158:ASN:C	1:A:158:ASN:HD22	2.00	0.64
1:A:58:THR:CB	1:A:59:PRO:HD2	2.29	0.62
1:B:14:ASP:HB2	1:B:15:PRO:HD2	1.82	0.61
1:B:33:TYR:CD2	1:D:264:VAL:HG12	2.40	0.57
1:D:239:MET:SD	1:D:263:LEU:HD11	2.45	0.57
1:B:113:LEU:C	1:B:113:LEU:HD23	2.25	0.56
1:A:188:ALA:O	1:A:190:ASP:N	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:MET:SD	1:D:263:LEU:CD1	2.93	0.56
1:A:4:PHE:CE1	1:A:111:ILE:HD11	2.41	0.56
1:A:140:VAL:HG12	1:C:239:MET:HB3	1.88	0.56
1:B:2:VAL:HG13	1:B:25:PHE:CZ	2.41	0.54
1:A:178:TYR:OH	1:A:217:THR:HG23	2.06	0.54
1:A:192:THR:C	1:A:194:LYS:N	2.58	0.54
1:A:55:VAL:HG13	1:A:61:ALA:HA	1.88	0.54
1:A:2:VAL:HG13	1:A:25:PHE:CZ	2.43	0.53
1:A:217:THR:HG21	1:A:220:LEU:CG	2.39	0.52
1:A:188:ALA:O	1:A:191:LYS:N	2.42	0.52
1:A:217:THR:HG21	1:A:220:LEU:HD12	1.92	0.52
1:A:158:ASN:ND2	1:A:158:ASN:C	2.64	0.51
1:B:60:THR:O	1:B:63:THR:HG22	2.11	0.50
1:A:4:PHE:CZ	1:A:111:ILE:HD11	2.46	0.50
1:A:217:THR:HG21	1:A:220:LEU:HG	1.95	0.49
1:B:51:TYR:OH	1:B:63:THR:HG23	2.13	0.48
1:A:14:ASP:HB2	1:A:15:PRO:HD2	1.96	0.48
1:A:113:LEU:HD23	1:A:113:LEU:C	2.35	0.46
1:B:33:TYR:HA	1:B:129:THR:O	2.15	0.46
1:A:4:PHE:CD2	1:A:111:ILE:HG13	2.52	0.45
1:D:240:THR:O	1:D:240:THR:HG23	2.17	0.45
1:B:149:PRO:N	1:B:229:ILE:HD11	2.32	0.45
1:B:228:ILE:HD13	1:B:228:ILE:HA	1.71	0.44
1:A:138:SER:HB3	1:C:239:MET:CE	2.47	0.43
1:A:138:SER:HB3	1:C:239:MET:HE1	2.01	0.43
1:B:82:THR:HA	1:B:83:PRO:HD3	1.89	0.43
1:A:217:THR:HG21	1:A:220:LEU:CD1	2.48	0.43
1:B:158:ASN:OD1	1:B:158:ASN:C	2.57	0.42
1:A:192:THR:O	1:A:194:LYS:N	2.53	0.42
1:B:55:VAL:O	1:B:58:THR:HG23	2.19	0.42
1:B:228:ILE:CG2	1:B:229:ILE:N	2.81	0.42
1:B:124:PHE:CE2	1:D:260:MET:CE	3.03	0.42
1:B:35:VAL:HG11	1:D:262:PHE:CZ	2.54	0.42
1:A:150:ALA:HB1	1:A:199:ILE:HG21	2.01	0.42
1:B:4:PHE:CG	1:B:111:ILE:HD11	2.54	0.42
1:C:252:THR:O	1:C:252:THR:HG23	2.19	0.42
1:A:60:THR:O	1:A:63:THR:CG2	2.58	0.42
1:A:217:THR:CG2	1:A:218:GLY:N	2.72	0.41
1:A:114:PRO:O	1:A:115:ASP:HB2	2.20	0.41
1:A:199:ILE:HG23	1:A:200:LEU:HG	2.03	0.41
1:B:14:ASP:HB2	1:B:15:PRO:CD	2.50	0.40

All (4) 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)
1:B:232:SER:O	1:D:233:LYS:N[12_565]	1.64	0.56
1:B:232:SER:O	1:D:233:LYS:CA[12_565]	1.67	0.53
1:B:232:SER:O	1:D:233:LYS:C[12_565]	1.80	0.40
1:B:232:SER:O	1:D:234:ALA:N[12_565]	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	204/338 (60%)	183 (90%)	12 (6%)	9 (4%)	3	5
1	B	205/338 (61%)	194 (95%)	9 (4%)	2 (1%)	19	41
1	C	31/338 (9%)	31 (100%)	0	0	100	100
1	D	31/338 (9%)	29 (94%)	2 (6%)	0	100	100
All	All	471/1352 (35%)	437 (93%)	23 (5%)	11 (2%)	8	17

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	PHE
1	B	31	PRO
1	A	188	ALA
1	A	194	LYS
1	A	202	ASP
1	A	177	PRO
1	A	192	THR
1	B	231	ALA
1	A	216	VAL
1	A	193	ARG
1	A	59	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	163/278 (59%)	149 (91%)	14 (9%)	13	26
1	B	175/278 (63%)	164 (94%)	11 (6%)	22	44
1	C	23/278 (8%)	22 (96%)	1 (4%)	35	63
1	D	23/278 (8%)	22 (96%)	1 (4%)	35	63
All	All	384/1112 (34%)	357 (93%)	27 (7%)	19	38

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	29	ILE
1	A	30	SER
1	A	58	THR
1	A	77	LYS
1	A	86	VAL
1	A	118	VAL
1	A	129	THR
1	A	158	ASN
1	A	163	GLU
1	A	199	ILE
1	A	222	SER
1	A	224	VAL
1	A	230	SER
1	B	7	THR
1	B	31	PRO
1	B	53	LYS
1	B	58	THR
1	B	63	THR
1	B	74	LYS
1	B	77	LYS
1	B	112	ILE
1	B	129	THR
1	B	136	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	169	MET
1	C	246	VAL
1	D	264	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	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 carbohydrates 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	210/338 (62%)	-0.39	0 100 100	43, 72, 102, 135	0
1	B	211/338 (62%)	-0.37	0 100 100	38, 62, 94, 109	0
1	C	33/338 (9%)	-0.01	0 100 100	49, 66, 99, 131	0
1	D	33/338 (9%)	-0.22	0 100 100	42, 58, 92, 129	0
All	All	487/1352 (36%)	-0.35	0 100 100	38, 66, 99, 135	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.