



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2017 – 01:41 PM EDT

PDB ID : 2HEU
Title : Atomic resolution structure of apo-form of RafE from *Streptococcus pneumoniae*
Authors : Paterson, N.G.; Riboldi-Tunncliffe, A.; Mitchell, T.J.; Isaacs, N.W.
Deposited on : unknown
Resolution : 1.04 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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
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) : rb-20030345

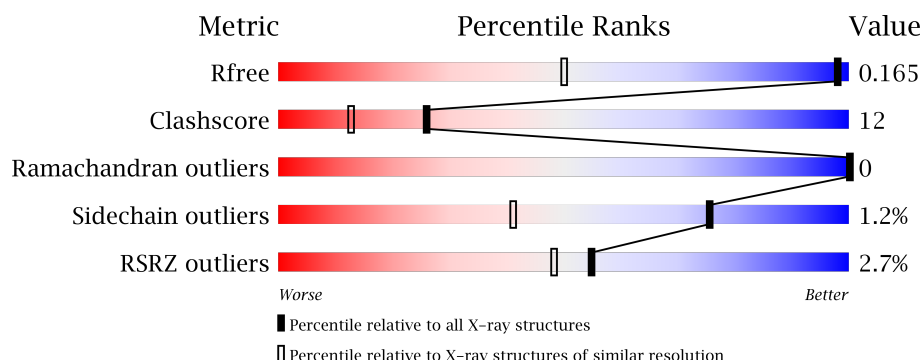
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.04 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	1186 (1.10-0.98)
Clashscore	112137	1267 (1.10-0.98)
Ramachandran outliers	110173	1192 (1.10-0.98)
Sidechain outliers	110143	1190 (1.10-0.98)
RSRZ outliers	101464	1191 (1.10-0.98)

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	401	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>• •</div> </div> </div>
1	B	401	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>• •</div> </div> </div>
1	C	401	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>• •</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TRS	C	5001	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12875 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 Sugar ABC transporter, sugar-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	41	0
			3467	2219	573	662	13			
1	B	390	Total	C	N	O	S	0	42	0
			3427	2190	561	664	12			
1	C	390	Total	C	N	O	S	0	35	0
			3416	2176	569	658	13			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP Q97NW2
A	2	HIS	-	EXPRESSION TAG	UNP Q97NW2
A	3	HIS	-	EXPRESSION TAG	UNP Q97NW2
A	4	HIS	-	EXPRESSION TAG	UNP Q97NW2
A	5	HIS	-	EXPRESSION TAG	UNP Q97NW2
A	6	HIS	-	EXPRESSION TAG	UNP Q97NW2
A	7	HIS	-	EXPRESSION TAG	UNP Q97NW2
A	8	LEU	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
A	9	GLU	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
A	10	VAL	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
A	11	LEU	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
A	12	PHE	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
A	13	GLN	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
A	14	GLY	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
A	15	PRO	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
A	16	SER	-	CLONING ARTIFACT	UNP Q97NW2
A	17	SER	-	CLONING ARTIFACT	UNP Q97NW2
A	401	MET	-	CLONING ARTIFACT	UNP Q97NW2
B	1	MET	-	INITIATING METHIONINE	UNP Q97NW2
B	2	HIS	-	EXPRESSION TAG	UNP Q97NW2
B	3	HIS	-	EXPRESSION TAG	UNP Q97NW2
B	4	HIS	-	EXPRESSION TAG	UNP Q97NW2
B	5	HIS	-	EXPRESSION TAG	UNP Q97NW2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	HIS	-	EXPRESSION TAG	UNP Q97NW2
B	7	HIS	-	EXPRESSION TAG	UNP Q97NW2
B	8	LEU	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
B	9	GLU	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
B	10	VAL	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
B	11	LEU	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
B	12	PHE	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
B	13	GLN	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
B	14	GLY	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
B	15	PRO	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
B	16	SER	-	CLONING ARTIFACT	UNP Q97NW2
B	17	SER	-	CLONING ARTIFACT	UNP Q97NW2
B	401	MET	-	CLONING ARTIFACT	UNP Q97NW2
C	1	MET	-	INITIATING METHIONINE	UNP Q97NW2
C	2	HIS	-	EXPRESSION TAG	UNP Q97NW2
C	3	HIS	-	EXPRESSION TAG	UNP Q97NW2
C	4	HIS	-	EXPRESSION TAG	UNP Q97NW2
C	5	HIS	-	EXPRESSION TAG	UNP Q97NW2
C	6	HIS	-	EXPRESSION TAG	UNP Q97NW2
C	7	HIS	-	EXPRESSION TAG	UNP Q97NW2
C	8	LEU	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
C	9	GLU	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
C	10	VAL	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
C	11	LEU	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
C	12	PHE	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
C	13	GLN	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
C	14	GLY	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
C	15	PRO	-	PROTEASE CLEAVAGE SITE	UNP Q97NW2
C	16	SER	-	CLONING ARTIFACT	UNP Q97NW2
C	17	SER	-	CLONING ARTIFACT	UNP Q97NW2
C	401	MET	-	CLONING ARTIFACT	UNP Q97NW2

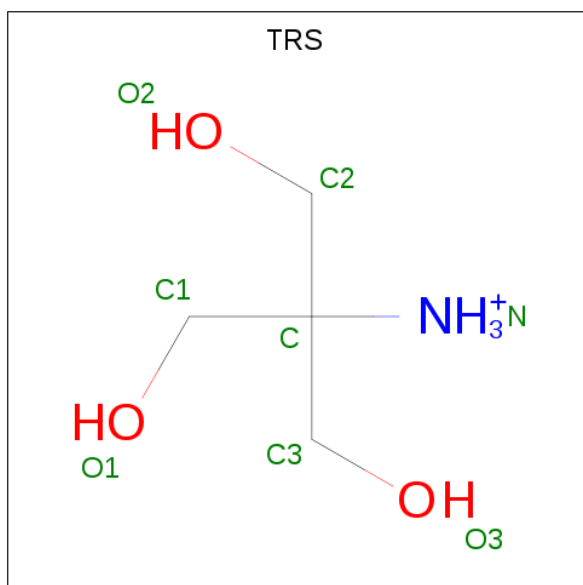
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Cl 2 2	0	0
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			8	4	1	3		

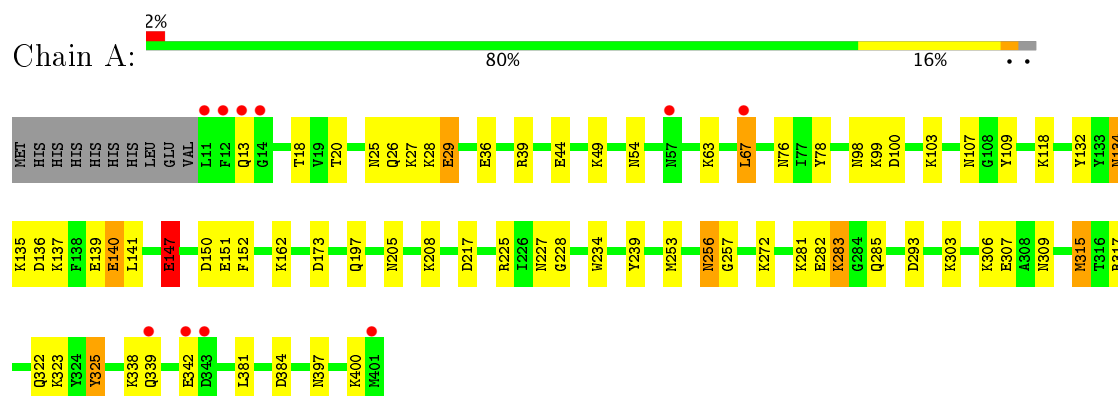
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	847	Total	O	0	3
			850	850		
5	B	837	Total	O	0	3
			840	840		
5	C	857	Total	O	0	5
			862	862		

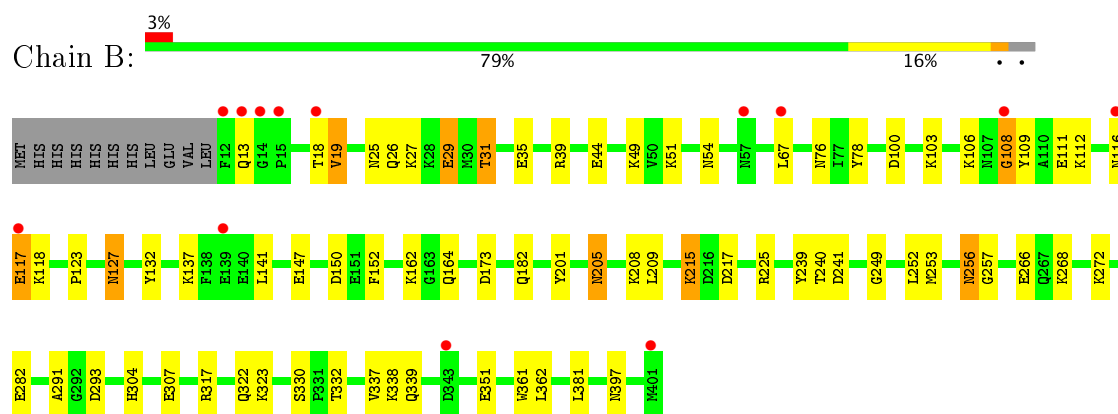
3 Residue-property plots [i](#)

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.

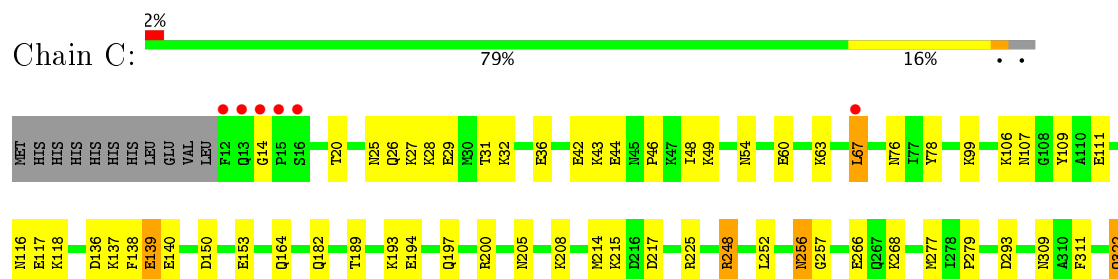
- Molecule 1: Sugar ABC transporter, sugar-binding protein

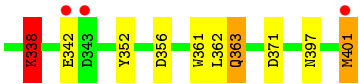


- Molecule 1: Sugar ABC transporter, sugar-binding protein



- Molecule 1: Sugar ABC transporter, sugar-binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	77.22Å 129.31Å 119.42Å 90.00° 94.21° 90.00°	Depositor
Resolution (Å)	19.82 – 1.04 19.82 – 1.04	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.82-1.04) 97.6 (19.82-1.04)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.04Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.130 , 0.157 0.139 , 0.165	Depositor DCC
R_{free} test set	27325 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	10.0	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12875	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: NA, TRS, CL

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	1.33	20/3567 (0.6%)	1.16	21/4812 (0.4%)
1	B	1.33	23/3525 (0.7%)	1.21	31/4763 (0.7%)
1	C	1.30	21/3491 (0.6%)	1.15	27/4709 (0.6%)
All	All	1.32	64/10583 (0.6%)	1.18	79/14284 (0.6%)

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	3

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	GLU	CB-CG	-16.41	1.21	1.52
1	B	147[A]	GLU	CG-CD	11.86	1.69	1.51
1	B	147[B]	GLU	CG-CD	11.86	1.69	1.51
1	B	147[C]	GLU	CG-CD	11.86	1.69	1.51
1	A	315	MET	SD-CE	-11.26	1.14	1.77

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	MET	CG-SD-CE	-12.09	80.85	100.20
1	C	352	TYR	CB-CG-CD2	9.37	126.62	121.00
1	B	266[A]	GLU	CG-CD-OE1	8.95	136.21	118.30
1	B	266[B]	GLU	CG-CD-OE1	8.95	136.21	118.30
1	B	208	LYS	CD-CE-NZ	8.78	131.90	111.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	GLU	Sidechain
1	A	400	LYS	Mainchain

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	3467	0	3456	91	2
1	B	3427	0	3380	76	2
1	C	3416	0	3369	78	4
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	C	8	0	12	0	0
5	A	850	0	0	32	7
5	B	840	0	0	28	9
5	C	862	0	0	29	8
All	All	12875	0	10217	245	18

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 12.

The worst 5 of 245 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:67:LEU:CD2	1:C:67:LEU:CG	1.75	1.61
1:A:283:LYS:CE	1:A:283:LYS:CD	1.75	1.55
1:A:315:MET:CG	1:A:315:MET:CE	1.95	1.44
1:B:240[B]:THR:HG22	5:B:3264:HOH:O	1.18	1.34
1:B:123[B]:PRO:HG3	5:B:3768:HOH:O	1.18	1.26

The worst 5 of 18 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:116[B]:ASN:OD1	1:C:107:ASN:ND2[3_555]	1.57	0.63
5:B:3203:HOH:O	5:C:5779:HOH:O[2_656]	1.82	0.38
1:C:208[B]:LYS:NZ	5:A:4516:HOH:O[3_545]	1.82	0.38
5:A:4405:HOH:O	5:A:4405:HOH:O[2_656]	1.92	0.28
1:A:107:ASN:ND2	1:C:116[B]:ASN:OD1[3_455]	1.93	0.27

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	435/401 (108%)	424 (98%)	11 (2%)	0	100	100
1	B	432/401 (108%)	418 (97%)	14 (3%)	0	100	100
1	C	427/401 (106%)	417 (98%)	10 (2%)	0	100	100
All	All	1294/1203 (108%)	1259 (97%)	35 (3%)	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	374/337 (111%)	369 (99%)	5 (1%)	73	37
1	B	370/337 (110%)	366 (99%)	4 (1%)	78	44
1	C	365/337 (108%)	359 (98%)	6 (2%)	68	29
All	All	1109/1011 (110%)	1094 (99%)	15 (1%)	75	35

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	117[B]	GLU
1	B	127	ASN
1	C	338[B]	LYS
1	B	117[A]	GLU
1	C	338[A]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	182	GLN
1	B	309	ASN
1	C	322	GLN
1	B	205	ASN
1	B	322	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 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	TRS	C	5001	-	7,7,7	1.18	1 (14%)	9,9,9	1.16	2 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRS	C	5001	-	-	0/9/9/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	5001	TRS	C-N	2.28	1.57	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5001	TRS	C3-C-C2	-2.06	105.23	111.06
4	C	5001	TRS	O3-C3-C	2.16	116.72	110.47

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	19[B]:VAL	C	20:THR	N	1.19

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	391/401 (97%)	-0.09	10 (2%) 56 49	8, 13, 22, 34	1 (0%)
1	B	390/401 (97%)	-0.04	13 (3%) 47 40	6, 11, 22, 31	0
1	C	390/401 (97%)	-0.09	9 (2%) 61 53	7, 12, 21, 36	0
All	All	1171/1203 (97%)	-0.07	32 (2%) 55 48	6, 12, 22, 36	1 (0%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	LEU	6.9
1	C	401	MET	5.2
1	B	12	PHE	4.8
1	A	12	PHE	4.7
1	C	14	GLY	4.2

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
4	TRS	C	5001	8/8	0.92	0.11	5.08	11,13,14,14	8
3	NA	C	4002	1/1	0.99	0.12	1.04	16,16,16,16	0
2	CL	A	3002	1/1	1.00	0.05	-1.05	12,12,12,12	1
2	CL	B	3001	1/1	1.00	0.07	-	8,8,8,8	1
2	CL	B	3003	1/1	0.99	0.06	-	13,13,13,13	1
3	NA	A	4001	1/1	0.99	0.13	-	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.