



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 07:33 PM GMT

PDB ID : 4TTV
Title : Crystal structure of human ThrRS complexing with a bioengineered macrolide BC194
Authors : Fang, P.; Guo, M.
Deposited on : 2014-06-23
Resolution : 2.80 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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-20026982

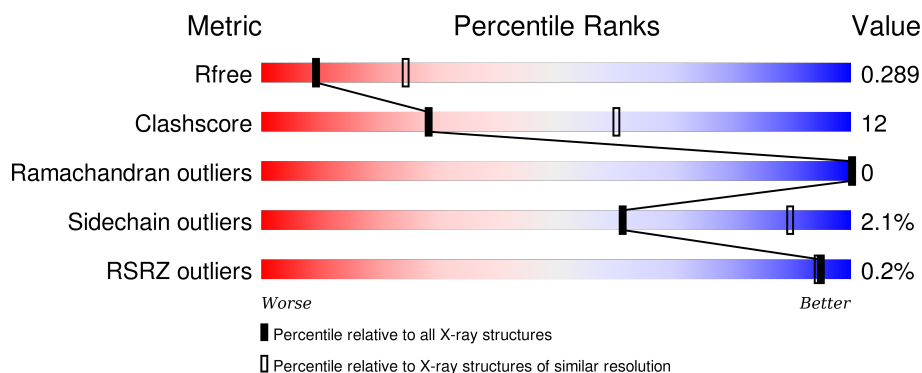
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	414	 77% 18% . .
1	B	414	 77% 19% . .
1	C	414	 76% 21% .
1	D	414	 74% 23% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13247 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 Threonine–tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3263	2083	570	594	16			
1	B	403	Total	C	N	O	S	0	0	0
			3269	2086	573	594	16			
1	C	403	Total	C	N	O	S	0	0	0
			3257	2080	571	590	16			
1	D	403	Total	C	N	O	S	0	0	0
			3256	2079	573	588	16			

There are 48 discrepancies between the modelled and reference sequences:

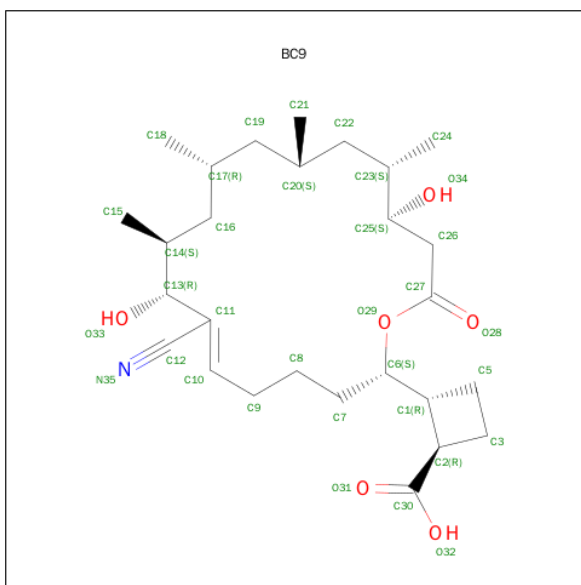
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	MET	-	initiating methionine	UNP P26639
A	311	GLY	-	expression tag	UNP P26639
A	312	SER	-	expression tag	UNP P26639
A	313	SER	-	expression tag	UNP P26639
A	314	HIS	-	expression tag	UNP P26639
A	315	HIS	-	expression tag	UNP P26639
A	316	HIS	-	expression tag	UNP P26639
A	317	HIS	-	expression tag	UNP P26639
A	318	HIS	-	expression tag	UNP P26639
A	319	HIS	-	expression tag	UNP P26639
A	320	SER	-	expression tag	UNP P26639
A	321	SER	-	expression tag	UNP P26639
B	310	MET	-	initiating methionine	UNP P26639
B	311	GLY	-	expression tag	UNP P26639
B	312	SER	-	expression tag	UNP P26639
B	313	SER	-	expression tag	UNP P26639
B	314	HIS	-	expression tag	UNP P26639
B	315	HIS	-	expression tag	UNP P26639
B	316	HIS	-	expression tag	UNP P26639
B	317	HIS	-	expression tag	UNP P26639
B	318	HIS	-	expression tag	UNP P26639

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Chain	Residue	Modelled	Actual	Comment	Reference
B	319	HIS	-	expression tag	UNP P26639
B	320	SER	-	expression tag	UNP P26639
B	321	SER	-	expression tag	UNP P26639
C	310	MET	-	initiating methionine	UNP P26639
C	311	GLY	-	expression tag	UNP P26639
C	312	SER	-	expression tag	UNP P26639
C	313	SER	-	expression tag	UNP P26639
C	314	HIS	-	expression tag	UNP P26639
C	315	HIS	-	expression tag	UNP P26639
C	316	HIS	-	expression tag	UNP P26639
C	317	HIS	-	expression tag	UNP P26639
C	318	HIS	-	expression tag	UNP P26639
C	319	HIS	-	expression tag	UNP P26639
C	320	SER	-	expression tag	UNP P26639
C	321	SER	-	expression tag	UNP P26639
D	310	MET	-	initiating methionine	UNP P26639
D	311	GLY	-	expression tag	UNP P26639
D	312	SER	-	expression tag	UNP P26639
D	313	SER	-	expression tag	UNP P26639
D	314	HIS	-	expression tag	UNP P26639
D	315	HIS	-	expression tag	UNP P26639
D	316	HIS	-	expression tag	UNP P26639
D	317	HIS	-	expression tag	UNP P26639
D	318	HIS	-	expression tag	UNP P26639
D	319	HIS	-	expression tag	UNP P26639
D	320	SER	-	expression tag	UNP P26639
D	321	SER	-	expression tag	UNP P26639

- Molecule 2 is (1R,2R)-2-[(2S,6E,8R,9S,11R,13S,15S,16S)-7-cyano-8,16-dihydroxy-9,11,13,15-tetramethyl-18-oxooxacyclooctadec-6-en-2-yl]cyclobutanecarboxylic acid (three-letter code: BC9) (formula: C₂₇H₄₃NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	27	1	6		
2	B	1	Total	C	N	O	0	0
			34	27	1	6		
2	C	1	Total	C	N	O	0	0
			34	27	1	6		
2	D	1	Total	C	N	O	0	0
			34	27	1	6		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		

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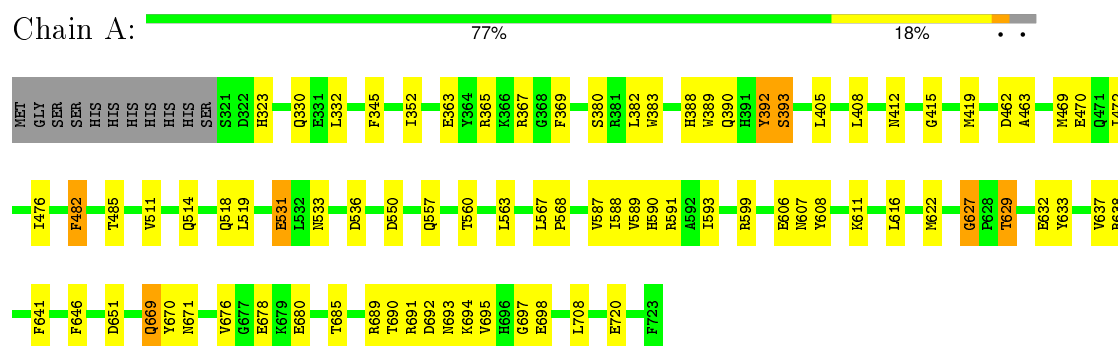
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	16	Total 16	O 16	0	0
4	C	11	Total 11	O 11	0	0
4	D	16	Total 16	O 16	0	0

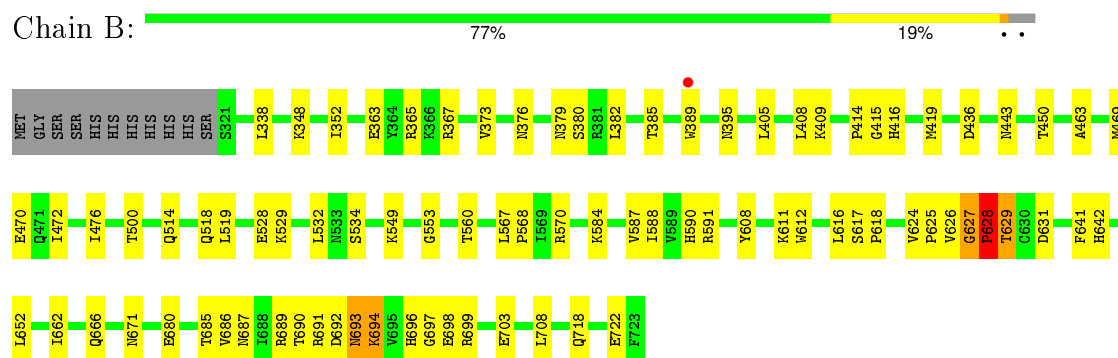
3 Residue-property plots

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

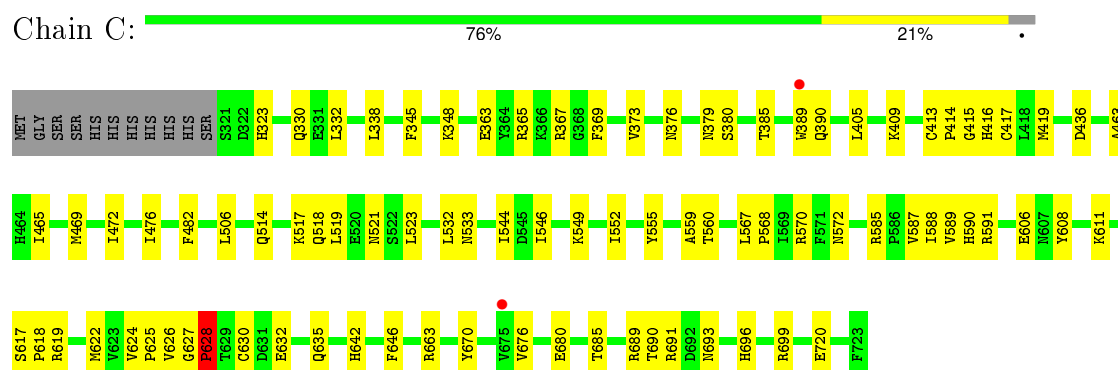
- Molecule 1: Threonine-tRNA ligase, cytoplasmic



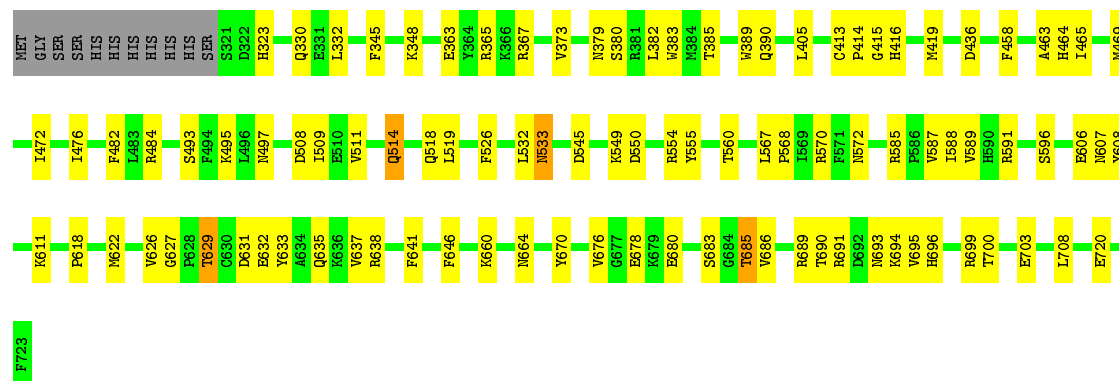
- Molecule 1: Threonine-tRNA ligase, cytoplasmic



- Molecule 1: Threonine-tRNA ligase, cytoplasmic



- Chain D:  74% 23% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.02Å 134.61Å 128.67Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	46.51 – 2.80 49.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.51-2.80) 87.3 (49.13-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.255 , 0.288 0.263 , 0.289	Depositor DCC
R_{free} test set	3872 reflections (6.02%)	DCC
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.749	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 20.9	EDS
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.439 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	4 of 77128 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13247	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.52 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.3945e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, BC9

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	0.42	0/3346	0.48	1/4523 (0.0%)
1	B	0.40	1/3352 (0.0%)	0.51	3/4530 (0.1%)
1	C	0.39	1/3340 (0.0%)	0.49	2/4515 (0.0%)
1	D	0.41	0/3339	0.48	1/4514 (0.0%)
All	All	0.40	2/13377 (0.0%)	0.49	7/18082 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	628	PRO	N-CD	5.48	1.55	1.47
1	B	628	PRO	N-CD	5.30	1.55	1.47

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	694	LYS	N-CA-C	-6.12	94.46	111.00
1	C	624	VAL	C-N-CD	6.00	140.99	128.40
1	B	624	VAL	C-N-CD	5.95	140.89	128.40
1	A	627	GLY	C-N-CD	5.72	140.41	128.40
1	D	627	GLY	C-N-CD	5.69	140.34	128.40

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	3263	0	3114	67	0
1	B	3269	0	3122	79	0
1	C	3257	0	3106	63	0
1	D	3256	0	3110	92	0
2	A	34	0	42	6	0
2	B	34	0	42	4	0
2	C	34	0	42	4	0
2	D	34	0	42	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	19	0	0	2	0
4	B	16	0	0	2	0
4	C	11	0	0	0	0
4	D	16	0	0	0	0
All	All	13247	0	12620	298	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 12.

The worst 5 of 298 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:D:611:LYS:CG	1:D:691:ARG:NH1	1.82	1.43
1:D:611:LYS:HG3	1:D:691:ARG:NH1	1.34	1.28
1:B:611:LYS:CG	1:B:691:ARG:NH1	1.98	1.27
1:B:611:LYS:HG2	1:B:691:ARG:NH1	1.57	1.19
1:D:611:LYS:HG2	1:D:691:ARG:HH12	1.10	1.13

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	401/414 (97%)	388 (97%)	13 (3%)	0	100	100
1	B	401/414 (97%)	382 (95%)	19 (5%)	0	100	100
1	C	401/414 (97%)	392 (98%)	9 (2%)	0	100	100
1	D	401/414 (97%)	386 (96%)	15 (4%)	0	100	100
All	All	1604/1656 (97%)	1548 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	342/368 (93%)	332 (97%)	10 (3%)	50	83
1	B	343/368 (93%)	338 (98%)	5 (2%)	72	93
1	C	340/368 (92%)	332 (98%)	8 (2%)	57	87
1	D	340/368 (92%)	334 (98%)	6 (2%)	66	91
All	All	1365/1472 (93%)	1336 (98%)	29 (2%)	61	90

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	629	THR
1	C	482	PHE
1	D	629	THR
1	B	693	ASN
1	C	506	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	693	ASN
1	D	696	HIS
1	D	664	ASN
1	A	669	GLN
1	D	533	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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
2	BC9	A	801	-	32,35,35	3.32	7 (21%)	31,48,48	1.77	4 (12%)
2	BC9	B	801	-	32,35,35	3.23	8 (25%)	31,48,48	2.09	6 (19%)
2	BC9	C	801	-	32,35,35	3.22	9 (28%)	31,48,48	2.25	8 (25%)
2	BC9	D	801	-	32,35,35	3.27	6 (18%)	31,48,48	2.24	8 (25%)

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
2	BC9	A	801	-	-	0/39/58/58	0/1/2/2
2	BC9	B	801	-	-	0/39/58/58	0/1/2/2
2	BC9	C	801	-	-	0/39/58/58	0/1/2/2
2	BC9	D	801	-	-	0/39/58/58	0/1/2/2

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	BC9	C12-C11	-15.91	1.23	1.43
2	D	801	BC9	C12-C11	-15.78	1.24	1.43
2	B	801	BC9	C12-C11	-15.50	1.24	1.43
2	C	801	BC9	C12-C11	-15.29	1.24	1.43
2	A	801	BC9	C8-C9	-5.51	1.31	1.52

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	BC9	C8-C9-C10	-3.96	103.79	113.04
2	B	801	BC9	C8-C9-C10	-3.81	104.14	113.04
2	A	801	BC9	C24-C23-C22	-3.18	105.89	110.69
2	B	801	BC9	C24-C23-C22	-3.00	106.16	110.69
2	C	801	BC9	O28-C27-C26	-2.98	118.44	124.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	BC9	6	0
2	B	801	BC9	4	0
2	C	801	BC9	4	0
2	D	801	BC9	2	0

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	403/414 (97%)	-0.22	0 100 100	32, 53, 78, 91	0
1	B	403/414 (97%)	-0.18	1 (0%) 95 94	33, 59, 88, 101	0
1	C	403/414 (97%)	-0.15	2 (0%) 91 88	33, 58, 89, 106	0
1	D	403/414 (97%)	-0.20	0 100 100	30, 53, 80, 93	0
All	All	1612/1656 (97%)	-0.19	3 (0%) 95 94	30, 56, 85, 106	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	675	VAL	2.7
1	B	389	TRP	2.3
1	C	389	TRP	2.1

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

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	BC9	B	801	34/34	0.95	0.22	1.46	50,52,53,54	0
2	BC9	D	801	34/34	0.94	0.22	1.41	45,48,50,50	0
2	BC9	C	801	34/34	0.95	0.23	1.21	49,50,52,53	0
2	BC9	A	801	34/34	0.95	0.20	0.54	41,46,49,49	0
3	ZN	D	802	1/1	0.95	0.13	-	61,61,61,61	0
3	ZN	B	802	1/1	0.97	0.12	-	57,57,57,57	0
3	ZN	A	802	1/1	0.97	0.10	-	71,71,71,71	0
3	ZN	C	802	1/1	0.98	0.11	-	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.