W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 16, 2017 – 11:15 PM EDT

PDB ID	:	4P3N
Title	:	Structural Basis for Full-Spectrum Inhibition of Threonyl-tRNA Synthetase by Borrelidin 1
Authors	:	Fang, P.; Yu, X.; Chen, K.; Chen, X.; Guo, M.
Deposited on	:	unknown
Resolution	:	2.60 Å(reported)

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

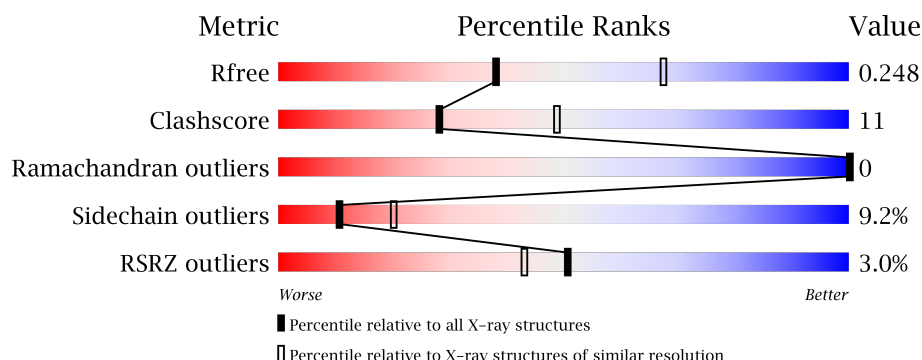|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	Percentile Ranks	Value
Rfree		0.248
Clashscore		11
Ramachandran outliers		0
Sidechain outliers		9.2%
RSRZ outliers		3.0%

Worse ... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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 <=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	415	.% 72% 22% • •
1	B	415	3% 70% 24% • •
1	C	415	4% 70% 22% 5% •
1	D	415	4% 72% 23% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13506 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	402	Total 3260	C 2081	N 571	O 592	S 16	0	0	0
1	B	402	Total 3253	C 2078	N 571	O 588	S 16	0	0	0
1	C	402	Total 3249	C 2077	N 566	O 590	S 16	0	0	0
1	D	402	Total 3211	C 2053	N 567	O 575	S 16	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	MET	-	expression tag	UNP P26639
A	310	GLY	-	expression tag	UNP P26639
A	311	SER	-	expression tag	UNP P26639
A	312	SER	-	expression tag	UNP P26639
A	313	HIS	-	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	SER	-	expression tag	UNP P26639
A	320	SER	-	expression tag	UNP P26639
A	321	GLY	-	expression tag	UNP P26639
B	309	MET	-	expression tag	UNP P26639
B	310	GLY	-	expression tag	UNP P26639
B	311	SER	-	expression tag	UNP P26639
B	312	SER	-	expression tag	UNP P26639
B	313	HIS	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	317	HIS	-	expression tag	UNP P26639
B	318	HIS	-	expression tag	UNP P26639
B	319	SER	-	expression tag	UNP P26639
B	320	SER	-	expression tag	UNP P26639
B	321	GLY	-	expression tag	UNP P26639
C	309	MET	-	expression tag	UNP P26639
C	310	GLY	-	expression tag	UNP P26639
C	311	SER	-	expression tag	UNP P26639
C	312	SER	-	expression tag	UNP P26639
C	313	HIS	-	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	SER	-	expression tag	UNP P26639
C	320	SER	-	expression tag	UNP P26639
C	321	GLY	-	expression tag	UNP P26639
D	309	MET	-	expression tag	UNP P26639
D	310	GLY	-	expression tag	UNP P26639
D	311	SER	-	expression tag	UNP P26639
D	312	SER	-	expression tag	UNP P26639
D	313	HIS	-	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	SER	-	expression tag	UNP P26639
D	320	SER	-	expression tag	UNP P26639
D	321	GLY	-	expression tag	UNP P26639

- Molecule 2 is (1R,2R)-2-[(2S,4E,6E,8R,9S,11R,13S,15S,16S)-7-cyano-8,16-dihydroxy-9,11,13,15-tetramethyl-18-oxooxacyclooctadeca-4,6-dien-2-yl]cyclopentanecarboxylic acid (three-letter code: 2CR) (formula: $C_{28}H_{43}NO_6$).
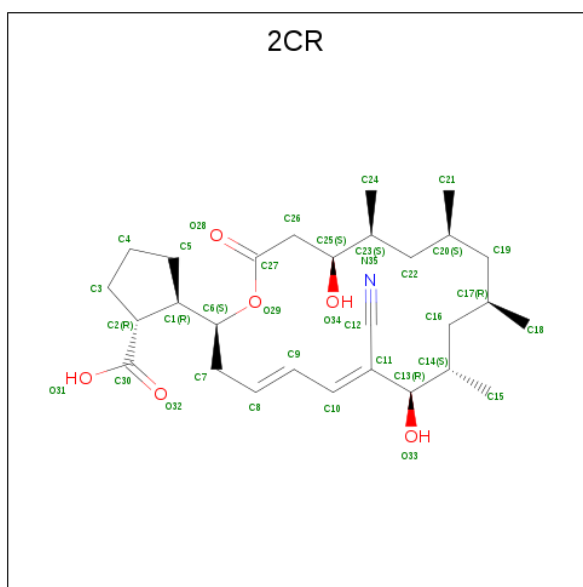
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total C N O				0	0
			35 28 1 6					
2	B	1	Total C N O				0	0
			35 28 1 6					
2	C	1	Total C N O				0	0
			35 28 1 6					
2	D	1	Total C N O				0	0
			35 28 1 6					

- 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	95	Total O		0	0
			95 95			

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	111	Total 111	O 111	0	0
4	C	90	Total 90	O 90	0	0
4	D	93	Total 93	O 93	0	0

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.
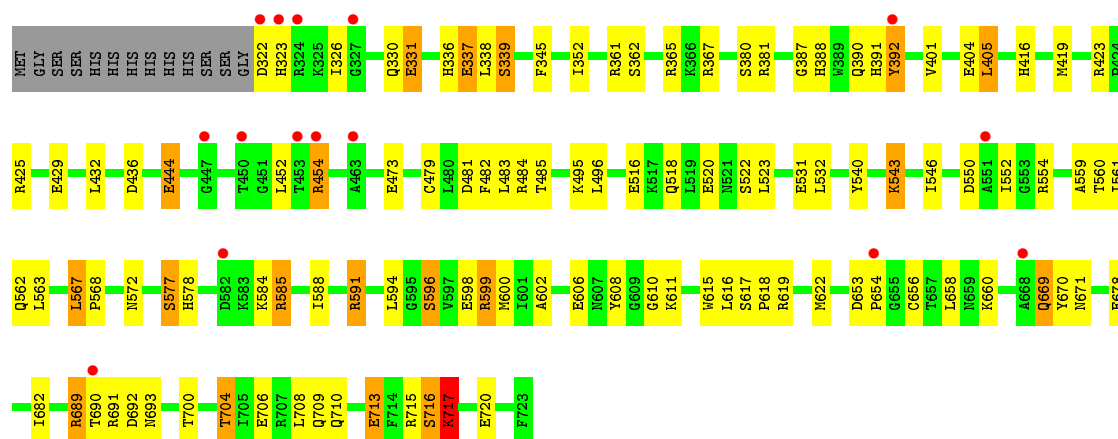
- Molecule 1: Threonine–tRNA ligase, cytoplasmic
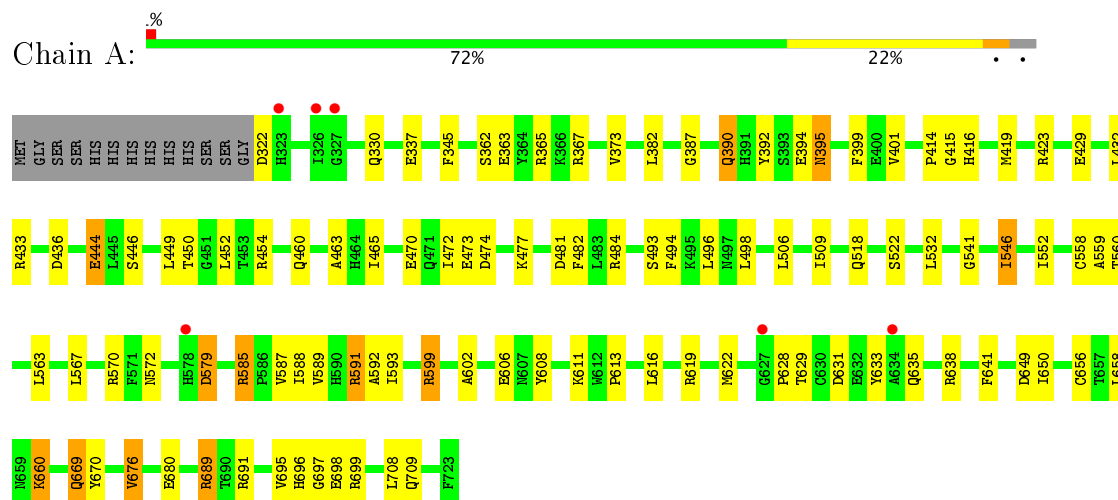
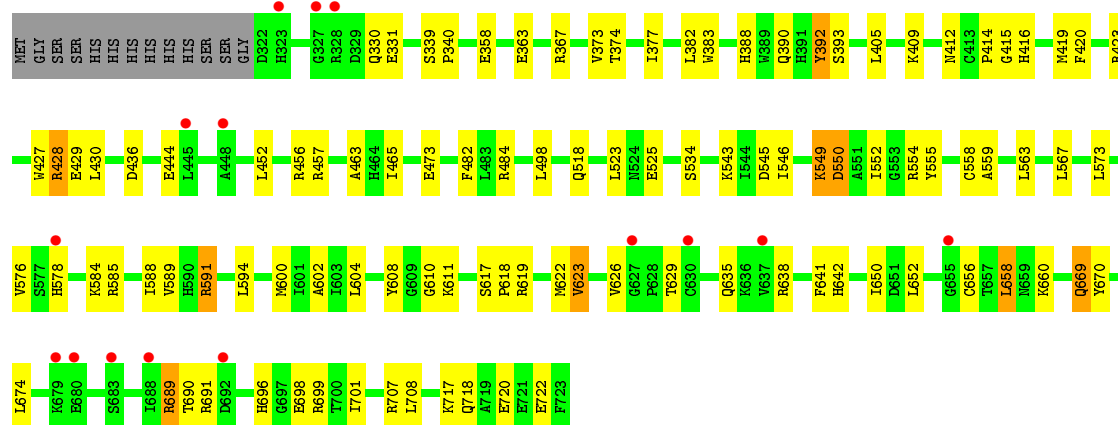- Molecule 1: Threonine–tRNA ligase, cytoplasmic

- Molecule 1: Threonine–tRNA ligase, cytoplasmic

• Molecule 1: Threonine–tRNA ligase, cytoplasmic

Chain D:
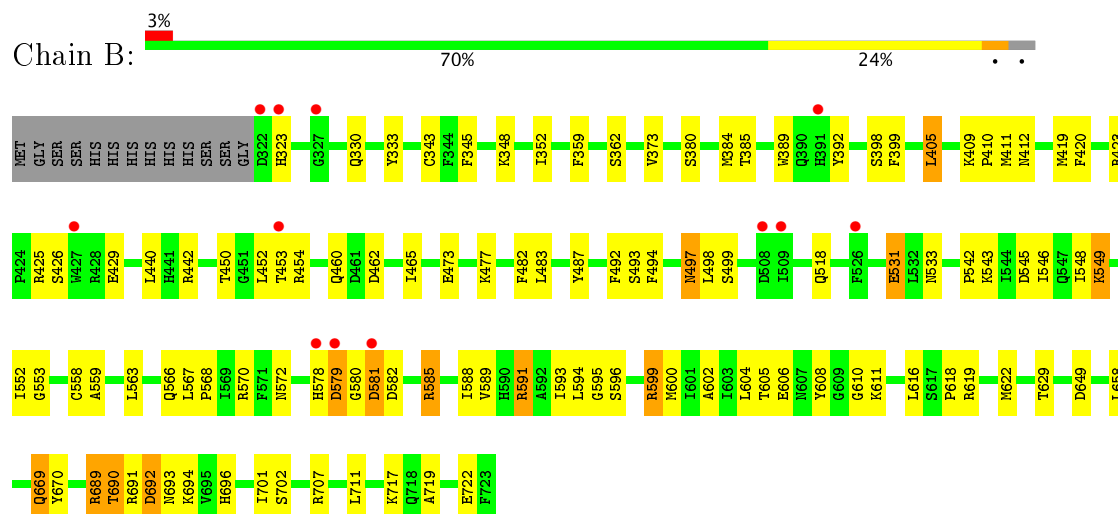
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	63.87Å 78.00Å 118.05Å 86.99° 83.32° 84.39°	Depositor
Resolution (Å)	47.71 – 2.60 63.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.7 (47.71-2.60) 94.5 (63.47-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.228 , 0.255 0.218 , 0.248	Depositor DCC
R_{free} test set	3366 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.802	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13506	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 2CR

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	0.35	0/3343	0.46	0/4520
1	B	0.44	0/3336	0.49	1/4510 (0.0%)
1	C	0.44	0/3332	0.51	0/4507
1	D	0.44	0/3294	0.51	1/4459 (0.0%)
All	All	0.42	0/13305	0.49	2/17996 (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	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	550	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	B	692	ASP	N-CA-C	5.11	124.79	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	717	LYS	Peptide

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	3260	0	3114	70	0
1	B	3253	0	3105	76	0
1	C	3249	0	3091	76	0
1	D	3211	0	3036	67	0
2	A	35	0	42	6	0
2	B	35	0	42	1	0
2	C	35	0	42	5	0
2	D	35	0	42	1	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	95	0	0	1	0
4	B	111	0	0	3	0
4	C	90	0	0	0	0
4	D	93	0	0	1	0
All	All	13506	0	12514	285	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 11.

The worst 5 of 285 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:331:GLU:OE1	1:D:423:ARG:NH1	1.81	1.13
1:A:689:ARG:HG3	1:A:689:ARG:HH21	0.96	1.09
1:C:444:GLU:OE1	1:C:454:ARG:NH1	1.99	0.96
1:A:395:ASN:N	1:A:395:ASN:HD22	1.58	0.95
1:A:689:ARG:NH2	1:A:689:ARG:HG3	1.77	0.94

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	400/415 (96%)	393 (98%)	7 (2%)	0	100	100
1	B	400/415 (96%)	393 (98%)	7 (2%)	0	100	100
1	C	400/415 (96%)	393 (98%)	7 (2%)	0	100	100
1	D	400/415 (96%)	393 (98%)	7 (2%)	0	100	100
All	All	1600/1660 (96%)	1572 (98%)	28 (2%)	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	342/368 (93%)	311 (91%)	31 (9%)	11	21
1	B	339/368 (92%)	312 (92%)	27 (8%)	14	27
1	C	338/368 (92%)	303 (90%)	35 (10%)	8	15
1	D	328/368 (89%)	297 (90%)	31 (10%)	10	19
All	All	1347/1472 (92%)	1223 (91%)	124 (9%)	11	20

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	702	SER
1	C	485	THR
1	D	622	MET

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Mol	Chain	Res	Type
1	B	717	LYS
1	C	392	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	497	ASN
1	B	666	GLN
1	D	422	HIS
1	B	460	GLN
1	C	497	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	2CR	A	800	-	32,36,36	3.21	8 (25%)	34,49,49	2.17	12 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	2CR	B	800	-	32,36,36	2.98	8 (25%)	34,49,49	2.11	9 (26%)
2	2CR	C	800	-	32,36,36	3.06	5 (15%)	34,49,49	1.72	7 (20%)
2	2CR	D	800	-	32,36,36	3.10	6 (18%)	34,49,49	1.89	8 (23%)

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	2CR	A	800	-	-	0/42/59/59	0/1/2/2
2	2CR	B	800	-	-	0/42/59/59	0/1/2/2
2	2CR	C	800	-	-	0/42/59/59	0/1/2/2
2	2CR	D	800	-	-	0/42/59/59	0/1/2/2

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	2CR	C12-C11	-15.53	1.25	1.43
2	D	800	2CR	C12-C11	-15.36	1.25	1.43
2	C	800	2CR	C12-C11	-14.84	1.25	1.43
2	B	800	2CR	C12-C11	-14.00	1.26	1.43
2	C	800	2CR	C23-C25	-4.45	1.50	1.53

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	800	2CR	C10-C9-C8	-6.42	108.22	123.75
2	B	800	2CR	C30-C2-C1	-6.04	105.78	116.27
2	D	800	2CR	C10-C9-C8	-5.05	111.54	123.75
2	B	800	2CR	C10-C9-C8	-5.04	111.57	123.75
2	A	800	2CR	C30-C2-C1	-4.02	109.29	116.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	2CR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	2CR	1	0
2	C	800	2CR	5	0
2	D	800	2CR	1	0

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(Å²)	Q<0.9
1	A	402/415 (96%)	0.29	6 (1%)	74	69	33, 51, 74, 95	0
1	B	402/415 (96%)	0.39	12 (2%)	51	43	35, 53, 72, 97	0
1	C	402/415 (96%)	0.38	15 (3%)	42	34	35, 58, 84, 100	0
1	D	402/415 (96%)	0.45	15 (3%)	42	34	36, 56, 89, 104	0
All	All	1608/1660 (96%)	0.38	48 (2%)	51	43	33, 54, 84, 104	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	HIS	4.9
1	B	322	ASP	4.2
1	C	322	ASP	3.9
1	C	327	GLY	3.9
1	D	679	LYS	3.8

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(Å^2)	Q<0.9
2	2CR	B	800	35/35	0.93	0.20	-0.26	45,46,50,51	0
2	2CR	D	800	35/35	0.91	0.21	-0.27	50,52,54,55	0
2	2CR	C	800	35/35	0.92	0.19	-0.34	52,53,55,55	0
2	2CR	A	800	35/35	0.94	0.16	-1.70	38,41,43,45	0
3	ZN	C	801	1/1	0.91	0.16	-	58,58,58,58	0
3	ZN	A	801	1/1	0.81	0.16	-	44,44,44,44	0
3	ZN	B	801	1/1	0.96	0.15	-	50,50,50,50	0
3	ZN	D	801	1/1	0.93	0.19	-	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.