WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 27, 2014 – 12:41 PM GMT

PDB ID   :   3IIQ
Title   :   Crystallographic analysis of bacterial signal peptidase in ternary complex with
               Arylomycin A2 and a beta-sultam inhibitor
Authors   :   Paetzel, M.
Deposited on :   2009-08-03
Resolution :   2.00 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1   Overall quality at a glance ⓘ

The reported resolution of this entry is 2.00 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		0.270
Clashscore		16
Ramachandran outliers		0.9%
Sidechain outliers		5.8%
RSRZ outliers		11.0%

Worse   *Better*

▊ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
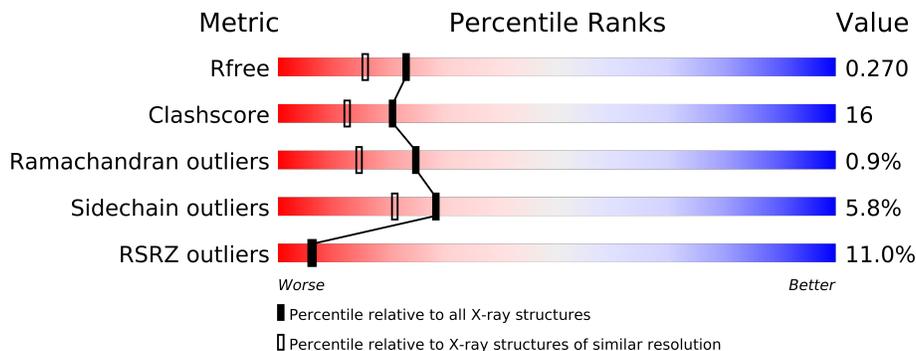
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	249	
1	B	249	
2	C	6	
2	D	6	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	JZA	A	324	-	X
3	JZA	B	324	-	X
4	TRT	A	325	-	X
4	TRT	B	325	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	GOL	A	326	-	X
5	GOL	A	327	-	X
5	GOL	A	328	-	X
5	GOL	A	329	-	X
6	CCN	A	330	-	X
6	CCN	A	331	-	X
7	M12	C	0	-	X
7	M12	D	0	-	X

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 3933 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SIGNAL PEPTIDASE I.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1726	1108	286	324	8			
1	B	224	Total	C	N	O	S	0	0	0
			1755	1121	295	331	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	MET	-	INITIATING METHIONINE	UNP P00803
B	75	MET	-	INITIATING METHIONINE	UNP P00803

- Molecule 2 is a protein called ARYLOMYCIN A2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			46	30	6	10			
2	D	6	Total	C	N	O	0	0	0
			46	30	6	10			

- Molecule 3 is 4-[(1,1-DIOXIDO-1,2-THIAZETIDIN-2-YL)CARBONYL]MORPHOLINE (three-letter code: JZA) (formula: $C_7H_{12}N_2O_4S$).
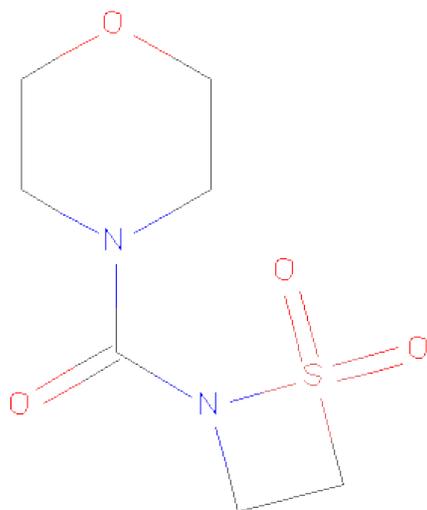
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			14	7	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			14	7	2	4	1		

- Molecule 4 is FRAGMENT OF TRITON X-100 (three-letter code: TRT) (formula: $C_{21}H_{36}O_4$).
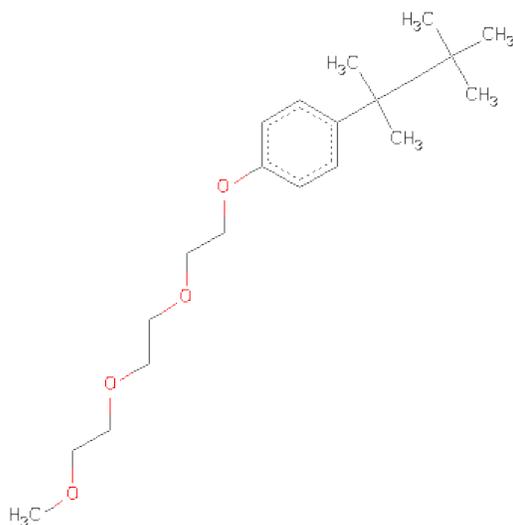
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	18	2		
4	B	1	Total	C	O	0	0
			20	18	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
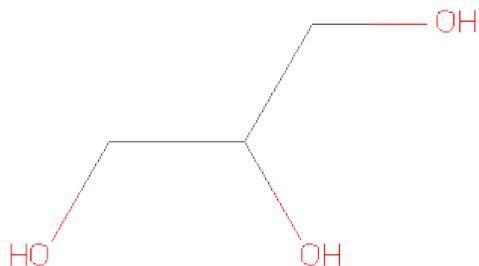
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 6	C 3	O 3	0	0
5	A	1	Total 6	C 3	O 3	0	0
5	A	1	Total 6	C 3	O 3	0	0
5	A	1	Total 6	C 3	O 3	0	0

- Molecule 6 is ACETONITRILE (three-letter code: CCN) (formula: C_2H_3N).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 3	C 2	N 1	0	0
6	A	1	Total 3	C 2	N 1	0	0

- Molecule 7 is 10-METHYLUNDECANOIC ACID (three-letter code: M12) (formula: $C_{12}H_{24}O_2$).
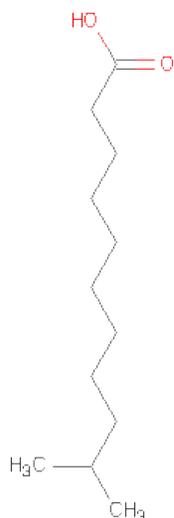
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total 13	C 12	O 1	0	0
7	D	1	Total 3	C 2	O 1	0	0

- Molecule 8 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	128	Total 128	O 128	0	0
8	B	111	Total 111	O 111	0	0
8	C	2	Total 2	O 2	0	0
8	D	5	Total 5	O 5	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: SIGNAL PEPTIDASE I
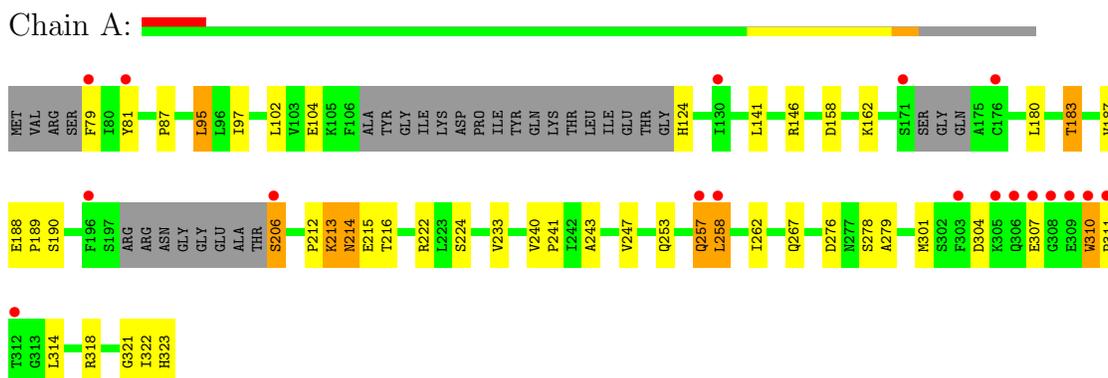
Chain A:

• Molecule 1: SIGNAL PEPTIDASE I

Chain B:

• Molecule 2: ARYLOMYCIN A2

Chain C:

• Molecule 2: ARYLOMYCIN A2

Chain D:
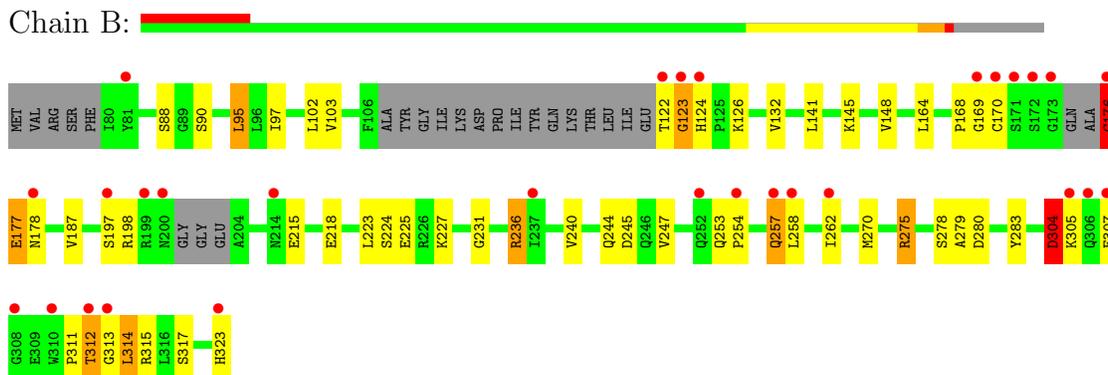
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	70.01Å 70.01Å 259.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.40 – 2.00 42.98 – 2.04	Depositor EDS
% Data completeness (in resolution range)	95.1 (67.40-2.00) 95.1 (42.98-2.04)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.207 , 0.250 0.234 , 0.270	Depositor DCC
R_{free} test set	2035 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	40.3	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	0 of 40272 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3933	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, DAL, 5PG, JZA, CCN, M12, DSE, TRT

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	1.17	5/1772 (0.3%)	0.96	5/2402 (0.2%)
1	B	1.29	13/1800 (0.7%)	0.96	5/2440 (0.2%)
2	C	1.90	0/21	2.16	0/24
2	D	1.58	0/21	1.78	0/24
All	All	1.24	18/3614 (0.5%)	0.97	10/4890 (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
1	A	0	1
1	B	0	3
2	C	0	1
2	D	0	1
All	All	0	6

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	177	GLU	CD-OE1	16.08	1.43	1.25
1	B	176	CYS	C-N	11.13	1.59	1.34
1	B	177	GLU	CG-CD	-9.56	1.37	1.51
1	B	177	GLU	C-O	9.21	1.40	1.23
1	A	216	THR	C-N	9.04	1.54	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	236	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	B	95	LEU	CB-CG-CD1	5.91	121.04	111.00
1	B	177	GLU	C-N-CA	-5.84	107.10	121.70
1	B	245	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	214	ASN	N-CA-CB	-5.62	100.49	110.60

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	310	TRP	Peptide
1	B	123	GLY	Peptide
1	B	176	CYS	Mainchain
1	B	198	ARG	Peptide
2	C	2	DAL	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1726	0	1676	44	0
1	B	1755	0	1698	53	0
2	C	46	0	37	1	0
2	D	46	0	37	2	0
3	A	14	0	12	3	0
3	B	14	0	12	7	0
4	A	20	0	27	2	0
4	B	20	0	27	9	0
5	A	24	0	32	14	0
6	A	6	0	6	7	0
7	C	13	0	23	1	0
7	D	3	0	0	0	0
8	A	128	0	0	6	0
8	B	111	0	0	5	0
8	C	2	0	0	0	0
8	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3933	0	3587	114	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

The worst 5 of 114 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:176:CYS:N	1:B:177:GLU:CG	1.75	1.46
1:B:168:PRO:HD2	1:B:178:ASN:O	1.30	1.23
1:B:176:CYS:N	1:B:177:GLU:HG2	0.86	1.18
4:B:325:TRT:H8C2	4:B:325:TRT:H3C3	1.34	1.07
1:B:123:GLY:HA2	1:B:124:HIS:CG	1.90	1.06

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	209/249 (84%)	203 (97%)	5 (2%)	1 (0%)	38	29
1	B	216/249 (87%)	205 (95%)	8 (4%)	3 (1%)	16	7
2	C	2/6 (33%)	2 (100%)	0	0	100	100
2	D	2/6 (33%)	2 (100%)	0	0	100	100
All	All	429/510 (84%)	412 (96%)	13 (3%)	4 (1%)	25	14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	PRO
1	B	312	THR
1	B	254	PRO
1	B	231	GLY

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	189/214 (88%)	178 (94%)	11 (6%)	28	21
1	B	190/214 (89%)	179 (94%)	11 (6%)	28	21
2	C	1/1 (100%)	1 (100%)	0	100	100
2	D	1/1 (100%)	1 (100%)	0	100	100
All	All	381/430 (89%)	359 (94%)	22 (6%)	28	21

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
1	B	102	LEU
1	B	305	LYS
1	A	304	ASP
1	B	95	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	HIS
1	B	85	GLN
1	B	252	GLN
1	A	291	ASN
1	B	253	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	DSE	C	1	2,7	6,6,7	7.99	2 (33%)	3,6,8	2.58	2 (66%)
2	DAL	C	2	2	4,4,5	18.77	2 (50%)	3,4,6	30.97	2 (66%)
2	5PG	C	4	2	12,12,13	5.62	2 (16%)	12,15,17	2.02	2 (16%)
2	DSE	D	1	2,7	6,6,7	7.89	3 (50%)	3,6,8	3.29	2 (66%)
2	DAL	D	2	2	4,4,5	19.41	2 (50%)	3,4,6	25.47	2 (66%)
2	5PG	D	4	2	12,12,13	6.54	5 (41%)	12,15,17	2.19	3 (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	DSE	C	1	2,7	-	1/4/6/8	0/0/0/0
2	DAL	C	2	2	-	0/0/2/4	0/0/0/0
2	5PG	C	4	2	-	1/6/8/10	0/1/1/1
2	DSE	D	1	2,7	-	1/4/6/8	0/0/0/0
2	DAL	D	2	2	-	0/0/2/4	0/0/0/0
2	5PG	D	4	2	-	1/6/8/10	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	DAL	O-C	38.62	1.38	1.11
2	C	2	DAL	O-C	37.36	1.37	1.11
2	D	4	5PG	O-C	21.71	1.26	1.11
2	C	1	DSE	O-C	19.20	1.24	1.11
2	D	1	DSE	O-C	18.77	1.24	1.11

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	DAL	C-CA-N	-48.37	107.79	113.27
2	D	2	DAL	C-CA-N	-41.28	108.59	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	DAL	CB-CA-C	23.21	118.81	108.46
2	D	2	DAL	CB-CA-C	15.57	115.41	108.46
2	D	4	5PG	CN-N-CA	6.40	124.85	113.53

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	DSE	CB-CA-N-CN
2	C	1	DSE	CB-CA-N-CN
2	C	4	5PG	C-CA-N-CN
2	D	4	5PG	C-CA-N-CN

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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	#$|Z| > 2$
3	JZA	A	324	-	15,15,15	3.53	6 (40%)	22,22,22	1.82	5 (22%)
4	TRT	A	325	-	20,20,25	1.39	2 (10%)	27,28,33	0.65	0
5	GOL	A	326	-	5,5,5	0.17	0	5,5,5	0.47	0
5	GOL	A	327	-	5,5,5	0.39	0	5,5,5	1.31	0
5	GOL	A	328	-	5,5,5	0.77	0	5,5,5	1.12	0
5	GOL	A	329	-	5,5,5	0.45	0	5,5,5	1.02	0
6	CCN	A	330	-	2,2,2	1.05	0	1,1,1	0.27	0
6	CCN	A	331	-	2,2,2	1.57	1 (50%)	1,1,1	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	JZA	B	324	-	15,15,15	5.16	6 (40%)	22,22,22	2.62	7 (31%)
4	TRT	B	325	-	20,20,25	1.73	4 (20%)	27,28,33	1.14	2 (7%)
7	M12	C	0	2	12,12,13	5.22	2 (16%)	10,12,14	0.49	0
7	M12	D	0	2	1,2,13	18.42	1 (100%)	0,1,14	0.00	-

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
3	JZA	A	324	-	-	0/4/28/28	0/1/2/2
4	TRT	A	325	-	-	0/18/18/23	0/1/1/1
5	GOL	A	326	-	-	0/4/4/4	0/0/0/0
5	GOL	A	327	-	-	0/4/4/4	0/0/0/0
5	GOL	A	328	-	-	0/4/4/4	0/0/0/0
5	GOL	A	329	-	-	0/4/4/4	0/0/0/0
6	CCN	A	330	-	-	0/0/0/0	0/0/0/0
6	CCN	A	331	-	-	0/0/0/0	0/0/0/0
3	JZA	B	324	-	-	0/4/28/28	0/1/2/2
4	TRT	B	325	-	-	0/18/18/23	0/1/1/1
7	M12	C	0	2	-	0/9/10/11	0/0/0/0
7	M12	D	0	2	-	0/0/0/11	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	0	M12	O1-C1	18.42	1.24	1.11
7	C	0	M12	O1-C1	17.62	1.23	1.11
3	B	324	JZA	C5-N6	13.75	1.62	1.49
3	B	324	JZA	O3-S1	8.03	1.52	1.43
3	B	324	JZA	O2-S1	7.48	1.52	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	324	JZA	C5-N6-C7	-7.78	95.60	125.83
3	B	324	JZA	C5-C4-S1	4.49	91.87	88.67
3	B	324	JZA	O2-S1-N6	4.29	117.05	112.64
3	A	324	JZA	C5-N6-C7	-3.89	110.74	125.83
3	B	324	JZA	O3-S1-N6	3.56	116.30	112.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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(Å²)	Q<0.9
1	A	217/249 (87%)	0.58	18 (8%)	11	11	19, 35, 51, 71	0
1	B	224/249 (89%)	0.77	29 (12%)	4	4	20, 36, 69, 78	0
2	C	6/6 (100%)	1.27	2 (33%)	1	1	0, 0, 38, 51	2 (33%)
2	D	6/6 (100%)	0.54	0	100	100	34, 37, 46, 65	2 (33%)
All	All	453/510 (88%)	0.68	49 (10%)	6	6	0, 35, 63, 78	4 (0%)

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	310	TRP	9.0
1	B	122	THR	7.2
1	B	200	ASN	7.2
1	B	172	SER	6.6
1	B	123	GLY	6.3

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

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	RSR	LLDF	B-factors(Å²)	Q<0.9
2	DSE	D	1	7/8	0.27	8.82	59,62,66,69	5
2	DAL	C	2	5/6	0.22	3.06	33,37,39,39	5
2	DAL	D	2	5/6	0.16	2.73	42,43,46,52	5
2	DSE	C	1	7/8	0.24	2.71	42,49,56,57	5
2	5PG	C	4	12/13	0.16	0.58	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	5PG	D	4	12/13	0.13	-0.41	31,33,37,39	0

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	M12	D	0	3/14	0.34	65.29	66,66,66,66	3
5	GOL	A	329	6/6	0.44	41.00	64,68,69,70	0
5	GOL	A	328	6/6	0.34	15.85	52,59,64,66	0
7	M12	C	0	13/14	0.32	8.86	60,77,83,85	3
3	JZA	A	324	14/14	0.56	5.43	161,162,163,163	0
5	GOL	A	327	6/6	0.40	5.43	83,86,88,88	0
6	CCN	A	331	3/3	0.36	5.13	26,26,35,48	0
5	GOL	A	326	6/6	0.27	5.12	82,83,83,86	0
4	TRT	B	325	20/25	0.38	5.09	92,97,101,101	0
3	JZA	B	324	14/14	0.40	4.45	135,138,141,142	0
4	TRT	A	325	20/25	0.36	4.25	121,133,137,138	0
6	CCN	A	330	3/3	0.24	2.70	27,27,30,37	0

6.5 Other polymers (i)

There are no such residues in this entry.