



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2017 – 08:01 PM EST

PDB ID : 5I5B
Title : quasi racemic structure of allo-Thr13-ShK and D-ShK
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Deposited on : 2016-02-15
Resolution : 0.90 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 : 1.7.1 (RC1), CSD as537be (2016)
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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DAR	B	1	-	-	X	-
2	DCY	B	3	-	-	X	-
5	GOL	B	102	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 756 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.

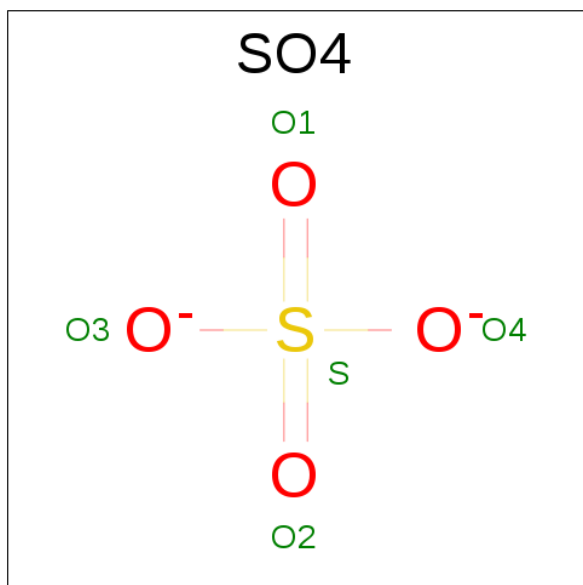
- Molecule 1 is a protein called Kappa-stichotoxin-She3a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	35	Total	C	N	O	S	0	4	0
			305	189	59	50	7			

- Molecule 2 is a protein (with D amino acids) called D-ShK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	35	Total	C	N	O	S	0	6	0
			314	198	58	50	8			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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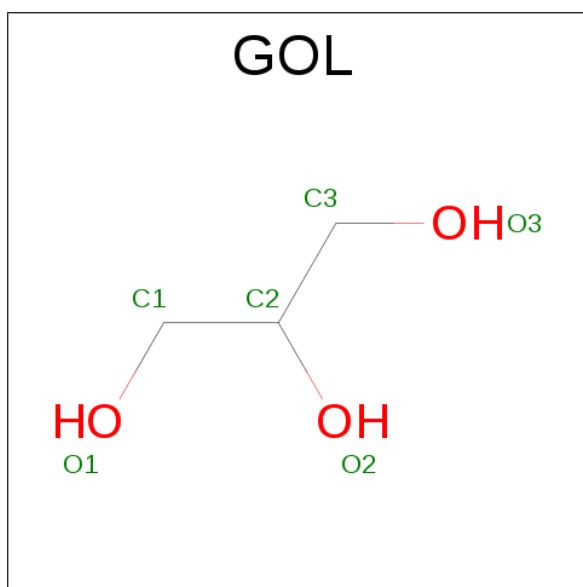
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is LITHIUM ION (three-letter code: LI) (formula: Li).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Li	0	0
			1	1		
4	A	3	Total	Li	0	0
			3	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		


- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	48	Total	O	0	3
			51	51		
6	B	54	Total	O	0	2
			56	56		

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: Kappa-stichotoxin-She3a

Chain A:  83% 14% .



- Molecule 2: D-ShK

Chain B:  86% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	21.46 Å 24.93 Å 29.93 Å 113.82° 90.42° 98.98°	Depositor
Resolution (Å)	27.30 – 0.90 27.30 – 0.90	Depositor EDS
% Data completeness (in resolution range)	85.4 (27.30-0.90) 73.8 (27.30-0.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.48 (at 0.90 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.112 , 0.128 0.113 , 0.129	Depositor DCC
R_{free} test set	1810 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	5.4	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.59$, $\langle L^2 \rangle = 0.43$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	756	wwPDB-VP
Average B, all atoms (Å ²)	9.0	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 23.37 % 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 4.7288e-03. 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, 0.333 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: DIL, GOL, DTH, DSN, DPR, DHI, ALO, DAL, DCY, DGN, LI, DLE, DTY, SO4, DAR, DAS, DPN, DLY, MED

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	1.14	0/316	1.35	6/414 (1.4%)
2	B	0.79	0/3	0.77	0/2
All	All	1.13	0/319	1.35	6/416 (1.4%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	A	18[A]	LYS	CD-CE-NZ	-6.52	96.69	111.70
1	A	18[B]	LYS	CD-CE-NZ	-6.52	96.69	111.70
1	A	21	MET	CG-SD-CE	-6.08	90.48	100.20
1	A	1	ARG	CB-CG-CD	6.02	127.24	111.60
1	A	1	ARG	NE-CZ-NH1	5.14	122.87	120.30

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	305	0	309	1	0
2	B	314	0	299	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	15	0	0	1	0
3	B	5	0	0	0	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
5	B	6	0	8	0	0
6	A	51	0	0	2	1
6	B	56	0	0	0	0
All	All	756	0	616	12	1

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 (12) 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)
3:A:103:SO4:O3	6:A:201:HOH:O	1.67	1.11
2:B:1:DAR:HD2	2:B:3:DCY:N	1.64	1.10
2:B:1:DAR:CD	2:B:3:DCY:N	2.35	0.89
2:B:1:DAR:HD3	2:B:1:DAR:C	2.19	0.73
2:B:1:DAR:HD2	2:B:3:DCY:CA	2.28	0.63
2:B:1:DAR:HD2	2:B:3:DCY:CB	2.31	0.60
2:B:1:DAR:HD2	2:B:3:DCY:HB3	1.88	0.54
2:B:21[B]:MED:HG3	2:B:25:DLE:HD12	1.95	0.49
6:A:224:HOH:O	2:B:9[B]:DLY:HD2	2.14	0.47
2:B:21[B]:MED:HE1	2:B:21[B]:MED:HA	2.00	0.43
1:A:16:GLN:HB3	1:A:23[A]:TYR:CG	2.55	0.41

All (1) 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)
6:A:227:HOH:O	6:A:239:HOH:O[1_455]	2.19	0.01

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	36/35 (103%)	34 (94%)	2 (6%)	0	100	100
2	B	1/35 (3%)	1 (100%)	0	0	100	100
All	All	37/70 (53%)	35 (95%)	2 (5%)	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	36/32 (112%)	35 (97%)	1 (3%)	51	12

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

41 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
1	ALO	A	13	1	5,6,7	1.18	1 (20%)	5,7,9	1.40	1 (20%)
2	DAR	B	1	2	5,10,11	2.03	2 (40%)	5,11,13	2.34	2 (40%)
2	DSN	B	10	2	3,5,6	0.70	0	3,5,7	2.12	1 (33%)
2	DAR	B	11	2	5,10,11	0.97	0	5,11,13	0.95	0
2	DCY	B	12	2	3,5,6	1.09	0	3,5,7	0.66	0
2	DTH	B	13	2	5,6,7	0.69	0	5,7,9	1.44	1 (20%)
2	DAL	B	14	2	1,4,5	1.04	0	1,4,6	0.01	0
2	DPN	B	15	2	9,11,12	1.17	1 (11%)	11,13,15	1.53	2 (18%)
2	DGN	B	16	2	6,8,9	0.62	0	7,9,11	0.68	0
2	DCY	B	17	2	3,5,6	0.65	0	3,5,7	1.75	1 (33%)
2	DLY	B	18	2	6,8,9	1.66	1 (16%)	6,8,10	1.37	2 (33%)
2	DHI	B	19[A]	-	4,10,11	0.60	0	4,12,14	1.36	1 (25%)
2	DHI	B	19[B]	-	4,10,11	1.11	0	4,12,14	1.27	0
2	DSN	B	2[A]	-	3,5,6	1.26	0	3,5,7	0.94	0
2	DSN	B	2[B]	-	3,5,6	0.64	0	3,5,7	1.92	1 (33%)
2	DSN	B	20	2	3,5,6	0.78	0	3,5,7	0.68	0
2	MED	B	21[A]	-	5,7,8	2.67	1 (20%)	4,7,9	1.62	1 (25%)
2	MED	B	21[B]	-	5,7,8	1.59	1 (20%)	4,7,9	1.28	0
2	DLY	B	22	2	6,8,9	0.81	0	6,8,10	0.80	0
2	DTY	B	23[A]	-	10,12,13	1.02	0	13,15,17	1.28	1 (7%)
2	DTY	B	23[B]	-	10,12,13	1.22	2 (20%)	13,15,17	1.33	2 (15%)
2	DAR	B	24	2	5,10,11	0.89	0	5,11,13	1.04	1 (20%)
2	DLE	B	25	2	5,7,8	0.43	0	6,8,10	1.12	1 (16%)
2	DSN	B	26	2	3,5,6	1.09	0	3,5,7	1.76	1 (33%)
2	DPN	B	27	2	9,11,12	0.89	0	11,13,15	1.32	1 (9%)
2	DCY	B	28	2	3,5,6	0.73	0	3,5,7	0.98	0
2	DAR	B	29	2	5,10,11	0.86	0	5,11,13	0.88	0
2	DCY	B	3	2	3,5,6	1.29	1 (33%)	3,5,7	1.05	0
2	DLY	B	30[A]	-	6,8,9	0.63	0	6,8,10	0.70	0
2	DLY	B	30[B]	-	6,8,9	0.94	0	6,8,10	0.70	0
2	DTH	B	31	2	5,6,7	0.53	0	5,7,9	1.41	1 (20%)
2	DCY	B	32	2	3,5,6	1.19	0	3,5,7	1.63	1 (33%)
2	DTH	B	34	2	5,6,7	1.63	1 (20%)	5,7,9	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DCY	B	35	2	3,6,6	2.00	1 (33%)	2,7,7	0.14	0
2	DIL	B	4	2	6,7,8	0.44	0	7,8,10	1.89	3 (42%)
2	DAS	B	5	2	2,7,8	1.77	1 (50%)	2,8,10	1.44	0
2	DTH	B	6	2	5,6,7	0.86	0	5,7,9	1.49	2 (40%)
2	DIL	B	7	2	6,7,8	0.72	0	7,8,10	0.86	0
2	DPR	B	8	2	5,7,8	0.49	0	7,8,10	0.97	0
2	DLY	B	9[A]	-	6,8,9	0.70	0	6,8,10	1.85	3 (50%)
2	DLY	B	9[B]	-	6,8,9	1.39	1 (16%)	6,8,10	0.83	0

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
1	ALO	A	13	1	-	0/4/6/8	0/0/0/0
2	DAR	B	1	2	-	0/5/9/11	0/0/0/0
2	DSN	B	10	2	-	0/2/4/6	0/0/0/0
2	DAR	B	11	2	-	0/5/9/11	0/0/0/0
2	DCY	B	12	2	-	0/1/4/6	0/0/0/0
2	DTH	B	13	2	-	0/4/6/8	0/0/0/0
2	DAL	B	14	2	-	0/0/2/4	0/0/0/0
2	DPN	B	15	2	-	0/4/6/8	0/1/1/1
2	DGN	B	16	2	-	0/5/7/9	0/0/0/0
2	DCY	B	17	2	-	0/1/4/6	0/0/0/0
2	DLY	B	18	2	-	0/5/7/9	0/0/0/0
2	DHI	B	19[A]	-	-	0/4/6/8	0/1/1/1
2	DHI	B	19[B]	-	-	0/4/6/8	0/1/1/1
2	DSN	B	2[A]	-	-	0/2/4/6	0/0/0/0
2	DSN	B	2[B]	-	-	0/2/4/6	0/0/0/0
2	DSN	B	20	2	-	0/2/4/6	0/0/0/0
2	MED	B	21[A]	-	-	0/4/6/8	0/0/0/0
2	MED	B	21[B]	-	-	0/4/6/8	0/0/0/0
2	DLY	B	22	2	-	0/5/7/9	0/0/0/0
2	DTY	B	23[A]	-	-	0/4/6/8	0/1/1/1
2	DTY	B	23[B]	-	-	0/4/6/8	0/1/1/1
2	DAR	B	24	2	-	0/5/9/11	0/0/0/0
2	DLE	B	25	2	-	0/4/6/8	0/0/0/0
2	DSN	B	26	2	-	0/2/4/6	0/0/0/0
2	DPN	B	27	2	-	0/4/6/8	0/1/1/1
2	DCY	B	28	2	-	0/1/4/6	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DAR	B	29	2	-	0/5/9/11	0/0/0/0
2	DCY	B	3	2	-	0/1/4/6	0/0/0/0
2	DLY	B	30[A]	-	-	0/5/7/9	0/0/0/0
2	DLY	B	30[B]	-	-	0/5/7/9	0/0/0/0
2	DTH	B	31	2	-	0/4/6/8	0/0/0/0
2	DCY	B	32	2	-	0/1/4/6	0/0/0/0
2	DTH	B	34	2	-	0/4/6/8	0/0/0/0
2	DCY	B	35	2	-	0/2/6/6	0/0/0/0
2	DIL	B	4	2	-	0/6/8/10	0/0/0/0
2	DAS	B	5	2	-	0/2/6/8	0/0/0/0
2	DTH	B	6	2	-	0/4/6/8	0/0/0/0
2	DIL	B	7	2	-	0/6/8/10	0/0/0/0
2	DPR	B	8	2	-	0/0/9/11	0/1/1/1
2	DLY	B	9[A]	-	-	0/5/7/9	0/0/0/0
2	DLY	B	9[B]	-	-	0/5/7/9	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	21[A]	MED	CE-SD	-5.73	1.44	1.78
2	B	18	DLY	CB-CA	-3.53	1.48	1.53
2	B	35	DCY	CB-CA	-2.66	1.50	1.52
2	B	23[B]	DTY	CE2-CZ	-2.64	1.33	1.38
2	B	9[B]	DLY	CB-CA	-2.62	1.50	1.53
2	B	21[B]	MED	CB-CA	-2.47	1.50	1.53
2	B	5	DAS	CB-CA	-2.29	1.48	1.53
2	B	3	DCY	CB-SG	-2.23	1.76	1.81
2	B	1	DAR	CD-NE	-2.16	1.42	1.46
1	A	13	ALO	OG1-CB	-2.15	1.36	1.43
2	B	15	DPN	O-C	2.02	1.29	1.19
2	B	23[B]	DTY	CB-CG	2.03	1.56	1.51
2	B	34	DTH	CG2-CB	3.34	1.61	1.51
2	B	1	DAR	CB-CA	3.82	1.58	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	15	DPN	O-C-CA	-3.30	116.88	125.72
2	B	10	DSN	O-C-CA	-3.19	117.18	125.72
2	B	23[A]	DTY	CG-CB-CA	-2.90	107.44	114.12
2	B	27	DPN	O-C-CA	-2.67	118.58	125.72
2	B	25	DLE	O-C-CA	-2.66	118.58	125.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	23[B]	DTY	CD2-CG-CD1	-2.56	113.93	118.15
2	B	32	DCY	O-C-CA	-2.56	118.87	125.72
2	B	18	DLY	O-C-CA	-2.50	119.03	125.72
2	B	17	DCY	O-C-CA	-2.49	119.05	125.72
2	B	19[A]	DHI	O-C-CA	-2.36	119.40	125.72
2	B	24	DAR	O-C-CA	-2.30	119.55	125.72
2	B	23[B]	DTY	O-C-CA	-2.26	119.65	125.72
2	B	9[A]	DLY	O-C-CA	-2.23	119.73	125.72
2	B	26	DSN	O-C-CA	-2.22	119.76	125.72
2	B	21[A]	MED	CE-SD-CG	-2.22	92.66	100.36
2	B	9[A]	DLY	CG-CB-CA	-2.14	105.07	114.00
2	B	6	DTH	O-C-CA	-2.13	119.88	125.69
2	B	31	DTH	O-C-CA	-2.01	120.19	125.69
2	B	6	DTH	OG1-CB-CG2	2.05	115.66	109.56
2	B	15	DPN	CZ-CE1-CD1	2.06	123.07	120.20
2	B	4	DIL	CG1-CB-CA	2.06	116.89	111.23
2	B	18	DLY	CD-CG-CB	2.15	121.28	113.67
1	A	13	ALO	CG2-CB-CA	2.20	116.29	112.42
2	B	13	DTH	OG1-CB-CG2	2.35	116.54	109.56
2	B	4	DIL	CG2-CB-CA	2.43	117.72	111.12
2	B	1	DAR	CG-CD-NE	2.55	121.74	112.30
2	B	2[B]	DSN	CB-CA-N	2.84	116.40	109.79
2	B	9[A]	DLY	CB-CA-N	3.08	119.21	110.54
2	B	4	DIL	CG2-CB-CG1	3.61	121.01	111.81
2	B	1	DAR	CG-CB-CA	3.97	130.57	114.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	DAR	7	0
2	B	21[B]	MED	2	0
2	B	25	DLE	1	0
2	B	3	DCY	5	0
2	B	9[B]	DLY	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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
3	SO4	A	101	-	4,4,4	0.61	0	6,6,6	0.38	0
3	SO4	A	102	-	4,4,4	0.56	0	6,6,6	0.73	0
3	SO4	A	103	-	4,4,4	2.14	1 (25%)	6,6,6	1.26	2 (33%)
3	SO4	B	101	-	4,4,4	0.89	0	6,6,6	0.46	0
5	GOL	B	102	-	5,5,5	0.97	1 (20%)	5,5,5	1.06	0

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	SO4	A	101	-	-	0/0/0/0	0/0/0/0
3	SO4	A	102	-	-	0/0/0/0	0/0/0/0
3	SO4	A	103	-	-	0/0/0/0	0/0/0/0
3	SO4	B	101	-	-	0/0/0/0	0/0/0/0
5	GOL	B	102	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	103	SO4	O2-S	-3.63	1.34	1.47
5	B	102	GOL	O2-C2	2.02	1.49	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	103	SO4	O4-S-O3	-2.15	100.41	109.09
3	A	103	SO4	O2-S-O1	2.03	116.38	109.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	103	SO4	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(Å ²)	Q<0.9
1	A	34/35 (97%)	-0.34	0 100 100	4, 6, 11, 14	0
2	B	1/35 (2%)	-0.69	0 100 100	7, 7, 7, 7	0
All	All	35/70 (50%)	-0.35	0 100 100	4, 6, 11, 14	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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	DTH	B	13	7/8	0.99	0.05	-	6,6,9,10	0
2	DHI	B	19[A]	10/11	0.97	0.08	-	4,5,7,9	7
2	DAR	B	29	11/12	0.98	0.06	-	4,4,6,8	0
2	DLY	B	30[B]	9/10	0.99	0.05	-	3,4,8,10	6
2	DSN	B	10	6/7	0.99	0.04	-	5,6,7,8	0
2	DLY	B	22	9/10	0.98	0.07	-	3,3,8,11	0
2	DPN	B	15	11/12	0.97	0.07	-	5,7,8,8	0
2	DCY	B	28	6/7	1.00	0.03	-	3,3,4,4	0
2	DCY	B	32	6/7	1.00	0.03	-	4,5,6,8	0
2	DTY	B	23[A]	12/13	0.98	0.08	-	2,3,4,4	9
2	DCY	B	3	6/7	0.99	0.09	-	7,8,8,8	0
2	DPR	B	8	7/8	0.98	0.06	-	4,5,6,7	0
2	DTH	B	31	7/8	0.99	0.06	-	3,4,5,5	0
2	DTY	B	23[B]	12/13	0.98	0.08	-	3,4,6,6	9
2	DAR	B	24	11/12	0.98	0.06	-	3,4,7,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	DTH	B	6	7/8	0.99	0.04	-	3,3,5,7	0
2	DCY	B	35	7/7	0.98	0.10	-	7,8,9,11	0
2	MED	B	21[B]	8/9	0.98	0.07	-	3,4,8,16	5
2	DSN	B	26	6/7	0.99	0.05	-	4,4,5,6	0
2	MED	B	21[A]	8/9	0.98	0.07	-	3,4,7,19	5
2	DLY	B	18	9/10	0.97	0.07	-	5,7,12,14	0
2	DLY	B	9[B]	9/10	0.97	0.10	-	5,7,12,13	6
2	DAL	B	14	5/6	0.98	0.04	-	6,6,7,11	0
2	DTH	B	34	7/8	0.98	0.05	-	6,6,8,9	0
2	DLY	B	9[A]	9/10	0.97	0.10	-	5,6,14,18	6
2	DLE	B	25	8/9	0.99	0.05	-	3,4,5,6	0
1	ALO	A	13	7/8	0.98	0.06	-	5,6,14,14	0
2	DAS	B	5	8/9	0.99	0.05	-	4,4,5,5	0
2	DIL	B	7	8/9	0.99	0.06	-	3,4,5,6	0
2	DGN	B	16	9/10	0.99	0.05	-	4,5,5,6	0
2	DCY	B	12	6/7	1.00	0.03	-	4,5,5,7	0
2	DSN	B	20	6/7	0.99	0.05	-	3,3,4,4	0
2	DSN	B	2[A]	6/7	0.95	0.15	-	9,11,11,12	3
2	DIL	B	4	8/9	0.97	0.07	-	5,8,11,11	0
2	DCY	B	17	6/7	0.99	0.04	-	4,5,6,6	0
2	DAR	B	11	11/12	0.99	0.05	-	3,4,5,7	0
2	DAR	B	1	11/12	0.86	0.21	-	11,15,27,31	0
2	DSN	B	2[B]	6/7	0.95	0.15	-	9,12,15,18	3
2	DHI	B	19[B]	10/11	0.97	0.08	-	3,4,5,7	7
2	DPN	B	27	11/12	0.99	0.05	-	3,4,6,6	0
2	DLY	B	30[A]	9/10	0.99	0.05	-	3,4,6,7	6

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
5	GOL	B	102	6/6	0.93	0.17	2.54	9,10,13,13	0
3	SO4	A	102	5/5	0.99	0.08	0.92	11,13,16,17	0
3	SO4	A	103	5/5	0.98	0.10	0.71	18,19,28,38	0
3	SO4	A	101	5/5	1.00	0.03	-2.99	4,4,7,8	0
4	LI	A	104	1/1	0.98	0.15	-	7,7,7,7	0
3	SO4	B	101	5/5	1.00	0.03	-	4,4,5,6	0
4	LI	A	105	1/1	0.96	0.33	-	7,7,7,7	0
4	LI	B	103	1/1	0.94	0.31	-	8,8,8,8	0
4	LI	A	106	1/1	0.21	1.66	-	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.