WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2025 – 11:02 PM EDT

PDB ID : 4RY8 / pdb_00004ry8

Title : Crystal structure of 5-methylthioribose transporter solute binding protein TLET_1677 from Thermotoga lettingae TMO TARGET EFI-511109 in complex with 5-methylthioribose

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Deposited on : 2014-12-13

Resolution : 1.75 Å(reported)

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

|		
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance ⓘ

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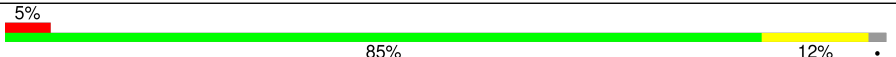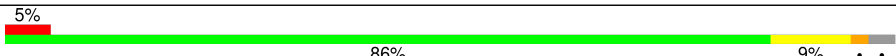*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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.
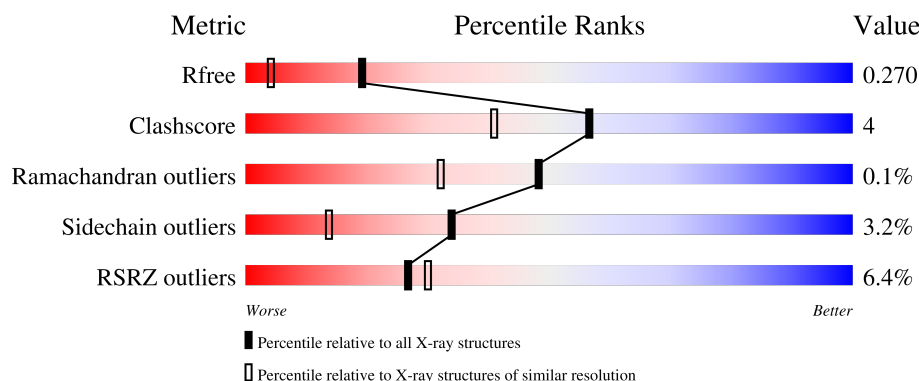
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	329	8% / 86% / 9% · ·
1	B	329	5% / 85% / 12% ·
1	C	329	5% / 86% / 9% · ·

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Mol	Chain	Length	Quality of chain
1	D	329	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 10412 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 Periplasmic binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	1	0
			2435	1551	418	453	13			
1	B	321	Total	C	N	O	S	0	1	0
			2501	1592	431	465	13			
1	C	319	Total	C	N	O	S	0	1	0
			2473	1579	424	457	13			
1	D	321	Total	C	N	O	S	0	0	0
			2483	1582	425	463	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	SER	-	expression tag	UNP A8F7U7
A	21	MET	-	expression tag	UNP A8F7U7
B	20	SER	-	expression tag	UNP A8F7U7
B	21	MET	-	expression tag	UNP A8F7U7
C	20	SER	-	expression tag	UNP A8F7U7
C	21	MET	-	expression tag	UNP A8F7U7
D	20	SER	-	expression tag	UNP A8F7U7
D	21	MET	-	expression tag	UNP A8F7U7

- Molecule 2 is 5-S-methyl-5-thio-alpha-D-ribofuranose (CCD ID: SR1) (formula: $C_6H_{12}O_4S$).
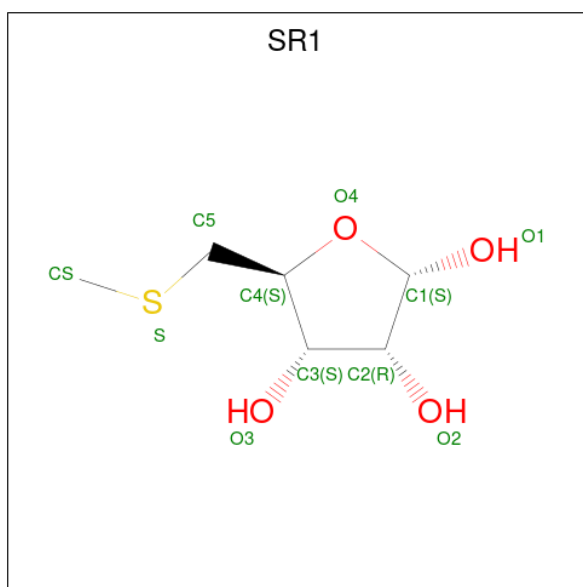
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 11	C 6	O 4	S 1	0	0
2	B	1	Total 11	C 6	O 4	S 1	0	0
2	C	1	Total 11	C 6	O 4	S 1	0	0
2	D	1	Total 11	C 6	O 4	S 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	113	Total 113	O 113	0	0
3	B	125	Total 125	O 125	0	0
3	C	121	Total 121	O 121	0	0
3	D	117	Total 117	O 117	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Periplasmic binding protein
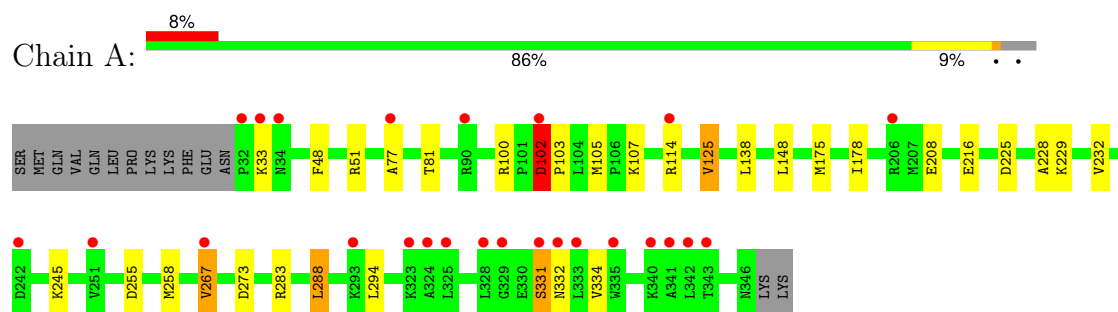
- Molecule 1: Periplasmic binding protein
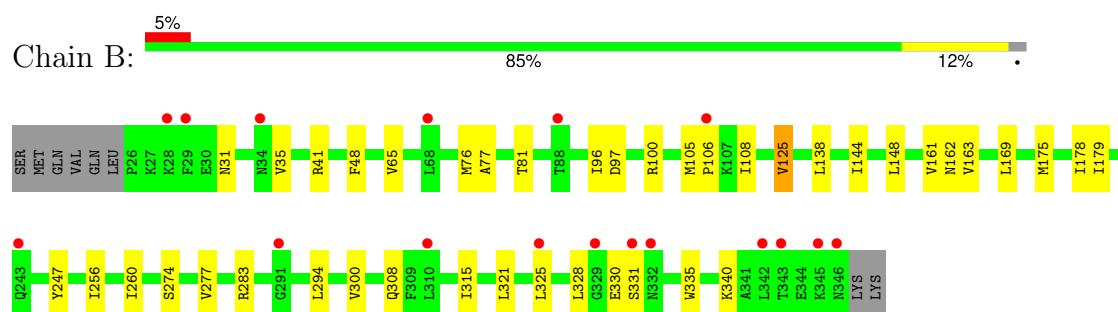
- Molecule 1: Periplasmic binding protein
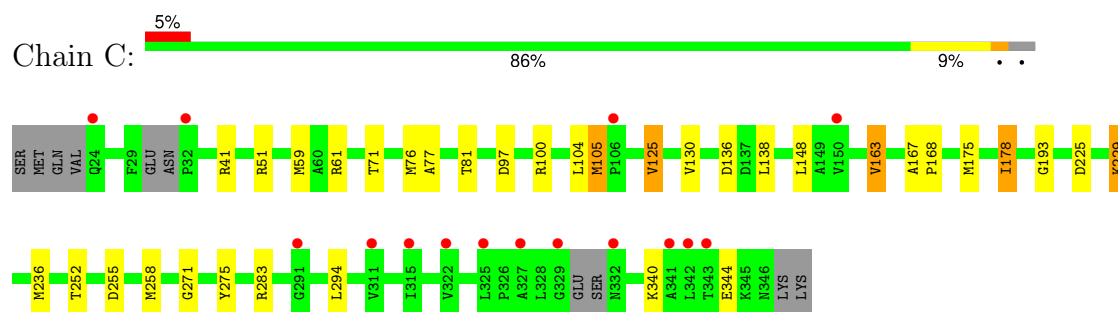
- Molecule 1: Periplasmic binding protein
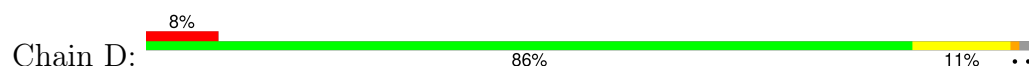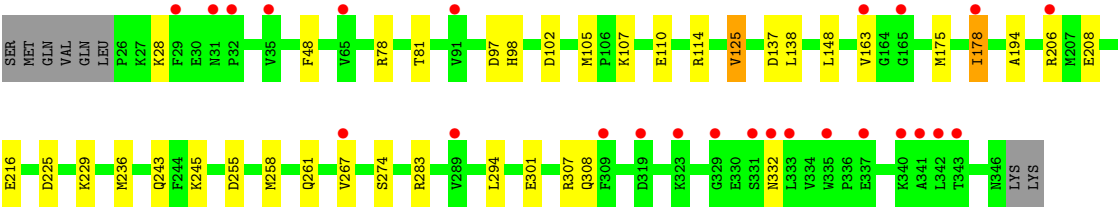
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	57.62Å 67.85Å 83.65Å 91.83° 92.39° 89.93°	Depositor
Resolution (Å)	50.00 – 1.75 50.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.0 (50.00-1.75) 96.9 (50.00-1.75)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.49 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.214 , 0.264 0.224 , 0.270	Depositor DCC
R_{free} test set	3773 reflections (3.05%)	wwPDB-VP
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	1.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.5	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.130 for -h,k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10412	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.61% 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: SR1

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	0.95	1/2480 (0.0%)	1.04	4/3364 (0.1%)
1	B	0.94	0/2548	1.04	4/3453 (0.1%)
1	C	0.92	0/2518	1.01	2/3412 (0.1%)
1	D	0.91	0/2527	1.01	1/3427 (0.0%)
All	All	0.93	1/10073 (0.0%)	1.03	11/13656 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	ASP	N-CA	-5.58	1.41	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	332	ASN	N-CA-C	7.22	119.15	111.28
1	A	331	SER	CA-C-N	6.25	128.65	120.28
1	A	331	SER	C-N-CA	6.25	128.65	120.28
1	A	267	VAL	CB-CA-C	-6.18	104.15	111.94
1	D	137	ASP	N-CA-C	5.48	118.01	111.71
1	C	271	GLY	N-CA-C	5.27	118.83	111.19
1	B	328	LEU	CA-C-N	5.22	125.06	120.10
1	B	328	LEU	C-N-CA	5.22	125.06	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	ASN	CA-C-N	5.17	125.47	119.47
1	B	31	ASN	C-N-CA	5.17	125.47	119.47
1	C	136	ASP	N-CA-C	-5.04	105.01	110.91

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	331	SER	Peptide

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	2435	0	2465	23	0
1	B	2501	0	2538	25	0
1	C	2473	0	2506	22	0
1	D	2483	0	2510	27	0
2	A	11	0	0	0	0
2	B	11	0	0	0	0
2	C	11	0	0	0	0
2	D	11	0	0	0	0
3	A	113	0	0	1	0
3	B	125	0	0	0	0
3	C	121	0	0	1	0
3	D	117	0	0	3	0
All	All	10412	0	10019	89	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 4.

All (89) 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:A:51[B]:ARG:HH21	1:A:51[B]:ARG:HG3	1.26	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:ILE:C	1:D:178:ILE:HD12	2.02	0.84
1:D:78:ARG:NH2	1:D:81:THR:OG1	2.23	0.71
1:A:51[B]:ARG:HH21	1:A:51[B]:ARG:CG	2.04	0.71
1:A:51[B]:ARG:HG3	1:A:51[B]:ARG:NH2	2.05	0.65
1:B:105:MET:HE1	1:B:125:VAL:HG23	1.81	0.63
1:A:229:LYS:HG2	1:A:258:MET:SD	2.40	0.60
1:C:229:LYS:HD2	1:C:258:MET:SD	2.42	0.60
1:A:148:LEU:HD23	1:A:148:LEU:C	2.27	0.59
1:B:283:ARG:HH11	1:B:283:ARG:HG3	1.67	0.59
1:A:105:MET:HE1	1:A:125:VAL:HB	1.87	0.57
1:D:148:LEU:C	1:D:148:LEU:HD23	2.30	0.56
1:B:178:ILE:HD11	1:D:178:ILE:CG2	2.35	0.56
1:A:178:ILE:HD11	1:C:178:ILE:HD13	1.87	0.55
1:C:236:MET:HE3	3:C:580:HOH:O	2.07	0.55
1:A:208:GLU:HG3	3:A:611:HOH:O	2.07	0.54
1:D:229:LYS:HD2	1:D:258:MET:SD	2.48	0.54
1:A:288:LEU:CD1	1:A:294:LEU:HD22	2.39	0.52
1:C:125:VAL:HG11	1:C:130:VAL:HG11	1.92	0.51
1:B:148:LEU:C	1:B:148:LEU:HD23	2.36	0.51
1:D:332:ASN:O	1:D:332:ASN:ND2	2.41	0.50
1:B:105:MET:HE1	1:B:125:VAL:CG2	2.41	0.50
1:C:77:ALA:O	1:C:81:THR:HG23	2.10	0.50
1:B:77:ALA:O	1:B:81:THR:HG23	2.11	0.50
1:A:51[B]:ARG:NH1	1:A:273:ASP:OD1	2.44	0.50
1:B:162:ASN:OD1	1:B:169:LEU:HB3	2.12	0.50
1:B:138:LEU:HB3	1:B:175:MET:HE2	1.94	0.49
1:C:167:ALA:HB3	1:C:168:PRO:CD	2.42	0.49
1:D:105:MET:HE1	1:D:125:VAL:HB	1.95	0.49
1:A:288:LEU:HD13	1:A:294:LEU:HD22	1.96	0.48
1:D:225:ASP:OD2	1:D:255:ASP:OD2	2.32	0.48
1:B:35:VAL:HB	1:B:65:VAL:HG12	1.96	0.48
1:C:41:ARG:HA	1:C:97:ASP:HB3	1.95	0.48
1:B:48:PHE:CE2	1:B:274:SER:HB3	2.50	0.47
1:B:178:ILE:CD1	1:D:178:ILE:HG21	2.44	0.47
1:A:245:LYS:HB3	1:A:267:VAL:HG21	1.95	0.47
1:C:148:LEU:C	1:C:148:LEU:HD23	2.39	0.47
1:D:225:ASP:O	1:D:229:LYS:HG3	2.15	0.47
1:D:110:GLU:O	1:D:114:ARG:HG2	2.15	0.47
1:D:178:ILE:C	1:D:178:ILE:CD1	2.77	0.47
1:B:138:LEU:HD13	1:D:178:ILE:HD11	1.97	0.47
1:C:76:MET:HG3	1:C:100:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:PHE:CE2	1:D:274:SER:HB3	2.49	0.47
1:A:77:ALA:O	1:A:81:THR:HG23	2.16	0.46
1:C:138:LEU:HB3	1:C:175:MET:HE2	1.98	0.46
1:C:105:MET:HE1	1:C:125:VAL:HG23	1.98	0.46
1:D:261:GLN:O	1:D:307:ARG:NH2	2.43	0.46
1:A:102:ASP:HB2	1:A:103:PRO:HD3	1.97	0.46
1:B:96:ILE:HD12	1:B:108:ILE:HG12	1.97	0.46
1:A:178:ILE:HD11	1:C:178:ILE:CD1	2.45	0.45
1:B:178:ILE:HD11	1:D:178:ILE:HG21	1.97	0.45
1:B:138:LEU:HD22	1:D:178:ILE:HD13	1.99	0.45
1:A:283:ARG:HD2	1:A:334:VAL:O	2.16	0.45
1:C:225:ASP:OD2	1:C:255:ASP:OD2	2.35	0.45
1:A:225:ASP:OD2	1:A:255:ASP:OD2	2.36	0.44
1:A:102:ASP:HB3	3:D:518:HOH:O	2.18	0.43
1:A:51[B]:ARG:CG	1:A:51[B]:ARG:NH2	2.67	0.43
1:C:76:MET:HE1	1:C:104:LEU:HD21	2.00	0.43
1:D:194:ALA:HB3	1:D:206:ARG:NH2	2.33	0.43
1:D:245:LYS:HD2	1:D:267:VAL:HG21	2.00	0.43
1:C:51[B]:ARG:HG2	1:C:275:TYR:HB2	2.00	0.43
1:B:41:ARG:HA	1:B:97:ASP:HB3	1.99	0.43
1:B:315:ILE:HD13	1:B:321:LEU:HA	2.01	0.43
1:C:252:THR:H	1:C:255:ASP:HB2	1.83	0.43
1:A:48:PHE:C	1:A:48:PHE:CD1	2.96	0.43
1:B:256:ILE:O	1:B:260:ILE:HG12	2.19	0.43
1:B:138:LEU:HD13	1:D:178:ILE:CD1	2.49	0.42
1:D:178:ILE:HD12	1:D:178:ILE:O	2.17	0.42
1:C:163:VAL:HG12	1:C:193:GLY:O	2.19	0.42
1:C:225:ASP:O	1:C:229:LYS:HG2	2.19	0.42
1:D:283:ARG:HH11	1:D:283:ARG:HG3	1.84	0.42
1:D:208:GLU:HG2	3:D:616:HOH:O	2.19	0.42
1:B:144:ILE:HD11	1:B:247:TYR:HB3	2.02	0.42
1:D:243:GLN:HB3	3:D:609:HOH:O	2.19	0.42
1:B:76:MET:HG3	1:B:100:ARG:HH21	1.85	0.42
1:D:138:LEU:HB3	1:D:175:MET:HE2	2.02	0.41
1:C:340:LYS:O	1:C:344:GLU:HG2	2.20	0.41
1:D:97:ASP:O	1:D:98:HIS:HB2	2.20	0.41
1:A:138:LEU:HB3	1:A:175:MET:HE2	2.01	0.41
1:B:335:TRP:HB3	1:B:340:LYS:HE3	2.01	0.41
1:C:41:ARG:HD3	1:C:71:THR:OG1	2.19	0.41
1:C:59:MET:SD	1:C:283:ARG:HG3	2.60	0.41
1:A:245:LYS:HD2	1:A:267:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:MET:HE1	1:D:261:GLN:OE1	2.21	0.41
1:B:283:ARG:HG3	1:B:283:ARG:NH1	2.34	0.41
1:C:167:ALA:HB3	1:C:168:PRO:HD3	2.01	0.41
1:A:228:ALA:O	1:A:232:VAL:HG23	2.21	0.41
1:B:105:MET:N	1:B:106:PRO:CD	2.85	0.40
1:B:277:VAL:HG22	1:B:300:VAL:HG21	2.03	0.40

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	314/329 (95%)	307 (98%)	7 (2%)	0	100	100
1	B	320/329 (97%)	313 (98%)	6 (2%)	1 (0%)	37	22
1	C	314/329 (95%)	308 (98%)	6 (2%)	0	100	100
1	D	319/329 (97%)	310 (97%)	9 (3%)	0	100	100
All	All	1267/1316 (96%)	1238 (98%)	28 (2%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	331	SER

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	254/272 (93%)	246 (97%)	8 (3%)	35	15
1	B	263/272 (97%)	255 (97%)	8 (3%)	36	15
1	C	258/272 (95%)	251 (97%)	7 (3%)	40	19
1	D	260/272 (96%)	250 (96%)	10 (4%)	28	10
All	All	1035/1088 (95%)	1002 (97%)	33 (3%)	34	14

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	100	ARG
1	A	102	ASP
1	A	107	LYS
1	A	114	ARG
1	A	125	VAL
1	A	216	GLU
1	A	288	LEU
1	B	125	VAL
1	B	161	VAL
1	B	163	VAL
1	B	179	ILE
1	B	294	LEU
1	B	308	GLN
1	B	325	LEU
1	B	330	GLU
1	C	61	ARG
1	C	105	MET
1	C	125	VAL
1	C	163	VAL
1	C	178	ILE
1	C	229	LYS
1	C	294	LEU
1	D	28	LYS
1	D	102	ASP
1	D	107	LYS
1	D	125	VAL
1	D	163	VAL
1	D	178	ILE
1	D	216	GLU
1	D	294	LEU

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Mol	Chain	Res	Type
1	D	301	GLU
1	D	308	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	73	HIS
1	A	85	ASN
1	A	157	ASN
1	B	34	ASN
1	B	73	HIS
1	B	85	ASN
1	B	157	ASN
1	B	262	GLN
1	C	34	ASN
1	C	85	ASN
1	C	155	ASN
1	C	157	ASN
1	C	261	GLN
1	D	34	ASN
1	D	85	ASN
1	D	157	ASN
1	D	303	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	#$|Z| > 2$
2	SR1	C	401	-	11,11,11	0.92	1 (9%)	14,15,15	1.63	4 (28%)
2	SR1	D	401	-	11,11,11	0.71	0	14,15,15	1.53	3 (21%)
2	SR1	B	401	-	11,11,11	0.80	0	14,15,15	1.85	1 (7%)
2	SR1	A	401	-	11,11,11	0.71	0	14,15,15	1.73	2 (14%)

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	SR1	C	401	-	-	0/3/19/19	0/1/1/1
2	SR1	D	401	-	-	0/3/19/19	0/1/1/1
2	SR1	B	401	-	-	0/3/19/19	0/1/1/1
2	SR1	A	401	-	-	0/3/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	SR1	O4-C4	-2.48	1.39	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	SR1	O1-C1-O4	-6.09	103.36	111.12
2	A	401	SR1	O1-C1-O4	-4.62	105.23	111.12
2	D	401	SR1	O1-C1-O4	-3.58	106.56	111.12
2	C	401	SR1	O4-C1-C2	3.44	109.44	104.67
2	C	401	SR1	O1-C1-O4	-3.01	107.29	111.12
2	C	401	SR1	C2-C3-C4	2.93	108.26	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	SR1	O4-C1-C2	2.65	108.35	104.67
2	D	401	SR1	C2-C3-C4	2.48	107.40	102.61
2	A	401	SR1	C1-C2-C3	2.17	104.96	102.29
2	C	401	SR1	O2-C2-C1	2.01	117.43	111.85

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 ⓘ

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	315/329 (95%)	0.81	25 (7%)	20	23	17, 30, 55, 84	1 (0%)
1	B	321/329 (97%)	0.78	17 (5%)	33	36	16, 30, 57, 85	1 (0%)
1	C	319/329 (96%)	0.79	15 (4%)	37	41	17, 30, 57, 87	1 (0%)
1	D	321/329 (97%)	0.83	25 (7%)	20	23	17, 30, 61, 82	0
All	All	1276/1316 (96%)	0.80	82 (6%)	27	30	16, 30, 59, 87	3 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	331	SER	5.5
1	D	329	GLY	4.6
1	C	332	ASN	4.6
1	D	341	ALA	4.5
1	D	331	SER	4.0
1	A	331	SER	3.9
1	A	343	THR	3.9
1	A	32	PRO	3.7
1	A	33	LYS	3.6
1	C	329	GLY	3.4
1	A	341	ALA	3.2
1	A	329	GLY	3.1
1	A	335	TRP	3.0
1	D	267	VAL	2.9
1	C	291	GLY	2.9
1	B	329	GLY	2.8
1	D	343	THR	2.8
1	A	325	LEU	2.8
1	D	163	VAL	2.8
1	A	77	ALA	2.8
1	A	333	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	342	LEU	2.7
1	C	327	ALA	2.6
1	B	332	ASN	2.6
1	C	32	PRO	2.6
1	A	323	LYS	2.6
1	C	322	VAL	2.6
1	C	24	GLN	2.6
1	D	65	VAL	2.5
1	A	342	LEU	2.5
1	C	342	LEU	2.5
1	A	324	ALA	2.5
1	B	343	THR	2.4
1	D	337	GLU	2.4
1	D	332	ASN	2.4
1	D	319	ASP	2.4
1	D	178	ILE	2.4
1	A	114	ARG	2.4
1	B	243	GLN	2.4
1	B	291	GLY	2.4
1	B	346	ASN	2.3
1	C	311	VAL	2.3
1	D	165	GLY	2.3
1	B	325	LEU	2.3
1	C	106	PRO	2.3
1	D	206	ARG	2.3
1	C	343	THR	2.3
1	A	34	ASN	2.3
1	A	340	LYS	2.3
1	D	323	LYS	2.3
1	A	328	LEU	2.3
1	B	310	LEU	2.3
1	C	325	LEU	2.3
1	C	315	ILE	2.2
1	A	102	ASP	2.2
1	C	341	ALA	2.2
1	B	68	LEU	2.2
1	D	335	TRP	2.2
1	D	309	PHE	2.2
1	A	267	VAL	2.2
1	B	345	LYS	2.1
1	B	29	PHE	2.1
1	B	88	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	31	ASN	2.1
1	D	333	LEU	2.1
1	D	29	PHE	2.1
1	D	289	VAL	2.1
1	D	342	LEU	2.1
1	A	90	ARG	2.1
1	D	340	LYS	2.1
1	A	251	VAL	2.1
1	C	150	VAL	2.1
1	D	91	VAL	2.1
1	A	206	ARG	2.0
1	B	106	PRO	2.0
1	D	32	PRO	2.0
1	D	35	VAL	2.0
1	A	293	LYS	2.0
1	B	28	LYS	2.0
1	A	242	ASP	2.0
1	A	332	ASN	2.0
1	B	34	ASN	2.0

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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	SR1	A	401	11/11	0.93	0.10	17,22,35,37	0
2	SR1	B	401	11/11	0.93	0.11	18,21,30,31	0
2	SR1	C	401	11/11	0.93	0.12	20,22,30,43	0
2	SR1	D	401	11/11	0.94	0.10	19,21,30,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.