



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:22 PM GMT

PDB ID : 4EO4
Title : Crystal structure of the yeast mitochondrial threonyl-tRNA synthetase (MST1) in complex with seryl sulfamoyl adenylate
Authors : Peterson, K.M.; Ling, J.; Simonovic, I.; Soll, D.; Simonovic, M.
Deposited on : 2012-04-13
Resolution : 2.87 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

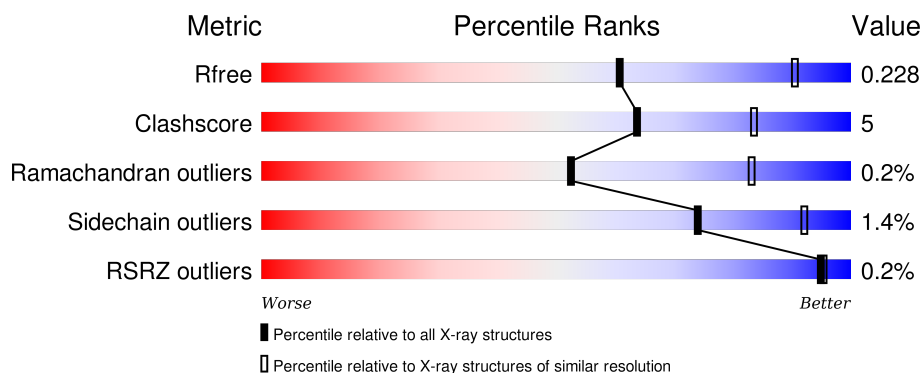
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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	460	 78% 12% 9%
1	B	460	 75% 14% 10%
1	C	460	 77% 13% 10%
1	D	460	 76% 13% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14113 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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	1	0
			3423	2214	577	615	17			
1	B	413	Total	C	N	O	S	0	2	0
			3377	2191	565	604	17			
1	C	416	Total	C	N	O	S	0	3	0
			3401	2200	568	616	17			
1	D	414	Total	C	N	O	S	3	1	0
			3335	2159	555	604	17			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	INITIATING METHIONINE	UNP P07236
A	4	GLY	-	EXPRESSION TAG	UNP P07236
A	5	SER	-	EXPRESSION TAG	UNP P07236
A	6	SER	-	EXPRESSION TAG	UNP P07236
A	7	HIS	-	EXPRESSION TAG	UNP P07236
A	8	HIS	-	EXPRESSION TAG	UNP P07236
A	9	HIS	-	EXPRESSION TAG	UNP P07236
A	10	HIS	-	EXPRESSION TAG	UNP P07236
A	11	HIS	-	EXPRESSION TAG	UNP P07236
A	12	HIS	-	EXPRESSION TAG	UNP P07236
A	13	SER	-	EXPRESSION TAG	UNP P07236
A	14	SER	-	EXPRESSION TAG	UNP P07236
A	15	GLY	-	EXPRESSION TAG	UNP P07236
A	16	LEU	-	EXPRESSION TAG	UNP P07236
A	17	VAL	-	EXPRESSION TAG	UNP P07236
A	18	PRO	-	EXPRESSION TAG	UNP P07236
A	19	ARG	-	EXPRESSION TAG	UNP P07236
A	20	GLY	-	EXPRESSION TAG	UNP P07236
A	21	SER	-	EXPRESSION TAG	UNP P07236
A	22	HIS	-	EXPRESSION TAG	UNP P07236
A	23	MET	-	INITIATING METHIONINE	UNP P07236

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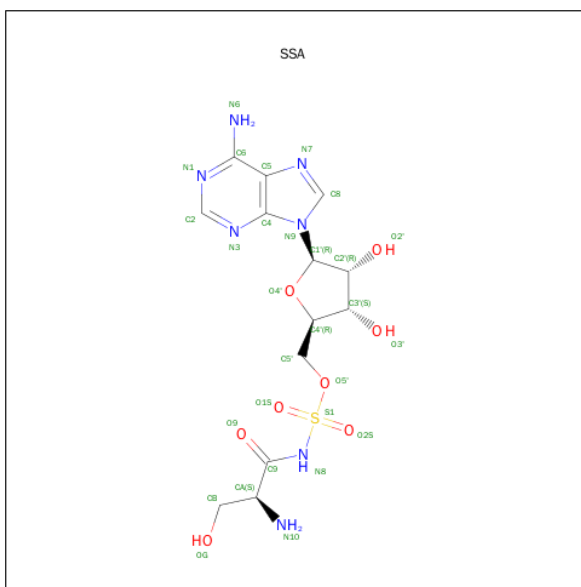
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ALA	-	EXPRESSION TAG	UNP P07236
A	25	SER	-	EXPRESSION TAG	UNP P07236
B	3	MET	-	EXPRESSION TAG	UNP P07236
B	4	GLY	-	EXPRESSION TAG	UNP P07236
B	5	SER	-	EXPRESSION TAG	UNP P07236
B	6	SER	-	EXPRESSION TAG	UNP P07236
B	7	HIS	-	EXPRESSION TAG	UNP P07236
B	8	HIS	-	EXPRESSION TAG	UNP P07236
B	9	HIS	-	EXPRESSION TAG	UNP P07236
B	10	HIS	-	EXPRESSION TAG	UNP P07236
B	11	HIS	-	EXPRESSION TAG	UNP P07236
B	12	HIS	-	EXPRESSION TAG	UNP P07236
B	13	SER	-	EXPRESSION TAG	UNP P07236
B	14	SER	-	EXPRESSION TAG	UNP P07236
B	15	GLY	-	EXPRESSION TAG	UNP P07236
B	16	LEU	-	EXPRESSION TAG	UNP P07236
B	17	VAL	-	EXPRESSION TAG	UNP P07236
B	18	PRO	-	EXPRESSION TAG	UNP P07236
B	19	ARG	-	EXPRESSION TAG	UNP P07236
B	20	GLY	-	EXPRESSION TAG	UNP P07236
B	21	SER	-	EXPRESSION TAG	UNP P07236
B	22	HIS	-	EXPRESSION TAG	UNP P07236
B	23	MET	-	EXPRESSION TAG	UNP P07236
B	24	ALA	-	EXPRESSION TAG	UNP P07236
B	25	SER	-	EXPRESSION TAG	UNP P07236
C	3	MET	-	INITIATING METHIONINE	UNP P07236
C	4	GLY	-	EXPRESSION TAG	UNP P07236
C	5	SER	-	EXPRESSION TAG	UNP P07236
C	6	SER	-	EXPRESSION TAG	UNP P07236
C	7	HIS	-	EXPRESSION TAG	UNP P07236
C	8	HIS	-	EXPRESSION TAG	UNP P07236
C	9	HIS	-	EXPRESSION TAG	UNP P07236
C	10	HIS	-	EXPRESSION TAG	UNP P07236
C	11	HIS	-	EXPRESSION TAG	UNP P07236
C	12	HIS	-	EXPRESSION TAG	UNP P07236
C	13	SER	-	EXPRESSION TAG	UNP P07236
C	14	SER	-	EXPRESSION TAG	UNP P07236
C	15	GLY	-	EXPRESSION TAG	UNP P07236
C	16	LEU	-	EXPRESSION TAG	UNP P07236
C	17	VAL	-	EXPRESSION TAG	UNP P07236
C	18	PRO	-	EXPRESSION TAG	UNP P07236
C	19	ARG	-	EXPRESSION TAG	UNP P07236

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	GLY	-	EXPRESSION TAG	UNP P07236
C	21	SER	-	EXPRESSION TAG	UNP P07236
C	22	HIS	-	EXPRESSION TAG	UNP P07236
C	23	MET	-	EXPRESSION TAG	UNP P07236
C	24	ALA	-	EXPRESSION TAG	UNP P07236
C	25	SER	-	EXPRESSION TAG	UNP P07236
D	3	MET	-	INITIATING METHIONINE	UNP P07236
D	4	GLY	-	EXPRESSION TAG	UNP P07236
D	5	SER	-	EXPRESSION TAG	UNP P07236
D	6	SER	-	EXPRESSION TAG	UNP P07236
D	7	HIS	-	EXPRESSION TAG	UNP P07236
D	8	HIS	-	EXPRESSION TAG	UNP P07236
D	9	HIS	-	EXPRESSION TAG	UNP P07236
D	10	HIS	-	EXPRESSION TAG	UNP P07236
D	11	HIS	-	EXPRESSION TAG	UNP P07236
D	12	HIS	-	EXPRESSION TAG	UNP P07236
D	13	SER	-	EXPRESSION TAG	UNP P07236
D	14	SER	-	EXPRESSION TAG	UNP P07236
D	15	GLY	-	EXPRESSION TAG	UNP P07236
D	16	LEU	-	EXPRESSION TAG	UNP P07236
D	17	VAL	-	EXPRESSION TAG	UNP P07236
D	18	PRO	-	EXPRESSION TAG	UNP P07236
D	19	ARG	-	EXPRESSION TAG	UNP P07236
D	20	GLY	-	EXPRESSION TAG	UNP P07236
D	21	SER	-	EXPRESSION TAG	UNP P07236
D	22	HIS	-	EXPRESSION TAG	UNP P07236
D	23	MET	-	EXPRESSION TAG	UNP P07236
D	24	ALA	-	EXPRESSION TAG	UNP P07236
D	25	SER	-	EXPRESSION TAG	UNP P07236

- Molecule 2 is 5'-O-(N-(L-SERYL)-SULFAMOYL)ADENOSINE (three-letter code: SSA) (formula: C₁₃H₁₉N₇O₈S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			29	13	7	8	1		
2	A	1	Total	C	N	O	S	0	0
			29	13	7	8	1		
2	B	1	Total	C	N	O	S	0	0
			29	13	7	8	1		
2	B	1	Total	C	N	O	S	0	0
			29	13	7	8	1		
2	C	1	Total	C	N	O	S	0	0
			29	13	7	8	1		
2	C	1	Total	C	N	O	S	0	0
			29	13	7	8	1		
2	D	1	Total	C	N	O	S	0	0
			29	13	7	8	1		
2	D	1	Total	C	N	O	S	0	0
			29	13	7	8	1		

- 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		

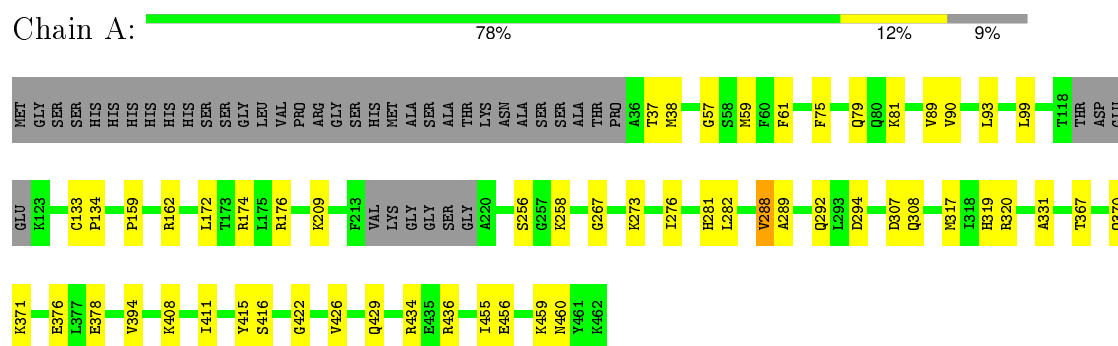
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total 121	O 121	0	0
4	B	96	Total 96	O 96	0	0
4	C	66	Total 66	O 66	0	0
4	D	58	Total 58	O 58	0	0

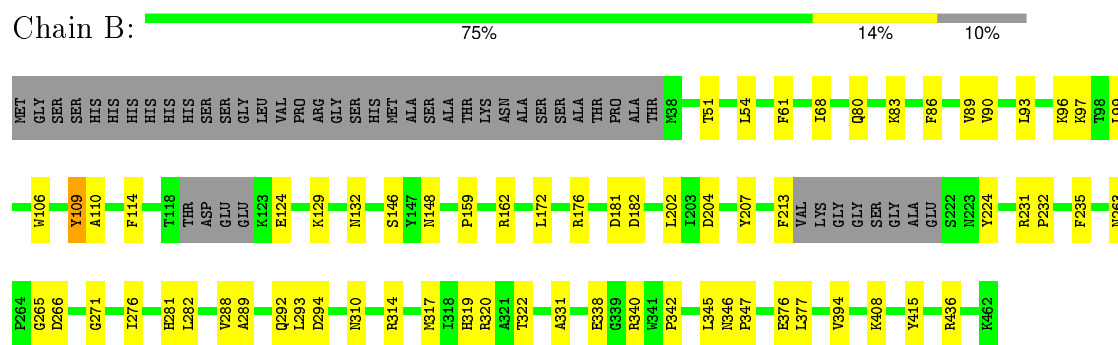
3 Residue-property plots

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.

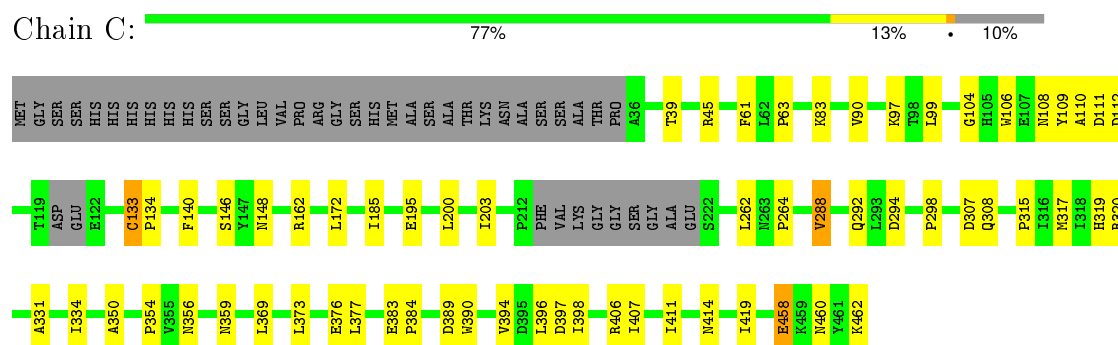
- Molecule 1: Threonine-tRNA ligase, mitochondrial



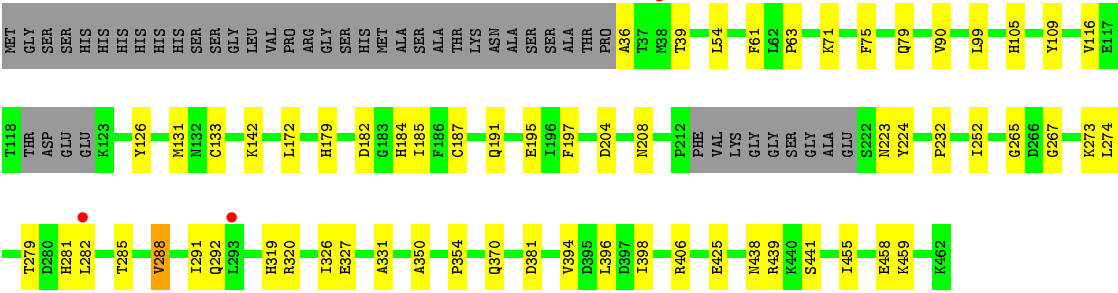
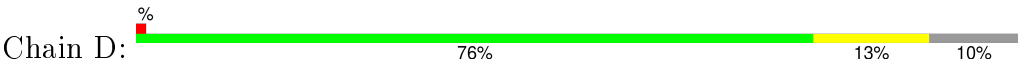
- Molecule 1: Threonine-tRNA ligase, mitochondrial



- Molecule 1: Threonine-tRNA ligase, mitochondrial



- Molecule 1: Threonine-tRNA ligase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	213.23 Å 107.50 Å 153.39 Å 90.00° 130.05° 90.00°	Depositor
Resolution (Å)	49.72 – 2.87 49.72 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.72-2.87) 98.9 (49.72-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.86 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.175 , 0.229 0.176 , 0.228	Depositor DCC
R_{free} test set	3053 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 60274 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14113	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, SSA

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	0.27	0/3516	0.43	1/4748 (0.0%)
1	B	0.26	0/3472	0.44	2/4692 (0.0%)
1	C	0.26	0/3496	0.42	0/4727
1	D	0.26	0/3427	0.43	0/4643
All	All	0.26	0/13911	0.43	3/18810 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	GLU	CB-CA-C	-10.41	89.58	110.40
1	A	376	GLU	CB-CA-C	-7.84	94.72	110.40
1	B	377	LEU	N-CA-C	5.52	125.91	111.00

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	3423	0	3338	34	0
1	B	3377	0	3293	40	0
1	C	3401	0	3287	37	0
1	D	3335	0	3180	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	58	0	38	4	0
2	B	58	0	38	1	0
2	C	58	0	37	1	0
2	D	58	0	38	3	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	121	0	0	4	0
4	B	96	0	0	2	0
4	C	66	0	0	0	0
4	D	58	0	0	0	0
All	All	14113	0	13249	141	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 5.

All (141) 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:36:ALA:N	1:D:39:THR:HG1	1.75	0.84
1:D:292:GLN:HB2	1:D:319:HIS:HB2	1.66	0.77
1:D:172:LEU:HB2	1:D:331:ALA:HB2	1.69	0.73
1:B:292:GLN:HE22	2:B:1001:SSA:HN8	1.39	0.71
1:B:83:LYS:NZ	1:D:381:ASP:OD1	2.26	0.68
1:D:116:VAL:HB	1:D:126:TYR:HB2	1.76	0.66
1:B:109:TYR:OH	1:B:162:ARG:HD3	1.97	0.65
1:D:279:THR:HG22	1:D:285:THR:HG22	1.80	0.64
1:B:232:PRO:HA	1:B:265:GLY:HA2	1.80	0.64
1:C:162:ARG:NH2	2:C:1001:SSA:O9	2.30	0.64
1:D:455:ILE:HG22	1:D:459:LYS:HE2	1.82	0.62
1:A:162:ARG:NH2	2:A:1001:SSA:O9	2.31	0.62
1:A:292:GLN:HB2	1:A:319:HIS:HB2	1.81	0.61
1:B:93:LEU:HD13	1:B:129:LYS:HE2	1.83	0.61
1:A:37:THR:OG1	1:A:38:MET:N	2.28	0.61
1:C:185:ILE:HG21	1:C:195:GLU:HG2	1.81	0.61
1:C:354:PRO:HD2	1:C:406:ARG:HH12	1.66	0.61
1:C:109:TYR:O	1:C:112:ASP:N	2.35	0.60
1:B:231:ARG:HD2	1:B:235:PHE:CZ	2.37	0.60
1:B:106:TRP:HA	1:B:110:ALA:HB2	1.84	0.59
1:B:51:THR:O	1:D:142:LYS:NZ	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ARG:NH2	1:C:414:ASN:OD1	2.31	0.59
1:B:90:VAL:HB	1:D:61:PHE:HB2	1.85	0.59
1:C:376:GLU:O	1:C:377:LEU:HD23	2.02	0.58
1:B:61:PHE:HB2	1:D:90:VAL:HB	1.84	0.58
1:B:281:HIS:CE1	1:B:282:LEU:HG	2.40	0.57
1:A:57:GLY:HA3	1:A:176:ARG:HG3	1.86	0.57
1:A:90:VAL:HB	1:C:61:PHE:HB2	1.87	0.57
1:B:172:LEU:HB2	1:B:331:ALA:HB2	1.87	0.57
1:C:104:GLY:O	1:C:108:ASN:ND2	2.31	0.56
1:B:294:ASP:HB3	1:B:317:MET:HB3	1.88	0.56
1:B:340:ARG:NH1	4:B:1187:HOH:O	2.30	0.55
1:A:307:ASP:OD1	1:A:308:GLN:N	2.34	0.55
1:D:274:LEU:HB2	1:D:291:ILE:HB	1.87	0.55
1:D:182:ASP:OD1	2:D:1001:SSA:OG	2.25	0.55
1:B:232:PRO:HG2	1:B:235:PHE:HB3	1.89	0.55
1:A:81:LYS:NZ	4:A:1119:HOH:O	2.40	0.55
1:B:54:LEU:HD13	1:D:99:LEU:HD12	1.89	0.55
1:D:71:LYS:NZ	1:D:458:GLU:OE1	2.37	0.54
1:B:114:PHE:HZ	1:B:176:ARG:HD3	1.72	0.54
1:C:172:LEU:HB2	1:C:331:ALA:HB2	1.88	0.54
1:A:294:ASP:HB3	1:A:317:MET:HB3	1.90	0.53
1:B:338:GLU:OE2	1:B:340:ARG:NH2	2.41	0.53
1:C:460:ASN:HB3	1:C:462:LYS:HG2	1.90	0.53
1:A:367:THR:HG22	1:A:371:LYS:HE2	1.90	0.53
1:D:354:PRO:O	1:D:406:ARG:NH2	2.42	0.52
1:C:185:ILE:HD13	1:C:195:GLU:HG3	1.92	0.52
1:A:408:LYS:NZ	4:A:1220:HOH:O	2.43	0.51
1:D:204:ASP:OD1	1:D:224:TYR:OH	2.26	0.51
1:C:356:ASN:HB3	1:C:359:ASN:HB2	1.92	0.51
1:D:396:LEU:HG	1:D:398:ILE:HG23	1.93	0.51
1:C:292:GLN:HB2	1:C:319:HIS:HB2	1.93	0.51
1:A:61:PHE:HB2	1:C:90:VAL:HB	1.93	0.51
1:C:294:ASP:HB3	1:C:317:MET:HB2	1.91	0.51
1:B:96:LYS:HE2	1:D:54:LEU:HA	1.92	0.50
1:C:298:PRO:HG3	1:C:317:MET:HG3	1.94	0.50
1:B:93:LEU:HD11	1:B:159:PRO:HG2	1.94	0.49
1:A:273:LYS:HG2	1:A:292:GLN:HG2	1.94	0.49
1:A:292:GLN:HE22	2:A:1001:SSA:HN8	1.59	0.49
1:D:292:GLN:HE22	2:D:1001:SSA:HN8	1.58	0.49
1:C:146:SER:OG	1:C:148:ASN:OD1	2.29	0.48
1:C:373:LEU:HD23	1:C:394:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ASN:ND2	1:D:223:ASN:OD1	2.47	0.48
1:A:172:LEU:HB2	1:A:331:ALA:HB2	1.95	0.48
1:A:93:LEU:HD21	1:A:159:PRO:HG2	1.95	0.48
1:B:292:GLN:HB2	1:B:319:HIS:HB2	1.95	0.48
1:B:263:ASN:ND2	1:B:266:ASP:OD2	2.47	0.48
1:A:426:VAL:O	1:A:429:GLN:NE2	2.39	0.48
1:B:68:ILE:HG23	1:B:345:LEU:HD22	1.96	0.48
1:D:204:ASP:O	1:D:208:ASN:HB2	2.13	0.47
1:A:455:ILE:HG22	1:A:459:LYS:HE2	1.96	0.47
1:D:438:ASN:HB3	1:D:441:SER:HB3	1.95	0.47
1:A:370:GLN:HG3	1:A:394:VAL:HG23	1.97	0.47
1:C:397:ASP:O	1:C:406:ARG:NH1	2.46	0.47
1:B:80:GLN:HB3	1:B:86:PHE:HB2	1.95	0.47
1:C:99:LEU:HD21	1:C:134:PRO:HB2	1.97	0.47
1:C:200:LEU:HD23	1:C:203:ILE:HD12	1.97	0.46
1:B:408:LYS:NZ	4:B:1195:HOH:O	2.38	0.46
1:A:411:ILE:HD13	2:A:1002:SSA:C5	2.45	0.46
1:C:133:CYS:SG	1:C:134:PRO:HD3	2.56	0.46
1:D:281:HIS:CE1	1:D:282:LEU:HG	2.51	0.46
1:A:99:LEU:HD21	1:A:134:PRO:HB2	1.98	0.45
1:A:378:GLU:O	1:C:83:LYS:NZ	2.42	0.45
1:A:434:ARG:HH22	2:A:1002:SSA:HN61	1.63	0.45
1:C:262:LEU:HG	1:C:264:PRO:HD3	1.99	0.45
1:D:425:GLU:N	1:D:425:GLU:OE1	2.48	0.45
1:B:204:ASP:OD1	1:B:224:TYR:OH	2.30	0.45
1:B:342:PRO:HG2	1:B:345:LEU:HB2	1.99	0.45
1:B:294:ASP:HB2	1:B:319:HIS:HE2	1.82	0.45
1:C:390:TRP:HZ3	1:C:458:GLU:HG2	1.82	0.45
1:D:232:PRO:HA	1:D:265:GLY:HA2	1.98	0.45
1:C:39:THR:HA	1:C:334:ILE:HG21	1.98	0.44
1:D:197:PHE:HE1	1:D:252:ILE:HG23	1.81	0.44
1:B:202:LEU:HG	1:B:322:THR:HG21	1.99	0.44
1:D:350:ALA:HB3	1:D:394:VAL:HG12	1.98	0.44
1:A:209:LYS:NZ	4:A:1135:HOH:O	2.50	0.44
1:B:415:TYR:O	1:B:436:ARG:HB2	2.18	0.44
1:C:97:LYS:HG3	1:C:106:TRP:CE2	2.53	0.44
1:B:97:LYS:HG3	1:B:106:TRP:CE2	2.53	0.44
1:B:276:ILE:HB	1:B:289:ALA:HB3	1.99	0.44
1:D:185:ILE:HG21	1:D:195:GLU:HG2	1.99	0.44
1:C:407:ILE:O	1:C:411:ILE:HG12	2.17	0.44
1:A:456:GLU:O	1:A:460:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:VAL:HG12	1:C:63:PRO:HD3	1.99	0.43
1:B:132:ASN:HB2	1:B:182:ASP:OD2	2.18	0.43
1:D:75:PHE:O	1:D:79:GLN:HG2	2.18	0.43
1:A:281:HIS:CE1	1:A:282:LEU:HG	2.53	0.43
1:D:327:GLU:OE1	1:D:327:GLU:N	2.45	0.43
1:C:369:LEU:HD21	1:C:419:ILE:HD13	2.00	0.43
1:C:109:TYR:O	1:C:111:ASP:N	2.51	0.43
1:D:179:HIS:O	1:D:326:ILE:HG12	2.18	0.43
1:C:39:THR:HG21	1:C:172:LEU:HD13	2.00	0.43
1:C:350:ALA:HB3	1:C:394:VAL:HG22	2.01	0.43
1:D:439:ARG:HH12	2:D:1002:SSA:H2'	1.84	0.43
1:A:267:GLY:HA2	1:A:273:LYS:HE2	2.01	0.42
1:B:181:ASP:N	1:B:181:ASP:OD1	2.52	0.42
1:A:75:PHE:O	1:A:79:GLN:HG2	2.19	0.42
1:C:307:ASP:OD1	1:C:308:GLN:N	2.41	0.42
1:A:422:GLY:O	1:A:426:VAL:HG23	2.20	0.42
1:D:187:CYS:HB2	1:D:191:GLN:HB2	2.01	0.42
1:C:396:LEU:HG	1:C:398:ILE:HG23	1.99	0.42
1:D:197:PHE:CE1	1:D:252:ILE:HG23	2.55	0.42
1:C:140:PHE:CE2	1:C:315:PRO:HG3	2.54	0.42
1:B:271:GLY:HA3	1:B:293:LEU:O	2.20	0.41
1:B:346:ASN:HA	1:B:347:PRO:HD2	1.93	0.41
1:D:274:LEU:HA	1:D:274:LEU:HD23	1.92	0.41
1:B:146:SER:OG	1:B:148:ASN:OD1	2.32	0.41
1:B:207:TYR:HD1	1:B:213:PHE:HE2	1.67	0.41
1:D:105:HIS:NE2	1:D:131:MET:SD	2.82	0.41
1:D:133:CYS:HA	1:D:184:HIS:NE2	2.36	0.41
1:D:370:GLN:HG3	1:D:394:VAL:HG23	2.03	0.41
1:D:267:GLY:HA2	1:D:273:LYS:HG3	2.03	0.41
1:B:89:VAL:HG12	1:D:63:PRO:HD3	2.03	0.41
1:A:256:SER:HB2	1:A:258:LYS:HG2	2.02	0.41
1:B:294:ASP:HB2	1:B:319:HIS:NE2	2.36	0.41
1:D:185:ILE:HD13	1:D:195:GLU:HG3	2.03	0.41
1:A:276:ILE:HB	1:A:289:ALA:HB3	2.01	0.41
1:C:383:GLU:HA	1:C:384:PRO:HD3	1.80	0.40
1:A:59:MET:SD	1:A:172:LEU:HG	2.61	0.40
1:A:174:ARG:NH2	4:A:1103:HOH:O	2.47	0.40
1:A:415:TYR:O	1:A:436:ARG:HB2	2.21	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	412/460 (90%)	400 (97%)	11 (3%)	1 (0%)	52	83
1	B	409/460 (89%)	401 (98%)	8 (2%)	0	100	100
1	C	413/460 (90%)	396 (96%)	15 (4%)	2 (0%)	34	69
1	D	409/460 (89%)	396 (97%)	12 (3%)	1 (0%)	52	83
All	All	1643/1840 (89%)	1593 (97%)	46 (3%)	4 (0%)	52	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	110	ALA
1	D	288	VAL
1	A	288	VAL
1	C	288	VAL

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	369/416 (89%)	365 (99%)	4 (1%)	80	94
1	B	363/416 (87%)	355 (98%)	8 (2%)	60	87
1	C	364/416 (88%)	359 (99%)	5 (1%)	74	92
1	D	351/416 (84%)	348 (99%)	3 (1%)	84	95
All	All	1447/1664 (87%)	1427 (99%)	20 (1%)	74	92

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	CYS
1	A	288	VAL
1	A	320	ARG
1	A	416	SER
1	B	99	LEU
1	B	109	TYR
1	B	124	GLU
1	B	288	VAL
1	B	310	ASN
1	B	314	ARG
1	B	320	ARG
1	B	394	VAL
1	C	133	CYS
1	C	288	VAL
1	C	320	ARG
1	C	389	ASP
1	C	458	GLU
1	D	109	TYR
1	D	288	VAL
1	D	320	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	SSA	A	1001	3	24,31,31	1.80	6 (25%)	29,46,46	3.75	9 (31%)
2	SSA	A	1002	-	24,31,31	1.88	6 (25%)	29,46,46	3.73	9 (31%)
2	SSA	B	1001	3	24,31,31	1.81	6 (25%)	29,46,46	3.78	9 (31%)
2	SSA	B	1002	-	24,31,31	1.84	7 (29%)	29,46,46	3.70	8 (27%)
2	SSA	C	1001	3	24,31,31	1.81	5 (20%)	29,46,46	3.92	10 (34%)
2	SSA	C	1002	-	24,31,31	1.86	6 (25%)	29,46,46	3.70	9 (31%)
2	SSA	D	1001	3	24,31,31	1.85	6 (25%)	29,46,46	3.92	8 (27%)
2	SSA	D	1002	-	24,31,31	1.86	6 (25%)	29,46,46	3.66	7 (24%)

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	SSA	A	1001	3	-	0/15/37/37	0/3/3/3
2	SSA	A	1002	-	-	0/15/37/37	0/3/3/3
2	SSA	B	1001	3	-	0/15/37/37	0/3/3/3
2	SSA	B	1002	-	-	0/15/37/37	0/3/3/3
2	SSA	C	1001	3	-	0/15/37/37	0/3/3/3
2	SSA	C	1002	-	-	0/15/37/37	0/3/3/3
2	SSA	D	1001	3	-	0/15/37/37	0/3/3/3
2	SSA	D	1002	-	-	0/15/37/37	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	SSA	CB-CA	-2.12	1.48	1.52
2	A	1001	SSA	CB-CA	-2.11	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	SSA	CB-CA	-2.09	1.48	1.52
2	D	1001	SSA	CB-CA	-2.09	1.48	1.52
2	B	1001	SSA	CB-CA	-2.07	1.48	1.52
2	B	1001	SSA	C4-N3	2.00	1.38	1.35
2	B	1002	SSA	O2S-S1	2.03	1.44	1.42
2	D	1001	SSA	C4-N3	2.07	1.38	1.35
2	C	1001	SSA	C2-N3	2.11	1.35	1.32
2	A	1001	SSA	O2S-S1	2.13	1.44	1.42
2	D	1001	SSA	C2-N3	2.16	1.36	1.32
2	A	1002	SSA	C4-N3	2.18	1.38	1.35
2	B	1001	SSA	C2-N3	2.18	1.36	1.32
2	D	1002	SSA	C4-N3	2.18	1.38	1.35
2	D	1002	SSA	O2S-S1	2.19	1.44	1.42
2	B	1002	SSA	C4-N3	2.19	1.38	1.35
2	A	1001	SSA	C2-N3	2.20	1.36	1.32
2	A	1002	SSA	O2S-S1	2.20	1.44	1.42
2	C	1002	SSA	C2-N3	2.21	1.36	1.32
2	C	1002	SSA	O2S-S1	2.23	1.44	1.42
2	A	1002	SSA	C2-N3	2.26	1.36	1.32
2	B	1002	SSA	C2-N3	2.29	1.36	1.32
2	C	1002	SSA	C4-N3	2.30	1.39	1.35
2	D	1002	SSA	C2-N3	2.31	1.36	1.32
2	B	1002	SSA	C6-N6	3.10	1.44	1.34
2	D	1002	SSA	C6-N6	3.12	1.44	1.34
2	C	1001	SSA	C6-N6	3.17	1.44	1.34
2	C	1002	SSA	C6-N6	3.17	1.44	1.34
2	A	1002	SSA	C6-N6	3.17	1.44	1.34
2	B	1001	SSA	C6-N6	3.18	1.44	1.34
2	A	1001	SSA	C6-N6	3.20	1.44	1.34
2	D	1001	SSA	C6-N6	3.20	1.44	1.34
2	A	1002	SSA	O1S-S1	3.31	1.45	1.42
2	B	1002	SSA	O1S-S1	3.43	1.45	1.42
2	D	1002	SSA	O1S-S1	3.64	1.45	1.42
2	A	1001	SSA	O1S-S1	3.70	1.45	1.42
2	C	1001	SSA	O1S-S1	3.72	1.45	1.42
2	C	1002	SSA	O1S-S1	3.77	1.45	1.42
2	B	1001	SSA	O1S-S1	3.79	1.45	1.42
2	D	1001	SSA	O1S-S1	3.80	1.45	1.42
2	A	1001	SSA	C9-N8	4.98	1.45	1.37
2	B	1001	SSA	C9-N8	5.12	1.45	1.37
2	C	1001	SSA	C9-N8	5.20	1.45	1.37
2	C	1002	SSA	C9-N8	5.22	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1002	SSA	C9-N8	5.38	1.46	1.37
2	D	1001	SSA	C9-N8	5.43	1.46	1.37
2	B	1002	SSA	C9-N8	5.43	1.46	1.37
2	A	1002	SSA	C9-N8	5.68	1.46	1.37

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	SSA	O2S-S1-O1S	-17.29	100.06	120.77
2	C	1001	SSA	O2S-S1-O1S	-16.70	100.77	120.77
2	A	1002	SSA	O2S-S1-O1S	-16.30	101.24	120.77
2	B	1001	SSA	O2S-S1-O1S	-16.28	101.26	120.77
2	B	1002	SSA	O2S-S1-O1S	-16.27	101.28	120.77
2	C	1002	SSA	O2S-S1-O1S	-16.16	101.41	120.77
2	A	1001	SSA	O2S-S1-O1S	-16.07	101.51	120.77
2	D	1002	SSA	O2S-S1-O1S	-16.04	101.55	120.77
2	C	1001	SSA	N3-C2-N1	-9.28	121.79	128.89
2	A	1002	SSA	N3-C2-N1	-9.22	121.83	128.89
2	C	1002	SSA	N3-C2-N1	-9.07	121.95	128.89
2	D	1001	SSA	N3-C2-N1	-8.93	122.06	128.89
2	B	1002	SSA	N3-C2-N1	-8.92	122.07	128.89
2	B	1001	SSA	N3-C2-N1	-8.85	122.12	128.89
2	D	1002	SSA	N3-C2-N1	-8.84	122.12	128.89
2	A	1001	SSA	N3-C2-N1	-8.81	122.14	128.89
2	A	1001	SSA	C9-N8-S1	-4.15	118.24	124.05
2	C	1001	SSA	C9-N8-S1	-3.59	119.03	124.05
2	C	1001	SSA	C1'-N9-C4	-3.30	121.97	126.94
2	D	1001	SSA	C1'-N9-C4	-3.28	121.99	126.94
2	B	1001	SSA	C1'-N9-C4	-3.19	122.13	126.94
2	A	1001	SSA	C1'-N9-C4	-3.08	122.30	126.94
2	B	1001	SSA	C9-N8-S1	-3.00	119.86	124.05
2	B	1002	SSA	C1'-N9-C4	-2.66	122.93	126.94
2	D	1001	SSA	C4-C5-N7	-2.42	107.25	109.48
2	C	1001	SSA	C4-C5-N7	-2.41	107.26	109.48
2	B	1001	SSA	C4-C5-N7	-2.40	107.27	109.48
2	A	1002	SSA	C1'-N9-C4	-2.38	123.34	126.94
2	D	1002	SSA	C1'-N9-C4	-2.34	123.41	126.94
2	C	1002	SSA	C1'-N9-C4	-2.26	123.53	126.94
2	B	1002	SSA	C4-C5-N7	-2.12	107.53	109.48
2	D	1002	SSA	C4-C5-N7	-2.08	107.56	109.48
2	A	1001	SSA	C4-C5-N7	-2.06	107.59	109.48
2	C	1002	SSA	C4-C5-N7	-2.05	107.59	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1002	SSA	C4-C5-N7	-2.01	107.63	109.48
2	C	1001	SSA	O5'-S1-O1S	2.03	111.96	105.66
2	C	1002	SSA	O5'-S1-O1S	2.03	111.96	105.66
2	D	1002	SSA	O5'-C5'-C4'	2.04	111.82	107.90
2	A	1001	SSA	O1S-S1-N8	2.05	111.24	108.50
2	B	1002	SSA	O5'-S1-O1S	2.07	112.09	105.66
2	A	1002	SSA	O5'-C5'-C4'	2.07	111.89	107.90
2	C	1002	SSA	O5'-C5'-C4'	2.08	111.91	107.90
2	A	1002	SSA	CA-C9-N8	2.10	119.09	114.85
2	C	1002	SSA	O1S-S1-N8	2.22	111.45	108.50
2	D	1001	SSA	O1S-S1-N8	2.23	111.47	108.50
2	A	1002	SSA	O1S-S1-N8	2.33	111.60	108.50
2	A	1001	SSA	O2S-S1-N8	2.41	111.71	108.50
2	B	1002	SSA	O1S-S1-N8	2.53	111.88	108.50
2	A	1001	SSA	OG-CB-CA	2.57	116.64	111.16
2	B	1002	SSA	OG-CB-CA	2.64	116.79	111.16
2	C	1002	SSA	O2S-S1-N8	2.68	112.08	108.50
2	C	1001	SSA	O2S-S1-N8	2.70	112.10	108.50
2	D	1001	SSA	CA-C9-N8	2.71	120.32	114.85
2	B	1001	SSA	O2S-S1-N8	2.73	112.14	108.50
2	B	1001	SSA	CA-C9-N8	2.75	120.39	114.85
2	A	1002	SSA	O2S-S1-N8	2.83	112.28	108.50
2	A	1002	SSA	OG-CB-CA	2.85	117.24	111.16
2	C	1001	SSA	OG-CB-CA	2.87	117.28	111.16
2	B	1001	SSA	O1S-S1-N8	2.87	112.33	108.50
2	B	1002	SSA	O2S-S1-N8	2.89	112.36	108.50
2	B	1001	SSA	OG-CB-CA	2.90	117.34	111.16
2	A	1001	SSA	CA-C9-N8	2.97	120.85	114.85
2	D	1001	SSA	OG-CB-CA	2.97	117.50	111.16
2	C	1001	SSA	O1S-S1-N8	3.00	112.51	108.50
2	D	1002	SSA	OG-CB-CA	3.21	118.01	111.16
2	C	1001	SSA	CA-C9-N8	3.26	121.42	114.85
2	D	1002	SSA	O2S-S1-N8	3.26	112.86	108.50
2	C	1002	SSA	OG-CB-CA	3.34	118.27	111.16
2	D	1001	SSA	O2S-S1-N8	3.43	113.07	108.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	SSA	2	0
2	A	1002	SSA	2	0
2	B	1001	SSA	1	0
2	C	1001	SSA	1	0
2	D	1001	SSA	2	0
2	D	1002	SSA	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 ⓘ

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	417/460 (90%)	-0.49	0	100 100	24, 39, 68, 98	0
1	B	413/460 (89%)	-0.34	0	100 100	28, 45, 79, 112	0
1	C	416/460 (90%)	-0.26	0	100 100	29, 54, 84, 102	0
1	D	414/460 (90%)	-0.18	3 (0%)	89 88	32, 58, 85, 110	0
All	All	1660/1840 (90%)	-0.32	3 (0%)	95 95	24, 50, 80, 112	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	38	MET	2.6
1	D	293	LEU	2.2
1	D	282	LEU	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
3	ZN	A	1003	1/1	0.99	0.16	0.62	36,36,36,36	0
2	SSA	C	1002	29/29	0.87	0.20	0.06	17,73,98,122	0
2	SSA	A	1001	29/29	0.98	0.16	-0.16	22,35,51,53	0
2	SSA	C	1001	29/29	0.97	0.16	-0.25	39,51,70,81	0
2	SSA	D	1002	29/29	0.89	0.21	-0.37	17,67,99,104	0
2	SSA	D	1001	29/29	0.96	0.16	-0.72	44,58,65,73	0
2	SSA	B	1002	29/29	0.92	0.14	-0.87	28,43,58,70	0
2	SSA	B	1001	29/29	0.98	0.15	-0.89	33,42,60,73	0
2	SSA	A	1002	29/29	0.94	0.14	-1.18	19,42,53,61	0
3	ZN	B	1003	1/1	0.98	0.16	-1.25	62,62,62,62	0
3	ZN	C	1003	1/1	0.88	0.12	-2.41	61,61,61,61	0
3	ZN	D	1003	1/1	0.84	0.12	-2.82	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.