



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:56 AM GMT

PDB ID : 2C2B
Title : CRYSTALLOGRAPHIC STRUCTURE OF ARABIDOPSIS THALIANA
THREONINE SYNTHASE COMPLEXED WITH PYRIDOXAL PHOS-
PHATE AND S-ADENOSYLMETHIONINE
Authors : Mas-Droux, C.; Biou, V.; Dumas, R.
Deposited on : 2005-09-27
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

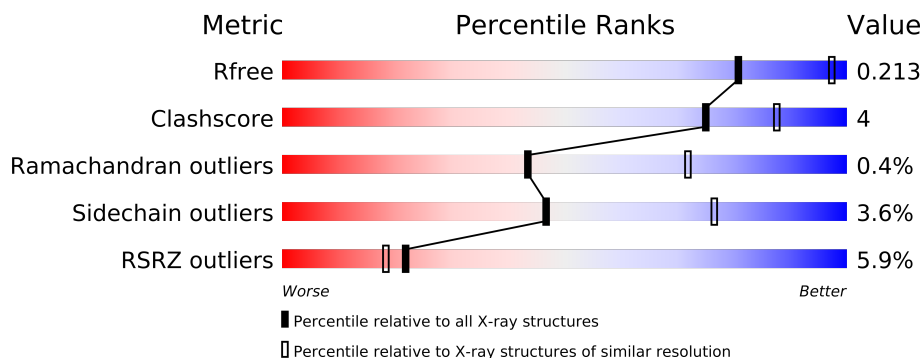
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	486	
1	B	486	
1	C	486	
1	D	486	
1	E	486	
1	F	486	

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	TRS	C	800	-	X

2 Entry composition i

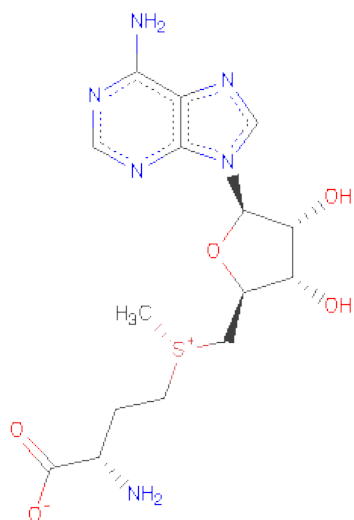
There are 4 unique types of molecules in this entry. The entry contains 20958 atoms, of which 0 are hydrogen and 0 are deuterium.

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 THREONINE SYNTHASE 1, CHLOROPLASTIC.

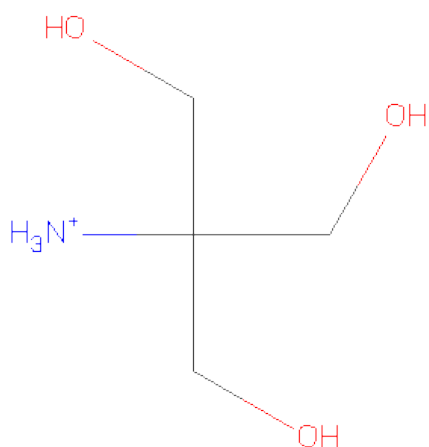
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	P	S	0	0	1
			3443	2197	577	645	1	23			
1	B	429	Total	C	N	O	P	S	0	0	1
			3320	2116	559	622	1	22			
1	C	444	Total	C	N	O	P	S	0	0	1
			3436	2192	576	644	1	23			
1	D	429	Total	C	N	O	P	S	0	0	1
			3320	2116	559	622	1	22			
1	E	431	Total	C	N	O	P	S	0	0	1
			3335	2124	562	626	1	22			
1	F	445	Total	C	N	O	P	S	0	0	1
			3443	2197	577	645	1	23			

- Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	E	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	E	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	F	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	F	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	C	1	Total	C	N	O	0	0
			8	4	1	3		
3	F	1	Total	C	N	O	0	0
			8	4	1	3		

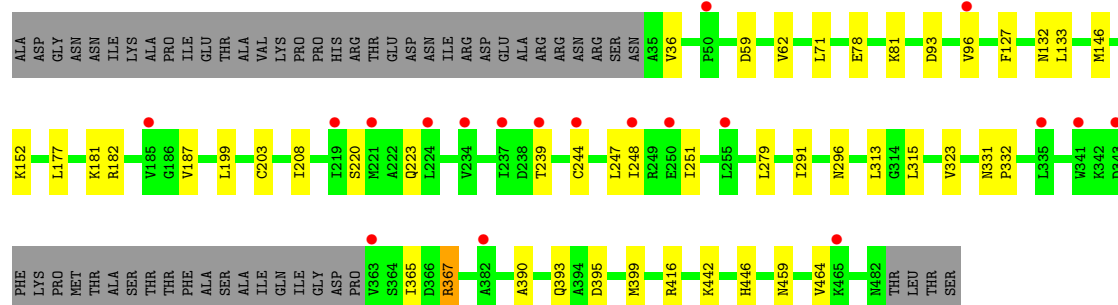
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	55	Total	O	0	0
			55	55		
4	C	52	Total	O	0	0
			52	52		
4	D	55	Total	O	0	0
			55	55		
4	E	44	Total	O	0	0
			44	44		
4	F	56	Total	O	0	0
			56	56		



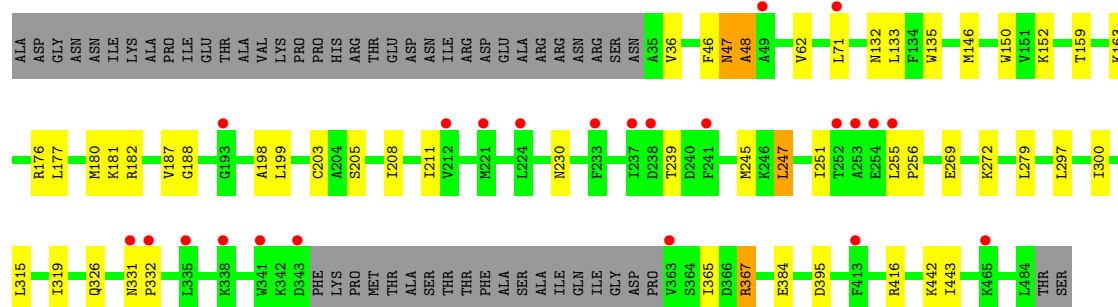
• Molecule 1: THREONINE SYNTHASE 1, CHLOROPLASTIC

Chain D:



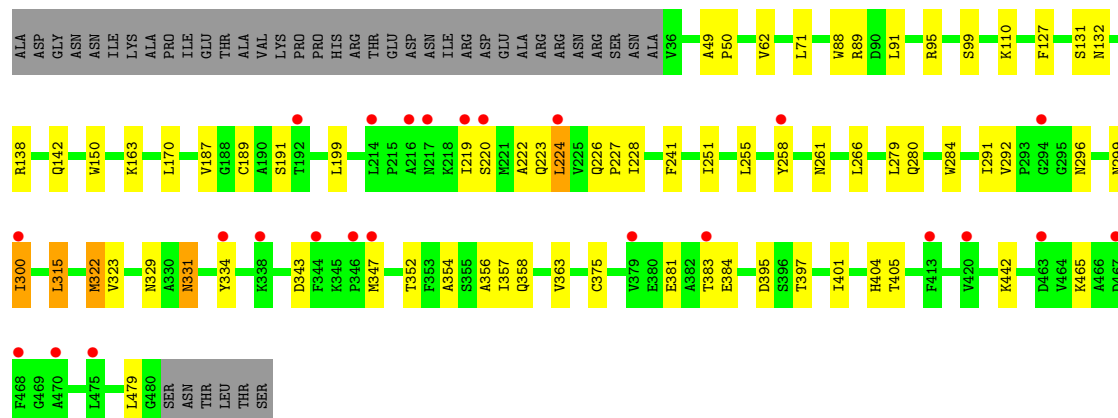
• Molecule 1: THREONINE SYNTHASE 1, CHLOROPLASTIC

Chain E:



• Molecule 1: THREONINE SYNTHASE 1, CHLOROPLASTIC

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	191.92Å 110.85Å 152.78Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	29.89 – 2.60 29.89 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.89-2.60) 99.6 (29.89-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.206 , 0.248 0.198 , 0.213	Depositor DCC
R_{free} test set	4904 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 20.1	EDS
Estimated twinning fraction	0.027 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.027 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.459 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.467 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.027 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 98158 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20958	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: TRS, LLP, SAM

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	0.34	1/3499 (0.0%)	0.47	0/4749
1	B	0.34	0/3371	0.47	0/4572
1	C	0.35	1/3492 (0.0%)	0.47	0/4739
1	D	0.34	0/3371	0.47	0/4572
1	E	0.34	0/3386	0.48	0/4593
1	F	0.35	1/3499 (0.0%)	0.48	0/4749
All	All	0.34	3/20618 (0.0%)	0.47	0/27974

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	479	LEU	C-N	-5.26	1.23	1.33
1	A	479	LEU	C-N	-5.24	1.23	1.33
1	C	479	LEU	C-N	-5.16	1.23	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3443	0	3390	23	0
1	B	3320	0	3265	20	0
1	C	3436	0	3381	27	0
1	D	3320	0	3265	26	0
1	E	3335	0	3278	32	0
1	F	3443	0	3390	38	0
2	A	54	0	44	1	0
2	B	54	0	44	0	0
2	C	54	0	44	2	0
2	D	54	0	44	1	0
2	E	54	0	44	5	0
2	F	54	0	44	7	0
3	A	8	0	12	0	0
3	C	8	0	12	0	0
3	F	8	0	12	0	0
4	A	51	0	0	0	0
4	B	55	0	0	1	0
4	C	52	0	0	0	0
4	D	55	0	0	1	0
4	E	44	0	0	0	0
4	F	56	0	0	0	0
All	All	20958	0	20269	164	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 4.

All (164) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:367:ARG:HH11	1:B:367:ARG:HG2	1.05	1.16
1:E:367:ARG:HH11	1:E:367:ARG:HG2	1.08	1.09
1:C:291:ILE:HG13	1:C:323:VAL:HB	1.57	0.85
1:B:367:ARG:HG2	1:B:367:ARG:NH1	1.85	0.84
1:E:367:ARG:HG2	1:E:367:ARG:NH1	1.88	0.83
2:F:500:SAM:H5'2	2:F:501:SAM:H2	1.61	0.82
1:E:150:TRP:CH2	2:F:500:SAM:HG2	2.14	0.81
1:B:367:ARG:HH11	1:B:367:ARG:CG	1.94	0.78
2:E:500:SAM:HG2	1:F:150:TRP:CH2	2.21	0.75
1:F:251:ILE:HG23	1:F:255:LEU:HD12	1.68	0.74
1:E:367:ARG:HH11	1:E:367:ARG:CG	1.96	0.73
1:F:219:ILE:HD11	1:F:223:GLN:HB2	1.70	0.72
1:B:46:PHE:O	1:B:47:ASN:HB2	1.90	0.72
1:F:331:ASN:HD22	1:F:331:ASN:H	1.38	0.72
1:C:331:ASN:H	1:C:331:ASN:HD22	1.37	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:195:THR:HG23	1:C:267:ARG:HH21	1.54	0.71
1:E:331:ASN:HB2	1:E:332:PRO:CD	2.20	0.71
1:D:331:ASN:HB2	1:D:332:PRO:CD	2.22	0.70
1:F:291:ILE:HG13	1:F:323:VAL:HB	1.73	0.70
1:A:331:ASN:H	1:A:331:ASN:HD22	1.38	0.70
1:C:251:ILE:HG23	1:C:255:LEU:HD12	1.75	0.68
1:D:446:HIS:HD2	1:D:459:ASN:H	1.38	0.68
1:D:367:ARG:HG2	1:D:367:ARG:HH11	1.57	0.68
1:E:46:PHE:O	1:E:47:ASN:HB2	1.92	0.68
1:A:251:ILE:HG23	1:A:255:LEU:HD12	1.75	0.68
1:A:131:SER:HB3	1:A:152:LYS:HE2	1.78	0.66
1:B:331:ASN:HB2	1:B:332:PRO:CD	2.25	0.66
1:A:291:ILE:HG13	1:A:323:VAL:HB	1.78	0.66
1:E:331:ASN:HB2	1:E:332:PRO:HD2	1.78	0.66
1:D:331:ASN:HB2	1:D:332:PRO:HD2	1.79	0.63
1:A:170:LEU:HD11	1:A:258:TYR:CE2	2.34	0.62
1:C:170:LEU:HD11	1:C:258:TYR:CE2	2.35	0.61
1:D:367:ARG:NH1	1:D:367:ARG:HG2	2.13	0.61
1:F:99:SER:HB2	2:F:500:SAM:HE3	1.82	0.61
1:B:331:ASN:HB2	1:B:332:PRO:HD2	1.86	0.58
1:E:443:ILE:HD11	1:F:222:ALA:HA	1.84	0.58
2:C:500:SAM:H8	1:D:132:ASN:HD21	1.71	0.56
1:C:386:GLU:HB3	1:C:410:THR:HG21	1.89	0.55
1:E:187:VAL:HG11	1:E:199:LEU:HD11	1.88	0.55
1:E:133:LEU:HD13	1:E:152:LYS:HD3	1.88	0.55
1:C:296:ASN:O	1:C:363:VAL:O	2.24	0.55
2:E:500:SAM:HG2	1:F:150:TRP:HH2	1.71	0.55
1:D:187:VAL:HG11	1:D:199:LEU:HD11	1.89	0.54
1:B:177:LEU:O	1:B:182:ARG:HB2	2.07	0.54
1:F:226:GLN:HB2	1:F:227:PRO:HD3	1.91	0.53
1:F:110:LYS:NZ	1:F:280:GLN:OE1	2.42	0.53
1:D:367:ARG:CG	1:D:367:ARG:HH11	2.21	0.53
2:E:500:SAM:H5'2	2:E:501:SAM:H2	1.92	0.52
1:F:356:ALA:H	1:F:404:HIS:HE1	1.58	0.52
1:B:187:VAL:HG11	1:B:199:LEU:HD11	1.92	0.52
1:E:135:TRP:CH2	2:F:501:SAM:HG2	2.45	0.51
1:E:163:LLP:O3	1:E:163:LLP:NZ	2.44	0.51
1:F:296:ASN:O	1:F:363:VAL:O	2.29	0.50
1:D:446:HIS:CD2	1:D:459:ASN:H	2.25	0.50
1:B:133:LEU:HD13	1:B:152:LYS:HD3	1.93	0.50
1:E:150:TRP:HH2	2:F:500:SAM:HG2	1.73	0.50
1:A:163:LLP:O3	1:A:163:LLP:NZ	2.44	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:354:ALA:O	1:F:357:ILE:HG22	2.11	0.49
1:A:214:LEU:HD22	1:A:219:ILE:HD11	1.94	0.49
1:C:356:ALA:H	1:C:404:HIS:HE1	1.60	0.49
1:A:397:THR:HG22	1:A:397:THR:O	2.13	0.49
1:E:132:ASN:ND2	2:F:500:SAM:H1'	2.27	0.49
1:A:356:ALA:H	1:A:404:HIS:HE1	1.60	0.49
1:D:244:CYS:O	1:D:248:ILE:HG12	2.13	0.49
1:F:49:ALA:HB1	1:F:50:PRO:HD2	1.96	0.48
1:C:163:LLP:NZ	1:C:163:LLP:O3	2.45	0.48
1:D:177:LEU:O	1:D:182:ARG:HB2	2.14	0.48
1:C:336:HIS:CD2	1:C:344:PHE:HB3	2.49	0.48
1:F:91:LEU:O	1:F:95:ARG:HG3	2.14	0.48
1:C:354:ALA:O	1:C:357:ILE:HG22	2.14	0.48
1:C:85:GLY:HA2	1:C:315:LEU:HD23	1.96	0.48
1:F:88:TRP:CB	1:F:315:LEU:HD11	2.44	0.48
1:C:88:TRP:HB2	1:C:315:LEU:CD2	2.44	0.48
1:F:331:ASN:HB2	1:F:334:TYR:HB3	1.95	0.47
1:C:88:TRP:HB2	1:C:315:LEU:HD21	1.97	0.47
1:C:190:ALA:HB3	1:C:245:MET:HE2	1.97	0.47
1:B:159:THR:HG21	1:B:198:ALA:HA	1.97	0.47
1:E:395:ASP:OD2	1:E:442:LYS:NZ	2.46	0.47
1:C:331:ASN:HB2	1:C:334:TYR:HB3	1.96	0.47
1:A:222:ALA:HA	1:B:443:ILE:HD11	1.97	0.47
1:E:205:SER:HA	1:F:397:THR:O	2.15	0.46
1:F:163:LLP:O3	1:F:163:LLP:NZ	2.48	0.46
2:A:500:SAM:H8	1:B:132:ASN:HD21	1.80	0.46
1:B:46:PHE:O	1:B:47:ASN:CB	2.62	0.46
1:F:170:LEU:HD11	1:F:258:TYR:CE2	2.51	0.46
1:C:91:LEU:O	1:C:95:ARG:HG3	2.15	0.46
1:A:331:ASN:HB2	1:A:334:TYR:HB3	1.97	0.46
1:E:247:LEU:O	1:E:251:ILE:HD12	2.15	0.45
1:E:132:ASN:HD21	2:F:500:SAM:H8	1.82	0.45
1:F:187:VAL:HG11	1:F:199:LEU:HD11	1.99	0.45
1:D:220:SER:HB3	1:D:223:GLN:HB2	1.98	0.45
1:F:138:ARG:O	1:F:142:GLN:HB2	2.17	0.45
1:F:401:ILE:HD13	1:F:405:THR:HB	1.99	0.45
1:C:132:ASN:HD21	2:D:500:SAM:H8	1.82	0.45
1:E:230:ASN:HA	1:F:395:ASP:O	2.16	0.45
1:D:247:LEU:O	1:D:251:ILE:HG12	2.17	0.45
1:A:226:GLN:HB2	1:A:227:PRO:HD3	1.98	0.45
1:A:352:THR:HG22	1:A:354:ALA:H	1.81	0.45
1:A:91:LEU:O	1:A:95:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:358:GLN:O	1:A:358:GLN:HG3	2.17	0.44
1:A:397:THR:CG2	1:A:397:THR:O	2.66	0.44
1:F:88:TRP:HB2	1:F:315:LEU:HD11	2.00	0.44
1:C:214:LEU:HD22	1:C:219:ILE:HD11	2.00	0.44
1:C:50:PRO:HG3	1:E:319:ILE:O	2.18	0.44
1:F:352:THR:HG22	1:F:354:ALA:H	1.82	0.44
1:E:188:GLY:HA2	1:E:211:ILE:O	2.18	0.44
1:F:322:MET:HB2	1:F:375:CYS:SG	2.58	0.44
1:E:177:LEU:O	1:E:182:ARG:HB2	2.17	0.44
1:D:395:ASP:OD2	1:D:442:LYS:NZ	2.49	0.43
1:E:297:LEU:HD21	1:E:326:GLN:NE2	2.33	0.43
1:A:137:GLU:HG3	1:A:141:LYS:HE2	1.99	0.43
1:E:269:GLU:O	1:E:272:LYS:HG2	2.18	0.43
1:D:203:CYS:HB3	1:D:208:ILE:O	2.18	0.43
1:B:391:MET:SD	1:B:442:LYS:NZ	2.86	0.43
1:D:291:ILE:HG12	1:D:323:VAL:HB	2.01	0.43
1:A:191:SER:HB3	1:A:195:THR:HB	2.00	0.43
1:E:159:THR:HG21	1:E:198:ALA:HA	2.00	0.43
1:F:261:ASN:HD22	1:F:261:ASN:HA	1.65	0.43
1:B:93:ASP:O	1:B:96:VAL:HG12	2.18	0.43
1:D:93:ASP:O	1:D:96:VAL:HG12	2.19	0.43
1:C:401:ILE:HD13	1:C:405:THR:HB	2.01	0.43
2:E:500:SAM:H8	1:F:132:ASN:HD21	1.84	0.42
2:E:500:SAM:HN1	2:E:501:SAM:H5'1	1.83	0.42
1:A:128:GLU:H	1:A:128:GLU:CD	2.23	0.42
1:B:296:ASN:ND2	4:B:2035:HOH:O	2.51	0.42
1:D:296:ASN:ND2	4:D:2038:HOH:O	2.52	0.42
1:C:85:GLY:HA3	1:C:314:GLY:O	2.19	0.42
1:D:395:ASP:HA	1:D:399:MET:O	2.19	0.42
1:F:191:SER:HA	1:F:241:PHE:HE1	1.85	0.42
1:F:138:ARG:HB3	1:F:397:THR:HG23	2.01	0.42
1:F:358:GLN:O	1:F:358:GLN:HG3	2.19	0.42
1:F:292:VAL:HB	1:F:300:ILE:HG12	2.01	0.42
1:D:390:ALA:HA	1:D:393:GLN:HE21	1.85	0.42
1:E:255:LEU:HA	1:E:256:PRO:HD3	1.93	0.42
1:F:331:ASN:N	1:F:331:ASN:HD22	2.08	0.41
1:E:176:ARG:O	1:E:180:MET:HG2	2.19	0.41
1:B:146:MET:SD	1:B:416:ARG:HD2	2.60	0.41
1:A:89:ARG:HD2	1:A:284:TRP:CD1	2.55	0.41
1:C:279:LEU:HD13	1:C:307:PHE:HE1	1.85	0.41
1:E:146:MET:SD	1:E:416:ARG:HD2	2.60	0.41
1:C:191:SER:HB3	1:C:195:THR:HB	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:59:ASP:HA	1:D:177:LEU:HD21	2.01	0.41
2:C:500:SAM:H8	1:D:132:ASN:ND2	2.35	0.41
1:D:81:LYS:HG3	1:D:313:LEU:HD23	2.01	0.41
1:E:47:ASN:HB3	1:E:48:ALA:H	1.58	0.41
1:B:135:TRP:HB2	1:B:150:TRP:CZ3	2.56	0.41
1:D:446:HIS:HD2	1:D:459:ASN:N	2.12	0.41
1:A:354:ALA:O	1:A:357:ILE:HG22	2.20	0.41
1:C:226:GLN:HB2	1:C:227:PRO:HD3	2.03	0.41
1:D:133:LEU:HD13	1:D:152:LYS:HD3	2.03	0.41
1:A:401:ILE:HD13	1:A:405:THR:HB	2.03	0.41
1:E:203:CYS:HB3	1:E:208:ILE:O	2.20	0.41
1:B:128:GLU:CD	1:B:128:GLU:H	2.24	0.41
1:F:89:ARG:HD2	1:F:284:TRP:CD1	2.56	0.41
1:C:203:CYS:HB3	1:C:208:ILE:O	2.21	0.41
1:F:329:ASN:HD21	1:F:384:GLU:HG3	1.86	0.41
1:E:135:TRP:HB2	1:E:150:TRP:CZ3	2.55	0.40
1:F:395:ASP:OD2	1:F:442:LYS:NZ	2.53	0.40
1:C:89:ARG:HD2	1:C:284:TRP:CD1	2.55	0.40
1:D:146:MET:SD	1:D:416:ARG:HD2	2.61	0.40
1:E:46:PHE:O	1:E:47:ASN:CB	2.67	0.40
1:F:224:LEU:O	1:F:228:ILE:HG12	2.21	0.40
1:A:178:ARG:HH11	1:A:208:ILE:HG12	1.86	0.40
1:B:188:GLY:HA2	1:B:211:ILE:O	2.22	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	442/486 (91%)	423 (96%)	18 (4%)	1 (0%)	56	82
1	B	424/486 (87%)	405 (96%)	17 (4%)	2 (0%)	38	67
1	C	441/486 (91%)	421 (96%)	18 (4%)	2 (0%)	38	67
1	D	424/486 (87%)	398 (94%)	25 (6%)	1 (0%)	56	82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	426/486 (88%)	399 (94%)	24 (6%)	3 (1%)	30	58
1	F	442/486 (91%)	419 (95%)	21 (5%)	2 (0%)	38	67
All	All	2599/2916 (89%)	2465 (95%)	123 (5%)	11 (0%)	43	72

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	47	ASN
1	E	47	ASN
1	A	220	SER
1	C	220	SER
1	F	220	SER
1	E	48	ALA
1	B	36	VAL
1	C	346	PRO
1	E	36	VAL
1	F	343	ASP
1	D	36	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	367/402 (91%)	353 (96%)	14 (4%)	44	74
1	B	353/402 (88%)	344 (98%)	9 (2%)	60	86
1	C	366/402 (91%)	352 (96%)	14 (4%)	44	74
1	D	353/402 (88%)	342 (97%)	11 (3%)	52	81
1	E	355/402 (88%)	343 (97%)	12 (3%)	49	78
1	F	367/402 (91%)	350 (95%)	17 (5%)	37	66
All	All	2161/2412 (90%)	2084 (96%)	77 (4%)	47	76

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	A	127	PHE
1	A	131	SER
1	A	144	LEU
1	A	218	LYS
1	A	224	LEU
1	A	239	THR
1	A	266	LEU
1	A	279	LEU
1	A	300	ILE
1	A	315	LEU
1	A	331	ASN
1	A	465	LYS
1	A	479	LEU
1	B	62	VAL
1	B	71	LEU
1	B	239	THR
1	B	247	LEU
1	B	315	LEU
1	B	365	ILE
1	B	367	ARG
1	B	384	GLU
1	B	465	LYS
1	C	62	VAL
1	C	71	LEU
1	C	127	PHE
1	C	224	LEU
1	C	239	THR
1	C	266	LEU
1	C	267	ARG
1	C	279	LEU
1	C	300	ILE
1	C	312	GLU
1	C	322	MET
1	C	331	ASN
1	C	342	LYS
1	C	465	LYS
1	D	62	VAL
1	D	71	LEU
1	D	78	GLU
1	D	127	PHE
1	D	181	LYS
1	D	239	THR

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Mol	Chain	Res	Type
1	D	279	LEU
1	D	315	LEU
1	D	365	ILE
1	D	367	ARG
1	D	464	VAL
1	E	62	VAL
1	E	71	LEU
1	E	181	LYS
1	E	239	THR
1	E	245	MET
1	E	247	LEU
1	E	279	LEU
1	E	300	ILE
1	E	315	LEU
1	E	365	ILE
1	E	367	ARG
1	E	384	GLU
1	F	62	VAL
1	F	71	LEU
1	F	127	PHE
1	F	131	SER
1	F	189	CYS
1	F	224	LEU
1	F	266	LEU
1	F	279	LEU
1	F	299	ASN
1	F	300	ILE
1	F	315	LEU
1	F	322	MET
1	F	331	ASN
1	F	347	MET
1	F	381	GLU
1	F	383	THR
1	F	465	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	226	GLN
1	A	230	ASN
1	A	261	ASN

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Mol	Chain	Res	Type
1	A	280	GLN
1	A	299	ASN
1	A	326	GLN
1	A	331	ASN
1	A	404	HIS
1	B	47	ASN
1	B	132	ASN
1	B	230	ASN
1	B	336	HIS
1	B	393	GLN
1	C	132	ASN
1	C	226	GLN
1	C	230	ASN
1	C	261	ASN
1	C	280	GLN
1	C	299	ASN
1	C	326	GLN
1	C	331	ASN
1	C	358	GLN
1	C	404	HIS
1	D	132	ASN
1	D	226	GLN
1	D	230	ASN
1	D	326	GLN
1	D	336	HIS
1	D	393	GLN
1	D	404	HIS
1	D	434	HIS
1	D	446	HIS
1	D	448	ASN
1	E	132	ASN
1	E	226	GLN
1	E	329	ASN
1	E	336	HIS
1	F	132	ASN
1	F	230	ASN
1	F	261	ASN
1	F	299	ASN
1	F	326	GLN
1	F	329	ASN
1	F	331	ASN
1	F	404	HIS

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$
1	LLP	A	163	1	24,24,25	4.02	5 (20%)	30,32,34	1.32	3 (10%)
1	LLP	B	163	1	24,24,25	4.02	5 (20%)	30,32,34	1.30	3 (10%)
1	LLP	C	163	1	24,24,25	4.01	5 (20%)	30,32,34	1.37	2 (6%)
1	LLP	D	163	1	24,24,25	4.07	5 (20%)	30,32,34	1.33	3 (10%)
1	LLP	E	163	1	24,24,25	4.07	5 (20%)	30,32,34	1.42	3 (10%)
1	LLP	F	163	1	24,24,25	3.93	5 (20%)	30,32,34	1.41	3 (10%)

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	LLP	A	163	1	-	0/15/17/19	0/1/1/1
1	LLP	B	163	1	-	0/15/17/19	0/1/1/1
1	LLP	C	163	1	-	0/15/17/19	0/1/1/1
1	LLP	D	163	1	-	0/15/17/19	0/1/1/1
1	LLP	E	163	1	-	0/15/17/19	0/1/1/1
1	LLP	F	163	1	-	0/15/17/19	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	163	LLP	O-C	18.27	1.24	1.11
1	D	163	LLP	O-C	18.24	1.24	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	LLP	O-C	18.03	1.23	1.11
1	B	163	LLP	O-C	18.00	1.23	1.11
1	C	163	LLP	O-C	17.93	1.23	1.11
1	F	163	LLP	O-C	17.54	1.23	1.11
1	A	163	LLP	O3-C3	-5.58	1.23	1.37
1	E	163	LLP	O3-C3	-5.55	1.23	1.37
1	C	163	LLP	O3-C3	-5.53	1.23	1.37
1	B	163	LLP	O3-C3	-5.52	1.23	1.37
1	D	163	LLP	O3-C3	-5.50	1.23	1.37
1	F	163	LLP	O3-C3	-5.45	1.23	1.37
1	C	163	LLP	CA-C	2.89	1.53	1.48
1	F	163	LLP	CA-C	2.80	1.53	1.48
1	E	163	LLP	CA-C	2.68	1.53	1.48
1	D	163	LLP	C2-N1	2.62	1.38	1.33
1	D	163	LLP	CA-C	2.61	1.53	1.48
1	E	163	LLP	C2-N1	2.59	1.38	1.33
1	B	163	LLP	C2-N1	2.56	1.38	1.33
1	A	163	LLP	CA-C	2.55	1.53	1.48
1	B	163	LLP	CA-C	2.49	1.52	1.48
1	E	163	LLP	C4'-NZ	-2.47	1.33	1.45
1	D	163	LLP	C4'-NZ	-2.46	1.33	1.45
1	B	163	LLP	C4'-NZ	-2.45	1.33	1.45
1	C	163	LLP	C2-N1	2.42	1.38	1.33
1	F	163	LLP	C2-N1	2.36	1.38	1.33
1	A	163	LLP	C2-N1	2.35	1.38	1.33
1	F	163	LLP	C4'-NZ	-2.35	1.33	1.45
1	C	163	LLP	C4'-NZ	-2.34	1.33	1.45
1	A	163	LLP	C4'-NZ	-2.33	1.33	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163	LLP	OP4-C5'-C5	5.56	120.57	109.26
1	F	163	LLP	OP4-C5'-C5	5.08	119.59	109.26
1	A	163	LLP	OP4-C5'-C5	4.90	119.23	109.26
1	E	163	LLP	OP4-C5'-C5	4.84	119.10	109.26
1	D	163	LLP	OP4-C5'-C5	4.41	118.22	109.26
1	B	163	LLP	OP4-C5'-C5	4.15	117.70	109.26
1	F	163	LLP	C6-C5-C4	2.90	120.31	118.10
1	A	163	LLP	C6-C5-C4	2.67	120.13	118.10
1	C	163	LLP	C6-C5-C4	2.37	119.90	118.10
1	E	163	LLP	C6-C5-C4	2.27	119.83	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	LLP	C5-C6-N1	-2.19	119.90	123.86
1	D	163	LLP	C5-C6-N1	-2.14	119.99	123.86
1	F	163	LLP	C5-C6-N1	-2.10	120.08	123.86
1	D	163	LLP	C6-C5-C4	2.09	119.69	118.10
1	B	163	LLP	C6-C5-C4	2.07	119.67	118.10
1	E	163	LLP	C5-C6-N1	-2.02	120.21	123.86
1	A	163	LLP	C5-C6-N1	-2.01	120.23	123.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

15 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	SAM	A	500	-	26,29,29	0.97	2 (7%)	38,42,42	2.23	7 (18%)
2	SAM	A	501	-	26,29,29	0.99	2 (7%)	38,42,42	2.12	5 (13%)
3	TRS	A	800	-	7,7,7	0.94	1 (14%)	9,9,9	0.24	0
2	SAM	B	500	-	26,29,29	0.97	2 (7%)	38,42,42	2.22	6 (15%)
2	SAM	B	501	-	26,29,29	0.99	2 (7%)	38,42,42	2.17	7 (18%)
2	SAM	C	500	-	26,29,29	0.97	2 (7%)	38,42,42	2.23	6 (15%)
2	SAM	C	501	-	26,29,29	0.99	2 (7%)	38,42,42	2.09	6 (15%)
3	TRS	C	800	-	7,7,7	0.93	1 (14%)	9,9,9	0.44	0
2	SAM	D	500	-	26,29,29	1.00	2 (7%)	38,42,42	2.33	8 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAM	D	501	-	26,29,29	1.00	2 (7%)	38,42,42	2.16	7 (18%)
2	SAM	E	500	-	26,29,29	0.97	2 (7%)	38,42,42	2.39	6 (15%)
2	SAM	E	501	-	26,29,29	0.99	2 (7%)	38,42,42	2.15	6 (15%)
2	SAM	F	500	-	26,29,29	0.97	2 (7%)	38,42,42	2.41	8 (21%)
2	SAM	F	501	-	26,29,29	0.98	2 (7%)	38,42,42	2.09	5 (13%)
3	TRS	F	800	-	7,7,7	0.89	1 (14%)	9,9,9	0.37	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
2	SAM	A	500	-	-	0/13/33/33	0/1/3/3
2	SAM	A	501	-	-	0/13/33/33	0/1/3/3
3	TRS	A	800	-	-	0/9/9/9	0/0/0/0
2	SAM	B	500	-	-	0/13/33/33	0/1/3/3
2	SAM	B	501	-	-	0/13/33/33	0/1/3/3
2	SAM	C	500	-	-	0/13/33/33	0/1/3/3
2	SAM	C	501	-	-	0/13/33/33	0/1/3/3
3	TRS	C	800	-	-	0/9/9/9	0/0/0/0
2	SAM	D	500	-	-	0/13/33/33	0/1/3/3
2	SAM	D	501	-	-	0/13/33/33	0/1/3/3
2	SAM	E	500	-	-	0/13/33/33	0/1/3/3
2	SAM	E	501	-	-	0/13/33/33	0/1/3/3
2	SAM	F	500	-	-	0/13/33/33	0/1/3/3
2	SAM	F	501	-	-	0/13/33/33	0/1/3/3
3	TRS	F	800	-	-	0/9/9/9	0/0/0/0

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	SAM	C2-N3	3.46	1.39	1.32
2	C	500	SAM	C2-N3	3.46	1.39	1.32
2	B	501	SAM	C2-N3	3.38	1.38	1.32
2	D	501	SAM	C2-N3	3.37	1.38	1.32
2	D	500	SAM	C2-N3	3.37	1.38	1.32
2	F	500	SAM	C2-N3	3.37	1.38	1.32
2	E	501	SAM	C2-N3	3.33	1.38	1.32
2	B	500	SAM	C2-N3	3.32	1.38	1.32
2	A	501	SAM	C2-N3	3.27	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	SAM	C2-N3	3.26	1.38	1.32
2	E	500	SAM	C2-N3	3.22	1.38	1.32
2	F	501	SAM	C2-N3	3.22	1.38	1.32
2	C	501	SAM	C2-N1	2.60	1.39	1.33
2	E	501	SAM	C2-N1	2.54	1.38	1.33
2	A	501	SAM	C2-N1	2.53	1.38	1.33
2	D	501	SAM	C2-N1	2.52	1.38	1.33
2	B	501	SAM	C2-N1	2.49	1.38	1.33
3	A	800	TRS	C-N	-2.43	1.47	1.50
2	F	501	SAM	C2-N1	2.40	1.38	1.33
2	B	500	SAM	C2-N1	2.38	1.38	1.33
3	C	800	TRS	C-N	-2.38	1.47	1.50
2	A	500	SAM	C2-N1	2.36	1.38	1.33
2	C	500	SAM	C2-N1	2.36	1.38	1.33
2	E	500	SAM	C2-N1	2.35	1.38	1.33
2	F	500	SAM	C2-N1	2.33	1.38	1.33
3	F	800	TRS	C-N	-2.29	1.47	1.50
2	D	500	SAM	C2-N1	2.28	1.38	1.33

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	SAM	N3-C2-N1	-10.96	119.54	128.71
2	E	500	SAM	N3-C2-N1	-10.96	119.54	128.71
2	F	500	SAM	N3-C2-N1	-10.81	119.67	128.71
2	C	500	SAM	N3-C2-N1	-10.73	119.74	128.71
2	B	500	SAM	N3-C2-N1	-10.67	119.79	128.71
2	A	500	SAM	N3-C2-N1	-10.64	119.81	128.71
2	A	501	SAM	N3-C2-N1	-10.42	120.00	128.71
2	E	501	SAM	N3-C2-N1	-10.38	120.03	128.71
2	B	501	SAM	N3-C2-N1	-10.33	120.08	128.71
2	D	501	SAM	N3-C2-N1	-10.31	120.09	128.71
2	F	501	SAM	N3-C2-N1	-10.19	120.19	128.71
2	C	501	SAM	N3-C2-N1	-10.12	120.25	128.71
2	F	500	SAM	CG-CB-CA	5.00	119.57	112.22
2	C	500	SAM	O4'-C1'-N9	4.63	112.75	108.44
2	A	500	SAM	O4'-C1'-N9	4.60	112.72	108.44
2	E	500	SAM	O4'-C1'-N9	4.52	112.64	108.44
2	B	500	SAM	N3-C4-N9	4.14	132.91	125.43
2	D	500	SAM	N3-C4-N9	4.13	132.89	125.43
2	E	500	SAM	N3-C4-N9	4.12	132.87	125.43
2	F	500	SAM	N3-C4-N9	4.10	132.84	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	SAM	N3-C4-N9	3.99	132.64	125.43
2	A	501	SAM	N3-C4-N9	3.96	132.58	125.43
2	D	500	SAM	CG-CB-CA	3.96	118.04	112.22
2	C	500	SAM	N3-C4-N9	3.95	132.56	125.43
2	C	501	SAM	N3-C4-N9	3.92	132.51	125.43
2	B	501	SAM	N3-C4-N9	3.85	132.39	125.43
2	D	501	SAM	N3-C4-N9	3.80	132.30	125.43
2	F	501	SAM	N3-C4-N9	3.80	132.30	125.43
2	E	501	SAM	N3-C4-N9	3.78	132.26	125.43
2	E	500	SAM	CG-CB-CA	3.77	117.76	112.22
2	B	500	SAM	O4'-C1'-N9	3.65	111.84	108.44
2	D	500	SAM	O4'-C1'-N9	3.37	111.58	108.44
2	F	500	SAM	O4'-C1'-N9	3.32	111.53	108.44
2	E	501	SAM	C3'-C2'-C1'	3.07	105.71	100.91
2	B	501	SAM	C3'-C2'-C1'	2.91	105.46	100.91
2	D	501	SAM	C3'-C2'-C1'	2.79	105.28	100.91
2	E	500	SAM	C5-C4-N3	-2.77	119.67	125.70
2	D	500	SAM	C5-C4-N3	-2.73	119.75	125.70
2	B	500	SAM	C5-C4-N3	-2.72	119.77	125.70
2	F	500	SAM	C5-C4-N3	-2.70	119.81	125.70
2	B	501	SAM	O4'-C1'-N9	2.63	110.89	108.44
2	B	501	SAM	C5-C4-N3	-2.61	120.02	125.70
2	F	501	SAM	C3'-C2'-C1'	2.61	104.99	100.91
2	E	500	SAM	C2-N3-C4	2.59	121.38	114.01
2	D	501	SAM	C5-C4-N3	-2.59	120.07	125.70
2	A	500	SAM	C5-C4-N3	-2.58	120.08	125.70
2	D	500	SAM	C2-N3-C4	2.57	121.32	114.01
2	C	501	SAM	C3'-C2'-C1'	2.54	104.88	100.91
2	C	500	SAM	C5-C4-N3	-2.53	120.20	125.70
2	C	501	SAM	C5-C4-N3	-2.52	120.21	125.70
2	E	501	SAM	C5-C4-N3	-2.52	120.21	125.70
2	A	501	SAM	C3'-C2'-C1'	2.51	104.84	100.91
2	A	501	SAM	C5-C4-N3	-2.50	120.26	125.70
2	F	501	SAM	C5-C4-N3	-2.49	120.28	125.70
2	C	501	SAM	CG-CB-CA	2.47	115.86	112.22
2	F	500	SAM	C2-N3-C4	2.47	121.03	114.01
2	B	500	SAM	C2-N3-C4	2.44	120.96	114.01
2	D	501	SAM	CG-CB-CA	2.41	115.77	112.22
2	D	501	SAM	O4'-C1'-N9	2.36	110.64	108.44
2	A	500	SAM	C2-N3-C4	2.34	120.67	114.01
2	C	500	SAM	C2-N3-C4	2.33	120.64	114.01
2	A	501	SAM	C2-N3-C4	2.28	120.51	114.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	SAM	C2-N3-C4	2.28	120.51	114.01
2	B	501	SAM	C2-N3-C4	2.27	120.47	114.01
2	E	501	SAM	C2-N3-C4	2.23	120.36	114.01
2	F	500	SAM	C3'-C2'-C1'	2.23	104.39	100.91
2	C	501	SAM	C2-N3-C4	2.22	120.33	114.01
2	F	500	SAM	C4-C5-N7	-2.21	107.62	109.52
2	F	501	SAM	C2-N3-C4	2.21	120.32	114.01
2	B	501	SAM	CG-CB-CA	2.21	115.47	112.22
2	D	500	SAM	C3'-C2'-C1'	2.07	104.15	100.91
2	B	500	SAM	C4-C5-N7	-2.06	107.76	109.52
2	A	500	SAM	C3'-C2'-C1'	2.04	104.10	100.91
2	C	500	SAM	C3'-C2'-C1'	2.04	104.10	100.91
2	D	500	SAM	N7-C8-N9	-2.03	108.61	114.36
2	E	501	SAM	C4'-O4'-C1'	2.03	111.95	109.75
2	A	500	SAM	C2'-C1'-N9	-2.02	108.08	113.27

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(Å ²)	Q<0.9
1	A	445/486 (91%)	0.66	36 (8%)	12 9	48, 58, 80, 94	0
1	B	429/486 (88%)	0.49	24 (5%)	24 20	51, 59, 77, 89	1 (0%)
1	C	444/486 (91%)	0.62	29 (6%)	18 15	48, 58, 79, 95	0
1	D	429/486 (88%)	0.47	19 (4%)	33 29	50, 59, 77, 89	1 (0%)
1	E	431/486 (88%)	0.45	23 (5%)	25 22	51, 59, 77, 91	1 (0%)
1	F	445/486 (91%)	0.61	24 (5%)	25 21	48, 58, 81, 94	0
All	All	2623/2916 (89%)	0.55	155 (5%)	22 18	48, 59, 79, 95	3 (0%)

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	237	ILE	5.6
1	A	387	LEU	5.5
1	D	465	LYS	4.6
1	A	334	TYR	4.5
1	A	466	ALA	4.5
1	E	238	ASP	4.5
1	C	221	MET	4.4
1	A	420	VAL	4.3
1	F	420	VAL	4.3
1	D	363	VAL	4.2
1	C	343	ASP	4.2
1	F	344	PHE	4.1
1	E	343	ASP	4.0
1	B	244	CYS	4.0
1	C	220	SER	3.8
1	F	470	ALA	3.8
1	F	294	GLY	3.8
1	D	237	ILE	3.8
1	A	214	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	255	LEU	3.7
1	E	241	PHE	3.7
1	B	253	ALA	3.6
1	A	220	SER	3.5
1	B	255	LEU	3.5
1	A	413	PHE	3.5
1	E	413	PHE	3.5
1	A	415	LEU	3.5
1	E	254	GLU	3.5
1	E	253	ALA	3.5
1	A	464	VAL	3.5
1	A	338	LYS	3.5
1	C	468	PHE	3.5
1	F	413	PHE	3.4
1	E	363	VAL	3.4
1	A	463	ASP	3.4
1	B	241	PHE	3.4
1	F	216	ALA	3.4
1	F	220	SER	3.3
1	F	463	ASP	3.3
1	C	344	PHE	3.2
1	B	329	ASN	3.2
1	B	252	THR	3.2
1	B	235	LEU	3.2
1	B	233	PHE	3.2
1	A	346	PRO	3.2
1	A	450	ILE	3.2
1	F	192	THR	3.1
1	D	343	ASP	3.1
1	D	335	LEU	3.1
1	F	468	PHE	3.1
1	A	221	MET	3.1
1	A	192	THR	3.0
1	A	224	LEU	3.0
1	C	217	ASN	3.0
1	C	323	VAL	3.0
1	E	338	LYS	3.0
1	E	224	LEU	3.0
1	C	454	ALA	3.0
1	F	338	LYS	3.0
1	A	468	PHE	2.9
1	C	413	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	337	TYR	2.9
1	A	216	ALA	2.9
1	A	237	ILE	2.8
1	F	346	PRO	2.8
1	C	317	ASP	2.8
1	B	237	ILE	2.8
1	D	219	ILE	2.8
1	B	465	LYS	2.8
1	D	50	PRO	2.8
1	A	462	VAL	2.8
1	B	185	VAL	2.7
1	D	185	VAL	2.7
1	C	409	LEU	2.6
1	C	466	ALA	2.6
1	F	217	ASN	2.6
1	E	255	LEU	2.6
1	A	344	PHE	2.6
1	B	413	PHE	2.6
1	E	233	PHE	2.6
1	A	449	ALA	2.6
1	C	214	LEU	2.5
1	E	221	MET	2.5
1	E	252	THR	2.5
1	E	465	LYS	2.5
1	E	212	VAL	2.5
1	E	335	LEU	2.5
1	C	378	ILE	2.5
1	F	383	THR	2.5
1	F	300	ILE	2.5
1	D	341	TRP	2.5
1	C	469	GLY	2.5
1	B	213	PHE	2.4
1	A	456	ARG	2.4
1	A	349	ALA	2.4
1	A	289	TRP	2.4
1	E	332	PRO	2.4
1	C	224	LEU	2.4
1	A	389	ASP	2.4
1	F	224	LEU	2.4
1	E	71	LEU	2.3
1	F	475	LEU	2.3
1	B	464	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	239	THR	2.3
1	A	325	ALA	2.3
1	B	219	ILE	2.3
1	C	219	ILE	2.3
1	B	343	ASP	2.3
1	F	214	LEU	2.3
1	D	244	CYS	2.3
1	A	311	GLN	2.3
1	A	465	LYS	2.3
1	B	249	ARG	2.3
1	A	136	ALA	2.3
1	D	234	VAL	2.2
1	D	248	ILE	2.2
1	F	258	TYR	2.2
1	F	334	TYR	2.2
1	A	475	LEU	2.2
1	F	347	MET	2.2
1	B	239	THR	2.2
1	A	217	ASN	2.2
1	C	467	ASP	2.2
1	A	411	ALA	2.2
1	A	313	LEU	2.2
1	C	334	TYR	2.2
1	C	333	LEU	2.2
1	C	353	PHE	2.2
1	D	382	ALA	2.2
1	C	347	MET	2.1
1	D	221	MET	2.1
1	C	335	LEU	2.1
1	E	193	GLY	2.1
1	C	379	VAL	2.1
1	A	219	ILE	2.1
1	C	237	ILE	2.1
1	B	254	GLU	2.1
1	E	341	TRP	2.1
1	B	36	VAL	2.1
1	C	357	ILE	2.1
1	F	219	ILE	2.1
1	E	331	ASN	2.1
1	B	332	PRO	2.1
1	C	462	VAL	2.1
1	D	96	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	450	ILE	2.1
1	C	415	LEU	2.1
1	D	250	GLU	2.1
1	B	341	TRP	2.1
1	D	224	LEU	2.1
1	E	49	ALA	2.0
1	F	467	ASP	2.0
1	A	453	MET	2.0
1	B	221	MET	2.0
1	F	379	VAL	2.0

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(Å ²)	Q<0.9
1	LLP	B	163	24/25	0.22	0.68	54,57,59,60	15
1	LLP	D	163	24/25	0.20	0.38	54,58,60,60	15
1	LLP	E	163	24/25	0.18	-0.18	54,58,60,61	15
1	LLP	C	163	24/25	0.17	-0.54	49,53,55,56	0
1	LLP	F	163	24/25	0.15	-1.11	48,54,56,57	0
1	LLP	A	163	24/25	0.14	-1.59	51,54,57,58	0

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	TRS	C	800	8/8	0.24	15.14	96,96,96,97	0
3	TRS	A	800	8/8	0.19	0.74	96,96,96,96	0
3	TRS	F	800	8/8	0.21	0.66	96,96,96,97	0
2	SAM	D	500	27/27	0.22	0.41	42,50,83,83	0
2	SAM	F	501	27/27	0.20	0.03	40,55,68,69	0
2	SAM	B	500	27/27	0.19	-0.10	47,55,75,76	0
2	SAM	C	500	27/27	0.19	-0.22	31,41,57,58	0
2	SAM	E	501	27/27	0.19	-0.54	52,63,81,81	0
2	SAM	D	501	27/27	0.18	-0.55	53,65,82,82	0
2	SAM	C	501	27/27	0.19	-0.58	49,58,65,65	0
2	SAM	E	500	27/27	0.18	-0.66	46,52,77,78	0
2	SAM	A	501	27/27	0.17	-0.79	45,56,68,68	0
2	SAM	B	501	27/27	0.18	-0.89	62,70,81,82	0
2	SAM	F	500	27/27	0.18	-1.16	36,43,64,65	0
2	SAM	A	500	27/27	0.15	-1.71	32,43,60,62	0

6.5 Other polymers ⓘ

There are no such residues in this entry.