



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 09:56 PM UTC

PDB ID : 9YBZ / pdb_00009ybz
Title : CRYSTAL STRUCTURE OF THE A149T VARIANT OF SERINE HYDROXYMETHYLTRANSFERASE 8 FROM SOYBEAN CULTIVAR ESSEX IN COMPLEX WITH PLP
Authors : Beamer, L.J.; Samarakoon, V.; Owuocha, L.F.
Deposited on : 2025-09-17
Resolution : 2.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

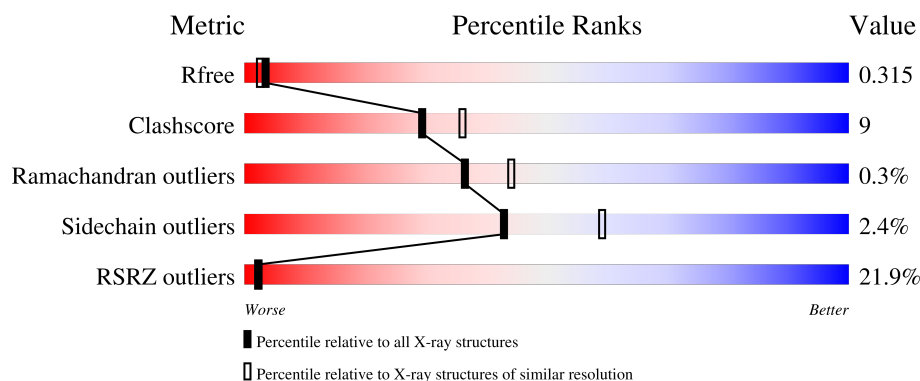
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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 $\leq 5\%$. 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	492	<div> <div>15%</div> <div>74%</div> <div>18%</div> <div>6%</div> </div>
1	B	492	<div> <div>10%</div> <div>75%</div> <div>17%</div> <div>7%</div> </div>
1	C	492	<div> <div>12%</div> <div>75%</div> <div>17%</div> <div>7%</div> </div>
1	D	492	<div> <div>13%</div> <div>76%</div> <div>18%</div> <div>6%</div> </div>
1	E	492	<div> <div>14%</div> <div>79%</div> <div>14%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	492	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (57%), green (74%), yellow (16%), and grey (9%). The segments are stacked horizontally, with the red segment starting from the left and ending at 57%, the green segment starting at 57% and ending at 74%, the yellow segment starting at 74% and ending at 16%, and the grey segment starting at 16% and ending at 9%.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20214 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 Serine hydroxymethyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	P	S	0	0	0
			3414	2159	588	649	1	17			
1	B	459	Total	C	N	O	P	S	0	0	0
			3409	2163	585	644	1	16			
1	C	460	Total	C	N	O	P	S	0	0	0
			3434	2180	584	652	1	17			
1	D	463	Total	C	N	O	P	S	0	0	0
			3419	2172	580	649	1	17			
1	E	461	Total	C	N	O	P	S	0	0	0
			3367	2137	578	635	1	16			
1	F	450	Total	C	N	O	P	S	0	0	0
			2972	1847	527	583	1	14			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP K4FZF8
A	-19	GLY	-	expression tag	UNP K4FZF8
A	-18	SER	-	expression tag	UNP K4FZF8
A	-17	SER	-	expression tag	UNP K4FZF8
A	-16	HIS	-	expression tag	UNP K4FZF8
A	-15	HIS	-	expression tag	UNP K4FZF8
A	-14	HIS	-	expression tag	UNP K4FZF8
A	-13	HIS	-	expression tag	UNP K4FZF8
A	-12	HIS	-	expression tag	UNP K4FZF8
A	-11	HIS	-	expression tag	UNP K4FZF8
A	-10	HIS	-	expression tag	UNP K4FZF8
A	-9	SER	-	expression tag	UNP K4FZF8
A	-8	SER	-	expression tag	UNP K4FZF8
A	-7	GLY	-	expression tag	UNP K4FZF8
A	-6	LEU	-	expression tag	UNP K4FZF8
A	-5	VAL	-	expression tag	UNP K4FZF8
A	-4	PRO	-	expression tag	UNP K4FZF8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ARG	-	expression tag	UNP K4FZF8
A	-2	GLY	-	expression tag	UNP K4FZF8
A	-1	SER	-	expression tag	UNP K4FZF8
A	0	ASN	-	expression tag	UNP K4FZF8
A	149	THR	ALA	engineered mutation	UNP K4FZF8
B	-20	MET	-	expression tag	UNP K4FZF8
B	-19	GLY	-	expression tag	UNP K4FZF8
B	-18	SER	-	expression tag	UNP K4FZF8
B	-17	SER	-	expression tag	UNP K4FZF8
B	-16	HIS	-	expression tag	UNP K4FZF8
B	-15	HIS	-	expression tag	UNP K4FZF8
B	-14	HIS	-	expression tag	UNP K4FZF8
B	-13	HIS	-	expression tag	UNP K4FZF8
B	-12	HIS	-	expression tag	UNP K4FZF8
B	-11	HIS	-	expression tag	UNP K4FZF8
B	-10	HIS	-	expression tag	UNP K4FZF8
B	-9	SER	-	expression tag	UNP K4FZF8
B	-8	SER	-	expression tag	UNP K4FZF8
B	-7	GLY	-	expression tag	UNP K4FZF8
B	-6	LEU	-	expression tag	UNP K4FZF8
B	-5	VAL	-	expression tag	UNP K4FZF8
B	-4	PRO	-	expression tag	UNP K4FZF8
B	-3	ARG	-	expression tag	UNP K4FZF8
B	-2	GLY	-	expression tag	UNP K4FZF8
B	-1	SER	-	expression tag	UNP K4FZF8
B	0	ASN	-	expression tag	UNP K4FZF8
B	149	THR	ALA	engineered mutation	UNP K4FZF8
C	-20	MET	-	expression tag	UNP K4FZF8
C	-19	GLY	-	expression tag	UNP K4FZF8
C	-18	SER	-	expression tag	UNP K4FZF8
C	-17	SER	-	expression tag	UNP K4FZF8
C	-16	HIS	-	expression tag	UNP K4FZF8
C	-15	HIS	-	expression tag	UNP K4FZF8
C	-14	HIS	-	expression tag	UNP K4FZF8
C	-13	HIS	-	expression tag	UNP K4FZF8
C	-12	HIS	-	expression tag	UNP K4FZF8
C	-11	HIS	-	expression tag	UNP K4FZF8
C	-10	HIS	-	expression tag	UNP K4FZF8
C	-9	SER	-	expression tag	UNP K4FZF8
C	-8	SER	-	expression tag	UNP K4FZF8
C	-7	GLY	-	expression tag	UNP K4FZF8
C	-6	LEU	-	expression tag	UNP K4FZF8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	VAL	-	expression tag	UNP K4FZF8
C	-4	PRO	-	expression tag	UNP K4FZF8
C	-3	ARG	-	expression tag	UNP K4FZF8
C	-2	GLY	-	expression tag	UNP K4FZF8
C	-1	SER	-	expression tag	UNP K4FZF8
C	0	ASN	-	expression tag	UNP K4FZF8
C	149	THR	ALA	engineered mutation	UNP K4FZF8
D	-20	MET	-	expression tag	UNP K4FZF8
D	-19	GLY	-	expression tag	UNP K4FZF8
D	-18	SER	-	expression tag	UNP K4FZF8
D	-17	SER	-	expression tag	UNP K4FZF8
D	-16	HIS	-	expression tag	UNP K4FZF8
D	-15	HIS	-	expression tag	UNP K4FZF8
D	-14	HIS	-	expression tag	UNP K4FZF8
D	-13	HIS	-	expression tag	UNP K4FZF8
D	-12	HIS	-	expression tag	UNP K4FZF8
D	-11	HIS	-	expression tag	UNP K4FZF8
D	-10	HIS	-	expression tag	UNP K4FZF8
D	-9	SER	-	expression tag	UNP K4FZF8
D	-8	SER	-	expression tag	UNP K4FZF8
D	-7	GLY	-	expression tag	UNP K4FZF8
D	-6	LEU	-	expression tag	UNP K4FZF8
D	-5	VAL	-	expression tag	UNP K4FZF8
D	-4	PRO	-	expression tag	UNP K4FZF8
D	-3	ARG	-	expression tag	UNP K4FZF8
D	-2	GLY	-	expression tag	UNP K4FZF8
D	-1	SER	-	expression tag	UNP K4FZF8
D	0	ASN	-	expression tag	UNP K4FZF8
D	149	THR	ALA	engineered mutation	UNP K4FZF8
E	-20	MET	-	expression tag	UNP K4FZF8
E	-19	GLY	-	expression tag	UNP K4FZF8
E	-18	SER	-	expression tag	UNP K4FZF8
E	-17	SER	-	expression tag	UNP K4FZF8
E	-16	HIS	-	expression tag	UNP K4FZF8
E	-15	HIS	-	expression tag	UNP K4FZF8
E	-14	HIS	-	expression tag	UNP K4FZF8
E	-13	HIS	-	expression tag	UNP K4FZF8
E	-12	HIS	-	expression tag	UNP K4FZF8
E	-11	HIS	-	expression tag	UNP K4FZF8
E	-10	HIS	-	expression tag	UNP K4FZF8
E	-9	SER	-	expression tag	UNP K4FZF8
E	-8	SER	-	expression tag	UNP K4FZF8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	GLY	-	expression tag	UNP K4FZF8
E	-6	LEU	-	expression tag	UNP K4FZF8
E	-5	VAL	-	expression tag	UNP K4FZF8
E	-4	PRO	-	expression tag	UNP K4FZF8
E	-3	ARG	-	expression tag	UNP K4FZF8
E	-2	GLY	-	expression tag	UNP K4FZF8
E	-1	SER	-	expression tag	UNP K4FZF8
E	0	ASN	-	expression tag	UNP K4FZF8
E	149	THR	ALA	engineered mutation	UNP K4FZF8
F	-20	MET	-	expression tag	UNP K4FZF8
F	-19	GLY	-	expression tag	UNP K4FZF8
F	-18	SER	-	expression tag	UNP K4FZF8
F	-17	SER	-	expression tag	UNP K4FZF8
F	-16	HIS	-	expression tag	UNP K4FZF8
F	-15	HIS	-	expression tag	UNP K4FZF8
F	-14	HIS	-	expression tag	UNP K4FZF8
F	-13	HIS	-	expression tag	UNP K4FZF8
F	-12	HIS	-	expression tag	UNP K4FZF8
F	-11	HIS	-	expression tag	UNP K4FZF8
F	-10	HIS	-	expression tag	UNP K4FZF8
F	-9	SER	-	expression tag	UNP K4FZF8
F	-8	SER	-	expression tag	UNP K4FZF8
F	-7	GLY	-	expression tag	UNP K4FZF8
F	-6	LEU	-	expression tag	UNP K4FZF8
F	-5	VAL	-	expression tag	UNP K4FZF8
F	-4	PRO	-	expression tag	UNP K4FZF8
F	-3	ARG	-	expression tag	UNP K4FZF8
F	-2	GLY	-	expression tag	UNP K4FZF8
F	-1	SER	-	expression tag	UNP K4FZF8
F	0	ASN	-	expression tag	UNP K4FZF8
F	149	THR	ALA	engineered mutation	UNP K4FZF8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	34	Total O 34 34	0	0
2	B	44	Total O 44 44	0	0
2	C	32	Total O 32 32	0	0
2	D	51	Total O 51 51	0	0

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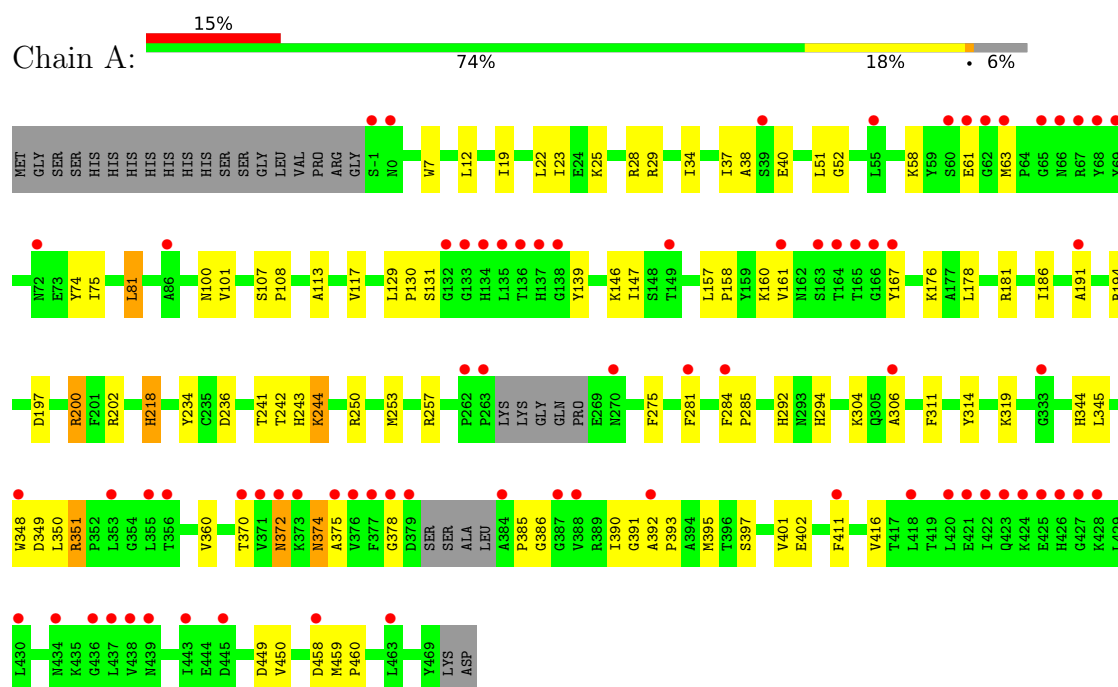
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	32	Total 32	O 32	0	0
2	F	6	Total 6	O 6	0	0

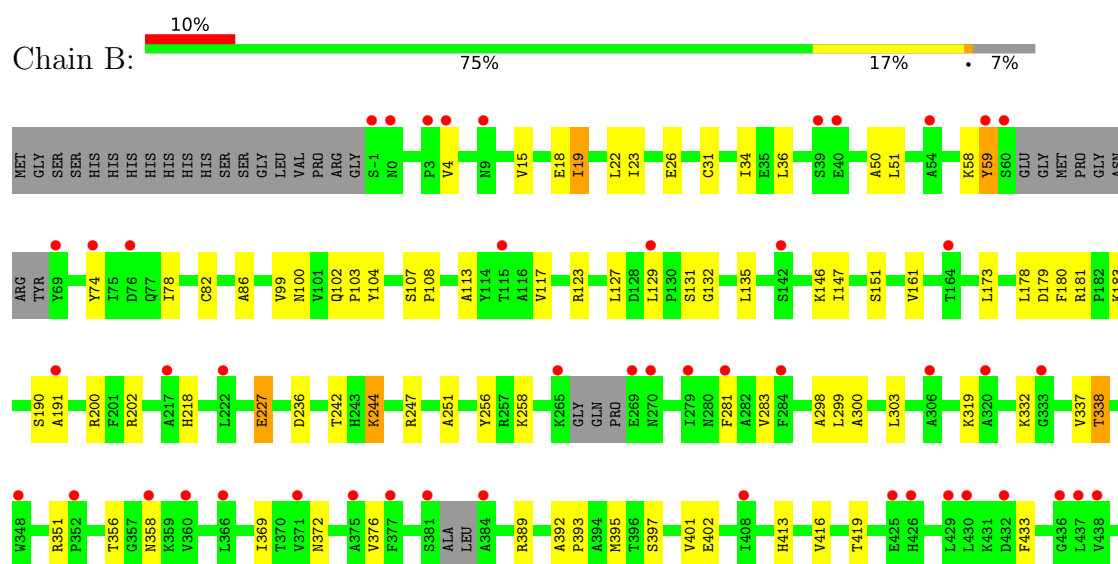
3 Residue-property plots [i](#)

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: Serine hydroxymethyltransferase

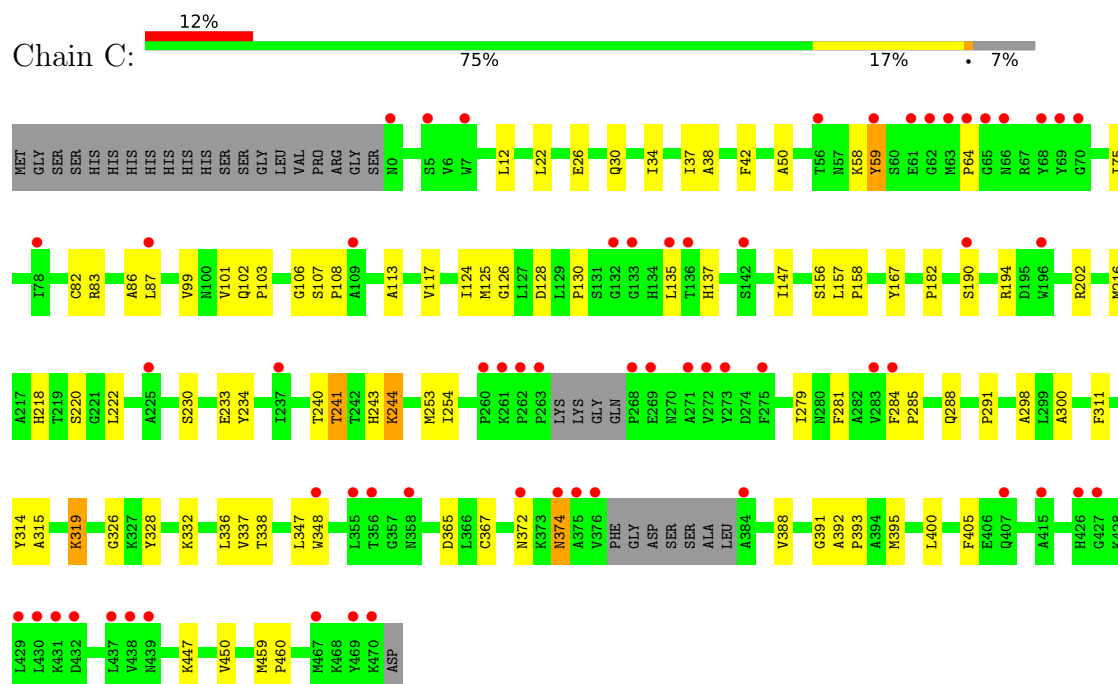


• Molecule 1: Serine hydroxymethyltransferase

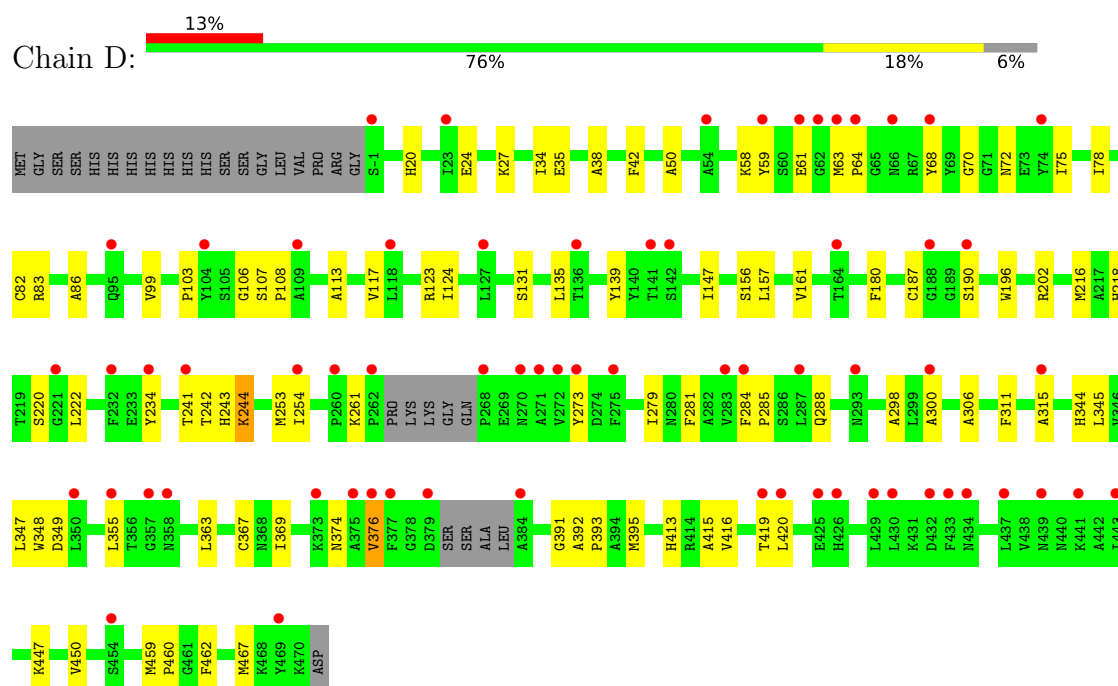




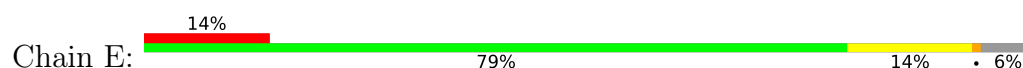
- Molecule 1: Serine hydroxymethyltransferase

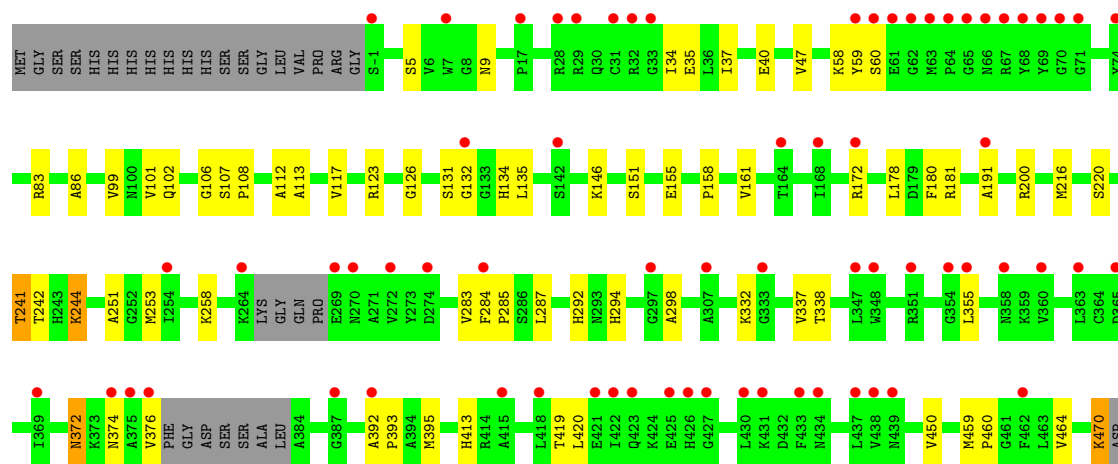


- Molecule 1: Serine hydroxymethyltransferase

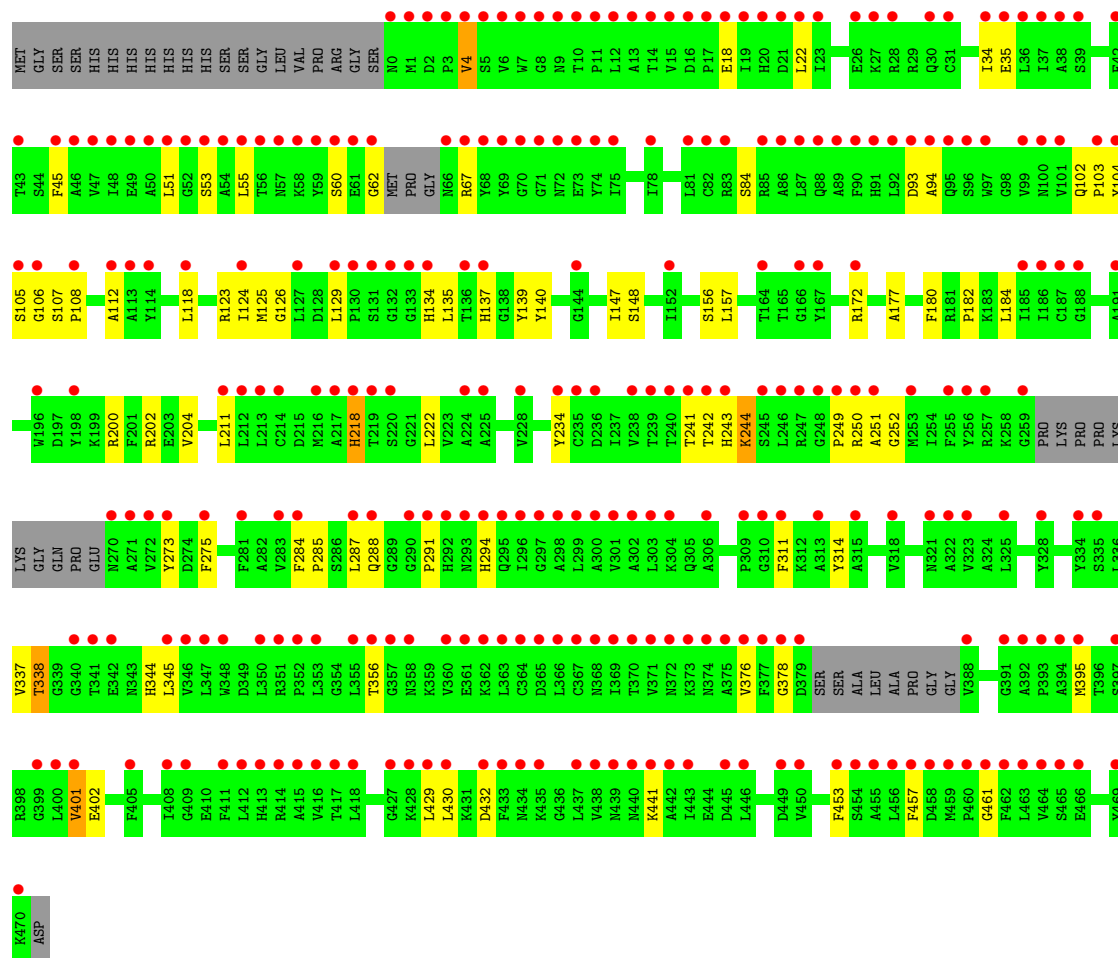
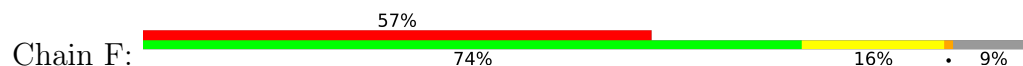


- Molecule 1: Serine hydroxymethyltransferase





• Molecule 1: Serine hydroxymethyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.32Å 174.32Å 184.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.54 – 2.28 48.54 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.54-2.28) 98.9 (48.54-2.28)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.272 , 0.313 0.276 , 0.315	Depositor DCC
R_{free} test set	7353 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20214	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.0390e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LLP

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	0.38	0/3468	0.61	0/4720
1	B	0.37	0/3461	0.61	0/4706
1	C	0.34	0/3490	0.57	0/4746
1	D	0.36	0/3472	0.59	0/4722
1	E	0.38	0/3418	0.60	0/4657
1	F	0.34	0/3003	0.61	0/4106
All	All	0.36	0/20312	0.60	0/27657

There are no bond length outliers.

There are no bond angle outliers.

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	3414	0	3144	75	0
1	B	3409	0	3178	62	0
1	C	3434	0	3216	61	0
1	D	3419	0	3173	59	0
1	E	3367	0	3109	46	0
1	F	2972	0	2362	56	0
2	A	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	0	0	0
2	C	32	0	0	0	0
2	D	51	0	0	3	0
2	E	32	0	0	0	0
2	F	6	0	0	0	0
All	All	20214	0	18182	330	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 9.

All (330) 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:C:125:MET:HE2	1:C:182:PRO:HG3	1.40	1.04
1:A:243:HIS:HE2	1:B:59:TYR:HE1	1.13	0.93
1:C:106:GLY:HA3	1:C:241:THR:HG22	1.56	0.86
1:D:34:ILE:HA	1:D:395:MET:HE2	1.58	0.84
1:E:37:ILE:HG23	1:E:372:ASN:HD21	1.44	0.82
1:F:125:MET:HE2	1:F:182:PRO:HG3	1.60	0.82
1:E:172:ARG:HH11	1:F:172:ARG:HH22	1.27	0.81
1:F:106:GLY:HA3	1:F:241:THR:HG22	1.62	0.81
1:C:64:PRO:HG2	1:C:83:ARG:HH12	1.50	0.77
1:A:34:ILE:HA	1:A:395:MET:HE2	1.66	0.76
1:A:34:ILE:HG13	1:A:450:VAL:HG13	1.65	0.76
1:A:374:ASN:HD22	1:A:375:ALA:H	1.32	0.75
1:A:74:TYR:HB2	1:B:26:GLU:HG2	1.67	0.75
1:F:62:GLY:HA3	1:F:67:ARG:HA	1.71	0.71
1:B:34:ILE:HA	1:B:395:MET:HE2	1.71	0.71
1:A:250:ARG:HH22	1:B:58:LYS:C	1.99	0.71
1:E:35:GLU:H	1:E:395:MET:HE2	1.56	0.70
1:C:107:SER:HB2	1:C:108:PRO:HD3	1.74	0.70
1:E:106:GLY:HA3	1:E:244:LLP:H5'1	1.73	0.69
1:E:178:LEU:O	1:E:181:ARG:HD3	1.95	0.67
1:A:130:PRO:HB2	1:A:378:GLY:HA2	1.77	0.67
1:D:58:LYS:HG2	1:D:75:ILE:HG13	1.77	0.66
1:B:372:ASN:HD21	1:B:389:ARG:HE	1.42	0.66
1:D:131:SER:HB3	1:D:161:VAL:HG13	1.77	0.66
1:D:107:SER:HB2	1:D:108:PRO:HD3	1.78	0.65
1:F:273:TYR:HD2	1:F:275:PHE:HE2	1.44	0.65
1:A:241:THR:HG21	1:A:244:LLP:HG2	1.78	0.65
1:A:52:GLY:HA2	1:B:51:LEU:HD23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ARG:HD3	1:B:376:VAL:HG21	1.80	0.64
1:E:241:THR:HG21	1:E:244:LLP:HE3	1.80	0.64
1:F:104:TYR:H	1:F:288:GLN:HE22	1.44	0.64
1:E:146:LYS:HD3	1:E:151:SER:O	1.98	0.64
1:A:107:SER:HB2	1:A:108:PRO:HD3	1.81	0.63
1:F:241:THR:HB	1:F:243:HIS:CE1	2.33	0.63
1:E:191:ALA:HB2	1:E:374:ASN:ND2	2.13	0.63
1:B:131:SER:HB3	1:B:161:VAL:HG13	1.79	0.63
1:F:126:GLY:HA3	1:F:137:HIS:HB3	1.81	0.62
1:B:146:LYS:HD3	1:B:151:SER:O	2.00	0.62
1:C:58:LYS:HG2	1:C:75:ILE:HG13	1.81	0.61
1:E:34:ILE:HG13	1:E:450:VAL:HG13	1.81	0.61
1:F:34:ILE:HA	1:F:395:MET:HE2	1.83	0.61
1:D:241:THR:HB	1:D:243:HIS:CE1	2.35	0.61
1:B:459:MET:SD	1:B:460:PRO:HD2	2.40	0.61
1:E:191:ALA:HB2	1:E:374:ASN:HD22	1.66	0.61
1:F:107:SER:HB2	1:F:108:PRO:HD3	1.83	0.60
1:F:125:MET:HG2	1:F:157:LEU:O	2.00	0.60
1:E:34:ILE:HA	1:E:395:MET:HE2	1.82	0.60
1:F:241:THR:HG21	1:F:244:LLP:H5'1	1.82	0.60
1:A:37:ILE:HD12	1:A:372:ASN:ND2	2.16	0.60
1:C:26:GLU:HG3	1:C:30:GLN:HE21	1.67	0.60
1:C:241:THR:HG21	1:C:244:LLP:H5'2	1.81	0.60
1:C:395:MET:HB3	1:C:400:LEU:HD22	1.82	0.60
1:F:273:TYR:HD2	1:F:275:PHE:CE2	2.20	0.60
1:D:106:GLY:HA3	1:D:241:THR:HG22	1.84	0.59
1:E:337:VAL:HG12	1:E:338:THR:HG23	1.84	0.59
1:E:58:LYS:HE3	1:E:59:TYR:O	2.02	0.59
1:E:459:MET:SD	1:E:460:PRO:HD2	2.43	0.59
1:F:125:MET:HE1	1:F:177:ALA:HA	1.85	0.59
1:F:311:PHE:O	1:F:314:TYR:HB3	2.04	0.58
1:D:34:ILE:HA	1:D:395:MET:CE	2.32	0.57
1:A:178:LEU:O	1:A:181:ARG:HD3	2.04	0.57
1:C:22:LEU:HD23	1:D:78:ILE:HG13	1.85	0.57
1:C:348:TRP:HB3	1:C:388:VAL:HG23	1.85	0.57
1:F:243:HIS:CG	1:F:250:ARG:HA	2.40	0.57
1:E:47:VAL:HG13	1:E:298:ALA:HB1	1.86	0.57
1:A:351:ARG:HD3	1:A:386:GLY:HA3	1.86	0.57
1:C:106:GLY:CA	1:C:241:THR:HG22	2.32	0.57
1:F:453:PHE:CE1	1:F:457:PHE:HE2	2.23	0.57
1:A:241:THR:CG2	1:A:244:LLP:HG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:ALA:HB3	1:E:99:VAL:HG11	1.88	0.56
1:C:38:ALA:HA	1:C:391:GLY:HA3	1.86	0.56
1:D:222:LEU:HD23	1:D:315:ALA:HB1	1.88	0.56
1:F:35:GLU:H	1:F:395:MET:HE2	1.71	0.56
1:F:200:ARG:O	1:F:204:VAL:HG23	2.07	0.55
1:B:337:VAL:HG12	1:B:338:THR:HG23	1.86	0.55
1:E:172:ARG:NH1	1:F:172:ARG:HH22	2.02	0.55
1:E:155:GLU:HB3	1:F:123:ARG:HH21	1.72	0.55
1:B:102:GLN:HB2	1:B:283:VAL:HG11	1.89	0.55
1:F:337:VAL:O	1:F:338:THR:HG22	2.07	0.54
1:D:392:ALA:N	1:D:393:PRO:HD3	2.22	0.54
1:A:374:ASN:O	1:A:385:PRO:HB2	2.07	0.54
1:A:459:MET:SD	1:A:460:PRO:HD2	2.47	0.54
1:C:216:MET:HG3	1:C:220:SER:HB3	1.87	0.54
1:F:124:ILE:CD1	1:F:184:LEU:HB3	2.38	0.54
1:B:82:CYS:HB2	1:B:300:ALA:HB2	1.88	0.54
1:A:242:THR:HG22	1:A:253:MET:HE2	1.89	0.54
1:B:356:THR:HG22	1:B:358:ASN:H	1.72	0.54
1:C:128:ASP:CG	1:C:130:PRO:HD2	2.33	0.54
1:D:82:CYS:HB2	1:D:300:ALA:HB2	1.90	0.54
1:F:34:ILE:HA	1:F:395:MET:CE	2.38	0.54
1:A:34:ILE:HG23	1:A:395:MET:HE2	1.90	0.53
1:A:350:LEU:HD22	1:A:360:VAL:HG21	1.90	0.53
1:F:118:LEU:HD11	1:F:124:ILE:HD11	1.90	0.53
1:D:218:HIS:HD2	1:D:244:LLP:O3	1.91	0.53
1:C:37:ILE:HG23	1:C:372:ASN:HD21	1.74	0.53
1:A:241:THR:HG21	1:A:244:LLP:HE3	1.89	0.53
1:A:37:ILE:HB	1:A:40:GLU:HB2	1.91	0.53
1:C:311:PHE:O	1:C:314:TYR:HB3	2.09	0.53
1:B:218:HIS:CD2	1:B:244:LLP:O3	2.62	0.53
1:B:356:THR:HG22	1:B:358:ASN:N	2.23	0.53
1:D:38:ALA:HA	1:D:391:GLY:HA3	1.90	0.53
1:C:125:MET:HG2	1:C:157:LEU:O	2.08	0.52
1:E:332:LYS:HG3	1:E:413:HIS:HD2	1.73	0.52
1:D:35:GLU:H	1:D:395:MET:HE2	1.74	0.52
1:B:107:SER:HB2	1:B:108:PRO:HD3	1.91	0.52
1:D:34:ILE:HG13	1:D:450:VAL:HG13	1.91	0.52
1:A:350:LEU:CD2	1:A:360:VAL:HG21	2.39	0.52
1:A:202:ARG:HB2	1:A:234:TYR:HB3	1.90	0.52
1:C:82:CYS:HB2	1:C:300:ALA:HB2	1.91	0.52
1:D:58:LYS:HE3	1:D:72:ASN:ND2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:MET:SD	1:D:460:PRO:HD2	2.50	0.52
1:D:467:MET:HG2	2:D:529:HOH:O	2.09	0.52
1:E:5:SER:HA	1:E:9:ASN:HB2	1.92	0.52
1:D:254:ILE:HG21	1:D:279:ILE:HD12	1.92	0.52
1:C:337:VAL:HG12	1:C:338:THR:HG23	1.91	0.51
1:A:61:GLU:HG2	1:A:284:PHE:CE1	2.44	0.51
1:A:167:TYR:CE1	1:A:194:ARG:HG3	2.46	0.51
1:C:58:LYS:HE3	1:C:59:TYR:O	2.11	0.51
1:D:61:GLU:HB3	1:D:284:PHE:CZ	2.45	0.51
1:D:344:HIS:NE2	1:D:345:LEU:HD23	2.25	0.51
1:B:372:ASN:ND2	1:B:389:ARG:HH21	2.09	0.51
1:D:27:LYS:HE3	1:D:462:PHE:CD2	2.45	0.51
1:F:284:PHE:CD1	1:F:285:PRO:HA	2.45	0.51
1:C:459:MET:SD	1:C:460:PRO:HD2	2.51	0.51
1:F:129:LEU:HD21	1:F:135:LEU:HD22	1.93	0.50
1:A:243:HIS:NE2	1:B:59:TYR:HE1	1.96	0.50
1:F:401:VAL:HG13	1:F:402:GLU:N	2.27	0.50
1:C:281:PHE:CZ	1:D:147:ILE:HD12	2.47	0.50
1:F:134:HIS:CD2	1:F:135:LEU:H	2.29	0.50
1:C:128:ASP:OD2	1:C:130:PRO:HD2	2.12	0.50
1:A:34:ILE:HA	1:A:395:MET:CE	2.39	0.50
1:C:102:GLN:OE1	1:C:291:PRO:HG3	2.11	0.50
1:D:413:HIS:C	1:D:413:HIS:CD2	2.91	0.49
1:A:306:ALA:HA	1:A:311:PHE:CG	2.48	0.49
1:E:355:LEU:HD22	1:E:419:THR:HG22	1.93	0.49
1:E:107:SER:HB2	1:E:108:PRO:HD3	1.94	0.49
1:F:123:ARG:HB3	1:F:180:PHE:CE2	2.48	0.49
1:C:365:ASP:OD1	1:D:70:GLY:HA3	2.13	0.49
1:C:392:ALA:N	1:C:393:PRO:CD	2.76	0.49
1:E:131:SER:HB3	1:E:161:VAL:HG13	1.95	0.49
1:A:38:ALA:HA	1:A:391:GLY:HA3	1.95	0.49
1:C:241:THR:CG2	1:C:244:LLP:H5'2	2.43	0.49
1:B:218:HIS:HD2	1:B:244:LLP:O3	1.96	0.48
1:A:200:ARG:HD2	1:A:200:ARG:HA	1.50	0.48
1:A:147:ILE:HD12	1:B:281:PHE:CZ	2.48	0.48
1:B:419:THR:HG23	1:B:433:PHE:HZ	1.78	0.48
1:E:241:THR:CG2	1:E:244:LLP:HG2	2.42	0.48
1:A:19:ILE:O	1:A:23:ILE:HG13	2.12	0.48
1:A:81:LEU:HD21	1:B:18:GLU:HG2	1.95	0.48
1:F:218:HIS:HB3	1:F:344:HIS:CE1	2.49	0.48
1:E:191:ALA:CB	1:E:374:ASN:HD22	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:HIS:HB3	1:E:294:HIS:CE1	2.48	0.48
1:A:51:LEU:O	1:A:294:HIS:HB2	2.14	0.48
1:C:202:ARG:HB2	1:C:234:TYR:HB3	1.96	0.47
1:E:392:ALA:N	1:E:393:PRO:CD	2.77	0.47
1:C:86:ALA:HB3	1:C:99:VAL:HG11	1.96	0.47
1:E:34:ILE:HA	1:E:395:MET:CE	2.44	0.47
1:F:22:LEU:HD23	1:F:22:LEU:HA	1.65	0.47
1:C:113:ALA:O	1:C:117:VAL:HG22	2.13	0.47
1:E:470:LYS:HE3	1:E:470:LYS:HB3	1.70	0.47
1:F:125:MET:HE1	1:F:177:ALA:CA	2.44	0.47
1:A:7:TRP:CH2	1:B:247:ARG:HD2	2.49	0.47
1:E:284:PHE:CD1	1:E:285:PRO:HA	2.50	0.47
1:C:124:ILE:O	1:C:156:SER:HA	2.15	0.47
1:A:37:ILE:HG12	1:A:370:THR:HG22	1.96	0.47
1:D:348:TRP:CH2	1:D:416:VAL:HG21	2.50	0.47
1:D:64:PRO:HD2	1:D:83:ARG:HH12	1.80	0.47
1:A:236:ASP:O	1:A:257:ARG:HG3	2.14	0.47
1:B:178:LEU:O	1:B:181:ARG:HD3	2.14	0.46
1:C:348:TRP:HB3	1:C:388:VAL:CG2	2.45	0.46
1:D:349:ASP:HA	1:D:376:VAL:HG11	1.97	0.46
1:A:131:SER:HB3	1:A:161:VAL:HG13	1.98	0.46
1:A:218:HIS:HD2	1:A:244:LLP:O3	1.97	0.46
1:E:112:ALA:HB2	1:E:287:LEU:HD23	1.97	0.46
1:A:147:ILE:HD12	1:B:281:PHE:HZ	1.81	0.46
1:C:34:ILE:HG13	1:C:450:VAL:HG13	1.97	0.46
1:C:190:SER:HA	1:C:218:HIS:CD2	2.50	0.46
1:A:101:VAL:HG12	1:A:253:MET:HG2	1.98	0.46
1:A:294:HIS:CD2	1:B:51:LEU:HD21	2.51	0.46
1:F:106:GLY:CA	1:F:241:THR:HG22	2.40	0.46
1:B:242:THR:OG1	1:B:251:ALA:HB3	2.15	0.46
1:C:202:ARG:HD2	1:C:234:TYR:O	2.15	0.46
1:D:355:LEU:HD21	1:D:420:LEU:HD23	1.97	0.46
1:A:113:ALA:O	1:A:117:VAL:HG22	2.15	0.46
1:A:218:HIS:HB3	1:A:344:HIS:CE1	2.51	0.46
1:C:230:SER:O	1:C:233:GLU:HG3	2.16	0.46
1:D:355:LEU:HD22	1:D:419:THR:HG22	1.96	0.46
1:B:86:ALA:HA	1:B:303:LEU:HD22	1.98	0.46
1:E:37:ILE:CG2	1:E:372:ASN:HD21	2.22	0.45
1:B:100:ASN:OD1	1:B:102:GLN:HG3	2.17	0.45
1:C:281:PHE:HZ	1:D:147:ILE:HD12	1.81	0.45
1:D:306:ALA:HA	1:D:311:PHE:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:VAL:HG13	1:B:467:MET:HE1	1.98	0.45
1:D:20:HIS:O	1:D:24:GLU:HG2	2.16	0.45
1:F:202:ARG:HB2	1:F:234:TYR:HB3	1.97	0.45
1:A:292:HIS:HB3	1:A:294:HIS:CE1	2.52	0.45
1:C:167:TYR:CE2	1:C:194:ARG:HG3	2.52	0.45
1:E:216:MET:HG3	1:E:220:SER:HB3	1.97	0.45
1:F:273:TYR:CD2	1:F:275:PHE:HE2	2.28	0.45
1:A:281:PHE:CE2	1:B:147:ILE:HD12	2.52	0.45
1:B:332:LYS:HG2	1:B:413:HIS:CD2	2.51	0.45
1:F:112:ALA:HB2	1:F:287:LEU:HD23	1.98	0.45
1:A:345:LEU:HD12	1:A:345:LEU:C	2.42	0.45
1:C:284:PHE:HD2	1:C:288:GLN:O	2.00	0.45
1:D:123:ARG:HB3	1:D:180:PHE:CE2	2.52	0.45
1:E:113:ALA:O	1:E:117:VAL:HG22	2.18	0.44
1:E:126:GLY:O	1:E:158:PRO:HA	2.18	0.44
1:F:102:GLN:N	1:F:103:PRO:CD	2.81	0.44
1:B:190:SER:HA	1:B:218:HIS:CD2	2.52	0.44
1:B:401:VAL:HG22	1:B:402:GLU:OE1	2.17	0.44
1:D:35:GLU:HG3	1:D:42:PHE:HZ	1.82	0.44
1:E:200:ARG:HA	1:E:200:ARG:HD2	1.80	0.44
1:B:179:ASP:HB3	1:D:157:LEU:HD11	1.99	0.44
1:C:126:GLY:HA3	1:C:137:HIS:HB3	1.99	0.44
1:C:26:GLU:HG3	1:C:30:GLN:NE2	2.32	0.44
1:D:50:ALA:HB3	1:D:298:ALA:HA	1.99	0.44
1:D:86:ALA:HB3	1:D:99:VAL:HG11	1.99	0.44
1:A:292:HIS:HE1	1:B:104:TYR:O	2.01	0.44
1:B:19:ILE:O	1:B:23:ILE:HG13	2.18	0.44
1:B:50:ALA:HB3	1:B:298:ALA:HA	2.00	0.44
1:D:347:LEU:HD11	1:D:374:ASN:HB3	1.99	0.44
1:F:105:SER:O	1:F:252:GLY:HA3	2.17	0.44
1:A:284:PHE:CD1	1:A:285:PRO:HA	2.53	0.44
1:F:147:ILE:HG22	1:F:148:SER:N	2.33	0.44
1:A:311:PHE:O	1:A:314:TYR:HB3	2.18	0.44
1:B:86:ALA:HB3	1:B:99:VAL:HG11	2.00	0.44
1:C:99:VAL:HG21	1:C:253:MET:HE2	2.00	0.43
1:C:254:ILE:HG21	1:C:279:ILE:HD13	1.99	0.43
1:C:395:MET:HB2	1:C:405:PHE:CZ	2.53	0.43
1:D:59:TYR:HA	2:D:528:HOH:O	2.18	0.43
1:F:242:THR:OG1	1:F:251:ALA:HB3	2.17	0.43
1:E:123:ARG:HB3	1:E:180:PHE:CE2	2.53	0.43
1:F:4:VAL:H	1:F:4:VAL:HG12	1.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:HIS:HA	1:F:244:LLP:HD3	2.00	0.43
1:B:113:ALA:O	1:B:117:VAL:HG22	2.18	0.43
1:C:319:LYS:HE3	1:C:319:LYS:HB3	1.72	0.43
1:F:453:PHE:CE1	1:F:457:PHE:CE2	3.06	0.43
1:B:132:GLY:HA2	1:B:191:ALA:HB3	2.00	0.43
1:D:363:LEU:HD12	1:D:415:ALA:HB1	2.00	0.43
1:F:51:LEU:O	1:F:294:HIS:HB2	2.18	0.43
1:C:42:PHE:HB3	1:C:460:PRO:HG2	2.01	0.43
1:C:328:TYR:CZ	1:C:332:LYS:HE2	2.54	0.43
1:A:197:ASP:CG	1:A:200:ARG:HB2	2.44	0.43
1:D:139:TYR:HA	2:D:546:HOH:O	2.19	0.43
1:C:222:LEU:HD23	1:C:315:ALA:HB1	2.01	0.42
1:D:218:HIS:CD2	1:D:244:LLP:O3	2.72	0.42
1:F:140:TYR:HE2	1:F:156:SER:O	2.02	0.42
1:F:243:HIS:HB3	1:F:249:PRO:C	2.44	0.42
1:F:243:HIS:ND1	1:F:243:HIS:N	2.67	0.42
1:C:86:ALA:CB	1:C:253:MET:HE1	2.49	0.42
1:D:218:HIS:HB3	1:D:344:HIS:CE1	2.54	0.42
1:D:392:ALA:N	1:D:393:PRO:CD	2.83	0.42
1:A:58:LYS:HG2	1:A:75:ILE:HG13	2.01	0.42
1:A:129:LEU:HD22	1:A:139:TYR:CD1	2.55	0.42
1:A:374:ASN:HD22	1:A:375:ALA:N	2.07	0.42
1:C:241:THR:HB	1:C:243:HIS:CE1	2.54	0.42
1:C:347:LEU:HD11	1:C:374:ASN:HB3	2.00	0.42
1:A:411:PHE:HE1	1:A:449:ASP:HB3	1.84	0.42
1:C:50:ALA:HB3	1:C:298:ALA:HA	2.02	0.42
1:E:83:ARG:O	1:E:86:ALA:HB3	2.20	0.42
1:E:101:VAL:HG12	1:E:253:MET:HE3	2.01	0.42
1:A:186:ILE:HD13	1:A:186:ILE:HG21	1.74	0.42
1:A:194:ARG:HD3	1:A:194:ARG:HA	1.83	0.42
1:B:200:ARG:HD2	1:B:200:ARG:HA	1.66	0.42
1:E:132:GLY:HA2	1:E:191:ALA:HB3	2.01	0.42
1:F:104:TYR:N	1:F:104:TYR:CD2	2.87	0.42
1:B:36:LEU:HD12	1:B:369:ILE:HG23	2.02	0.42
1:D:216:MET:HG3	1:D:220:SER:HB3	2.02	0.42
1:E:86:ALA:CB	1:E:99:VAL:HG11	2.49	0.42
1:E:355:LEU:HD11	1:E:420:LEU:HG	2.00	0.42
1:B:227:GLU:HG3	1:B:319:LYS:HD3	2.00	0.42
1:C:216:MET:HG2	1:C:240:THR:HB	2.00	0.42
1:D:63:MET:HB3	1:D:63:MET:HE3	1.78	0.42
1:D:187:CYS:HB2	1:D:196:TRP:CE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ALA:HB2	1:A:374:ASN:OD1	2.20	0.42
1:B:127:LEU:HD21	1:B:131:SER:O	2.20	0.42
1:A:349:ASP:OD1	1:A:351:ARG:HB2	2.20	0.42
1:A:401:VAL:HG22	1:A:402:GLU:H	1.84	0.42
1:F:243:HIS:HB3	1:F:249:PRO:O	2.20	0.42
1:A:12:LEU:HD12	1:A:12:LEU:O	2.20	0.41
1:A:22:LEU:HB3	1:B:78:ILE:HD11	2.02	0.41
1:B:102:GLN:N	1:B:103:PRO:CD	2.83	0.41
1:B:463:LEU:HD23	1:B:463:LEU:HA	1.72	0.41
1:A:160:LYS:HE3	1:A:176:LYS:NZ	2.34	0.41
1:E:242:THR:OG1	1:E:251:ALA:HB3	2.20	0.41
1:A:63:MET:HE1	1:A:100:ASN:HD21	1.84	0.41
1:C:128:ASP:HB2	1:C:158:PRO:HB2	2.02	0.41
1:D:68:TYR:CE2	1:D:284:PHE:HZ	2.38	0.41
1:B:242:THR:HB	1:B:299:LEU:HD13	2.02	0.41
1:B:392:ALA:N	1:B:393:PRO:CD	2.83	0.41
1:F:60:SER:O	1:F:291:PRO:HD2	2.20	0.41
1:A:348:TRP:CH2	1:A:416:VAL:HG21	2.55	0.41
1:C:285:PRO:HB2	1:D:135:LEU:CD1	2.51	0.41
1:D:124:ILE:O	1:D:156:SER:HA	2.20	0.41
1:C:326:GLY:HA2	1:C:336:LEU:HD11	2.02	0.41
1:D:113:ALA:O	1:D:117:VAL:HG22	2.21	0.41
1:A:285:PRO:HB2	1:B:135:LEU:HD13	2.02	0.41
1:A:392:ALA:N	1:A:393:PRO:CD	2.84	0.41
1:B:202:ARG:HH22	1:B:236:ASP:CG	2.29	0.41
1:C:101:VAL:HG12	1:C:253:MET:HE3	2.02	0.41
1:C:102:GLN:N	1:C:103:PRO:CD	2.84	0.41
1:D:261:LYS:HA	1:D:273:TYR:CE2	2.56	0.41
1:A:319:LYS:HB3	1:A:319:LYS:HE2	1.81	0.41
1:B:22:LEU:HD23	1:B:22:LEU:HA	1.92	0.41
1:B:123:ARG:HG2	1:B:180:PHE:CZ	2.56	0.41
1:B:256:TYR:HE1	1:B:258:LYS:HD3	1.86	0.41
1:C:135:LEU:CD1	1:D:285:PRO:HB2	2.51	0.41
1:E:102:GLN:HB2	1:E:283:VAL:HG11	2.02	0.41
1:E:134:HIS:CD2	1:E:135:LEU:H	2.39	0.41
1:F:53:SER:OG	1:F:55:LEU:HD23	2.21	0.41
1:D:202:ARG:HB2	1:D:234:TYR:HB3	2.02	0.41
1:A:29:ARG:HB2	1:B:74:TYR:HE2	1.86	0.40
1:E:413:HIS:ND1	1:E:413:HIS:C	2.79	0.40
1:F:45:PHE:N	1:F:461:GLY:HA2	2.35	0.40
1:A:304:LYS:HE2	1:B:15:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:CYS:HB3	1:B:459:MET:HE2	2.02	0.40
1:B:178:LEU:HD23	1:B:178:LEU:HA	1.89	0.40
1:A:25:LYS:HE2	1:B:74:TYR:CE1	2.57	0.40
1:A:236:ASP:HB3	1:A:275:PHE:CE2	2.56	0.40
1:D:242:THR:HG22	1:D:253:MET:HE2	2.03	0.40
1:F:184:LEU:HD12	1:F:211:LEU:O	2.22	0.40
1:A:157:LEU:HA	1:A:158:PRO:HD3	1.98	0.40
1:A:458:ASP:HB3	1:B:4:VAL:HG11	2.03	0.40
1:C:367:CYS:HA	1:C:447:LYS:HB2	2.02	0.40
1:D:103:PRO:HA	1:D:288:GLN:OE1	2.20	0.40
1:D:367:CYS:HA	1:D:447:LYS:HB2	2.04	0.40
1:F:243:HIS:CD2	1:F:250:ARG:HA	2.56	0.40
1:A:392:ALA:N	1:A:393:PRO:HD3	2.37	0.40
1:C:147:ILE:HD12	1:D:281:PHE:CZ	2.56	0.40
1:F:139:TYR:HD2	1:F:147:ILE:HB	1.86	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	455/492 (92%)	435 (96%)	20 (4%)	0	100	100
1	B	450/492 (92%)	432 (96%)	18 (4%)	0	100	100
1	C	453/492 (92%)	433 (96%)	20 (4%)	0	100	100
1	D	456/492 (93%)	433 (95%)	23 (5%)	0	100	100
1	E	454/492 (92%)	436 (96%)	18 (4%)	0	100	100
1	F	441/492 (90%)	410 (93%)	22 (5%)	9 (2%)	6	4
All	All	2709/2952 (92%)	2579 (95%)	121 (4%)	9 (0%)	36	44

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	94	ALA
1	F	429	LEU
1	F	430	LEU
1	F	432	ASP
1	F	376	VAL
1	F	441	LYS
1	F	93	ASP
1	F	378	GLY
1	F	18	GLU

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	327/403 (81%)	317 (97%)	10 (3%)	35	50
1	B	330/403 (82%)	321 (97%)	9 (3%)	39	55
1	C	337/403 (84%)	331 (98%)	6 (2%)	51	68
1	D	328/403 (81%)	325 (99%)	3 (1%)	70	82
1	E	318/403 (79%)	310 (98%)	8 (2%)	42	58
1	F	217/403 (54%)	209 (96%)	8 (4%)	30	43
All	All	1857/2418 (77%)	1813 (98%)	44 (2%)	43	59

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	81	LEU
1	A	146	LYS
1	A	200	ARG
1	A	218	HIS
1	A	351	ARG
1	A	372	ASN
1	A	374	ASN
1	A	390	ILE
1	A	397	SER

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Mol	Chain	Res	Type
1	B	19	ILE
1	B	59	TYR
1	B	129	LEU
1	B	173	LEU
1	B	183	LYS
1	B	227	GLU
1	B	338	THR
1	B	397	SER
1	B	416	VAL
1	C	12	LEU
1	C	59	TYR
1	C	87	LEU
1	C	241	THR
1	C	319	LYS
1	C	374	ASN
1	D	190	SER
1	D	369	ILE
1	D	376	VAL
1	E	40	GLU
1	E	60	SER
1	E	241	THR
1	E	258	LYS
1	E	372	ASN
1	E	376	VAL
1	E	464	VAL
1	E	470	LYS
1	F	4	VAL
1	F	84	SER
1	F	218	HIS
1	F	222	LEU
1	F	338	THR
1	F	345	LEU
1	F	356	THR
1	F	401	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	HIS
1	A	295	GLN
1	A	372	ASN
1	A	374	ASN

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Mol	Chain	Res	Type
1	A	434	ASN
1	B	321	ASN
1	B	372	ASN
1	C	372	ASN
1	C	407	GLN
1	C	434	ASN
1	C	440	ASN
1	D	9	ASN
1	D	72	ASN
1	D	226	GLN
1	D	295	GLN
1	D	407	GLN
1	D	413	HIS
1	E	77	GLN
1	E	293	ASN
1	E	295	GLN
1	E	321	ASN
1	E	372	ASN
1	E	374	ASN
1	E	407	GLN
1	F	226	GLN
1	F	288	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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	C	244	1	23,24,25	1.08	1 (4%)	25,32,34	1.64	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	D	244	1	23,24,25	1.17	3 (13%)	25,32,34	1.62	8 (32%)
1	LLP	B	244	1	23,24,25	1.16	2 (8%)	25,32,34	2.01	8 (32%)
1	LLP	A	244	1	23,24,25	1.14	1 (4%)	25,32,34	1.12	3 (12%)
1	LLP	E	244	1	23,24,25	1.18	2 (8%)	25,32,34	1.73	4 (16%)
1	LLP	F	244	1	23,24,25	1.17	1 (4%)	25,32,34	1.43	5 (20%)

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	C	244	1	-	13/16/17/19	0/1/1/1
1	LLP	D	244	1	-	11/16/17/19	0/1/1/1
1	LLP	B	244	1	-	8/16/17/19	0/1/1/1
1	LLP	A	244	1	-	11/16/17/19	0/1/1/1
1	LLP	E	244	1	-	11/16/17/19	0/1/1/1
1	LLP	F	244	1	-	10/16/17/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	244	LLP	P-OP4	4.37	1.74	1.60
1	E	244	LLP	P-OP4	3.94	1.72	1.60
1	D	244	LLP	P-OP4	3.70	1.72	1.60
1	A	244	LLP	P-OP4	3.66	1.71	1.60
1	C	244	LLP	P-OP4	3.54	1.71	1.60
1	B	244	LLP	P-OP4	3.42	1.71	1.60
1	B	244	LLP	O3-C3	-2.25	1.31	1.36
1	D	244	LLP	OP4-C5'	-2.17	1.36	1.44
1	D	244	LLP	O3-C3	-2.06	1.32	1.36
1	E	244	LLP	O3-C3	-2.03	1.32	1.36

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	LLP	C5-C4-C4'	4.68	128.69	121.47
1	B	244	LLP	C4-C3-C2	4.49	122.67	120.14
1	E	244	LLP	C5-C4-C4'	3.83	127.39	121.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	244	LLP	OP4-C5'-C5	3.66	116.22	109.36
1	C	244	LLP	OP3-P-OP2	3.61	121.35	107.80
1	E	244	LLP	C3-C4-C4'	-3.61	113.88	120.40
1	F	244	LLP	C5'-C5-C6	3.60	125.23	119.36
1	D	244	LLP	OP3-P-OP2	3.59	121.26	107.80
1	C	244	LLP	OP4-C5'-C5	3.36	115.66	109.36
1	F	244	LLP	OP4-C5'-C5	3.35	115.64	109.36
1	B	244	LLP	C3-C4-C4'	-3.04	114.92	120.40
1	F	244	LLP	C2'-C2-C3	-2.87	117.44	120.80
1	C	244	LLP	C5-C4-C4'	2.85	125.87	121.47
1	C	244	LLP	C5'-C5-C6	-2.82	114.77	119.36
1	B	244	LLP	OP2-P-OP4	-2.76	99.48	106.67
1	D	244	LLP	C2'-C2-C3	-2.74	117.59	120.80
1	B	244	LLP	OP3-P-OP2	2.74	118.06	107.80
1	B	244	LLP	C3-C4-C5	-2.65	116.15	118.28
1	D	244	LLP	OP4-P-OP1	-2.64	99.30	106.44
1	D	244	LLP	OP2-P-OP4	-2.62	99.83	106.67
1	E	244	LLP	OP3-P-OP2	2.54	117.33	107.80
1	D	244	LLP	C5'-C5-C6	2.47	123.39	119.36
1	B	244	LLP	OP4-P-OP1	-2.47	99.76	106.44
1	A	244	LLP	OP3-P-OP2	2.30	116.43	107.80
1	F	244	LLP	OP3-P-OP2	2.29	116.37	107.80
1	D	244	LLP	C4-C3-C2	2.24	121.40	120.14
1	D	244	LLP	C2'-C2-N1	2.23	121.84	117.64
1	D	244	LLP	C3-C4-C5	-2.23	116.49	118.28
1	A	244	LLP	C5-C4-C4'	2.22	124.89	121.47
1	F	244	LLP	C2'-C2-N1	2.14	121.68	117.64
1	B	244	LLP	CE-NZ-C4'	2.13	125.55	118.72
1	A	244	LLP	OP4-P-OP1	-2.07	100.85	106.44

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	244	LLP	C4-C4'-NZ-CE
1	A	244	LLP	C5'-OP4-P-OP1
1	A	244	LLP	C5'-OP4-P-OP2
1	A	244	LLP	C5'-OP4-P-OP3
1	A	244	LLP	O-C-CA-CB
1	B	244	LLP	C4-C4'-NZ-CE
1	B	244	LLP	O-C-CA-CB
1	C	244	LLP	C5-C4-C4'-NZ

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Mol	Chain	Res	Type	Atoms
1	C	244	LLP	C4-C4'-NZ-CE
1	C	244	LLP	C4-C5-C5'-OP4
1	C	244	LLP	C6-C5-C5'-OP4
1	C	244	LLP	C5'-OP4-P-OP1
1	C	244	LLP	O-C-CA-CB
1	D	244	LLP	C4-C4'-NZ-CE
1	D	244	LLP	C5'-OP4-P-OP1
1	D	244	LLP	C5'-OP4-P-OP2
1	D	244	LLP	C5'-OP4-P-OP3
1	D	244	LLP	O-C-CA-CB
1	E	244	LLP	C5-C4-C4'-NZ
1	E	244	LLP	C4-C4'-NZ-CE
1	E	244	LLP	C5'-OP4-P-OP1
1	E	244	LLP	C5'-OP4-P-OP2
1	E	244	LLP	C5'-OP4-P-OP3
1	E	244	LLP	O-C-CA-CB
1	F	244	LLP	C4-C4'-NZ-CE
1	F	244	LLP	C5'-OP4-P-OP2
1	F	244	LLP	C5'-OP4-P-OP3
1	F	244	LLP	O-C-CA-CB
1	A	244	LLP	CG-CD-CE-NZ
1	B	244	LLP	CG-CD-CE-NZ
1	C	244	LLP	CG-CD-CE-NZ
1	D	244	LLP	CG-CD-CE-NZ
1	E	244	LLP	CG-CD-CE-NZ
1	F	244	LLP	CG-CD-CE-NZ
1	B	244	LLP	C3-C4-C4'-NZ
1	D	244	LLP	C3-C4-C4'-NZ
1	F	244	LLP	C3-C4-C4'-NZ
1	D	244	LLP	C5-C4-C4'-NZ
1	A	244	LLP	C3-C4-C4'-NZ
1	C	244	LLP	C3-C4-C4'-NZ
1	E	244	LLP	C3-C4-C4'-NZ
1	F	244	LLP	C5'-OP4-P-OP1
1	A	244	LLP	C5-C4-C4'-NZ
1	B	244	LLP	C5-C4-C4'-NZ
1	E	244	LLP	CE-CD-CG-CB
1	A	244	LLP	CE-CD-CG-CB
1	B	244	LLP	CE-CD-CG-CB
1	C	244	LLP	CE-CD-CG-CB
1	A	244	LLP	CD-CE-NZ-C4'
1	B	244	LLP	CD-CE-NZ-C4'

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Mol	Chain	Res	Type	Atoms
1	F	244	LLP	CE-CD-CG-CB
1	D	244	LLP	CE-CD-CG-CB
1	C	244	LLP	CD-CE-NZ-C4'
1	D	244	LLP	CD-CE-NZ-C4'
1	F	244	LLP	CA-CB-CG-CD
1	E	244	LLP	CD-CE-NZ-C4'
1	F	244	LLP	CD-CE-NZ-C4'
1	B	244	LLP	CA-CB-CG-CD
1	C	244	LLP	C5'-OP4-P-OP2
1	C	244	LLP	C5'-OP4-P-OP3
1	E	244	LLP	CA-CB-CG-CD
1	C	244	LLP	CA-CB-CG-CD
1	A	244	LLP	CA-CB-CG-CD
1	D	244	LLP	CA-CB-CG-CD

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	244	LLP	2	0
1	D	244	LLP	2	0
1	B	244	LLP	2	0
1	A	244	LLP	4	0
1	E	244	LLP	3	0
1	F	244	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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	461/492 (93%)	1.13	75 (16%) 4 5	29, 46, 82, 118	0
1	B	458/492 (93%)	1.10	51 (11%) 10 11	26, 38, 71, 103	0
1	C	459/492 (93%)	1.17	61 (13%) 7 7	28, 44, 79, 108	0
1	D	462/492 (93%)	1.15	66 (14%) 6 6	28, 38, 76, 102	0
1	E	460/492 (93%)	1.11	69 (15%) 5 6	34, 48, 87, 110	0
1	F	449/492 (91%)	2.50	280 (62%) 0 0	53, 76, 109, 134	0
All	All	2749/2952 (93%)	1.36	602 (21%) 2 2	26, 47, 92, 134	0

All (602) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	74	TYR	9.6
1	F	460	PRO	8.5
1	F	54	ALA	8.3
1	F	240	THR	7.1
1	E	68	TYR	6.6
1	F	69	TYR	6.6
1	F	66	ASN	6.6
1	C	68	TYR	6.5
1	F	1	MET	6.3
1	A	68	TYR	6.2
1	E	69	TYR	6.2
1	B	381	SER	6.1
1	F	7	TRP	6.1
1	F	68	TYR	6.0
1	F	251	ALA	5.9
1	F	465	SER	5.9
1	F	376	VAL	5.8
1	F	454	SER	5.8
1	F	399	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
1	F	59	TYR	5.5
1	F	466	GLU	5.5
1	F	379	ASP	5.4
1	F	255	PHE	5.3
1	D	68	TYR	5.3
1	F	95	GLN	5.2
1	F	377	PHE	5.2
1	E	376	VAL	5.2
1	F	4	VAL	5.1
1	A	438	VAL	5.1
1	F	301	VAL	5.0
1	F	247	ARG	4.9
1	F	464	VAL	4.9
1	F	132	GLY	4.9
1	C	190	SER	4.8
1	E	60	SER	4.8
1	F	360	VAL	4.8
1	F	81	LEU	4.7
1	F	246	LEU	4.7
1	E	66	ASN	4.7
1	F	433	PHE	4.7
1	F	388	VAL	4.7
1	B	436	GLY	4.6
1	D	376	VAL	4.6
1	C	375	ALA	4.5
1	F	313	ALA	4.5
1	B	442	ALA	4.5
1	E	61	GLU	4.5
1	A	62	GLY	4.5
1	F	62	GLY	4.5
1	F	9	ASN	4.5
1	F	75	ILE	4.5
1	E	142	SER	4.4
1	C	69	TYR	4.4
1	F	243	HIS	4.4
1	F	70	GLY	4.4
1	F	0	ASN	4.4
1	F	13	ALA	4.3
1	F	12	LEU	4.3
1	D	74	TYR	4.3
1	F	61	GLU	4.3
1	F	462	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	35	GLU	4.3
1	F	196	TRP	4.2
1	B	-1	SER	4.1
1	F	83	ARG	4.1
1	F	304	LYS	4.1
1	C	376	VAL	4.1
1	E	65	GLY	4.1
1	F	439	ASN	4.1
1	F	16	ASP	4.0
1	F	371	VAL	4.0
1	F	17	PRO	4.0
1	F	56	THR	4.0
1	B	358	ASN	4.0
1	F	374	ASN	4.0
1	F	259	GLY	4.0
1	F	440	ASN	4.0
1	F	53	SER	4.0
1	C	384	ALA	3.9
1	F	284	PHE	3.9
1	F	458	ASP	3.9
1	F	11	PRO	3.9
1	D	377	PHE	3.9
1	F	291	PRO	3.9
1	F	469	TYR	3.9
1	F	129	LEU	3.9
1	A	60	SER	3.8
1	F	318	VAL	3.8
1	D	379	ASP	3.7
1	F	275	PHE	3.7
1	A	378	GLY	3.7
1	C	437	LEU	3.7
1	D	66	ASN	3.7
1	F	242	THR	3.7
1	F	96	SER	3.7
1	F	51	LEU	3.7
1	F	340	GLY	3.7
1	F	60	SER	3.7
1	F	292	HIS	3.7
1	F	31	CYS	3.6
1	F	270	ASN	3.6
1	A	377	PHE	3.6
1	F	23	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	248	GLY	3.6
1	B	129	LEU	3.6
1	A	426	HIS	3.6
1	F	294	HIS	3.6
1	F	104	TYR	3.6
1	F	19	ILE	3.6
1	F	250	ARG	3.6
1	F	351	ARG	3.6
1	A	439	ASN	3.6
1	F	303	LEU	3.6
1	F	47	VAL	3.6
1	F	18	GLU	3.6
1	D	63	MET	3.5
1	B	333	GLY	3.5
1	F	10	THR	3.5
1	F	14	THR	3.5
1	A	67	ARG	3.5
1	F	39	SER	3.5
1	E	347	LEU	3.5
1	E	358	ASN	3.5
1	F	241	THR	3.5
1	E	375	ALA	3.5
1	D	-1	SER	3.5
1	F	5	SER	3.5
1	B	59	TYR	3.5
1	C	66	ASN	3.5
1	C	439	ASN	3.5
1	F	34	ILE	3.4
1	F	48	ILE	3.4
1	F	405	PHE	3.4
1	F	216	MET	3.4
1	F	82	CYS	3.4
1	E	422	ILE	3.4
1	F	88	GLN	3.4
1	F	45	PHE	3.4
1	F	99	VAL	3.4
1	A	0	ASN	3.4
1	F	78	ILE	3.4
1	F	213	LEU	3.4
1	F	43	THR	3.4
1	C	142	SER	3.4
1	F	245	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	373	LYS	3.4
1	A	379	ASP	3.4
1	B	0	ASN	3.4
1	A	63	MET	3.3
1	F	28	ARG	3.3
1	A	384	ALA	3.3
1	F	89	ALA	3.3
1	F	283	VAL	3.3
1	F	450	VAL	3.3
1	A	132	GLY	3.3
1	D	437	LEU	3.3
1	E	363	LEU	3.3
1	F	456	LEU	3.3
1	F	356	THR	3.3
1	E	-1	SER	3.3
1	F	238	VAL	3.3
1	C	62	GLY	3.3
1	C	284	PHE	3.3
1	F	298	ALA	3.3
1	F	133	GLY	3.3
1	F	87	LEU	3.3
1	A	422	ILE	3.3
1	A	263	PRO	3.2
1	D	262	PRO	3.2
1	F	361	GLU	3.2
1	F	453	PHE	3.2
1	A	-1	SER	3.2
1	E	63	MET	3.2
1	F	392	ALA	3.2
1	F	219	THR	3.2
1	F	370	THR	3.2
1	F	397	SER	3.2
1	C	61	GLU	3.2
1	F	134	HIS	3.2
1	A	437	LEU	3.2
1	F	295	GLN	3.2
1	E	433	PHE	3.2
1	F	92	LEU	3.2
1	D	284	PHE	3.1
1	C	133	GLY	3.1
1	F	455	ALA	3.1
1	E	272	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	69	TYR	3.1
1	F	325	LEU	3.1
1	C	356	THR	3.1
1	F	428	LYS	3.1
1	F	461	GLY	3.1
1	F	375	ALA	3.1
1	B	269	GLU	3.1
1	E	423	GLN	3.1
1	F	94	ALA	3.1
1	F	191	ALA	3.1
1	F	416	VAL	3.1
1	B	429	LEU	3.1
1	C	263	PRO	3.1
1	E	67	ARG	3.1
1	F	212	LEU	3.1
1	F	299	LEU	3.1
1	F	366	LEU	3.1
1	E	264	LYS	3.1
1	D	358	ASN	3.1
1	F	437	LEU	3.1
1	D	419	THR	3.0
1	F	57	ASN	3.0
1	F	364	CYS	3.0
1	B	375	ALA	3.0
1	F	401	VAL	3.0
1	A	134	HIS	3.0
1	C	426	HIS	3.0
1	E	164	THR	3.0
1	F	8	GLY	3.0
1	F	72	ASN	3.0
1	A	388	VAL	3.0
1	A	356	THR	3.0
1	D	270	ASN	3.0
1	F	310	GLY	3.0
1	B	377	PHE	3.0
1	C	438	VAL	3.0
1	F	288	GLN	3.0
1	A	387	GLY	3.0
1	B	270	ASN	3.0
1	E	333	GLY	3.0
1	E	425	GLU	3.0
1	F	73	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	348	TRP	3.0
1	B	352	PRO	3.0
1	C	262	PRO	3.0
1	A	135	LEU	2.9
1	F	22	LEU	2.9
1	F	355	LEU	2.9
1	B	438	VAL	2.9
1	C	272	VAL	2.9
1	F	187	CYS	2.9
1	F	27	LYS	2.9
1	F	58	LYS	2.9
1	E	32	ARG	2.9
1	F	408	ILE	2.9
1	A	69	TYR	2.9
1	F	52	GLY	2.9
1	F	393	PRO	2.9
1	C	275	PHE	2.9
1	F	30	GLN	2.9
1	E	369	ILE	2.9
1	F	328	TYR	2.9
1	B	458	ASP	2.9
1	E	434	ASN	2.9
1	F	2	ASP	2.9
1	F	311	PHE	2.9
1	F	350	LEU	2.9
1	A	371	VAL	2.9
1	C	65	GLY	2.9
1	F	334	TYR	2.9
1	B	281	PHE	2.9
1	F	225	ALA	2.9
1	E	348	TRP	2.9
1	F	6	VAL	2.9
1	F	185	ILE	2.9
1	F	296	ILE	2.9
1	E	439	ASN	2.9
1	F	449	ASP	2.9
1	C	273	TYR	2.8
1	B	437	LEU	2.8
1	C	430	LEU	2.8
1	F	37	ILE	2.8
1	D	434	ASN	2.8
1	D	439	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	321	ASN	2.8
1	F	358	ASN	2.8
1	F	372	ASN	2.8
1	F	409	GLY	2.8
1	A	137	HIS	2.8
1	F	167	TYR	2.8
1	B	384	ALA	2.8
1	D	271	ALA	2.8
1	E	269	GLU	2.8
1	F	49	GLU	2.8
1	E	274	ASP	2.8
1	F	357	GLY	2.8
1	A	262	PRO	2.8
1	F	463	LEU	2.8
1	D	283	VAL	2.8
1	A	348	TRP	2.8
1	C	432	ASP	2.8
1	F	97	TRP	2.8
1	D	469	TYR	2.8
1	C	374	ASN	2.7
1	F	188	GLY	2.7
1	C	63	MET	2.7
1	B	54	ALA	2.7
1	D	273	TYR	2.7
1	F	315	ALA	2.7
1	A	133	GLY	2.7
1	B	60	SER	2.7
1	F	218	HIS	2.7
1	F	42	PHE	2.7
1	F	391	GLY	2.7
1	F	26	GLU	2.7
1	B	348	TRP	2.7
1	F	235	CYS	2.7
1	F	459	MET	2.7
1	A	420	LEU	2.7
1	E	430	LEU	2.7
1	E	437	LEU	2.7
1	F	363	LEU	2.7
1	A	191	ALA	2.7
1	B	426	HIS	2.7
1	E	191	ALA	2.7
1	D	104	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	431	LYS	2.7
1	F	445	ASP	2.7
1	B	279	ILE	2.7
1	B	3	PRO	2.7
1	A	353	LEU	2.7
1	E	418	LEU	2.7
1	D	384	ALA	2.6
1	F	394	ALA	2.6
1	F	442	ALA	2.6
1	D	234	TYR	2.6
1	A	61	GLU	2.6
1	A	434	ASN	2.6
1	F	228	VAL	2.6
1	A	165	THR	2.6
1	A	427	GLY	2.6
1	E	387	GLY	2.6
1	B	430	LEU	2.6
1	F	362	LYS	2.6
1	A	375	ALA	2.6
1	B	306	ALA	2.6
1	F	38	ALA	2.6
1	F	306	ALA	2.6
1	D	272	VAL	2.6
1	F	106	GLY	2.6
1	A	39	SER	2.6
1	B	455	ALA	2.6
1	C	271	ALA	2.6
1	F	86	ALA	2.6
1	F	224	ALA	2.6
1	F	21	ASP	2.6
1	D	59	TYR	2.6
1	E	59	TYR	2.6
1	F	249	PRO	2.6
1	D	23	ILE	2.6
1	F	335	SER	2.6
1	B	217	ALA	2.6
1	E	374	ASN	2.6
1	D	221	GLY	2.6
1	F	103	PRO	2.6
1	F	124	ILE	2.6
1	F	91	HIS	2.6
1	C	87	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	270	ASN	2.5
1	F	432	ASP	2.5
1	A	138	GLY	2.5
1	E	70	GLY	2.5
1	F	164	THR	2.5
1	F	457	PHE	2.5
1	D	373	LYS	2.5
1	F	470	LYS	2.5
1	F	369	ILE	2.5
1	F	273	TYR	2.5
1	A	425	GLU	2.5
1	F	430	LEU	2.5
1	E	31	CYS	2.5
1	F	112	ALA	2.5
1	F	113	ALA	2.5
1	F	300	ALA	2.5
1	F	434	ASN	2.5
1	F	130	PRO	2.5
1	D	275	PHE	2.5
1	A	376	VAL	2.5
1	F	412	LEU	2.5
1	D	375	ALA	2.5
1	C	268	PRO	2.5
1	F	20	HIS	2.5
1	F	378	GLY	2.5
1	B	284	PHE	2.5
1	C	196	TRP	2.5
1	F	429	LEU	2.5
1	A	72	ASN	2.5
1	F	50	ALA	2.5
1	F	271	ALA	2.5
1	C	64	PRO	2.5
1	E	297	GLY	2.5
1	F	309	PRO	2.5
1	F	105	SER	2.4
1	B	4	VAL	2.4
1	F	281	PHE	2.4
1	C	59	TYR	2.4
1	D	420	LEU	2.4
1	D	430	LEU	2.4
1	F	36	LEU	2.4
1	F	400	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	373	LYS	2.4
1	F	100	ASN	2.4
1	E	64	PRO	2.4
1	E	415	ALA	2.4
1	B	164	THR	2.4
1	F	136	THR	2.4
1	D	190	SER	2.4
1	D	454	SER	2.4
1	E	284	PHE	2.4
1	A	428	LYS	2.4
1	C	355	LEU	2.4
1	D	287	LEU	2.4
1	C	358	ASN	2.4
1	D	432	ASP	2.4
1	A	166	GLY	2.4
1	A	333	GLY	2.4
1	D	109	ALA	2.4
1	E	62	GLY	2.4
1	F	217	ALA	2.4
1	F	346	VAL	2.4
1	C	429	LEU	2.4
1	D	118	LEU	2.4
1	F	353	LEU	2.4
1	D	426	HIS	2.4
1	F	256	TYR	2.4
1	A	372	ASN	2.4
1	C	415	ALA	2.4
1	E	33	GLY	2.4
1	E	427	GLY	2.4
1	A	149	THR	2.4
1	C	56	THR	2.4
1	B	39	SER	2.4
1	A	281	PHE	2.4
1	F	15	VAL	2.4
1	F	186	ILE	2.4
1	F	214	CYS	2.4
1	E	426	HIS	2.4
1	C	269	GLU	2.4
1	A	458	ASP	2.3
1	F	198	TYR	2.3
1	D	268	PRO	2.3
1	F	3	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	62	GLY	2.3
1	D	357	GLY	2.3
1	F	166	GLY	2.3
1	A	306	ALA	2.3
1	F	302	ALA	2.3
1	F	441	LYS	2.3
1	A	370	THR	2.3
1	E	168	ILE	2.3
1	F	90	PHE	2.3
1	F	67	ARG	2.3
1	D	429	LEU	2.3
1	E	365	ASP	2.3
1	F	236	ASP	2.3
1	F	365	ASP	2.3
1	C	348	TRP	2.3
1	F	234	TYR	2.3
1	E	132	GLY	2.3
1	D	54	ALA	2.3
1	C	237	ILE	2.3
1	F	443	ILE	2.3
1	D	127	LEU	2.3
1	F	418	LEU	2.3
1	C	469	TYR	2.3
1	E	307	ALA	2.3
1	F	46	ALA	2.3
1	D	241	THR	2.3
1	E	421	GLU	2.3
1	A	161	VAL	2.3
1	E	360	VAL	2.3
1	F	55	LEU	2.3
1	F	347	LEU	2.3
1	F	435	LYS	2.3
1	F	446	LEU	2.3
1	A	445	ASP	2.3
1	E	17	PRO	2.3
1	C	427	GLY	2.3
1	E	74	TYR	2.3
1	F	322	ALA	2.3
1	F	415	ALA	2.3
1	A	164	THR	2.3
1	D	136	THR	2.3
1	D	164	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	95	GLN	2.3
1	E	355	LEU	2.2
1	F	411	PHE	2.2
1	D	188	GLY	2.2
1	F	414	ARG	2.2
1	F	341	THR	2.2
1	A	163	SER	2.2
1	B	360	VAL	2.2
1	B	371	VAL	2.2
1	F	211	LEU	2.2
1	D	260	PRO	2.2
1	D	425	GLU	2.2
1	B	265	LYS	2.2
1	B	115	THR	2.2
1	B	142	SER	2.2
1	F	131	SER	2.2
1	E	7	TRP	2.2
1	A	443	ILE	2.2
1	D	254	ILE	2.2
1	A	55	LEU	2.2
1	D	433	PHE	2.2
1	C	0	ASN	2.2
1	E	351	ARG	2.2
1	F	93	ASP	2.2
1	F	108	PRO	2.2
1	B	425	GLU	2.2
1	C	470	LYS	2.2
1	E	431	LYS	2.2
1	A	86	ALA	2.2
1	B	191	ALA	2.2
1	B	320	ALA	2.2
1	D	300	ALA	2.2
1	D	350	LEU	2.2
1	B	432	ASP	2.2
1	E	438	VAL	2.2
1	F	101	VAL	2.2
1	D	61	GLU	2.2
1	F	137	HIS	2.2
1	A	392	ALA	2.2
1	E	29	ARG	2.1
1	C	135	LEU	2.1
1	F	152	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	283	VAL	2.1
1	F	71	GLY	2.1
1	F	172	ARG	2.1
1	A	167	TYR	2.1
1	B	366	LEU	2.1
1	D	355	LEU	2.1
1	E	254	ILE	2.1
1	F	127	LEU	2.1
1	F	253	MET	2.1
1	B	76	ASP	2.1
1	F	293	ASN	2.1
1	F	438	VAL	2.1
1	A	284	PHE	2.1
1	A	411	PHE	2.1
1	A	423	GLN	2.1
1	C	132	GLY	2.1
1	C	136	THR	2.1
1	E	172	ARG	2.1
1	F	367	CYS	2.1
1	D	142	SER	2.1
1	E	392	ALA	2.1
1	F	220	SER	2.1
1	F	395	MET	2.1
1	B	222	LEU	2.1
1	F	342	GLU	2.1
1	B	408	ILE	2.1
1	F	352	PRO	2.1
1	E	71	GLY	2.1
1	F	290	GLY	2.1
1	F	427	GLY	2.1
1	E	28	ARG	2.1
1	F	257	ARG	2.1
1	C	5	SER	2.1
1	F	417	THR	2.1
1	C	261	LYS	2.1
1	D	315	ALA	2.1
1	B	40	GLU	2.1
1	A	418	LEU	2.1
1	F	118	LEU	2.1
1	A	66	ASN	2.1
1	D	293	ASN	2.1
1	F	413	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	64	PRO	2.1
1	F	114	TYR	2.1
1	A	436	GLY	2.1
1	E	354	GLY	2.1
1	E	462	PHE	2.1
1	F	297	GLY	2.1
1	C	7	TRP	2.1
1	F	85	ARG	2.1
1	A	424	LYS	2.0
1	D	141	THR	2.0
1	F	239	THR	2.0
1	C	225	ALA	2.0
1	C	467	MET	2.0
1	A	430	LEU	2.0
1	C	372	ASN	2.0
1	F	287	LEU	2.0
1	D	443	ILE	2.0
1	B	74	TYR	2.0
1	F	272	VAL	2.0
1	F	323	VAL	2.0
1	A	65	GLY	2.0
1	C	70	GLY	2.0
1	F	144	GLY	2.0
1	D	232	PHE	2.0
1	A	136	THR	2.0
1	A	421	GLU	2.0
1	C	109	ALA	2.0
1	C	407	GLN	2.0
1	A	270	ASN	2.0
1	A	355	LEU	2.0
1	A	463	LEU	2.0
1	B	9	ASN	2.0
1	F	345	LEU	2.0
1	F	368	ASN	2.0
1	C	78	ILE	2.0
1	C	260	PRO	2.0
1	D	441	LYS	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. 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
1	LLP	F	244	24/25	0.81	0.21	64,78,89,91	0
1	LLP	B	244	24/25	0.87	0.15	28,33,35,36	0
1	LLP	C	244	24/25	0.88	0.14	34,42,47,47	0
1	LLP	D	244	24/25	0.91	0.13	28,36,40,41	0
1	LLP	A	244	24/25	0.91	0.15	33,43,47,48	0
1	LLP	E	244	24/25	0.92	0.14	38,45,51,51	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.