Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2024 – 06:23 PM EDT

PDB ID	:	9CG8
Title	:	CRYSTAL STRUCTURE OF THE P285S VARIANT OF SERINE HYDRO XYMETHYLTRANSFERASE 8 FROM SOYBEAN CULTIVAR FORREST
Authors	:	Beamer, L.J.; Samarakoon, V.; Owuocha, L.F.
Deposited on	:	2024-06-28
Resolution	:	1.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

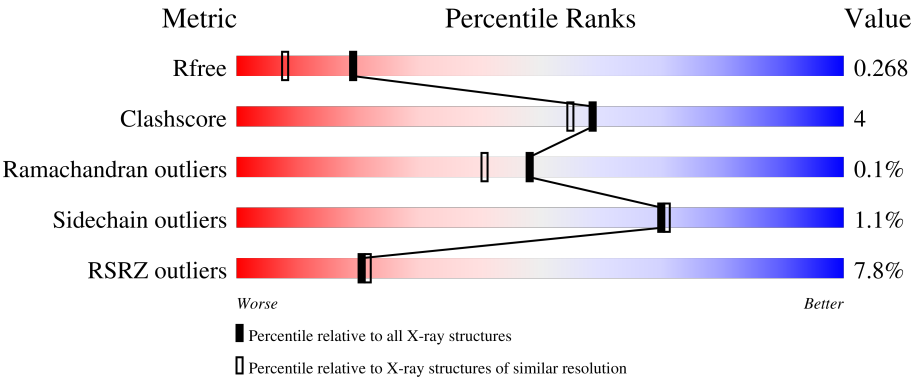
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	492	7% 82% 9% 8%
1	B	492	15% 80% 11% 8%
1	C	492	6% 83% 9% 8%
1	D	492	5% 83% 9% 8%
1	E	492	5% 81% 12% 7%

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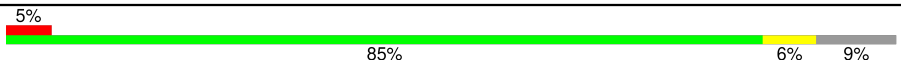
Mol	Chain	Length	Quality of chain
1	F	492	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 21398 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	451	Total	C	N	O	P	S	0	1	0
			3397	2155	580	644	1	17			
1	B	451	Total	C	N	O	P	S	0	2	0
			3358	2120	576	643	1	18			
1	C	452	Total	C	N	O	P	S	0	1	0
			3411	2168	585	640	1	17			
1	D	454	Total	C	N	O	P	S	0	1	0
			3476	2209	593	656	1	17			
1	E	458	Total	C	N	O	P	S	0	3	0
			3472	2204	589	659	1	19			
1	F	450	Total	C	N	O	P	S	0	2	0
			3419	2170	583	647	1	18			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP K4FW35
A	-19	GLY	-	expression tag	UNP K4FW35
A	-18	SER	-	expression tag	UNP K4FW35
A	-17	SER	-	expression tag	UNP K4FW35
A	-16	HIS	-	expression tag	UNP K4FW35
A	-15	HIS	-	expression tag	UNP K4FW35
A	-14	HIS	-	expression tag	UNP K4FW35
A	-13	HIS	-	expression tag	UNP K4FW35
A	-12	HIS	-	expression tag	UNP K4FW35
A	-11	HIS	-	expression tag	UNP K4FW35
A	-10	HIS	-	expression tag	UNP K4FW35
A	-9	SER	-	expression tag	UNP K4FW35
A	-8	SER	-	expression tag	UNP K4FW35
A	-7	GLY	-	expression tag	UNP K4FW35
A	-6	LEU	-	expression tag	UNP K4FW35
A	-5	VAL	-	expression tag	UNP K4FW35
A	-4	PRO	-	expression tag	UNP K4FW35

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ARG	-	expression tag	UNP K4FW35
A	-2	GLY	-	expression tag	UNP K4FW35
A	-1	SER	-	expression tag	UNP K4FW35
A	0	HIS	-	expression tag	UNP K4FW35
A	285	SER	PRO	engineered mutation	UNP K4FW35
B	-20	MET	-	expression tag	UNP K4FW35
B	-19	GLY	-	expression tag	UNP K4FW35
B	-18	SER	-	expression tag	UNP K4FW35
B	-17	SER	-	expression tag	UNP K4FW35
B	-16	HIS	-	expression tag	UNP K4FW35
B	-15	HIS	-	expression tag	UNP K4FW35
B	-14	HIS	-	expression tag	UNP K4FW35
B	-13	HIS	-	expression tag	UNP K4FW35
B	-12	HIS	-	expression tag	UNP K4FW35
B	-11	HIS	-	expression tag	UNP K4FW35
B	-10	HIS	-	expression tag	UNP K4FW35
B	-9	SER	-	expression tag	UNP K4FW35
B	-8	SER	-	expression tag	UNP K4FW35
B	-7	GLY	-	expression tag	UNP K4FW35
B	-6	LEU	-	expression tag	UNP K4FW35
B	-5	VAL	-	expression tag	UNP K4FW35
B	-4	PRO	-	expression tag	UNP K4FW35
B	-3	ARG	-	expression tag	UNP K4FW35
B	-2	GLY	-	expression tag	UNP K4FW35
B	-1	SER	-	expression tag	UNP K4FW35
B	0	HIS	-	expression tag	UNP K4FW35
B	285	SER	PRO	engineered mutation	UNP K4FW35
C	-20	MET	-	expression tag	UNP K4FW35
C	-19	GLY	-	expression tag	UNP K4FW35
C	-18	SER	-	expression tag	UNP K4FW35
C	-17	SER	-	expression tag	UNP K4FW35
C	-16	HIS	-	expression tag	UNP K4FW35
C	-15	HIS	-	expression tag	UNP K4FW35
C	-14	HIS	-	expression tag	UNP K4FW35
C	-13	HIS	-	expression tag	UNP K4FW35
C	-12	HIS	-	expression tag	UNP K4FW35
C	-11	HIS	-	expression tag	UNP K4FW35
C	-10	HIS	-	expression tag	UNP K4FW35
C	-9	SER	-	expression tag	UNP K4FW35
C	-8	SER	-	expression tag	UNP K4FW35
C	-7	GLY	-	expression tag	UNP K4FW35
C	-6	LEU	-	expression tag	UNP K4FW35

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	VAL	-	expression tag	UNP K4FW35
C	-4	PRO	-	expression tag	UNP K4FW35
C	-3	ARG	-	expression tag	UNP K4FW35
C	-2	GLY	-	expression tag	UNP K4FW35
C	-1	SER	-	expression tag	UNP K4FW35
C	0	HIS	-	expression tag	UNP K4FW35
C	285	SER	PRO	engineered mutation	UNP K4FW35
D	-20	MET	-	expression tag	UNP K4FW35
D	-19	GLY	-	expression tag	UNP K4FW35
D	-18	SER	-	expression tag	UNP K4FW35
D	-17	SER	-	expression tag	UNP K4FW35
D	-16	HIS	-	expression tag	UNP K4FW35
D	-15	HIS	-	expression tag	UNP K4FW35
D	-14	HIS	-	expression tag	UNP K4FW35
D	-13	HIS	-	expression tag	UNP K4FW35
D	-12	HIS	-	expression tag	UNP K4FW35
D	-11	HIS	-	expression tag	UNP K4FW35
D	-10	HIS	-	expression tag	UNP K4FW35
D	-9	SER	-	expression tag	UNP K4FW35
D	-8	SER	-	expression tag	UNP K4FW35
D	-7	GLY	-	expression tag	UNP K4FW35
D	-6	LEU	-	expression tag	UNP K4FW35
D	-5	VAL	-	expression tag	UNP K4FW35
D	-4	PRO	-	expression tag	UNP K4FW35
D	-3	ARG	-	expression tag	UNP K4FW35
D	-2	GLY	-	expression tag	UNP K4FW35
D	-1	SER	-	expression tag	UNP K4FW35
D	0	HIS	-	expression tag	UNP K4FW35
D	285	SER	PRO	engineered mutation	UNP K4FW35
E	-20	MET	-	expression tag	UNP K4FW35
E	-19	GLY	-	expression tag	UNP K4FW35
E	-18	SER	-	expression tag	UNP K4FW35
E	-17	SER	-	expression tag	UNP K4FW35
E	-16	HIS	-	expression tag	UNP K4FW35
E	-15	HIS	-	expression tag	UNP K4FW35
E	-14	HIS	-	expression tag	UNP K4FW35
E	-13	HIS	-	expression tag	UNP K4FW35
E	-12	HIS	-	expression tag	UNP K4FW35
E	-11	HIS	-	expression tag	UNP K4FW35
E	-10	HIS	-	expression tag	UNP K4FW35
E	-9	SER	-	expression tag	UNP K4FW35
E	-8	SER	-	expression tag	UNP K4FW35

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	GLY	-	expression tag	UNP K4FW35
E	-6	LEU	-	expression tag	UNP K4FW35
E	-5	VAL	-	expression tag	UNP K4FW35
E	-4	PRO	-	expression tag	UNP K4FW35
E	-3	ARG	-	expression tag	UNP K4FW35
E	-2	GLY	-	expression tag	UNP K4FW35
E	-1	SER	-	expression tag	UNP K4FW35
E	0	HIS	-	expression tag	UNP K4FW35
E	285	SER	PRO	engineered mutation	UNP K4FW35
F	-20	MET	-	expression tag	UNP K4FW35
F	-19	GLY	-	expression tag	UNP K4FW35
F	-18	SER	-	expression tag	UNP K4FW35
F	-17	SER	-	expression tag	UNP K4FW35
F	-16	HIS	-	expression tag	UNP K4FW35
F	-15	HIS	-	expression tag	UNP K4FW35
F	-14	HIS	-	expression tag	UNP K4FW35
F	-13	HIS	-	expression tag	UNP K4FW35
F	-12	HIS	-	expression tag	UNP K4FW35
F	-11	HIS	-	expression tag	UNP K4FW35
F	-10	HIS	-	expression tag	UNP K4FW35
F	-9	SER	-	expression tag	UNP K4FW35
F	-8	SER	-	expression tag	UNP K4FW35
F	-7	GLY	-	expression tag	UNP K4FW35
F	-6	LEU	-	expression tag	UNP K4FW35
F	-5	VAL	-	expression tag	UNP K4FW35
F	-4	PRO	-	expression tag	UNP K4FW35
F	-3	ARG	-	expression tag	UNP K4FW35
F	-2	GLY	-	expression tag	UNP K4FW35
F	-1	SER	-	expression tag	UNP K4FW35
F	0	HIS	-	expression tag	UNP K4FW35
F	285	SER	PRO	engineered mutation	UNP K4FW35

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	154	Total O 154 154	0	0
2	B	82	Total O 82 82	0	0
2	C	140	Total O 140 140	0	0
2	D	164	Total O 164 164	0	0

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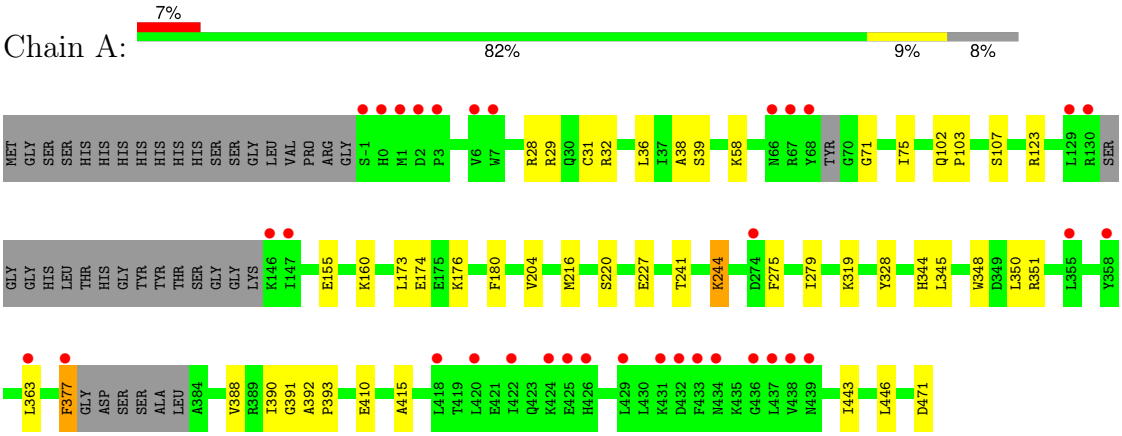
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	166	Total O 166 166	0	0
2	F	159	Total O 159 159	0	0

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.

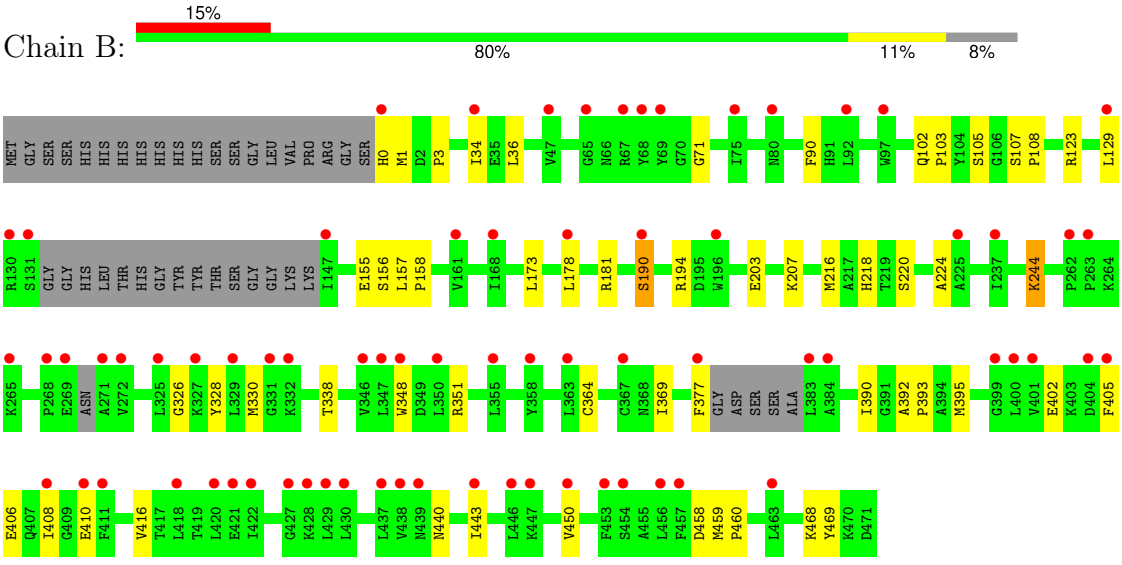
• Molecule 1: Serine hydroxymethyltransferase

Chain A:



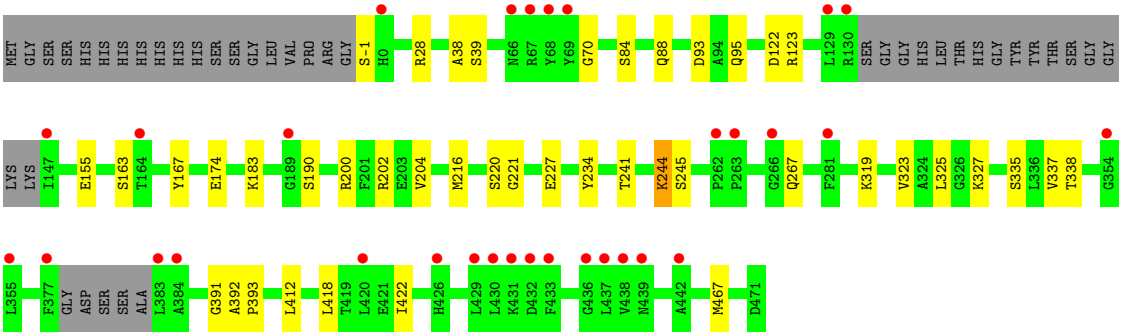
• Molecule 1: Serine hydroxymethyltransferase

Chain B:



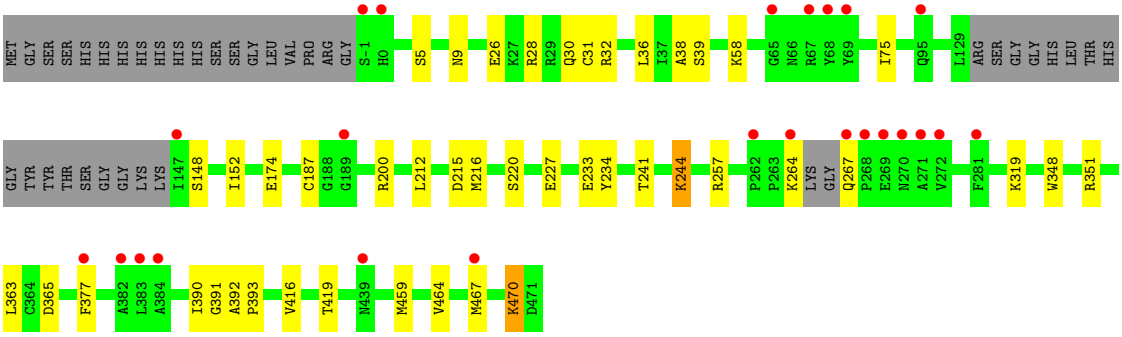
• Molecule 1: Serine hydroxymethyltransferase

Chain C:



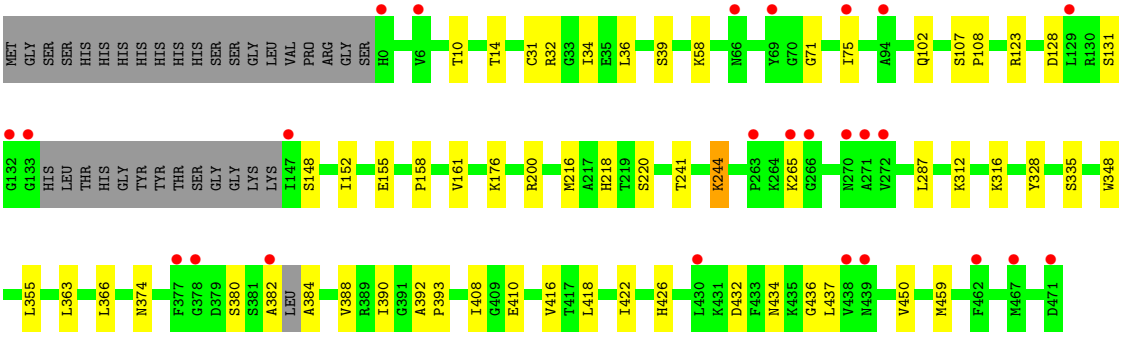
• Molecule 1: Serine hydroxymethyltransferase

Chain D:



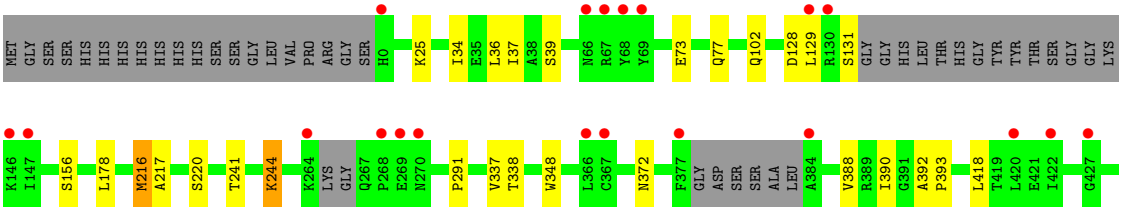
• Molecule 1: Serine hydroxymethyltransferase

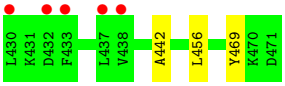
Chain E:



• Molecule 1: Serine hydroxymethyltransferase

Chain F:




L430
K431
D432
F433
L437
V438
A442
L456
Y469
K470
D471

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	174.18Å 174.18Å 183.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.50 – 1.90 48.50 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.50-1.90) 99.6 (48.50-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.227 , 0.266 0.231 , 0.268	Depositor DCC
R_{free} test set	12686 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 34.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21398	wwPDB-VP
Average B, all atoms (Å^2)	40.0	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 35.98 % 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 5.3619e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.41	1/3437 (0.0%)	0.61	0/4665
1	B	0.36	0/3403	0.58	0/4629
1	C	0.41	0/3453	0.61	0/4685
1	D	0.43	0/3518	0.62	0/4767
1	E	0.44	0/3518	0.63	0/4774
1	F	0.41	0/3464	0.62	0/4701
All	All	0.41	1/20793 (0.0%)	0.61	0/28221

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	CYS	CB-SG	-6.05	1.72	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3397	0	3209	30	0
1	B	3358	0	3064	37	0
1	C	3411	0	3244	24	0
1	D	3476	0	3365	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3472	0	3311	34	0
1	F	3419	0	3245	18	0
2	A	154	0	0	0	0
2	B	82	0	0	0	0
2	C	140	0	0	1	0
2	D	164	0	0	1	0
2	E	166	0	0	0	0
2	F	159	0	0	0	0
All	All	21398	0	19438	170	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (170) 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:B:0:HIS:HD2	1:B:1:MET:H	1.29	0.80
1:B:34:ILE:HG13	1:B:450:VAL:HG13	1.67	0.75
1:F:216:MET:HG3	1:F:220:SER:HB3	1.68	0.74
1:B:0:HIS:CD2	1:B:1:MET:H	2.05	0.74
1:E:34:ILE:HG13	1:E:450:VAL:HG13	1.69	0.72
1:B:459:MET:HG3	1:B:460:PRO:N	2.04	0.72
1:D:31:CYS:HB3	1:D:459:MET:HG2	1.71	0.70
1:D:58:LYS:HG2	1:D:75:ILE:HG13	1.73	0.70
1:B:34:ILE:HA	1:B:395:MET:HE1	1.76	0.67
1:B:34:ILE:HA	1:B:395:MET:CE	2.25	0.66
1:E:58:LYS:HE2	1:E:71:GLY:O	1.98	0.63
1:D:351:ARG:NH1	1:D:377:PHE:O	2.30	0.63
1:E:36:LEU:HB3	1:E:390:ILE:HG23	1.80	0.63
1:E:382:ALA:O	1:E:384:ALA:N	2.32	0.62
1:B:203:GLU:O	1:B:207:LYS:HG3	2.01	0.61
1:A:28:ARG:NE	1:A:471:ASP:O	2.33	0.60
1:D:39:SER:HB2	1:D:244[B]:LLP:HE3	1.83	0.60
1:D:363:LEU:HD13	1:D:419:THR:OG1	2.01	0.60
1:E:434:ASN:HA	1:E:437:LEU:HD12	1.82	0.60
1:D:39:SER:HB2	1:D:244[A]:LLP:HE3	1.84	0.60
1:B:351:ARG:HG3	1:B:351:ARG:HH11	1.67	0.60
1:E:131:SER:HB3	1:E:161:VAL:HG13	1.83	0.59
1:D:264:LYS:O	1:D:267:GLN:N	2.35	0.59
1:D:233:GLU:HG2	1:D:234:TYR:CE2	2.37	0.59
1:F:217:ALA:HB1	1:F:241:THR:HG22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:HG2	1:A:28:ARG:HH11	1.67	0.58
1:F:36:LEU:HB3	1:F:390:ILE:HG23	1.86	0.58
1:B:328:TYR:OH	1:B:410:GLU:OE1	2.21	0.58
1:E:328:TYR:OH	1:E:410:GLU:OE2	2.21	0.58
1:E:58:LYS:HG2	1:E:75:ILE:HG12	1.84	0.58
1:C:70:GLY:HA3	1:D:365:ASP:OD2	2.04	0.57
1:A:363:LEU:HD12	1:A:415:ALA:HB1	1.85	0.57
1:D:216:MET:HE3	1:D:220:SER:HB2	1.86	0.57
1:D:5:SER:HA	1:D:9:ASN:HD22	1.70	0.56
1:E:128:ASP:HB2	1:E:158:PRO:HB2	1.87	0.56
1:C:122:ASP:OD2	1:C:183:LYS:HE2	2.06	0.56
1:B:36:LEU:HB3	1:B:390:ILE:HG23	1.87	0.55
1:D:174:GLU:OE1	1:D:200:ARG:NH2	2.38	0.55
1:B:178:LEU:O	1:B:181:ARG:HD3	2.06	0.55
1:D:464:VAL:HA	1:D:467:MET:HG3	1.90	0.53
1:A:328:TYR:OH	1:A:410:GLU:OE1	2.27	0.53
1:D:227:GLU:HB3	1:D:319:LYS:HD3	1.90	0.53
1:C:84:SER:O	1:C:88:GLN:HG3	2.08	0.52
1:E:148:SER:O	1:E:152:ILE:HG13	2.08	0.52
1:C:337:VAL:HG12	1:C:338:THR:HG23	1.91	0.52
1:B:129:LEU:HD23	1:B:156:SER:HB2	1.90	0.52
1:E:363:LEU:HD11	1:E:418:LEU:HG	1.92	0.51
1:E:102:GLN:HB3	1:E:287:LEU:HD11	1.91	0.51
1:F:39:SER:HB2	1:F:244[A]:LLP:HE3	1.93	0.51
1:B:405:PHE:HA	1:B:408:ILE:HD12	1.92	0.50
1:F:39:SER:HB2	1:F:244[B]:LLP:HE3	1.92	0.50
1:D:348:TRP:CH2	1:D:416:VAL:HG21	2.46	0.50
1:C:216:MET:HG3	1:C:220:SER:HB3	1.92	0.50
1:A:363:LEU:HD21	1:A:443:ILE:HD11	1.93	0.50
1:B:216:MET:HG3	1:B:220:SER:HB3	1.94	0.50
1:B:218:HIS:HA	1:B:244[A]:LLP:HD2	1.94	0.49
1:A:377:PHE:N	1:A:377:PHE:CD1	2.79	0.49
1:A:241:THR:HG21	1:A:244[A]:LLP:HE2	1.95	0.48
1:F:102:GLN:OE1	1:F:291:PRO:HG3	2.14	0.48
1:A:28:ARG:CZ	1:A:32:ARG:HD2	2.43	0.48
1:C:325:LEU:HD11	1:C:412:LEU:HD12	1.96	0.48
1:A:275:PHE:HB3	1:A:279:ILE:HD12	1.95	0.48
1:C:39:SER:HB2	1:C:244[B]:LLP:HE3	1.96	0.48
1:D:148:SER:O	1:D:152:ILE:HG13	2.12	0.48
1:F:392:ALA:N	1:F:393:PRO:CD	2.77	0.47
1:A:39:SER:HB2	1:A:244[B]:LLP:HE3	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ARG:HG2	2:D:587:HOH:O	2.14	0.47
1:C:323:VAL:O	1:C:327:LYS:HG3	2.15	0.47
1:B:468:LYS:HD3	1:B:469:TYR:CE2	2.49	0.47
1:D:58:LYS:CG	1:D:75:ILE:HG13	2.44	0.47
1:F:25:LYS:HG3	1:F:469:TYR:CE2	2.50	0.47
1:B:402:GLU:O	1:B:406:GLU:HG3	2.14	0.46
1:F:418:LEU:HD21	1:F:442:ALA:HB1	1.98	0.46
1:C:392:ALA:N	1:C:393:PRO:HD3	2.30	0.46
1:E:366:LEU:HD12	1:E:437:LEU:HD22	1.97	0.46
1:E:392:ALA:N	1:E:393:PRO:CD	2.79	0.46
1:D:233:GLU:HG2	1:D:234:TYR:CD2	2.50	0.46
1:B:90:PHE:CE1	1:B:224:ALA:HB2	2.51	0.46
1:A:58:LYS:HG2	1:A:75:ILE:HG12	1.97	0.46
1:B:190:SER:HB2	1:B:244[A]:LLP:H5'2	1.98	0.46
1:D:58:LYS:HG2	1:D:75:ILE:CG1	2.44	0.46
1:C:174:GLU:HG3	1:C:204:VAL:HG22	1.98	0.46
1:E:123:ARG:HA	1:E:155:GLU:O	2.15	0.46
1:E:107:SER:HB3	1:E:108:PRO:HD3	1.98	0.46
1:D:470:LYS:HB3	1:D:470:LYS:HE3	1.45	0.45
1:A:58:LYS:HE2	1:A:71:GLY:O	2.16	0.45
1:F:392:ALA:N	1:F:393:PRO:HD3	2.31	0.45
1:A:227:GLU:HB3	1:A:319:LYS:HD3	1.99	0.45
1:E:312:LYS:HE3	1:E:316:LYS:HE2	1.98	0.45
1:A:348:TRP:HB3	1:A:388:VAL:HG23	1.98	0.45
1:C:93:ASP:OD2	1:C:95:GLN:HB2	2.16	0.45
1:A:415:ALA:HB2	1:A:446:LEU:HD21	1.97	0.45
1:C:183:LYS:HB3	1:C:183:LYS:HE3	1.63	0.45
1:E:31[B]:CYS:O	1:E:32:ARG:HD3	2.17	0.45
1:E:216:MET:HG3	1:E:220:SER:HB3	1.99	0.45
1:A:174:GLU:HG3	1:A:204:VAL:HG22	1.99	0.45
1:D:36:LEU:HB3	1:D:390:ILE:HG23	1.99	0.45
1:B:348:TRP:CH2	1:B:416:VAL:HG21	2.52	0.44
1:B:218:HIS:HA	1:B:244[B]:LLP:HD2	1.99	0.44
1:E:426:HIS:O	1:E:432:ASP:HB3	2.17	0.44
1:A:36:LEU:HB3	1:A:390:ILE:HG23	1.98	0.44
1:A:344:HIS:CE1	1:A:345:LEU:HD23	2.53	0.44
1:B:364:CYS:HB3	1:B:369:ILE:HB	2.00	0.44
1:C:123:ARG:HA	1:C:155:GLU:O	2.18	0.44
1:E:34:ILE:HD13	1:E:408:ILE:HG12	2.00	0.44
1:B:157:LEU:HD12	1:B:158:PRO:HD2	2.00	0.44
1:A:392:ALA:N	1:A:393:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:GLU:O	1:F:77:GLN:HG3	2.18	0.44
1:F:129:LEU:HG	1:F:156:SER:HB2	2.00	0.44
1:A:102:GLN:N	1:A:103:PRO:CD	2.81	0.43
1:E:31[B]:CYS:SG	1:E:459:MET:HB2	2.58	0.43
1:D:38:ALA:HA	1:D:391:GLY:HA3	2.00	0.43
1:A:39:SER:HB2	1:A:244[A]:LLP:HE3	2.01	0.43
1:B:34:ILE:HA	1:B:395:MET:HE2	2.01	0.43
1:C:39:SER:HB2	1:C:244[A]:LLP:HE3	2.00	0.43
1:D:392:ALA:N	1:D:393:PRO:CD	2.82	0.43
1:C:38:ALA:HA	1:C:391:GLY:HA3	2.00	0.43
1:C:221:GLY:N	1:C:245:SER:OG	2.48	0.43
1:E:218:HIS:HA	1:E:244[A]:LLP:HD2	2.01	0.43
1:E:348:TRP:HB3	1:E:388:VAL:HG23	2.01	0.42
1:F:216:MET:HG3	1:F:216:MET:O	2.18	0.42
1:D:187:CYS:SG	1:D:212:LEU:HD11	2.59	0.42
1:A:351:ARG:HE	1:A:351:ARG:HB2	1.51	0.42
1:D:28:ARG:CZ	1:D:32:ARG:HG3	2.50	0.42
1:E:10:THR:HG22	1:E:14:THR:OG1	2.20	0.42
1:F:178:LEU:HD23	1:F:178:LEU:HA	1.80	0.42
1:B:3:PRO:HG2	1:E:335:SER:OG	2.19	0.42
1:B:102:GLN:N	1:B:103:PRO:CD	2.83	0.42
1:B:440:ASN:HD22	1:B:443:ILE:H	1.67	0.42
1:F:34:ILE:HG22	1:F:36:LEU:HG	2.00	0.42
1:D:26:GLU:O	1:D:30:GLN:HG3	2.20	0.42
1:E:392:ALA:N	1:E:393:PRO:HD3	2.35	0.42
1:E:392:ALA:H	1:E:393:PRO:HD3	1.85	0.42
1:C:190:SER:HB3	1:C:244[A]:LLP:H5'2	2.02	0.42
1:A:38:ALA:HA	1:A:391:GLY:HA3	2.02	0.41
1:A:392:ALA:N	1:A:393:PRO:HD3	2.35	0.41
1:C:227:GLU:HB3	1:C:319:LYS:HD3	2.02	0.41
1:B:459:MET:HG3	1:B:460:PRO:CD	2.49	0.41
1:E:218:HIS:HA	1:E:244[B]:LLP:HD2	2.02	0.41
1:A:350:LEU:HD11	1:A:388:VAL:HG13	2.03	0.41
1:D:58:LYS:HD2	1:D:58:LYS:HA	1.83	0.41
1:B:194:ARG:NH2	1:B:338:THR:O	2.53	0.41
1:C:167:TYR:HB3	2:C:607:HOH:O	2.20	0.41
1:F:37:ILE:HG23	1:F:372:ASN:OD1	2.19	0.41
1:F:348:TRP:HB3	1:F:388:VAL:HG23	2.02	0.41
1:A:123:ARG:HB3	1:A:180:PHE:CE2	2.55	0.41
1:A:244[A]:LLP:H4'1	1:A:244[A]:LLP:OP3	2.20	0.41
1:B:105:SER:O	1:B:108:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:SER:HB3	1:B:108:PRO:HD3	2.03	0.41
1:B:326:GLY:O	1:B:330:MET:HB2	2.21	0.41
1:E:200:ARG:HD2	1:E:200:ARG:HA	1.87	0.41
1:A:29:ARG:HD2	1:B:71:GLY:HA2	2.03	0.41
1:F:337:VAL:HG12	1:F:338:THR:HG23	2.03	0.41
1:A:123:ARG:HA	1:A:155:GLU:O	2.21	0.41
1:B:123:ARG:HA	1:B:155:GLU:O	2.20	0.41
1:B:190:SER:HB2	1:B:244[A]:LLP:C5'	2.51	0.41
1:C:28:ARG:HA	1:C:467:MET:HE1	2.03	0.41
1:B:392:ALA:N	1:B:393:PRO:CD	2.84	0.41
1:D:215:ASP:OD2	1:D:244[A]:LLP:H2'3	2.21	0.41
1:E:355:LEU:HD23	1:E:355:LEU:HA	1.93	0.41
1:C:200:ARG:HA	1:C:200:ARG:HD2	1.86	0.40
1:E:39:SER:HB2	1:E:244[B]:LLP:HE3	2.03	0.40
1:D:392:ALA:N	1:D:393:PRO:HD3	2.36	0.40
1:A:216:MET:HG3	1:A:220:SER:HB3	2.03	0.40
1:C:392:ALA:N	1:C:393:PRO:CD	2.84	0.40
1:C:202:ARG:HB2	1:C:234:TYR:HB3	2.04	0.40
1:E:348:TRP:CH2	1:E:416:VAL:HG21	2.56	0.40
1:C:418:LEU:O	1:C:422:ILE:HG13	2.21	0.40
1:E:422:ILE:HG23	1:E:436:GLY:HA3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/492 (90%)	433 (98%)	9 (2%)	0	100	100
1	B	443/492 (90%)	423 (96%)	20 (4%)	0	100	100
1	C	445/492 (90%)	437 (98%)	8 (2%)	0	100	100
1	D	447/492 (91%)	431 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	453/492 (92%)	439 (97%)	13 (3%)	1 (0%)	44 36
1	F	442/492 (90%)	429 (97%)	12 (3%)	1 (0%)	44 36
All	All	2672/2952 (90%)	2592 (97%)	78 (3%)	2 (0%)	48 41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	128	ASP
1	E	265	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	334/402 (83%)	329 (98%)	5 (2%)	60 59
1	B	320/402 (80%)	316 (99%)	4 (1%)	65 65
1	C	336/402 (84%)	331 (98%)	5 (2%)	60 59
1	D	354/402 (88%)	352 (99%)	2 (1%)	84 86
1	E	348/402 (87%)	344 (99%)	4 (1%)	70 71
1	F	341/402 (85%)	338 (99%)	3 (1%)	75 77
All	All	2033/2412 (84%)	2010 (99%)	23 (1%)	70 71

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	SER
1	A	160	LYS
1	A	173	LEU
1	A	176	LYS
1	A	377	PHE
1	B	173	LEU
1	B	190	SER
1	B	377	PHE

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Mol	Chain	Res	Type
1	B	458	ASP
1	C	-1	SER
1	C	163	SER
1	C	241	THR
1	C	267	GLN
1	C	335	SER
1	D	241	THR
1	D	470	LYS
1	E	176	LYS
1	E	241	THR
1	E	374	ASN
1	E	380	SER
1	F	131	SER
1	F	216	MET
1	F	456	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	B	0	HIS
1	B	440	ASN
1	C	88	GLN
1	C	267	GLN
1	D	9	ASN
1	E	9	ASN
1	F	434	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 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	E	244[A]	1	23,24,25	2.51	6 (26%)	25,32,34	1.57	6 (24%)
1	LLP	B	244[A]	1	23,24,25	2.59	6 (26%)	25,32,34	1.60	6 (24%)
1	LLP	D	244[A]	1	23,24,25	2.58	7 (30%)	25,32,34	1.48	6 (24%)
1	LLP	F	244[A]	1	23,24,25	2.63	6 (26%)	25,32,34	1.40	4 (16%)
1	LLP	C	244[A]	1	23,24,25	2.53	6 (26%)	25,32,34	1.28	3 (12%)
1	LLP	A	244[B]	1	7,8,25	0.73	0	3,8,34	0.56	0
1	LLP	A	244[A]	1	23,24,25	2.54	6 (26%)	25,32,34	1.55	5 (20%)
1	LLP	E	244[B]	1	7,8,25	0.69	0	3,8,34	0.66	0
1	LLP	F	244[B]	1	7,8,25	0.66	0	3,8,34	0.58	0
1	LLP	B	244[B]	1	7,8,25	0.68	0	3,8,34	0.63	0
1	LLP	D	244[B]	1	7,8,25	0.71	0	3,8,34	0.50	0
1	LLP	C	244[B]	1	7,8,25	0.66	0	3,8,34	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	E	244[A]	1	-	7/16/17/19	0/1/1/1
1	LLP	B	244[A]	1	-	6/16/17/19	0/1/1/1
1	LLP	D	244[A]	1	-	4/16/17/19	0/1/1/1
1	LLP	F	244[A]	1	-	2/16/17/19	0/1/1/1
1	LLP	C	244[A]	1	-	4/16/17/19	0/1/1/1
1	LLP	A	244[B]	1	-	1/6/7/19	-
1	LLP	A	244[A]	1	-	7/16/17/19	0/1/1/1
1	LLP	E	244[B]	1	-	2/6/7/19	-
1	LLP	F	244[B]	1	-	1/6/7/19	-
1	LLP	B	244[B]	1	-	2/6/7/19	-
1	LLP	D	244[B]	1	-	1/6/7/19	-
1	LLP	C	244[B]	1	-	2/6/7/19	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	244[A]	LLP	C4-C4'	7.79	1.63	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	244[A]	LLP	C4-C4'	7.54	1.62	1.46
1	C	244[A]	LLP	C4-C4'	7.49	1.62	1.46
1	E	244[A]	LLP	C4-C4'	7.38	1.62	1.46
1	B	244[A]	LLP	C4-C4'	7.16	1.61	1.46
1	A	244[A]	LLP	C4-C4'	7.06	1.61	1.46
1	B	244[A]	LLP	C4'-NZ	5.05	1.44	1.27
1	F	244[A]	LLP	C4'-NZ	5.04	1.44	1.27
1	E	244[A]	LLP	C4'-NZ	4.95	1.43	1.27
1	C	244[A]	LLP	C4'-NZ	4.89	1.43	1.27
1	A	244[A]	LLP	C4'-NZ	4.88	1.43	1.27
1	D	244[A]	LLP	C4'-NZ	4.71	1.42	1.27
1	B	244[A]	LLP	C4-C5	-4.23	1.36	1.42
1	D	244[A]	LLP	C4-C5	-4.19	1.36	1.42
1	B	244[A]	LLP	C2'-C2	4.06	1.56	1.50
1	A	244[A]	LLP	C4-C5	-4.02	1.36	1.42
1	D	244[A]	LLP	C2'-C2	3.88	1.56	1.50
1	F	244[A]	LLP	C4-C5	-3.83	1.36	1.42
1	F	244[A]	LLP	C2'-C2	3.81	1.56	1.50
1	A	244[A]	LLP	C2'-C2	3.81	1.56	1.50
1	E	244[A]	LLP	C4-C5	-3.70	1.36	1.42
1	C	244[A]	LLP	C2'-C2	3.68	1.56	1.50
1	E	244[A]	LLP	C2'-C2	3.62	1.56	1.50
1	C	244[A]	LLP	C4-C5	-3.61	1.36	1.42
1	D	244[A]	LLP	C6-N1	3.59	1.41	1.34
1	B	244[A]	LLP	C6-N1	3.55	1.41	1.34
1	F	244[A]	LLP	C6-N1	3.49	1.41	1.34
1	A	244[A]	LLP	C6-N1	3.41	1.41	1.34
1	E	244[A]	LLP	C6-N1	3.34	1.41	1.34
1	C	244[A]	LLP	C6-N1	3.22	1.41	1.34
1	C	244[A]	LLP	C3-C2	2.32	1.43	1.41
1	F	244[A]	LLP	C3-C2	2.23	1.43	1.41
1	E	244[A]	LLP	C6-C5	2.12	1.41	1.37
1	B	244[A]	LLP	O3-C3	2.07	1.41	1.36
1	D	244[A]	LLP	C6-C5	2.05	1.41	1.37
1	D	244[A]	LLP	C5'-C5	2.03	1.56	1.50
1	A	244[A]	LLP	C5'-C5	2.03	1.56	1.50

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	244[A]	LLP	C4-C4'-NZ	-3.56	107.64	124.04
1	B	244[A]	LLP	C4-C4'-NZ	-3.32	108.70	124.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	244[A]	LLP	C4-C4'-NZ	-3.16	109.48	124.04
1	C	244[A]	LLP	C4-C4'-NZ	-3.14	109.53	124.04
1	D	244[A]	LLP	CE-NZ-C4'	-3.14	108.65	118.72
1	E	244[A]	LLP	C2'-C2-C3	-3.06	117.21	120.80
1	A	244[A]	LLP	CE-NZ-C4'	-2.96	109.25	118.72
1	F	244[A]	LLP	C4-C4'-NZ	-2.95	110.43	124.04
1	E	244[A]	LLP	C4-C4'-NZ	-2.91	110.61	124.04
1	B	244[A]	LLP	CE-NZ-C4'	-2.90	109.44	118.72
1	F	244[A]	LLP	C5-C6-N1	-2.89	119.13	123.83
1	C	244[A]	LLP	CE-NZ-C4'	-2.85	109.59	118.72
1	B	244[A]	LLP	C5-C6-N1	-2.81	119.26	123.83
1	B	244[A]	LLP	C3-C4-C5	2.77	120.50	118.28
1	A	244[A]	LLP	OP4-P-OP1	2.70	113.75	106.44
1	E	244[A]	LLP	CE-NZ-C4'	-2.68	110.12	118.72
1	E	244[A]	LLP	C2'-C2-N1	2.67	122.68	117.64
1	F	244[A]	LLP	CE-NZ-C4'	-2.64	110.27	118.72
1	A	244[A]	LLP	C3-C4-C5	2.59	120.35	118.28
1	E	244[A]	LLP	C5-C6-N1	-2.50	119.76	123.83
1	A	244[A]	LLP	C5-C6-N1	-2.50	119.76	123.83
1	C	244[A]	LLP	C5-C6-N1	-2.43	119.89	123.83
1	D	244[A]	LLP	C5-C6-N1	-2.41	119.91	123.83
1	B	244[A]	LLP	C2'-C2-N1	2.38	122.12	117.64
1	D	244[A]	LLP	C2'-C2-N1	2.26	121.90	117.64
1	B	244[A]	LLP	C2'-C2-C3	-2.24	118.18	120.80
1	E	244[A]	LLP	C4-C3-C2	2.19	121.38	120.14
1	D	244[A]	LLP	C2'-C2-C3	-2.18	118.25	120.80
1	D	244[A]	LLP	OP3-P-OP4	2.16	112.30	106.67
1	F	244[A]	LLP	C2'-C2-N1	2.02	121.44	117.64

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	244[A]	LLP	C5'-OP4-P-OP2
1	A	244[A]	LLP	C5'-OP4-P-OP3
1	A	244[A]	LLP	O-C-CA-CB
1	A	244[B]	LLP	O-C-CA-CB
1	B	244[A]	LLP	C5'-OP4-P-OP1
1	B	244[A]	LLP	C5'-OP4-P-OP2
1	B	244[A]	LLP	C5'-OP4-P-OP3
1	B	244[A]	LLP	C-CA-CB-CG
1	B	244[A]	LLP	O-C-CA-CB

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

There are no ring outliers.

12 monomers are involved in 20 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	244[B]	LLP	2	0
1	F	244[B]	LLP	1	0
1	B	244[B]	LLP	1	0
1	D	244[B]	LLP	1	0
1	C	244[B]	LLP	1	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 (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, 95^{th} 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	450/492 (91%)	0.56	34 (7%) 21 22	23, 38, 63, 82	0
1	B	450/492 (91%)	1.14	73 (16%) 5 5	25, 47, 72, 81	1 (0%)
1	C	451/492 (91%)	0.63	31 (6%) 24 25	24, 38, 67, 82	0
1	D	453/492 (92%)	0.38	24 (5%) 33 34	22, 35, 56, 80	0
1	E	457/492 (92%)	0.51	25 (5%) 32 33	18, 34, 56, 83	2 (0%)
1	F	449/492 (91%)	0.50	25 (5%) 31 32	21, 37, 62, 75	1 (0%)
All	All	2710/2952 (91%)	0.62	212 (7%) 20 21	18, 38, 65, 83	4 (0%)

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	383	LEU	6.4
1	A	422	ILE	4.7
1	F	377	PHE	4.5
1	D	147	ILE	4.3
1	B	129	LEU	4.3
1	E	129	LEU	4.2
1	F	69	TYR	4.2
1	B	383	LEU	4.2
1	D	264	LYS	4.1
1	C	69	TYR	4.1
1	B	438	VAL	4.1
1	A	-1	SER	4.0
1	B	422	ILE	4.0
1	C	438	VAL	3.9
1	C	147	ILE	3.9
1	B	329	LEU	3.9
1	C	68	TYR	3.9
1	B	272	VAL	3.8
1	B	377	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	68	TYR	3.8
1	A	130	ARG	3.8
1	B	68	TYR	3.6
1	A	429	LEU	3.6
1	A	67	ARG	3.6
1	B	437	LEU	3.5
1	B	439	ASN	3.4
1	B	420	LEU	3.4
1	F	420	LEU	3.4
1	C	129	LEU	3.4
1	F	422	ILE	3.4
1	B	350	LEU	3.4
1	E	270	ASN	3.3
1	F	129	LEU	3.3
1	F	130	ARG	3.3
1	B	69	TYR	3.3
1	F	264	LYS	3.3
1	D	384	ALA	3.3
1	A	433	PHE	3.3
1	A	355	LEU	3.3
1	B	443	ILE	3.3
1	C	432	ASP	3.2
1	D	272	VAL	3.2
1	A	437	LEU	3.2
1	B	67	ARG	3.2
1	C	437	LEU	3.2
1	C	164	THR	3.2
1	A	0	HIS	3.2
1	B	399	GLY	3.2
1	E	147	ILE	3.2
1	B	263	PRO	3.1
1	A	66	ASN	3.1
1	E	69	TYR	3.1
1	A	436	GLY	3.1
1	E	377	PHE	3.0
1	B	271	ALA	3.0
1	D	383	LEU	3.0
1	B	325	LEU	3.0
1	C	67	ARG	3.0
1	C	429	LEU	3.0
1	E	265	LYS	3.0
1	B	418	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	161	VAL	2.9
1	B	147	ILE	2.9
1	F	147	ILE	2.9
1	F	68	TYR	2.9
1	A	377	PHE	2.9
1	A	424	LYS	2.9
1	B	265	LYS	2.9
1	D	270	ASN	2.9
1	C	377	PHE	2.8
1	A	438	VAL	2.8
1	F	66	ASN	2.8
1	B	348	TRP	2.8
1	C	436	GLY	2.8
1	D	69	TYR	2.8
1	D	439	ASN	2.8
1	F	367	CYS	2.8
1	F	0	HIS	2.8
1	A	432	ASP	2.8
1	A	6	VAL	2.7
1	C	384	ALA	2.7
1	B	408	ILE	2.7
1	B	363	LEU	2.7
1	F	438	VAL	2.7
1	C	439	ASN	2.7
1	C	130	ARG	2.7
1	A	7	TRP	2.7
1	B	411	PHE	2.7
1	E	462	PHE	2.7
1	D	271	ALA	2.7
1	A	439	ASN	2.7
1	E	132	GLY	2.6
1	B	0	HIS	2.6
1	B	400	LEU	2.6
1	B	196	TRP	2.6
1	D	269	GLU	2.6
1	F	268	PRO	2.6
1	C	430	LEU	2.6
1	E	439	ASN	2.6
1	B	427	GLY	2.6
1	D	95	GLN	2.6
1	E	378	GLY	2.6
1	A	363	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	0	HIS	2.5
1	B	75	ILE	2.5
1	B	225	ALA	2.5
1	C	266	GLY	2.5
1	B	130	ARG	2.5
1	E	271	ALA	2.5
1	B	428	LYS	2.5
1	E	430	LEU	2.5
1	C	66	ASN	2.5
1	B	450	VAL	2.5
1	D	268	PRO	2.4
1	A	147	ILE	2.4
1	D	382	ALA	2.4
1	A	425	GLU	2.4
1	B	47	VAL	2.4
1	C	426	HIS	2.4
1	B	65	GLY	2.4
1	A	434	ASN	2.4
1	F	384	ALA	2.4
1	B	453	PHE	2.4
1	A	129	LEU	2.4
1	F	67	ARG	2.4
1	E	382	ALA	2.4
1	F	146	LYS	2.4
1	B	454	SER	2.4
1	A	2	ASP	2.4
1	A	3	PRO	2.4
1	E	266	GLY	2.4
1	C	433	PHE	2.4
1	D	281	PHE	2.4
1	B	347	LEU	2.3
1	B	355	LEU	2.3
1	E	467	MET	2.3
1	C	0	HIS	2.3
1	B	405	PHE	2.3
1	B	457	PHE	2.3
1	A	1	MET	2.3
1	B	269	GLU	2.3
1	C	262	PRO	2.3
1	C	263	PRO	2.3
1	E	263	PRO	2.3
1	D	-1	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	75	ILE	2.3
1	E	94	ALA	2.3
1	B	262	PRO	2.3
1	B	331	GLY	2.3
1	C	354	GLY	2.3
1	D	65	GLY	2.3
1	A	420	LEU	2.3
1	B	430	LEU	2.3
1	D	467	MET	2.2
1	D	267	GLN	2.2
1	F	269	GLU	2.2
1	D	67	ARG	2.2
1	B	92	LEU	2.2
1	F	366	LEU	2.2
1	B	168	ILE	2.2
1	D	0	HIS	2.2
1	A	418	LEU	2.2
1	B	178	LEU	2.2
1	A	146	LYS	2.2
1	B	80	ASN	2.2
1	E	66	ASN	2.2
1	D	68	TYR	2.2
1	B	237	ILE	2.2
1	A	431	LYS	2.2
1	F	270	ASN	2.2
1	F	427	GLY	2.2
1	B	429	LEU	2.2
1	B	463	LEU	2.2
1	C	442	ALA	2.2
1	F	437	LEU	2.2
1	A	358	TYR	2.2
1	B	34	ILE	2.2
1	B	131	SER	2.1
1	B	190	SER	2.1
1	B	327	LYS	2.1
1	C	431	LYS	2.1
1	B	346	VAL	2.1
1	C	189	GLY	2.1
1	B	446	LEU	2.1
1	C	355	LEU	2.1
1	B	384	ALA	2.1
1	B	404	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	432	ASP	2.1
1	B	410	GLU	2.1
1	E	133	GLY	2.1
1	B	401	VAL	2.1
1	E	6	VAL	2.1
1	A	274	ASP	2.1
1	E	471	ASP	2.1
1	B	456	LEU	2.1
1	F	430	LEU	2.1
1	F	433	PHE	2.1
1	B	447	LYS	2.1
1	B	358	TYR	2.1
1	B	421	GLU	2.1
1	A	426	HIS	2.0
1	B	367	CYS	2.0
1	E	272	VAL	2.0
1	D	262	PRO	2.0
1	C	281	PHE	2.0
1	D	377	PHE	2.0
1	B	97	TRP	2.0
1	D	189	GLY	2.0
1	B	332	LYS	2.0
1	B	268	PRO	2.0
1	E	438	VAL	2.0
1	C	420	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	B	244[A]	24/25	0.80	0.17	37,51,59,66	24
1	LLP	B	244[B]	9/25	0.80	0.17	37,39,46,50	9
1	LLP	F	244[A]	24/25	0.87	0.15	28,44,57,60	24
1	LLP	F	244[B]	9/25	0.87	0.15	28,29,37,42	9
1	LLP	C	244[A]	24/25	0.89	0.12	28,40,51,52	24
1	LLP	C	244[B]	9/25	0.89	0.12	28,30,36,39	9
1	LLP	E	244[A]	24/25	0.89	0.12	25,38,47,53	24
1	LLP	E	244[B]	9/25	0.89	0.12	24,28,35,37	9

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LLP	A	244[A]	24/25	0.89	0.13	27,42,51,53	24
1	LLP	A	244[B]	9/25	0.89	0.13	29,32,36,39	9
1	LLP	D	244[A]	24/25	0.90	0.11	25,37,45,48	24
1	LLP	D	244[B]	9/25	0.90	0.11	24,28,34,35	9

6.3 Carbohydrates (i)

There are no monosaccharides 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.