



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2022 – 12:23 PM EDT

PDB ID : 7MDL
Title : High-resolution crystal structure of human SepSecS-tRNA^{Sec} complex
Authors : Puppala, A.; French, R.L.; Simonovic, M.
Deposited on : 2021-04-05
Resolution : 2.32 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

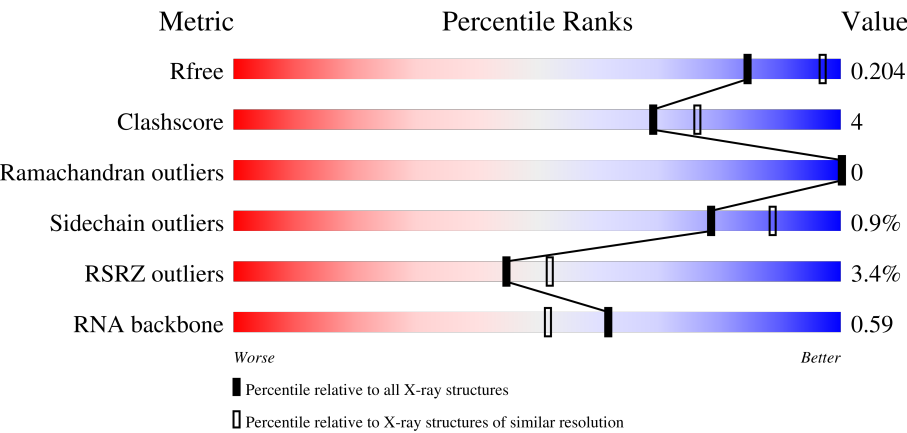
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)
RNA backbone	3102	1031 (2.70-1.94)

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	521	<div><div>3%</div><div>82%9%9%</div></div>
1	B	521	<div><div>%</div><div>80%6%14%</div></div>
1	C	521	<div><div>4%</div><div>84%7%9%</div></div>
1	D	521	<div><div></div><div>81%5%14%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	90	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FLC	A	1002	-	X	-	-
4	FLC	C	1002	-	-	X	-
4	FLC	D	1002	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19300 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 O-phosphoseryl-tRNA(Sec) selenium transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	6	0
			3678	2328	648	674	28			
1	B	447	Total	C	N	O	S	0	5	0
			3470	2201	611	631	27			
1	C	473	Total	C	N	O	S	0	8	0
			3675	2326	646	673	30			
1	D	448	Total	C	N	O	S	0	9	0
			3496	2219	615	634	28			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q9HD40
A	-18	GLY	-	expression tag	UNP Q9HD40
A	-17	SER	-	expression tag	UNP Q9HD40
A	-16	SER	-	expression tag	UNP Q9HD40
A	-15	HIS	-	expression tag	UNP Q9HD40
A	-14	HIS	-	expression tag	UNP Q9HD40
A	-13	HIS	-	expression tag	UNP Q9HD40
A	-12	HIS	-	expression tag	UNP Q9HD40
A	-11	HIS	-	expression tag	UNP Q9HD40
A	-10	HIS	-	expression tag	UNP Q9HD40
A	-9	SER	-	expression tag	UNP Q9HD40
A	-8	SER	-	expression tag	UNP Q9HD40
A	-7	GLY	-	expression tag	UNP Q9HD40
A	-6	LEU	-	expression tag	UNP Q9HD40
A	-5	VAL	-	expression tag	UNP Q9HD40
A	-4	PRO	-	expression tag	UNP Q9HD40
A	-3	ARG	-	expression tag	UNP Q9HD40
A	-2	GLY	-	expression tag	UNP Q9HD40
A	-1	SER	-	expression tag	UNP Q9HD40
A	0	HIS	-	expression tag	UNP Q9HD40
A	491	ALA	VAL	engineered mutation	UNP Q9HD40

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP Q9HD40
B	-18	GLY	-	expression tag	UNP Q9HD40
B	-17	SER	-	expression tag	UNP Q9HD40
B	-16	SER	-	expression tag	UNP Q9HD40
B	-15	HIS	-	expression tag	UNP Q9HD40
B	-14	HIS	-	expression tag	UNP Q9HD40
B	-13	HIS	-	expression tag	UNP Q9HD40
B	-12	HIS	-	expression tag	UNP Q9HD40
B	-11	HIS	-	expression tag	UNP Q9HD40
B	-10	HIS	-	expression tag	UNP Q9HD40
B	-9	SER	-	expression tag	UNP Q9HD40
B	-8	SER	-	expression tag	UNP Q9HD40
B	-7	GLY	-	expression tag	UNP Q9HD40
B	-6	LEU	-	expression tag	UNP Q9HD40
B	-5	VAL	-	expression tag	UNP Q9HD40
B	-4	PRO	-	expression tag	UNP Q9HD40
B	-3	ARG	-	expression tag	UNP Q9HD40
B	-2	GLY	-	expression tag	UNP Q9HD40
B	-1	SER	-	expression tag	UNP Q9HD40
B	0	HIS	-	expression tag	UNP Q9HD40
B	491	ALA	VAL	engineered mutation	UNP Q9HD40
C	-19	MET	-	initiating methionine	UNP Q9HD40
C	-18	GLY	-	expression tag	UNP Q9HD40
C	-17	SER	-	expression tag	UNP Q9HD40
C	-16	SER	-	expression tag	UNP Q9HD40
C	-15	HIS	-	expression tag	UNP Q9HD40
C	-14	HIS	-	expression tag	UNP Q9HD40
C	-13	HIS	-	expression tag	UNP Q9HD40
C	-12	HIS	-	expression tag	UNP Q9HD40
C	-11	HIS	-	expression tag	UNP Q9HD40
C	-10	HIS	-	expression tag	UNP Q9HD40
C	-9	SER	-	expression tag	UNP Q9HD40
C	-8	SER	-	expression tag	UNP Q9HD40
C	-7	GLY	-	expression tag	UNP Q9HD40
C	-6	LEU	-	expression tag	UNP Q9HD40
C	-5	VAL	-	expression tag	UNP Q9HD40
C	-4	PRO	-	expression tag	UNP Q9HD40
C	-3	ARG	-	expression tag	UNP Q9HD40
C	-2	GLY	-	expression tag	UNP Q9HD40
C	-1	SER	-	expression tag	UNP Q9HD40
C	0	HIS	-	expression tag	UNP Q9HD40
C	491	ALA	VAL	engineered mutation	UNP Q9HD40

Continued on next page...

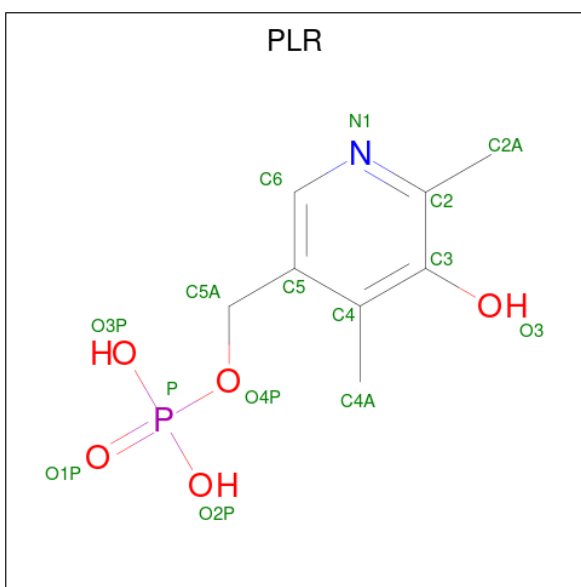
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP Q9HD40
D	-18	GLY	-	expression tag	UNP Q9HD40
D	-17	SER	-	expression tag	UNP Q9HD40
D	-16	SER	-	expression tag	UNP Q9HD40
D	-15	HIS	-	expression tag	UNP Q9HD40
D	-14	HIS	-	expression tag	UNP Q9HD40
D	-13	HIS	-	expression tag	UNP Q9HD40
D	-12	HIS	-	expression tag	UNP Q9HD40
D	-11	HIS	-	expression tag	UNP Q9HD40
D	-10	HIS	-	expression tag	UNP Q9HD40
D	-9	SER	-	expression tag	UNP Q9HD40
D	-8	SER	-	expression tag	UNP Q9HD40
D	-7	GLY	-	expression tag	UNP Q9HD40
D	-6	LEU	-	expression tag	UNP Q9HD40
D	-5	VAL	-	expression tag	UNP Q9HD40
D	-4	PRO	-	expression tag	UNP Q9HD40
D	-3	ARG	-	expression tag	UNP Q9HD40
D	-2	GLY	-	expression tag	UNP Q9HD40
D	-1	SER	-	expression tag	UNP Q9HD40
D	0	HIS	-	expression tag	UNP Q9HD40
D	491	ALA	VAL	engineered mutation	UNP Q9HD40

- Molecule 2 is a RNA chain called RNA (90-MER).

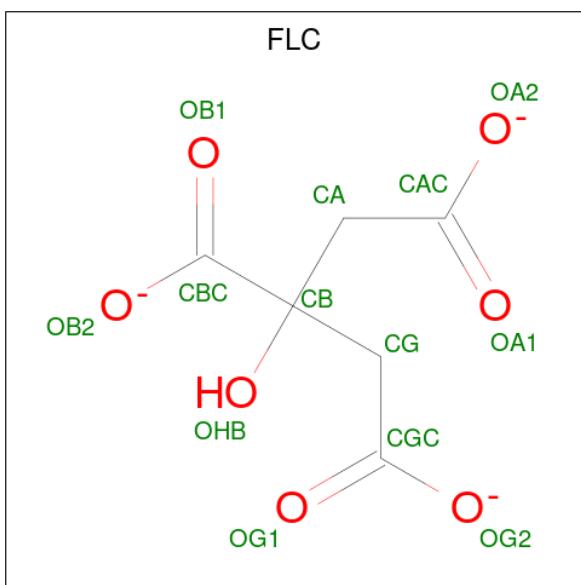
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	84	Total	C	N	O	P	0	84	0
			3558	1582	621	1187	168			

- Molecule 3 is (5-HYDROXY-4,6-DIMETHYLPYRIDIN-3-YL)METHYL DIHYDROGEN PHOSPHATE (three-letter code: PLR) (formula: C₈H₁₂NO₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0
4	C	1	Total C O 13 6 7	0	0
4	D	1	Total C O 13 6 7	0	0

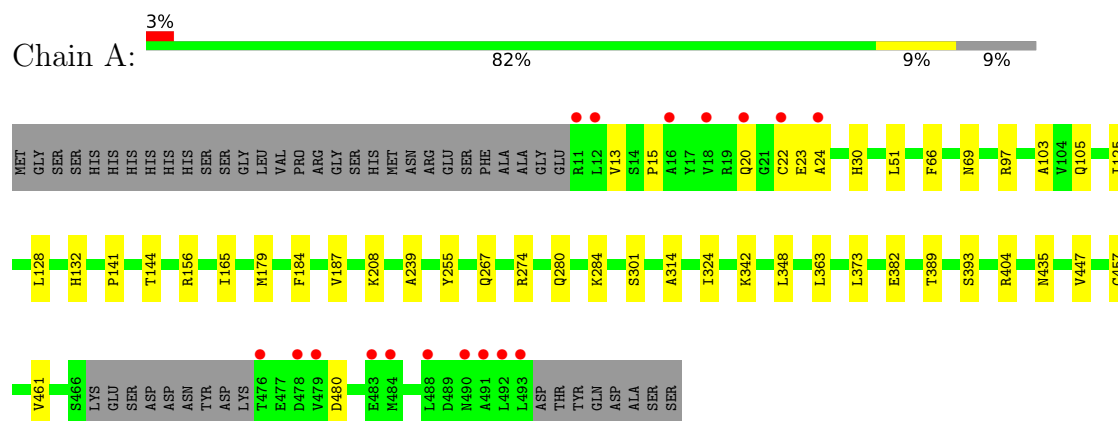
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	339	Total O 339 339	0	0
5	B	314	Total O 315 315	0	1
5	C	336	Total O 336 336	0	0
5	D	311	Total O 312 312	0	1
5	E	9	Total O 9 9	0	0

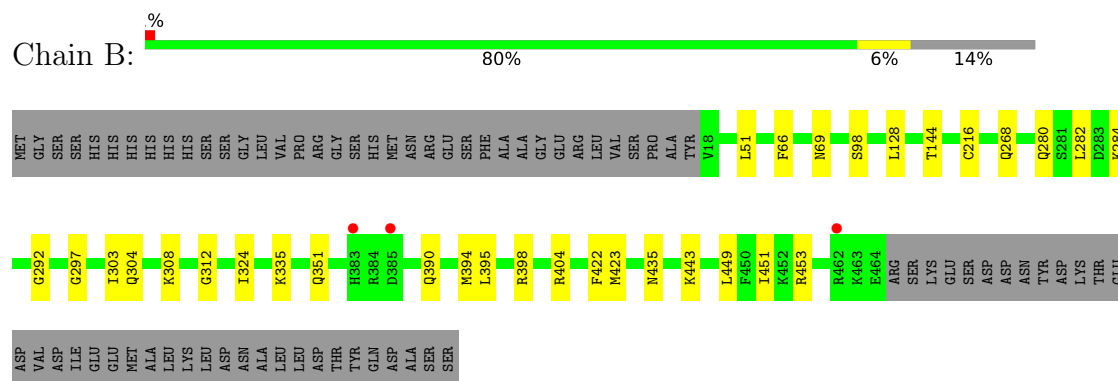
3 Residue-property plots [i](#)

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.

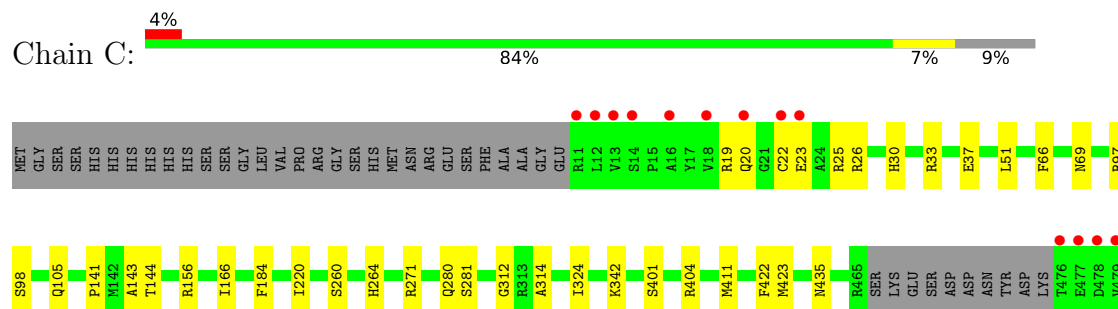
- Molecule 1: O-phosphoseryl-tRNA(Sec) selenium transferase

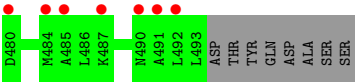


- Molecule 1: O-phosphoseryl-tRNA(Sec) selenium transferase

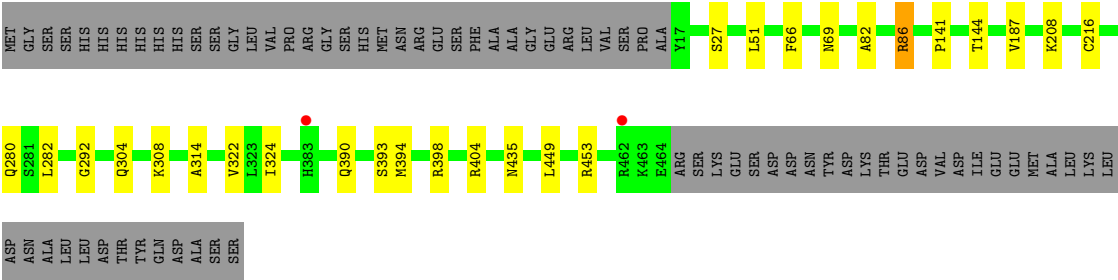
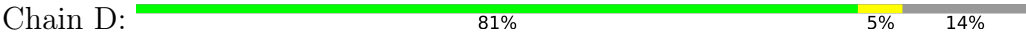


- Molecule 1: O-phosphoseryl-tRNA(Sec) selenium transferase

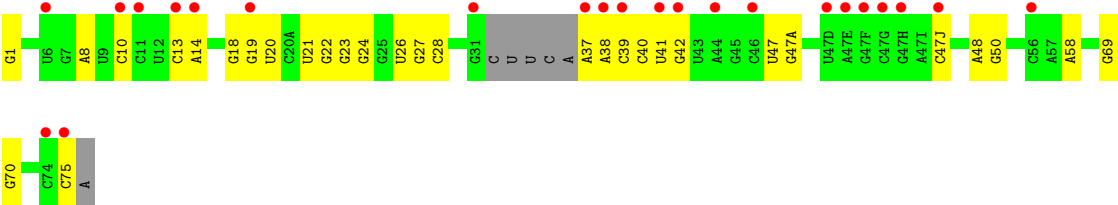




● Molecule 1: O-phosphoseryl-tRNA(Sec) selenium transferase



● Molecule 2: RNA (90-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	167.06Å 167.06Å 239.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.60 – 2.32 41.60 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.60-2.32) 89.9 (41.60-2.29)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.77 (at 2.29Å)	Xtriage
Refinement program	PHENIX 3951	Depositor
R, R_{free}	0.176 , 0.203 0.177 , 0.204	Depositor DCC
R_{free} test set	2051 reflections (1.21%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.479 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19300	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: FLC, PLR

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	0.25	0/3761	0.49	0/5081
1	B	0.25	0/3549	0.48	0/4791
1	C	0.26	0/3761	0.50	0/5083
1	D	0.25	0/3584	0.48	0/4840
2	E	36.10	4/3978 (0.1%)	1.51	8/6190 (0.1%)
All	All	16.68	4/18633 (0.0%)	0.85	8/25985 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	10[A]	C	C1'-N1	1610.05	25.63	1.48
2	E	10[B]	C	C1'-N1	1610.05	25.63	1.48
2	E	1[A]	G	OP3-P	-10.48	1.48	1.61
2	E	1[B]	G	OP3-P	-10.48	1.48	1.61

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	10[A]	C	N1-C1'-C2'	-61.46	34.10	114.00
2	E	10[B]	C	N1-C1'-C2'	-61.46	34.10	114.00
2	E	10[A]	C	C6-N1-C1'	-34.38	79.54	120.80
2	E	10[B]	C	C6-N1-C1'	-34.38	79.54	120.80
2	E	10[A]	C	C2-N1-C1'	-20.55	96.20	118.80
2	E	10[B]	C	C2-N1-C1'	-20.55	96.20	118.80
2	E	10[A]	C	O4'-C1'-N1	-14.37	96.70	108.20
2	E	10[B]	C	O4'-C1'-N1	-14.37	96.70	108.20

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	3678	0	3707	28	0
1	B	3470	0	3511	22	0
1	C	3675	0	3694	28	0
1	D	3496	0	3549	16	0
2	E	3558	0	1756	37	0
3	A	15	0	8	4	0
3	B	15	0	8	3	0
3	C	15	0	8	3	0
3	D	15	0	8	2	0
4	A	13	0	5	2	0
4	B	13	0	5	1	0
4	C	13	0	5	4	0
4	D	13	0	5	1	0
5	A	339	0	0	2	0
5	B	315	0	0	2	0
5	C	336	0	0	1	0
5	D	312	0	0	1	0
5	E	9	0	0	0	0
All	All	19300	0	16269	126	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 (126) 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:271:ARG:HH12	2:E:47(J)[B]:C:H4'	1.31	0.93
1:D:216:CYS:SG	5:D:1320:HOH:O	2.44	0.75
1:B:144:THR:HB	3:B:1001:PLR:H5A1	1.68	0.74
1:A:66:PHE:HB2	1:A:69:ASN:HB2	1.71	0.71
1:C:33:ARG:NH2	2:E:42[A]:G:OP1	2.24	0.70
1:C:66:PHE:HB2	1:C:69:ASN:HB2	1.73	0.70
1:B:216:CYS:SG	5:B:1358:HOH:O	2.51	0.69
1:D:82:ALA:HB1	1:D:86[A]:ARG:HH21	1.58	0.67
1:C:271:ARG:NH1	2:E:47(J)[B]:C:H4'	2.08	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:ARG:HB3	1:C:435:ASN:HB2	1.77	0.66
1:B:304:GLN:HG2	1:B:308:LYS:HE3	1.78	0.65
1:A:404:ARG:HB3	1:A:435:ASN:HB2	1.80	0.64
1:D:144:THR:HB	3:D:1001:PLR:H5A1	1.80	0.63
1:C:342:LYS:NZ	5:C:1106:HOH:O	2.31	0.62
1:A:97:ARG:HB3	4:A:1002:FLC:HA1	1.80	0.62
1:A:132:HIS:HD2	1:A:267:GLN:HE22	1.48	0.62
1:A:20:GLN:HG3	1:A:24:ALA:H	1.66	0.60
1:B:404:ARG:HB3	1:B:435:ASN:HB2	1.83	0.60
1:D:141:PRO:HG2	1:D:314:ALA:HB1	1.83	0.59
1:C:166:ILE:HB	1:C:220:ILE:HD13	1.84	0.58
1:C:19:ARG:NE	2:E:75[B]:C:H41	2.01	0.58
1:C:98:SER:HB2	4:C:1002:FLC:HG1	1.84	0.58
1:C:33:ARG:NH1	1:C:37:GLU:OE1	2.37	0.57
1:A:165:ILE:HD12	1:A:179:MET:HB3	1.87	0.57
2:E:37[A]:A:H3'	2:E:38[A]:A:H8	1.69	0.57
1:C:105:GLN:HE22	4:C:1002:FLC:HA1	1.70	0.56
1:B:398:ARG:HH22	2:E:38[B]:A:H4'	1.71	0.56
1:A:30[B]:HIS:CE1	2:E:41[B]:U:H4'	2.40	0.55
1:C:20:GLN:HG3	1:C:23:GLU:HB3	1.88	0.55
1:B:390:GLN:O	1:B:394:MET:HG3	2.06	0.55
1:B:268:GLN:NE2	5:B:1107:HOH:O	2.40	0.55
2:E:48[A]:A:H4'	2:E:50[A]:G:H5''	1.89	0.55
1:B:128:LEU:HD11	1:B:335:LYS:HE3	1.89	0.54
1:C:144:THR:HB	3:C:1001:PLR:H5A1	1.90	0.54
2:E:39[A]:C:H2'	2:E:40[A]:C:C6	2.43	0.53
1:A:342:LYS:HE3	5:A:1352:HOH:O	2.08	0.53
1:C:97:ARG:HB3	4:C:1002:FLC:HG2	1.90	0.53
4:D:1002:FLC:OG2	4:D:1002:FLC:OHB	2.26	0.52
1:D:66:PHE:HB2	1:D:69:ASN:HB2	1.91	0.52
1:A:30[B]:HIS:NE2	2:E:41[B]:U:H4'	2.25	0.51
1:C:30[A]:HIS:CE1	2:E:41[A]:U:H4'	2.45	0.51
1:D:282:LEU:HD22	1:D:322[A]:VAL:HG21	1.91	0.51
2:E:21[A]:U:H2'	2:E:22[A]:G:C8	2.46	0.51
1:A:284:LYS:NZ	3:A:1001:PLR:O3	2.44	0.50
1:B:51:LEU:HD21	1:B:324:ILE:HG23	1.93	0.50
2:E:47[B]:U:H2'	2:E:47(A)[B]:G:C8	2.46	0.50
1:B:66:PHE:HB2	1:B:69:ASN:HB2	1.94	0.50
2:E:37[A]:A:H3'	2:E:38[A]:A:C8	2.47	0.49
1:D:404:ARG:HB3	1:D:435:ASN:HB2	1.95	0.49
1:B:98[A]:SER:HA	1:B:312:GLY:HA2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:GLN:O	1:D:308:LYS:HG2	2.13	0.49
2:E:21[A]:U:H2'	2:E:22[A]:G:H8	1.78	0.49
1:D:394:MET:O	1:D:398:ARG:HD2	2.12	0.49
1:C:98:SER:HA	1:C:312:GLY:HA2	1.94	0.49
1:A:363:LEU:HD11	1:A:373:LEU:HD22	1.94	0.49
1:B:282:LEU:HD12	1:B:292:GLY:HA3	1.95	0.49
2:E:38[B]:A:H2'	2:E:39[B]:C:C6	2.48	0.49
1:B:98[B]:SER:HA	1:B:312:GLY:HA2	1.96	0.48
2:E:19[A]:G:H4'	2:E:20[A]:U:O5'	2.13	0.48
1:B:98[B]:SER:HB3	4:B:1002:FLC:HA1	1.94	0.48
1:C:97:ARG:HH21	4:C:1002:FLC:HOB	1.62	0.48
1:A:51:LEU:HD21	1:A:324:ILE:HG23	1.96	0.47
1:D:82:ALA:CB	1:D:86[A]:ARG:HH21	2.27	0.47
2:E:26[A]:U:H2'	2:E:27[A]:G:C8	2.48	0.47
1:C:51:LEU:HD21	1:C:324:ILE:HG23	1.95	0.47
1:A:105:GLN:HE22	4:A:1002:FLC:HG2	1.78	0.47
1:C:22:CYS:HA	1:C:25:ARG:HB3	1.95	0.47
1:D:187:VAL:HG11	1:D:208:LYS:HG2	1.96	0.47
2:E:47[A]:U:H2'	2:E:47(A)[A]:G:C8	2.50	0.47
1:D:393:SER:HA	2:E:75[B]:C:OP1	2.14	0.47
2:E:48[B]:A:H4'	2:E:50[B]:G:H5''	1.95	0.47
1:C:156:ARG:HB2	1:C:184:PHE:HZ	1.78	0.47
1:D:282:LEU:HD12	1:D:292:GLY:HA3	1.95	0.46
2:E:27[A]:G:O2'	2:E:28[A]:C:OP1	2.31	0.46
1:A:457:CYS:O	1:A:461:VAL:HG23	2.15	0.46
1:A:141:PRO:HG3	1:A:314:ALA:HB1	1.98	0.46
1:D:390:GLN:O	1:D:394:MET:HG3	2.16	0.45
3:B:1001:PLR:H4A1	3:B:1001:PLR:H5A2	1.49	0.45
1:A:348:LEU:HD13	1:A:447:VAL:HG22	1.98	0.45
1:A:382:GLU:OE2	1:A:389:THR:OG1	2.34	0.45
1:C:260:SER:O	1:C:264[A]:HIS:ND1	2.46	0.45
1:B:297:GLY:HA3	1:B:303:ILE:HD11	1.99	0.44
1:B:422:PHE:O	1:B:423:MET:HB2	2.17	0.44
1:C:20:GLN:HA	1:C:23:GLU:HB3	1.99	0.44
2:E:18[A]:G:N2	2:E:58[A]:A:OP2	2.50	0.44
2:E:41[A]:U:H2'	2:E:42[A]:G:C8	2.52	0.44
1:A:156:ARG:HB2	1:A:184:PHE:HZ	1.83	0.44
3:C:1001:PLR:H4A1	3:C:1001:PLR:H5A2	1.51	0.44
1:D:51:LEU:HD21	1:D:324:ILE:HG23	1.99	0.44
2:E:23[A]:G:H2'	2:E:24[A]:G:C8	2.53	0.44
2:E:47[B]:U:H2'	2:E:47(A)[B]:G:H8	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:HG3	1:A:103:ALA:HB3	2.00	0.43
1:A:187:VAL:HG11	1:A:208:LYS:HG2	2.00	0.43
2:E:13[B]:C:H2'	2:E:14[B]:A:C8	2.54	0.43
1:A:20:GLN:HG3	1:A:23:GLU:HB3	2.00	0.43
1:A:141:PRO:CG	1:A:314:ALA:HB1	2.48	0.43
1:B:304:GLN:O	1:B:308:LYS:HG3	2.19	0.43
1:B:443:LYS:HD3	1:B:443:LYS:HA	1.86	0.43
1:A:125:ILE:HD13	1:A:128:LEU:HD21	2.01	0.43
1:C:30[A]:HIS:CD2	2:E:41[A]:U:H5'	2.53	0.43
2:E:41[B]:U:H2'	2:E:42[B]:G:C8	2.54	0.43
1:C:23:GLU:O	1:C:26:ARG:HB2	2.18	0.42
1:D:449:LEU:O	1:D:453:ARG:HG3	2.19	0.42
2:E:19[A]:G:N2	2:E:20[A]:U:O4	2.53	0.42
1:B:284:LYS:NZ	3:B:1001:PLR:O3	2.53	0.42
3:A:1001:PLR:O3P	5:A:1101:HOH:O	2.21	0.42
1:A:13:VAL:O	1:A:15:PRO:HD3	2.20	0.42
1:A:144:THR:HB	3:A:1001:PLR:H5A1	2.02	0.42
1:C:141:PRO:CG	1:C:314:ALA:HB1	2.50	0.42
2:E:27[A]:G:HO2'	2:E:28[A]:C:P	2.41	0.42
1:A:255:TYR:HB3	1:A:284:LYS:HB3	2.02	0.41
1:B:351:GLN:HB3	1:B:451:ILE:HG13	2.02	0.41
3:D:1001:PLR:H5A2	3:D:1001:PLR:H4A1	1.46	0.41
1:B:395:LEU:HD23	1:B:395:LEU:HA	1.86	0.41
1:B:449:LEU:O	1:B:453:ARG:HG3	2.21	0.41
2:E:40[A]:C:H2'	2:E:41[A]:U:C6	2.56	0.41
2:E:69[A]:G:H2'	2:E:70[A]:G:H8	1.86	0.41
1:C:422:PHE:O	1:C:423:MET:HB2	2.20	0.41
2:E:47[A]:U:H2'	2:E:47(A)[A]:G:H8	1.85	0.41
2:E:23[A]:G:H2'	2:E:24[A]:G:H8	1.85	0.41
1:C:143:ALA:HB1	3:C:1001:PLR:O1P	2.21	0.41
2:E:27[A]:G:H2'	2:E:28[A]:C:C6	2.56	0.41
1:A:144:THR:HB	3:A:1001:PLR:C5A	2.51	0.40
1:C:404:ARG:NH1	1:C:435:ASN:OD1	2.53	0.40
1:A:239:ALA:HB1	1:A:274:ARG:H	1.87	0.40
2:E:8[B]:A:H1'	2:E:48[B]:A:N3	2.37	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	476/521 (91%)	459 (96%)	17 (4%)	0	100	100
1	B	450/521 (86%)	438 (97%)	12 (3%)	0	100	100
1	C	477/521 (92%)	463 (97%)	14 (3%)	0	100	100
1	D	455/521 (87%)	442 (97%)	13 (3%)	0	100	100
All	All	1858/2084 (89%)	1802 (97%)	56 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	399/446 (90%)	394 (99%)	5 (1%)	69	81
1	B	376/446 (84%)	375 (100%)	1 (0%)	92	96
1	C	397/446 (89%)	393 (99%)	4 (1%)	76	87
1	D	380/446 (85%)	376 (99%)	4 (1%)	73	85
All	All	1552/1784 (87%)	1538 (99%)	14 (1%)	78	89

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	CYS
1	A	280	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	301	SER
1	A	393	SER
1	A	480	ASP
1	B	280	GLN
1	C	280	GLN
1	C	281	SER
1	C	401	SER
1	C	411	MET
1	D	27	SER
1	D	86[A]	ARG
1	D	86[B]	ARG
1	D	280	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	B	350	ASN
1	D	20	GLN
1	D	445	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	0/90	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLR	B	1001	1	15,15,15	1.18	2 (13%)	20,22,22	1.37	3 (15%)
3	PLR	D	1001	1	15,15,15	1.22	2 (13%)	20,22,22	1.40	4 (20%)
4	FLC	B	1002	-	12,12,12	1.06	0	17,17,17	1.46	3 (17%)
4	FLC	D	1002	-	12,12,12	1.13	0	17,17,17	4.79	10 (58%)
3	PLR	A	1001	1	15,15,15	1.09	1 (6%)	20,22,22	1.15	3 (15%)
4	FLC	C	1002	-	12,12,12	1.00	0	17,17,17	1.40	2 (11%)
3	PLR	C	1001	1	15,15,15	1.22	2 (13%)	20,22,22	1.42	3 (15%)
4	FLC	A	1002	-	12,12,12	1.23	1 (8%)	17,17,17	4.66	10 (58%)

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
3	PLR	B	1001	1	-	3/6/6/6	0/1/1/1
3	PLR	D	1001	1	-	4/6/6/6	0/1/1/1
4	FLC	B	1002	-	-	7/16/16/16	-
4	FLC	D	1002	-	-	8/16/16/16	-
3	PLR	A	1001	1	-	0/6/6/6	0/1/1/1
4	FLC	C	1002	-	-	6/16/16/16	-
3	PLR	C	1001	1	-	3/6/6/6	0/1/1/1
4	FLC	A	1002	-	-	9/16/16/16	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1001	PLR	C2-N1	2.69	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	PLR	C2-N1	2.67	1.38	1.33
3	D	1001	PLR	C2-N1	2.66	1.38	1.33
3	A	1001	PLR	C2-N1	2.48	1.38	1.33
4	A	1002	FLC	CG-CB	2.16	1.56	1.53
3	C	1001	PLR	C6-N1	2.13	1.38	1.34
3	D	1001	PLR	C6-N1	2.09	1.38	1.34
3	B	1001	PLR	C6-N1	2.08	1.38	1.34

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1002	FLC	CG-CB-CBC	-10.45	87.65	110.11
4	A	1002	FLC	OHB-CB-CG	-9.96	86.10	109.40
4	D	1002	FLC	OHB-CB-CG	-9.54	87.07	109.40
4	A	1002	FLC	CG-CB-CBC	-8.82	91.16	110.11
4	D	1002	FLC	OHB-CB-CBC	8.25	120.45	108.86
4	A	1002	FLC	OHB-CB-CBC	7.54	119.44	108.86
4	A	1002	FLC	CG-CB-CA	-7.21	90.34	109.16
4	D	1002	FLC	CG-CB-CA	-7.14	90.52	109.16
4	A	1002	FLC	CA-CB-CBC	5.09	121.04	110.11
4	D	1002	FLC	OHB-CB-CA	4.53	120.01	109.40
4	A	1002	FLC	OHB-CB-CA	4.30	119.46	109.40
4	D	1002	FLC	CA-CB-CBC	4.29	119.31	110.11
4	C	1002	FLC	OB1-CBC-CB	-3.92	116.71	122.25
4	A	1002	FLC	OB1-CBC-CB	-3.77	116.92	122.25
4	B	1002	FLC	OB1-CBC-CB	-3.74	116.95	122.25
4	D	1002	FLC	OB1-CBC-CB	-3.36	117.50	122.25
3	C	1001	PLR	C6-C5-C4	3.30	120.75	118.16
3	D	1001	PLR	C6-C5-C4	3.14	120.63	118.16
3	B	1001	PLR	C6-C5-C4	2.88	120.43	118.16
3	C	1001	PLR	C5-C6-N1	-2.72	119.28	123.82
3	D	1001	PLR	C5-C6-N1	-2.67	119.36	123.82
3	A	1001	PLR	C6-C5-C4	2.63	120.23	118.16
3	B	1001	PLR	C5-C6-N1	-2.51	119.63	123.82
4	C	1002	FLC	OB2-CBC-CB	2.46	117.32	113.05
3	A	1001	PLR	C5-C6-N1	-2.35	119.91	123.82
4	B	1002	FLC	OG1-CGC-CG	-2.32	116.18	122.94
4	B	1002	FLC	OB2-CBC-CB	2.31	117.07	113.05
4	A	1002	FLC	OB2-CBC-CB	2.28	117.00	113.05
3	A	1001	PLR	O4P-C5A-C5	2.21	113.55	109.35
3	C	1001	PLR	C5A-C5-C6	2.21	123.00	119.37
3	D	1001	PLR	C4A-C4-C5	-2.15	118.72	120.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1002	FLC	OB2-CBC-CB	2.11	116.72	113.05
4	A	1002	FLC	OG1-CGC-CG	-2.10	116.80	122.94
4	D	1002	FLC	OG1-CGC-CG	-2.09	116.82	122.94
4	A	1002	FLC	OA1-CAC-CA	-2.09	116.83	122.94
3	D	1001	PLR	C5A-C5-C6	2.09	122.81	119.37
3	B	1001	PLR	O4P-C5A-C5	2.03	113.21	109.35
4	D	1002	FLC	OA1-CAC-CA	-2.02	117.05	122.94

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1001	PLR	C5A-O4P-P-O1P
3	B	1001	PLR	C5A-O4P-P-O2P
3	B	1001	PLR	C5A-O4P-P-O3P
3	C	1001	PLR	C5A-O4P-P-O1P
3	C	1001	PLR	C5A-O4P-P-O2P
3	C	1001	PLR	C5A-O4P-P-O3P
3	D	1001	PLR	C5A-O4P-P-O2P
3	D	1001	PLR	C5A-O4P-P-O3P
4	A	1002	FLC	CA-CB-CBC-OB1
4	A	1002	FLC	CA-CB-CBC-OB2
4	B	1002	FLC	CA-CB-CBC-OB2
4	B	1002	FLC	OHB-CB-CBC-OB2
4	C	1002	FLC	CG-CB-CBC-OB2
4	D	1002	FLC	OHB-CB-CBC-OB1
4	D	1002	FLC	OHB-CB-CBC-OB2
4	A	1002	FLC	CAC-CA-CB-OHB
4	D	1002	FLC	CAC-CA-CB-OHB
4	B	1002	FLC	CA-CB-CBC-OB1
4	D	1002	FLC	CA-CB-CBC-OB1
4	D	1002	FLC	CAC-CA-CB-CBC
3	D	1001	PLR	C5A-O4P-P-O1P
4	A	1002	FLC	OHB-CB-CBC-OB1
4	C	1002	FLC	OHB-CB-CBC-OB2
4	B	1002	FLC	CG-CB-CBC-OB1
4	B	1002	FLC	CG-CB-CBC-OB2
4	C	1002	FLC	CG-CB-CBC-OB1
4	D	1002	FLC	CA-CB-CBC-OB2
4	A	1002	FLC	CAC-CA-CB-CBC
4	A	1002	FLC	OHB-CB-CG-CGC
4	C	1002	FLC	CAC-CA-CB-OHB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	1002	FLC	OHB-CB-CG-CGC
4	C	1002	FLC	CA-CB-CBC-OB2
4	A	1002	FLC	OHB-CB-CBC-OB2
4	B	1002	FLC	OHB-CB-CBC-OB1
4	C	1002	FLC	CA-CB-CBC-OB1
4	A	1002	FLC	CB-CA-CAC-OA2
3	D	1001	PLR	C6-C5-C5A-O4P
4	A	1002	FLC	CB-CA-CAC-OA1
4	D	1002	FLC	CB-CG-CGC-OG1
4	D	1002	FLC	CB-CG-CGC-OG2

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1001	PLR	3	0
3	D	1001	PLR	2	0
4	B	1002	FLC	1	0
4	D	1002	FLC	1	0
3	A	1001	PLR	4	0
4	C	1002	FLC	4	0
3	C	1001	PLR	3	0
4	A	1002	FLC	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	474/521 (90%)	-0.36	17 (3%) 42 49	25, 37, 103, 173	0
1	B	447/521 (85%)	-0.47	3 (0%) 87 91	25, 38, 74, 118	0
1	C	473/521 (90%)	-0.35	20 (4%) 36 43	25, 37, 99, 157	0
1	D	448/521 (85%)	-0.47	2 (0%) 92 95	24, 38, 74, 116	0
2	E	84/90 (93%)	1.69	23 (27%) 0 0	44, 76, 96, 99	1 (1%)
All	All	1926/2174 (88%)	-0.32	65 (3%) 45 52	24, 38, 94, 173	1 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	47(G)[A]	C	10.2
1	A	16	ALA	8.9
2	E	74[A]	C	7.6
2	E	47(F)[A]	G	6.5
1	C	13	VAL	5.8
2	E	47(H)[A]	G	5.4
1	A	476	THR	5.3
1	C	476	THR	5.3
1	C	16	ALA	5.1
2	E	47(E)[A]	A	5.0
1	A	492	LEU	4.9
1	A	18	VAL	4.9
1	C	11	ARG	4.6
1	C	492	LEU	4.6
2	E	75[A]	C	4.5
1	C	12	LEU	4.2
1	A	22	CYS	4.1
1	A	11	ARG	4.0
2	E	42[A]	G	4.0
1	A	493	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	490	ASN	3.9
2	E	6[A]	U	3.7
1	A	12	LEU	3.7
1	C	484	MET	3.7
1	C	480	ASP	3.6
1	C	22	CYS	3.6
1	A	484	MET	3.5
1	C	479	VAL	3.5
2	E	14[A]	A	3.5
1	A	491	ALA	3.5
1	A	24	ALA	3.4
2	E	13[A]	C	3.3
2	E	38[A]	A	3.3
1	C	491	ALA	3.2
1	A	490	ASN	3.1
2	E	37[A]	A	3.1
1	A	479	VAL	3.1
2	E	19[A]	G	3.0
2	E	41[A]	U	2.9
2	E	11[A]	C	2.9
1	C	478	ASP	2.8
1	C	18	VAL	2.8
2	E	10[A]	C	2.7
1	A	20	GLN	2.7
1	B	385	ASP	2.6
2	E	47(D)[A]	U	2.5
2	E	31[A]	G	2.5
1	D	462	ARG	2.4
2	E	47(J)[A]	C	2.4
1	C	20	GLN	2.4
1	C	23	GLU	2.4
1	C	477	GLU	2.4
1	B	383	HIS	2.3
1	A	483	GLU	2.3
1	A	478	ASP	2.2
2	E	56[A]	C	2.2
1	A	488	LEU	2.2
1	D	383	HIS	2.2
2	E	39[A]	C	2.2
1	B	462	ARG	2.1
2	E	44[A]	A	2.1
1	C	487	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	485	ALA	2.0
1	C	14	SER	2.0
2	E	46[A]	C	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [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, 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(\AA^2)	Q<0.9
4	FLC	C	1002	13/13	0.84	0.14	64,79,87,89	0
4	FLC	B	1002	13/13	0.87	0.23	58,83,94,96	0
4	FLC	A	1002	13/13	0.88	0.15	75,83,93,99	0
4	FLC	D	1002	13/13	0.92	0.25	57,76,91,106	0
3	PLR	A	1001	15/15	0.99	0.11	28,34,41,43	0
3	PLR	B	1001	15/15	0.99	0.11	27,35,39,43	0
3	PLR	C	1001	15/15	0.99	0.12	26,35,40,42	0
3	PLR	D	1001	15/15	0.99	0.10	26,35,41,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.