



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:06 AM GMT

PDB ID : 3ISS
Title : Crystal structure of enolpyruvyl-UDP-GlcNAcsynthase (MurA):UDP-N-acetyl-muramic acid:phosphite from Escherichia coli
Authors : Jackson, S.G.; Zhang, F.; Chindemi, P.; Junop, M.S.; Berti, P.J.
Deposited on : 2009-08-27
Resolution : 2.50 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

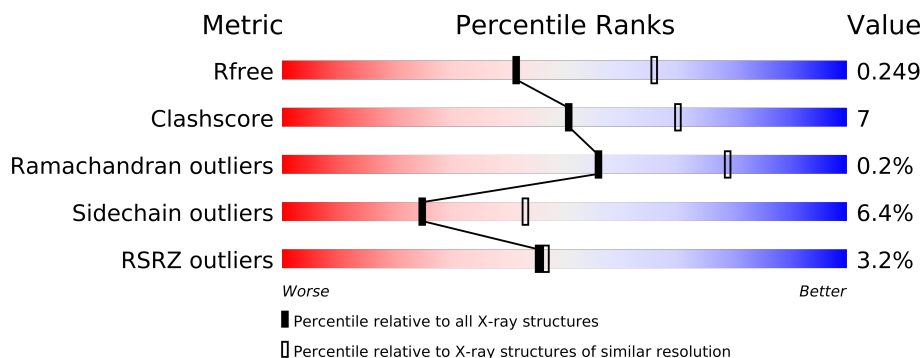
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	418	
1	B	418	
1	C	418	
1	D	418	
1	E	418	
1	F	418	
1	G	418	
1	H	418	
1	I	418	
1	J	418	
1	K	418	
1	L	418	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PO3	A	501	-	X
2	PO3	C	502	-	X
2	PO3	E	504	-	X
2	PO3	H	508	-	X
2	PO3	I	509	-	X
2	PO3	J	510	-	X
2	PO3	K	511	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 39025 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called UDP-N-acetylglucosamine1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	B	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	C	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	D	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	E	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	F	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	G	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	H	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	I	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	J	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	K	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	L	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			

There are 12 discrepancies between the modelled and reference sequences:

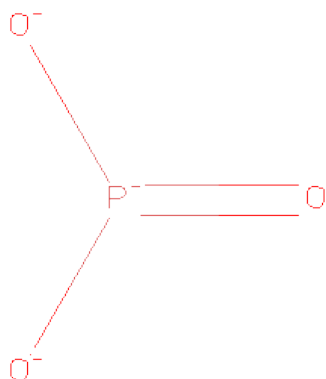
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ASP	ASN	ENGINEERED	UNP P0A749
B	67	ASP	ASN	ENGINEERED	UNP P0A749
C	67	ASP	ASN	ENGINEERED	UNP P0A749
D	67	ASP	ASN	ENGINEERED	UNP P0A749
E	67	ASP	ASN	ENGINEERED	UNP P0A749

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	67	ASP	ASN	ENGINEERED	UNP P0A749
G	67	ASP	ASN	ENGINEERED	UNP P0A749
H	67	ASP	ASN	ENGINEERED	UNP P0A749
I	67	ASP	ASN	ENGINEERED	UNP P0A749
J	67	ASP	ASN	ENGINEERED	UNP P0A749
K	67	ASP	ASN	ENGINEERED	UNP P0A749
L	67	ASP	ASN	ENGINEERED	UNP P0A749

- Molecule 2 is PHOSPHITE ION (three-letter code: PO3) (formula: O₃P).



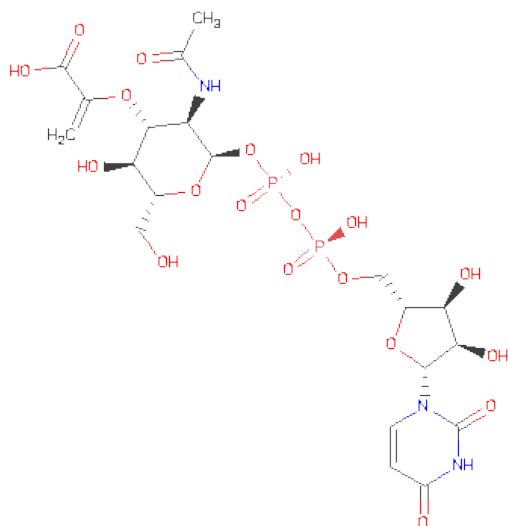
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			4	3	1		
2	B	1	Total	O	P	0	0
			4	3	1		
2	C	1	Total	O	P	0	0
			4	3	1		
2	D	1	Total	O	P	0	0
			4	3	1		
2	E	1	Total	O	P	0	0
			4	3	1		
2	F	1	Total	O	P	0	0
			4	3	1		
2	G	1	Total	O	P	0	0
			4	3	1		
2	H	1	Total	O	P	0	0
			4	3	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	O	P	0	0
			4	3	1		
2	J	1	Total	O	P	0	0
			4	3	1		
2	K	1	Total	O	P	0	0
			4	3	1		
2	L	1	Total	O	P	0	0
			4	3	1		

- Molecule 3 is URIDINE-DIPHOSPHATE-2(N-ACETYLGLUCOSAMINYL)BUTYRIC ACID (three-letter code: EPU) (formula: C₂₀H₂₉N₃O₁₉P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	B	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	C	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	D	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	E	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	F	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	G	1	Total	C	N	O	P	0	0
			44	20	3	19	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	I	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	J	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	K	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	L	1	Total	C	N	O	P	0	0
			44	20	3	19	2		

- Molecule 4 is water.

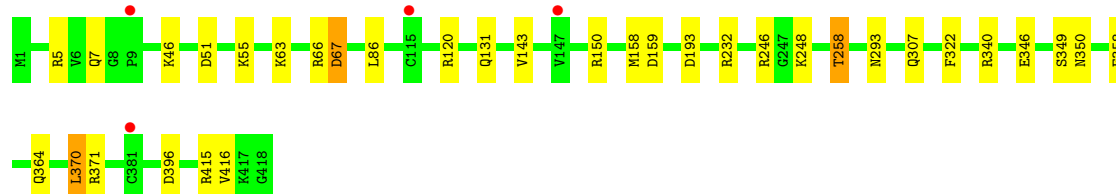
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	63	Total	O	0	0
			63	63		
4	C	112	Total	O	0	0
			112	112		
4	D	106	Total	O	0	0
			106	106		
4	E	83	Total	O	0	0
			83	83		
4	F	69	Total	O	0	0
			69	69		
4	G	54	Total	O	0	0
			54	54		
4	H	84	Total	O	0	0
			84	84		
4	I	43	Total	O	0	0
			43	43		
4	J	55	Total	O	0	0
			55	55		
4	K	69	Total	O	0	0
			69	69		
4	L	36	Total	O	0	0
			36	36		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

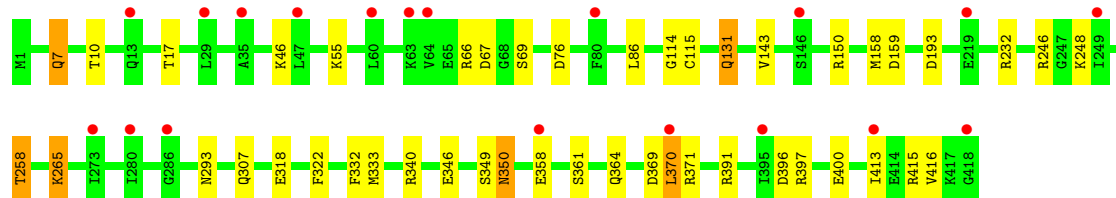
- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain A: 



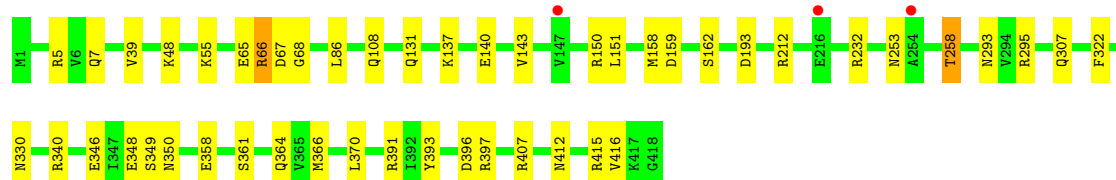
- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain B: 



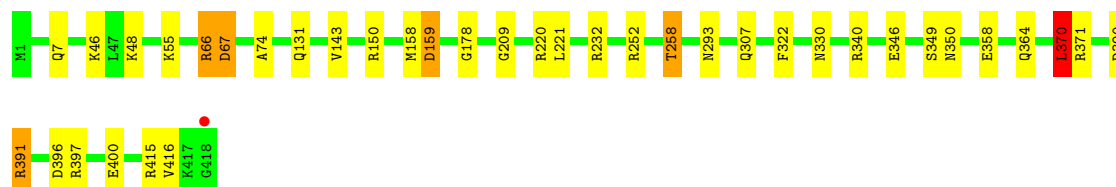
- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain C: 



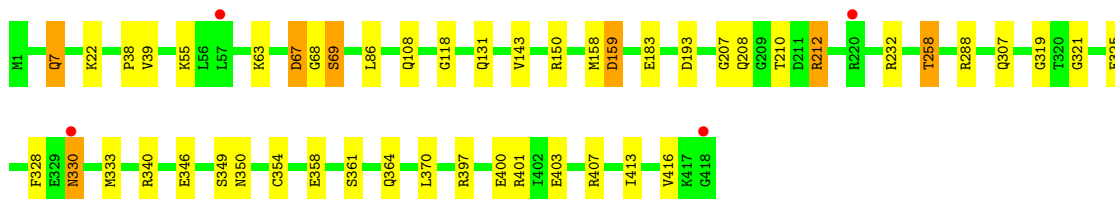
- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain D: 



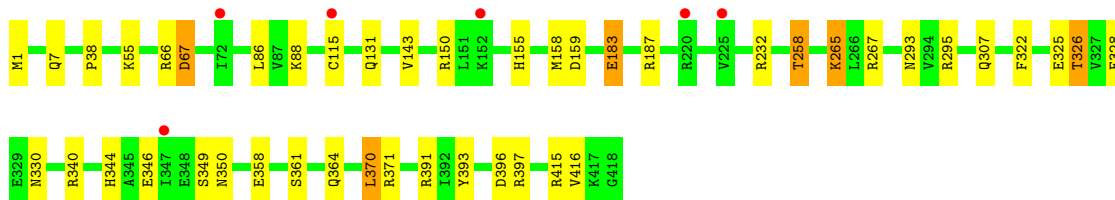
- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain E:



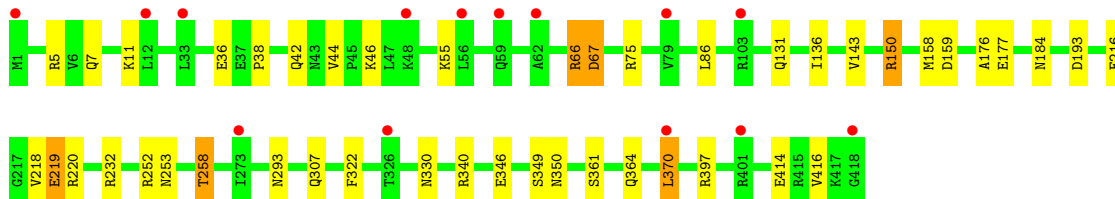
- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain F:



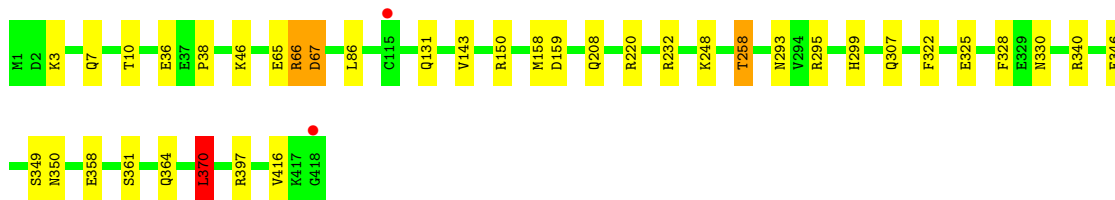
- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain G:



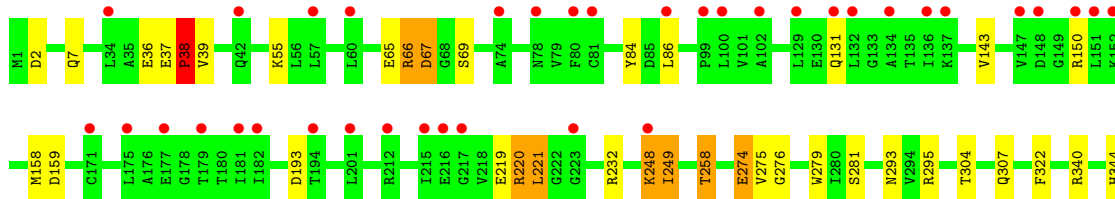
- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain H:



- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

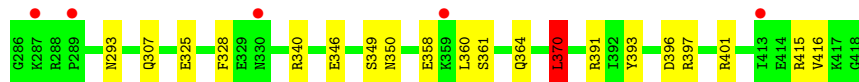
Chain I:





- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain J:



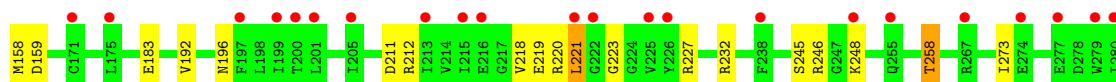
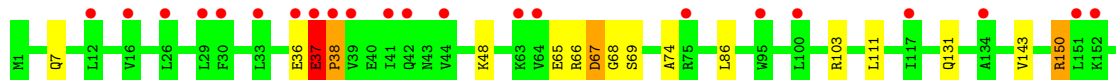
- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain K:



- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.51Å 120.91Å 139.73Å 111.52° 104.44° 90.19°	Depositor
Resolution (Å)	47.48 – 2.50 47.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.48-2.50) 97.6 (47.48-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.222 , 0.254 0.217 , 0.249	Depositor DCC
R_{free} test set	8364 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 167326 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	39025	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPU, PO3

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	0.49	0/3176	0.61	1/4298 (0.0%)
1	B	0.51	1/3176 (0.0%)	0.60	3/4298 (0.1%)
1	C	0.54	0/3176	0.63	3/4298 (0.1%)
1	D	0.53	0/3176	0.62	2/4298 (0.0%)
1	E	0.51	0/3176	0.65	1/4298 (0.0%)
1	F	0.56	1/3176 (0.0%)	0.60	1/4298 (0.0%)
1	G	0.50	0/3176	0.62	2/4298 (0.0%)
1	H	0.53	0/3176	0.59	3/4298 (0.1%)
1	I	0.52	0/3176	0.59	1/4298 (0.0%)
1	J	0.48	0/3176	0.58	2/4298 (0.0%)
1	K	0.51	0/3176	0.59	2/4298 (0.0%)
1	L	0.52	0/3176	0.61	1/4298 (0.0%)
All	All	0.52	2/38112 (0.0%)	0.61	22/51576 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	115	CYS	CB-SG	-5.21	1.73	1.81
1	B	115	CYS	C-N	-5.09	1.22	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	67	ASP	CB-CG-OD1	18.46	134.91	118.30
1	A	67	ASP	CB-CG-OD1	17.43	133.98	118.30
1	G	67	ASP	CB-CG-OD1	14.32	131.18	118.30
1	D	67	ASP	N-CA-CB	-14.03	85.34	110.60
1	C	67	ASP	N-CA-CB	-10.81	91.13	110.60
1	J	67	ASP	CB-CA-C	-7.38	95.64	110.40
1	C	67	ASP	CB-CA-C	-6.38	97.63	110.40
1	K	67	ASP	CB-CA-C	-5.97	98.47	110.40
1	L	37	GLU	C-N-CD	-5.92	107.58	120.60
1	I	369	ASP	CB-CA-C	5.82	122.04	110.40
1	C	68	GLY	N-CA-C	-5.80	98.61	113.10
1	H	370	LEU	CB-CA-C	-5.72	99.34	110.20
1	H	67	ASP	CB-CG-OD1	5.62	123.36	118.30
1	K	370	LEU	CB-CA-C	-5.45	99.84	110.20
1	H	67	ASP	CB-CA-C	-5.43	99.54	110.40
1	B	114	GLY	O-C-N	-5.39	114.07	122.70
1	B	115	CYS	O-C-N	-5.21	114.36	122.70
1	B	370	LEU	CB-CA-C	-5.10	100.50	110.20
1	D	370	LEU	CB-CA-C	-5.10	100.52	110.20
1	J	370	LEU	CB-CA-C	-5.08	100.54	110.20
1	F	370	LEU	CB-CA-C	-5.04	100.63	110.20
1	G	370	LEU	CB-CA-C	-5.03	100.64	110.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	66	ARG	Peptide
1	D	66	ARG	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3133	0	0	12	0
1	B	3133	0	0	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3133	0	0	22	0
1	D	3133	0	0	22	0
1	E	3133	0	0	26	0
1	F	3133	0	0	23	0
1	G	3133	0	0	25	0
1	H	3133	0	0	17	0
1	I	3133	0	0	23	0
1	J	3133	0	0	26	0
1	K	3133	0	2	36	0
1	L	3133	0	0	32	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0
2	J	4	0	0	0	0
2	K	4	0	0	0	0
2	L	4	0	0	0	0
3	A	44	0	26	0	0
3	B	44	0	26	0	0
3	C	44	0	26	2	0
3	D	44	0	26	0	0
3	E	44	0	26	1	0
3	F	44	0	26	2	0
3	G	44	0	26	0	0
3	H	44	0	26	2	0
3	I	44	0	26	0	0
3	J	44	0	26	0	0
3	K	44	0	26	0	0
3	L	44	0	26	1	0
4	A	79	0	0	5	0
4	B	63	0	0	13	0
4	C	112	0	0	11	0
4	D	106	0	0	9	0
4	E	83	0	0	6	0
4	F	69	0	0	6	0
4	G	54	0	0	10	0
4	H	84	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	43	0	0	7	0
4	J	55	0	0	11	0
4	K	69	0	0	10	0
4	L	36	0	0	8	0
All	All	39025	0	314	283	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (283) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:248:LYS:CD	1:K:283:ASP:CA	2.28	1.09
1:B:370:LEU:CD1	1:B:397:ARG:CB	2.40	1.00
1:E:370:LEU:CD1	1:E:397:ARG:CB	2.41	0.98
1:G:370:LEU:CD1	1:G:397:ARG:CB	2.42	0.97
1:J:370:LEU:CD1	1:J:397:ARG:CB	2.44	0.96
1:H:370:LEU:CD1	1:H:397:ARG:CB	2.43	0.95
1:D:370:LEU:CD1	1:D:397:ARG:CB	2.45	0.95
1:C:370:LEU:CD1	1:C:397:ARG:CB	2.45	0.93
1:I:37:GLU:CG	1:I:38:PRO:CD	2.47	0.92
1:F:370:LEU:CD1	1:F:397:ARG:CB	2.47	0.92
1:K:370:LEU:CD1	1:K:397:ARG:CB	2.48	0.92
3:C:603:EPU:O4	3:C:603:EPU:HE31	1.69	0.91
1:L:370:LEU:CD1	1:L:397:ARG:CB	2.48	0.91
1:K:248:LYS:CA	1:K:248:LYS:CE	2.50	0.90
1:F:391:ARG:NH1	1:F:393:TYR:CE2	2.42	0.87
1:G:218:VAL:CG1	1:G:219:GLU:N	2.38	0.87
1:K:247:GLY:O	1:K:248:LYS:CE	2.23	0.86
1:J:293:ASN:CB	4:J:760:HOH:O	2.22	0.86
1:K:330:ASN:CB	4:K:714:HOH:O	2.26	0.83
1:L:48:LYS:CE	4:L:761:HOH:O	2.26	0.82
3:H:608:EPU:HE31	3:H:608:EPU:O4	1.79	0.82
1:L:67:ASP:CG	1:L:69:SER:N	2.29	0.80
1:L:67:ASP:CB	1:L:69:SER:O	2.30	0.80
1:G:11:LYS:CE	4:G:796:HOH:O	2.29	0.80
1:I:248:LYS:O	1:I:249:ILE:CG2	2.30	0.79
1:E:330:ASN:N	1:E:330:ASN:ND2	2.30	0.79
1:I:84:TYR:CE2	4:I:824:HOH:O	2.34	0.79
3:C:603:EPU:C3E	3:C:603:EPU:O4	2.32	0.78
1:J:66:ARG:C	1:J:67:ASP:O	2.14	0.78
1:L:36:GLU:O	1:L:37:GLU:CB	2.32	0.77
1:K:247:GLY:O	1:K:248:LYS:NZ	2.19	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:66:ARG:O	1:J:67:ASP:O	2.03	0.75
1:K:248:LYS:CD	1:K:282:LEU:O	2.36	0.74
1:K:212:ARG:NH1	4:K:735:HOH:O	2.20	0.74
1:B:246:ARG:CD	4:B:786:HOH:O	2.36	0.74
1:E:183:GLU:OE2	1:E:212:ARG:CZ	2.36	0.73
1:F:88:LYS:NZ	4:F:637:HOH:O	2.20	0.73
1:D:221:LEU:N	4:D:440:HOH:O	2.22	0.72
1:L:357:VAL:CG1	1:L:358:GLU:N	2.53	0.72
1:D:67:ASP:O	1:D:67:ASP:CG	2.24	0.72
1:L:67:ASP:CG	1:L:67:ASP:OXT	2.29	0.71
1:G:75:ARG:NH1	4:G:813:HOH:O	2.23	0.71
1:F:326:THR:O	1:F:326:THR:CG2	2.39	0.71
1:I:248:LYS:C	1:I:249:ILE:CG2	2.59	0.71
1:E:183:GLU:OE2	1:E:212:ARG:NH2	2.25	0.70
1:A:46:LYS:NZ	1:A:67:ASP:OXT	2.25	0.69
1:F:155:HIS:NE2	1:F:183:GLU:OE1	2.25	0.69
1:K:152:LYS:CE	1:K:177:GLU:OE1	2.40	0.69
1:D:209:GLY:N	4:D:438:HOH:O	2.25	0.69
1:L:67:ASP:CB	1:L:69:SER:N	2.55	0.69
1:K:248:LYS:CE	1:K:282:LEU:O	2.40	0.69
1:H:340:ARG:NH2	4:H:453:HOH:O	2.25	0.69
1:H:3:LYS:NZ	4:H:498:HOH:O	2.25	0.69
1:K:340:ARG:NH1	1:K:364:GLN:O	2.25	0.69
1:I:220:ARG:CG	1:I:221:LEU:N	2.56	0.69
1:F:1:MET:CE	1:F:391:ARG:NH1	2.57	0.68
1:D:371:ARG:NH2	4:D:459:HOH:O	2.27	0.68
1:E:403:GLU:CG	4:E:756:HOH:O	2.40	0.67
1:K:248:LYS:NZ	1:K:284:MET:N	2.42	0.67
1:A:371:ARG:NH2	4:A:426:HOH:O	2.26	0.67
1:E:288:ARG:NH2	4:E:433:HOH:O	2.28	0.66
1:I:401:ARG:CA	4:I:436:HOH:O	2.44	0.66
1:J:283:ASP:OD1	1:J:285:HIS:N	2.30	0.65
1:J:267:ARG:NH1	4:J:697:HOH:O	2.29	0.65
1:L:290:LYS:CB	4:L:743:HOH:O	2.45	0.65
1:L:67:ASP:OD1	1:L:69:SER:N	2.30	0.65
1:I:66:ARG:NH2	1:I:67:ASP:OD1	2.30	0.65
1:A:66:ARG:NH2	1:A:67:ASP:OD1	2.30	0.64
1:C:108:GLN:NE2	4:C:444:HOH:O	2.30	0.64
1:J:103:ARG:NH2	4:J:561:HOH:O	2.30	0.64
1:C:330:ASN:ND2	1:C:330:ASN:O	2.30	0.64
1:F:88:LYS:CE	4:F:637:HOH:O	2.46	0.64
1:L:150:ARG:NH2	1:L:218:VAL:O	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:46:LYS:NZ	4:B:434:HOH:O	2.29	0.64
1:G:44:VAL:O	1:G:66:ARG:NH2	2.31	0.63
1:L:67:ASP:OD1	1:L:68:GLY:C	2.35	0.63
1:K:394:HIS:CE1	4:K:811:HOH:O	2.52	0.63
1:C:340:ARG:NH1	1:C:364:GLN:O	2.32	0.62
1:D:46:LYS:NZ	1:D:67:ASP:O	2.33	0.62
1:F:187:ARG:NH1	4:F:454:HOH:O	2.32	0.62
1:F:344:HIS:N	4:F:434:HOH:O	2.33	0.61
1:G:11:LYS:CD	4:G:796:HOH:O	2.48	0.60
1:I:344:HIS:N	4:I:428:HOH:O	2.33	0.60
1:L:273:ILE:CB	4:L:704:HOH:O	2.49	0.60
1:C:330:ASN:CG	1:D:330:ASN:ND2	2.55	0.60
1:D:67:ASP:O	1:D:67:ASP:OD1	2.19	0.60
1:G:42:GLN:NE2	4:G:420:HOH:O	2.33	0.60
1:J:66:ARG:CG	1:J:67:ASP:O	2.50	0.60
1:G:340:ARG:NH1	1:G:364:GLN:O	2.35	0.60
1:B:333:MET:N	4:B:427:HOH:O	2.34	0.60
1:J:283:ASP:OD2	1:J:285:HIS:CE1	2.55	0.60
1:G:177:GLU:N	4:G:433:HOH:O	2.34	0.60
1:J:284:MET:O	1:J:285:HIS:C	2.40	0.59
1:L:36:GLU:O	1:L:37:GLU:CG	2.51	0.59
1:C:151:LEU:N	4:C:462:HOH:O	2.35	0.59
1:K:187:ARG:NH2	4:K:452:HOH:O	2.34	0.59
1:C:295:ARG:NE	4:C:430:HOH:O	2.34	0.59
1:C:212:ARG:NH1	4:C:437:HOH:O	2.34	0.59
1:L:211:ASP:N	1:L:211:ASP:OD1	2.33	0.59
1:B:332:PHE:N	4:B:427:HOH:O	2.35	0.59
1:E:67:ASP:OD1	1:E:69:SER:N	2.36	0.59
1:B:350:ASN:ND2	4:B:437:HOH:O	2.35	0.58
1:A:120:ARG:CD	4:A:780:HOH:O	2.51	0.58
1:H:66:ARG:NE	1:H:67:ASP:O	2.36	0.58
1:K:42:GLN:NE2	4:K:434:HOH:O	2.36	0.58
1:K:159:ASP:N	4:K:453:HOH:O	2.37	0.58
1:F:371:ARG:NH2	4:F:427:HOH:O	2.36	0.58
1:E:67:ASP:OD1	1:E:68:GLY:C	2.37	0.58
3:F:606:EPU:O4	3:F:606:EPU:HE31	2.03	0.58
1:J:55:LYS:NZ	4:J:442:HOH:O	2.35	0.57
1:B:246:ARG:NE	4:B:786:HOH:O	2.37	0.57
1:E:108:GLN:NE2	4:E:453:HOH:O	2.38	0.57
1:D:178:GLY:N	4:D:486:HOH:O	2.36	0.57
1:L:245:SER:O	1:L:246:ARG:CB	2.53	0.57
1:F:340:ARG:NH1	1:F:364:GLN:O	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:3:LYS:CD	4:H:498:HOH:O	2.53	0.57
1:C:407:ARG:NH1	4:C:463:HOH:O	2.38	0.57
1:E:7:GLN:OE1	1:K:179:THR:OG1	2.23	0.56
1:L:397:ARG:NH1	4:L:618:HOH:O	2.39	0.56
1:E:400:GLU:O	1:E:401:ARG:CB	2.52	0.56
1:E:22:LYS:NZ	3:E:605:EPU:O2E	2.39	0.56
1:J:23:ASN:N	4:J:423:HOH:O	2.39	0.55
1:A:46:LYS:CE	1:A:67:ASP:OXT	2.55	0.55
1:I:402:ILE:N	4:I:436:HOH:O	2.38	0.55
1:B:369:ASP:C	1:B:369:ASP:OD1	2.45	0.54
3:H:608:EPU:C3E	3:H:608:EPU:O4	2.55	0.54
1:B:17:THR:N	4:B:426:HOH:O	2.41	0.53
1:J:360:LEU:N	4:J:419:HOH:O	2.40	0.53
1:G:36:GLU:OE1	1:G:220:ARG:CZ	2.56	0.53
1:G:150:ARG:NH2	4:G:752:HOH:O	2.41	0.53
1:B:131:GLN:CG	4:B:720:HOH:O	2.56	0.53
1:H:3:LYS:CE	4:H:498:HOH:O	2.57	0.53
1:K:212:ARG:NH2	4:K:738:HOH:O	2.40	0.52
1:K:184:ASN:N	4:K:450:HOH:O	2.42	0.52
1:L:192:VAL:C	4:L:433:HOH:O	2.48	0.52
1:E:325:GLU:CG	1:E:328:PHE:O	2.58	0.52
1:C:330:ASN:CG	1:C:330:ASN:O	2.48	0.52
1:L:219:GLU:O	1:L:220:ARG:CG	2.58	0.52
1:G:176:ALA:C	4:G:433:HOH:O	2.49	0.51
1:L:196:ASN:ND2	4:L:433:HOH:O	2.43	0.51
1:J:46:LYS:NZ	1:J:67:ASP:OXT	2.43	0.51
1:H:340:ARG:NH1	1:H:364:GLN:O	2.43	0.51
1:L:218:VAL:CG2	1:L:219:GLU:N	2.72	0.51
1:L:192:VAL:CG1	4:L:433:HOH:O	2.58	0.51
1:G:177:GLU:CA	4:G:433:HOH:O	2.57	0.51
1:A:340:ARG:NH1	1:A:364:GLN:O	2.44	0.51
1:B:76:ASP:N	4:B:425:HOH:O	2.44	0.51
1:B:369:ASP:OD1	1:B:371:ARG:N	2.43	0.51
1:E:330:ASN:CB	1:H:330:ASN:CG	2.79	0.50
1:C:150:ARG:CB	4:C:462:HOH:O	2.59	0.50
1:I:340:ARG:NH1	1:I:364:GLN:O	2.44	0.50
1:J:340:ARG:NH1	1:J:364:GLN:O	2.45	0.50
1:B:66:ARG:O	1:B:67:ASP:OXT	2.30	0.50
1:G:66:ARG:O	1:G:67:ASP:O	2.30	0.50
1:F:325:GLU:CG	1:F:328:PHE:O	2.59	0.50
1:D:252:ARG:NH2	4:D:428:HOH:O	2.43	0.50
1:F:1:MET:CE	1:F:391:ARG:CZ	2.89	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:391:ARG:CG	1:C:393:TYR:CE2	2.95	0.50
1:I:66:ARG:O	1:I:67:ASP:OXT	2.29	0.50
1:F:66:ARG:O	1:F:67:ASP:O	2.30	0.50
1:I:66:ARG:O	1:I:67:ASP:C	2.50	0.49
1:K:248:LYS:NZ	1:K:284:MET:CG	2.75	0.49
1:G:184:ASN:ND2	4:G:421:HOH:O	2.45	0.49
1:B:400:GLU:N	4:B:431:HOH:O	2.45	0.49
1:H:232:ARG:CB	1:H:258:THR:CG2	2.90	0.49
1:I:2:ASP:OD1	1:I:417:LYS:CD	2.61	0.49
1:K:152:LYS:CD	1:K:177:GLU:OE1	2.61	0.49
1:H:67:ASP:C	1:H:67:ASP:OD1	2.51	0.49
1:L:74:ALA:O	1:L:103:ARG:NH1	2.46	0.48
1:L:396:ASP:OD2	1:L:415:ARG:NH2	2.46	0.48
1:E:340:ARG:NH1	1:E:364:GLN:O	2.46	0.48
1:L:340:ARG:NH1	1:L:364:GLN:O	2.47	0.48
1:E:321:GLY:N	4:E:425:HOH:O	2.47	0.47
1:G:5:ARG:CD	1:G:414:GLU:OE2	2.62	0.47
1:J:401:ARG:NH2	4:J:438:HOH:O	2.47	0.47
1:K:247:GLY:C	1:K:248:LYS:CE	2.83	0.47
1:B:340:ARG:NH1	1:B:364:GLN:O	2.47	0.47
1:E:319:GLY:N	4:E:451:HOH:O	2.47	0.47
1:G:66:ARG:CG	1:G:67:ASP:O	2.62	0.47
1:D:232:ARG:CB	1:D:258:THR:CG2	2.93	0.47
1:A:396:ASP:OD2	1:A:415:ARG:NH2	2.47	0.47
1:I:293:ASN:ND2	1:I:322:PHE:N	2.62	0.47
1:C:330:ASN:ND2	1:D:330:ASN:ND2	2.63	0.47
1:C:253:ASN:OD1	4:C:484:HOH:O	2.20	0.47
1:H:65:GLU:OE2	4:H:446:HOH:O	2.20	0.47
1:D:159:ASP:OD1	1:F:265:LYS:NZ	2.47	0.47
1:F:232:ARG:CB	1:F:258:THR:CG2	2.93	0.47
1:L:232:ARG:CB	1:L:258:THR:CG2	2.92	0.47
1:F:293:ASN:ND2	1:F:322:PHE:N	2.64	0.46
1:C:293:ASN:ND2	1:C:322:PHE:N	2.63	0.46
1:D:400:GLU:N	4:D:475:HOH:O	2.49	0.46
1:K:407:ARG:NH1	1:K:413:ILE:O	2.48	0.46
1:B:232:ARG:CB	1:B:258:THR:CG2	2.93	0.46
1:A:232:ARG:CB	1:A:258:THR:CG2	2.94	0.46
1:I:232:ARG:CB	1:I:258:THR:CG2	2.93	0.46
1:K:248:LYS:CG	1:K:283:ASP:OD1	2.63	0.46
1:G:232:ARG:CB	1:G:258:THR:CG2	2.94	0.46
1:H:299:HIS:O	4:H:447:HOH:O	2.21	0.46
1:D:74:ALA:N	4:D:464:HOH:O	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:227:ARG:NH2	4:L:421:HOH:O	2.49	0.46
1:I:304:THR:N	4:I:419:HOH:O	2.48	0.46
1:E:118:GLY:CA	1:E:330:ASN:OD1	2.64	0.45
1:J:285:HIS:N	4:J:444:HOH:O	2.48	0.45
1:B:391:ARG:CD	4:B:607:HOH:O	2.64	0.45
1:B:265:LYS:NZ	1:E:159:ASP:OD1	2.50	0.45
1:H:293:ASN:ND2	1:H:322:PHE:N	2.65	0.45
1:D:252:ARG:NH1	4:D:454:HOH:O	2.49	0.45
1:G:67:ASP:OXT	1:G:67:ASP:OD1	2.34	0.45
1:B:396:ASP:OD2	1:B:415:ARG:NH2	2.50	0.45
1:K:66:ARG:NE	1:K:67:ASP:O	2.50	0.45
1:B:293:ASN:ND2	1:B:322:PHE:N	2.64	0.45
1:C:396:ASP:OD2	1:C:415:ARG:NH2	2.49	0.45
1:H:325:GLU:CG	1:H:328:PHE:O	2.65	0.45
1:J:232:ARG:CB	1:J:258:THR:CG2	2.94	0.45
1:I:295:ARG:N	4:I:422:HOH:O	2.48	0.45
1:L:38:PRO:O	1:L:223:GLY:CA	2.65	0.45
1:D:390:ASP:O	1:D:391:ARG:CB	2.63	0.45
1:H:295:ARG:NE	4:H:451:HOH:O	2.50	0.45
1:C:412:ASN:N	4:C:476:HOH:O	2.49	0.45
1:I:219:GLU:O	1:I:219:GLU:CG	2.65	0.45
1:I:275:VAL:CG2	1:I:275:VAL:O	2.65	0.45
1:E:67:ASP:CG	1:E:69:SER:N	2.70	0.44
1:E:207:GLY:O	1:E:210:THR:OG1	2.36	0.44
1:F:396:ASP:OD2	1:F:415:ARG:NH2	2.49	0.44
1:C:232:ARG:CB	1:C:258:THR:CG2	2.94	0.44
1:C:5:ARG:NH1	4:C:428:HOH:O	2.50	0.44
1:A:246:ARG:NE	4:A:432:HOH:O	2.51	0.44
1:G:252:ARG:O	1:G:253:ASN:CB	2.65	0.44
1:K:248:LYS:NZ	1:K:282:LEU:CD2	2.81	0.44
1:G:150:ARG:NE	4:G:433:HOH:O	2.50	0.44
1:K:46:LYS:C	1:K:47:LEU:CD2	2.86	0.43
1:G:66:ARG:C	1:G:67:ASP:O	2.55	0.43
1:L:183:GLU:OE2	1:L:212:ARG:CZ	2.65	0.43
1:J:187:ARG:N	4:J:435:HOH:O	2.51	0.43
1:L:371:ARG:NH1	1:L:398:GLY:O	2.51	0.43
1:D:340:ARG:NH1	1:D:364:GLN:O	2.51	0.43
1:C:162:SER:N	4:C:450:HOH:O	2.52	0.43
1:K:66:ARG:CG	1:K:67:ASP:O	2.67	0.43
1:I:276:GLY:CA	1:I:279:TRP:CE2	3.01	0.43
1:H:36:GLU:OE1	1:H:220:ARG:NH2	2.51	0.43
1:E:232:ARG:CB	1:E:258:THR:CG2	2.96	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:396:ASP:OD2	1:J:415:ARG:NH2	2.51	0.43
1:J:283:ASP:OD1	1:J:284:MET:N	2.52	0.43
1:I:274:GLU:O	1:I:281:SER:N	2.52	0.43
1:K:67:ASP:C	1:K:67:ASP:OD1	2.57	0.43
1:F:267:ARG:NH1	4:F:432:HOH:O	2.51	0.43
1:F:391:ARG:NH1	1:F:393:TYR:OH	2.52	0.42
1:I:37:GLU:CG	1:I:38:PRO:N	2.82	0.42
1:G:293:ASN:ND2	1:G:322:PHE:N	2.67	0.42
1:K:396:ASP:OD2	1:K:415:ARG:NH2	2.52	0.42
1:K:232:ARG:CB	1:K:258:THR:CG2	2.97	0.42
1:E:208:GLN:N	1:E:208:GLN:OE1	2.52	0.42
1:C:366:MET:O	4:C:436:HOH:O	2.22	0.42
1:J:325:GLU:CG	1:J:328:PHE:O	2.67	0.42
1:G:46:LYS:CE	1:G:67:ASP:OD1	2.67	0.42
3:F:606:EPU:O4	3:F:606:EPU:C3E	2.67	0.42
1:K:247:GLY:O	1:K:248:LYS:CG	2.68	0.41
1:C:348:GLU:CG	1:F:322:PHE:CE2	3.03	0.41
1:F:391:ARG:NH1	1:F:393:TYR:CZ	2.87	0.41
1:E:354:CYS:O	4:E:425:HOH:O	2.22	0.41
1:D:66:ARG:O	1:D:67:ASP:OXT	2.39	0.41
1:B:318:GLU:OE2	4:B:814:HOH:O	2.21	0.41
1:K:204:LYS:N	4:K:433:HOH:O	2.54	0.41
1:L:36:GLU:N	1:L:221:LEU:O	2.54	0.41
1:J:391:ARG:CG	1:J:393:TYR:CE2	3.04	0.41
1:I:401:ARG:N	4:I:436:HOH:O	2.52	0.41
1:D:396:ASP:OD2	1:D:415:ARG:NH2	2.54	0.41
1:J:16:VAL:CB	4:J:425:HOH:O	2.69	0.41
1:D:220:ARG:CD	4:D:733:HOH:O	2.69	0.41
1:F:330:ASN:CG	1:G:330:ASN:CG	2.79	0.41
1:K:386:THR:N	4:K:436:HOH:O	2.53	0.41
1:B:7:GLN:NE2	4:B:449:HOH:O	2.54	0.41
3:L:612:EPU:O2A	3:L:612:EPU:O1B	2.37	0.41
1:A:293:ASN:ND2	1:A:322:PHE:N	2.69	0.41
1:K:247:GLY:O	1:K:248:LYS:CD	2.69	0.40
1:K:340:ARG:NE	1:L:111:LEU:O	2.54	0.40
1:H:208:GLN:OE1	1:H:208:GLN:N	2.55	0.40
1:E:403:GLU:OE2	1:J:277:GLU:OE2	2.39	0.40
1:A:51:ASP:OD1	4:A:434:HOH:O	2.22	0.40
1:J:277:GLU:CG	4:J:783:HOH:O	2.70	0.40
1:D:293:ASN:ND2	1:D:322:PHE:N	2.69	0.40
1:A:5:ARG:CD	4:A:420:HOH:O	2.70	0.40
1:E:407:ARG:NH1	1:E:413:ILE:O	2.54	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	414/418 (99%)	403 (97%)	10 (2%)	1 (0%)	56	79
1	B	414/418 (99%)	404 (98%)	10 (2%)	0	100	100
1	C	414/418 (99%)	401 (97%)	13 (3%)	0	100	100
1	D	414/418 (99%)	404 (98%)	9 (2%)	1 (0%)	56	79
1	E	414/418 (99%)	403 (97%)	11 (3%)	0	100	100
1	F	414/418 (99%)	404 (98%)	10 (2%)	0	100	100
1	G	414/418 (99%)	402 (97%)	12 (3%)	0	100	100
1	H	414/418 (99%)	403 (97%)	10 (2%)	1 (0%)	56	79
1	I	414/418 (99%)	399 (96%)	13 (3%)	2 (0%)	38	60
1	J	414/418 (99%)	404 (98%)	9 (2%)	1 (0%)	56	79
1	K	414/418 (99%)	403 (97%)	11 (3%)	0	100	100
1	L	414/418 (99%)	400 (97%)	12 (3%)	2 (0%)	38	60
All	All	4968/5016 (99%)	4830 (97%)	130 (3%)	8 (0%)	56	79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	37	GLU
1	L	38	PRO
1	A	370	LEU
1	H	370	LEU
1	I	38	PRO
1	J	370	LEU
1	D	370	LEU
1	I	39	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/331 (100%)	312 (94%)	19 (6%)	29	50
1	B	331/331 (100%)	309 (93%)	22 (7%)	24	41
1	C	331/331 (100%)	309 (93%)	22 (7%)	24	41
1	D	331/331 (100%)	315 (95%)	16 (5%)	35	60
1	E	331/331 (100%)	307 (93%)	24 (7%)	20	36
1	F	331/331 (100%)	309 (93%)	22 (7%)	24	41
1	G	331/331 (100%)	310 (94%)	21 (6%)	25	44
1	H	331/331 (100%)	311 (94%)	20 (6%)	27	47
1	I	331/331 (100%)	303 (92%)	28 (8%)	15	28
1	J	331/331 (100%)	309 (93%)	22 (7%)	24	41
1	K	331/331 (100%)	312 (94%)	19 (6%)	29	50
1	L	331/331 (100%)	311 (94%)	20 (6%)	27	47
All	All	3972/3972 (100%)	3717 (94%)	255 (6%)	25	43

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	55	LYS
1	A	63	LYS
1	A	86	LEU
1	A	131	GLN
1	A	143	VAL
1	A	150	ARG
1	A	158	MET
1	A	159	ASP
1	A	193	ASP
1	A	248	LYS
1	A	258	THR
1	A	307	GLN
1	A	346	GLU
1	A	349	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	350	ASN
1	A	358	GLU
1	A	370	LEU
1	A	416	VAL
1	B	7	GLN
1	B	10	THR
1	B	55	LYS
1	B	69	SER
1	B	86	LEU
1	B	131	GLN
1	B	143	VAL
1	B	150	ARG
1	B	158	MET
1	B	159	ASP
1	B	193	ASP
1	B	248	LYS
1	B	258	THR
1	B	265	LYS
1	B	307	GLN
1	B	346	GLU
1	B	349	SER
1	B	350	ASN
1	B	358	GLU
1	B	361	SER
1	B	413	ILE
1	B	416	VAL
1	C	7	GLN
1	C	39	VAL
1	C	48	LYS
1	C	55	LYS
1	C	65	GLU
1	C	66	ARG
1	C	86	LEU
1	C	131	GLN
1	C	137	LYS
1	C	140	GLU
1	C	143	VAL
1	C	158	MET
1	C	159	ASP
1	C	193	ASP
1	C	258	THR
1	C	307	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	346	GLU
1	C	349	SER
1	C	350	ASN
1	C	358	GLU
1	C	361	SER
1	C	416	VAL
1	D	7	GLN
1	D	48	LYS
1	D	55	LYS
1	D	131	GLN
1	D	143	VAL
1	D	150	ARG
1	D	158	MET
1	D	159	ASP
1	D	258	THR
1	D	307	GLN
1	D	346	GLU
1	D	349	SER
1	D	350	ASN
1	D	358	GLU
1	D	391	ARG
1	D	416	VAL
1	E	7	GLN
1	E	38	PRO
1	E	39	VAL
1	E	55	LYS
1	E	63	LYS
1	E	69	SER
1	E	86	LEU
1	E	131	GLN
1	E	143	VAL
1	E	150	ARG
1	E	158	MET
1	E	159	ASP
1	E	193	ASP
1	E	212	ARG
1	E	258	THR
1	E	307	GLN
1	E	330	ASN
1	E	333	MET
1	E	346	GLU
1	E	349	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	350	ASN
1	E	358	GLU
1	E	361	SER
1	E	416	VAL
1	F	7	GLN
1	F	38	PRO
1	F	55	LYS
1	F	67	ASP
1	F	86	LEU
1	F	131	GLN
1	F	143	VAL
1	F	150	ARG
1	F	158	MET
1	F	159	ASP
1	F	183	GLU
1	F	258	THR
1	F	265	LYS
1	F	295	ARG
1	F	307	GLN
1	F	326	THR
1	F	346	GLU
1	F	349	SER
1	F	350	ASN
1	F	358	GLU
1	F	361	SER
1	F	416	VAL
1	G	7	GLN
1	G	38	PRO
1	G	55	LYS
1	G	66	ARG
1	G	86	LEU
1	G	131	GLN
1	G	136	ILE
1	G	143	VAL
1	G	150	ARG
1	G	158	MET
1	G	159	ASP
1	G	193	ASP
1	G	216	GLU
1	G	219	GLU
1	G	258	THR
1	G	307	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	346	GLU
1	G	349	SER
1	G	350	ASN
1	G	361	SER
1	G	416	VAL
1	H	7	GLN
1	H	10	THR
1	H	38	PRO
1	H	46	LYS
1	H	66	ARG
1	H	86	LEU
1	H	131	GLN
1	H	143	VAL
1	H	150	ARG
1	H	158	MET
1	H	159	ASP
1	H	248	LYS
1	H	258	THR
1	H	307	GLN
1	H	346	GLU
1	H	349	SER
1	H	350	ASN
1	H	358	GLU
1	H	361	SER
1	H	416	VAL
1	I	7	GLN
1	I	36	GLU
1	I	38	PRO
1	I	55	LYS
1	I	65	GLU
1	I	66	ARG
1	I	67	ASP
1	I	69	SER
1	I	86	LEU
1	I	131	GLN
1	I	143	VAL
1	I	150	ARG
1	I	158	MET
1	I	159	ASP
1	I	193	ASP
1	I	220	ARG
1	I	221	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	248	LYS
1	I	249	ILE
1	I	258	THR
1	I	274	GLU
1	I	307	GLN
1	I	346	GLU
1	I	349	SER
1	I	350	ASN
1	I	358	GLU
1	I	361	SER
1	I	416	VAL
1	J	7	GLN
1	J	55	LYS
1	J	63	LYS
1	J	65	GLU
1	J	66	ARG
1	J	67	ASP
1	J	69	SER
1	J	86	LEU
1	J	131	GLN
1	J	143	VAL
1	J	150	ARG
1	J	158	MET
1	J	159	ASP
1	J	193	ASP
1	J	258	THR
1	J	307	GLN
1	J	346	GLU
1	J	349	SER
1	J	350	ASN
1	J	358	GLU
1	J	361	SER
1	J	416	VAL
1	K	7	GLN
1	K	55	LYS
1	K	86	LEU
1	K	131	GLN
1	K	143	VAL
1	K	150	ARG
1	K	158	MET
1	K	159	ASP
1	K	216	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	248	LYS
1	K	258	THR
1	K	307	GLN
1	K	346	GLU
1	K	349	SER
1	K	350	ASN
1	K	358	GLU
1	K	361	SER
1	K	413	ILE
1	K	416	VAL
1	L	7	GLN
1	L	37	GLU
1	L	65	GLU
1	L	66	ARG
1	L	67	ASP
1	L	86	LEU
1	L	131	GLN
1	L	143	VAL
1	L	150	ARG
1	L	158	MET
1	L	159	ASP
1	L	221	LEU
1	L	248	LYS
1	L	258	THR
1	L	307	GLN
1	L	346	GLU
1	L	349	SER
1	L	350	ASN
1	L	361	SER
1	L	416	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PO3	A	501	-	1,3,3	4.13	1 (100%)	0,3,3	0.00	-
3	EPU	A	601	-	46,46,46	1.95	14 (30%)	65,69,69	2.14	13 (20%)
2	PO3	B	502	-	1,3,3	4.23	1 (100%)	0,3,3	0.00	-
3	EPU	B	602	-	46,46,46	1.79	8 (17%)	65,69,69	2.36	14 (21%)
2	PO3	C	502	-	1,3,3	4.18	1 (100%)	0,3,3	0.00	-
3	EPU	C	603	-	46,46,46	2.02	14 (30%)	65,69,69	2.25	16 (24%)
2	PO3	D	503	-	1,3,3	4.14	1 (100%)	0,3,3	0.00	-
3	EPU	D	604	-	46,46,46	1.90	13 (28%)	65,69,69	2.32	18 (27%)
2	PO3	E	504	-	1,3,3	4.19	1 (100%)	0,3,3	0.00	-
3	EPU	E	605	-	46,46,46	1.94	11 (23%)	65,69,69	2.07	20 (30%)
2	PO3	F	506	-	1,3,3	0.67	0	0,3,3	0.00	-
3	EPU	F	606	-	46,46,46	1.95	17 (36%)	65,69,69	2.06	16 (24%)
2	PO3	G	507	-	1,3,3	4.19	1 (100%)	0,3,3	0.00	-
3	EPU	G	607	-	46,46,46	1.82	10 (21%)	65,69,69	2.08	14 (21%)
2	PO3	H	508	-	1,3,3	4.19	1 (100%)	0,3,3	0.00	-
3	EPU	H	608	-	46,46,46	1.81	11 (23%)	65,69,69	2.40	15 (23%)
2	PO3	I	509	-	1,3,3	0.14	0	0,3,3	0.00	-
3	EPU	I	609	-	46,46,46	1.99	14 (30%)	65,69,69	2.23	14 (21%)
2	PO3	J	510	-	1,3,3	2.23	1 (100%)	0,3,3	0.00	-
3	EPU	J	610	-	46,46,46	1.89	10 (21%)	65,69,69	2.41	20 (30%)
2	PO3	K	511	-	1,3,3	1.04	0	0,3,3	0.00	-
3	EPU	K	611	-	46,46,46	1.84	11 (23%)	65,69,69	2.07	15 (23%)
2	PO3	L	512	-	1,3,3	4.16	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EPU	L	612	-	46,46,46	1.80	9 (19%)	65,69,69	2.30	17 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO3	A	501	-	-	0/0/0/0	0/0/0/0
3	EPU	A	601	-	-	3/32/71/71	0/3/3/3
2	PO3	B	502	-	-	0/0/0/0	0/0/0/0
3	EPU	B	602	-	-	3/32/71/71	0/3/3/3
2	PO3	C	502	-	-	0/0/0/0	0/0/0/0
3	EPU	C	603	-	-	2/32/71/71	0/3/3/3
2	PO3	D	503	-	-	0/0/0/0	0/0/0/0
3	EPU	D	604	-	-	1/32/71/71	0/3/3/3
2	PO3	E	504	-	-	0/0/0/0	0/0/0/0
3	EPU	E	605	-	-	2/32/71/71	0/3/3/3
2	PO3	F	506	-	-	0/0/0/0	0/0/0/0
3	EPU	F	606	-	-	1/32/71/71	0/3/3/3
2	PO3	G	507	-	-	0/0/0/0	0/0/0/0
3	EPU	G	607	-	-	1/32/71/71	0/3/3/3
2	PO3	H	508	-	-	0/0/0/0	0/0/0/0
3	EPU	H	608	-	-	1/32/71/71	0/3/3/3
2	PO3	I	509	-	-	0/0/0/0	0/0/0/0
3	EPU	I	609	-	-	3/32/71/71	0/3/3/3
2	PO3	J	510	-	-	0/0/0/0	0/0/0/0
3	EPU	J	610	-	-	1/32/71/71	0/3/3/3
2	PO3	K	511	-	-	0/0/0/0	0/0/0/0
3	EPU	K	611	-	-	3/32/71/71	0/3/3/3
2	PO3	L	512	-	-	0/0/0/0	0/0/0/0
3	EPU	L	612	-	-	3/32/71/71	0/3/3/3

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	611	EPU	C3E-C2E	7.06	1.52	1.31
3	E	605	EPU	C3E-C2E	7.05	1.52	1.31
3	J	610	EPU	C3E-C2E	6.97	1.51	1.31
3	B	602	EPU	C3E-C2E	6.93	1.51	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	609	EPU	C3E-C2E	6.90	1.51	1.31
3	A	601	EPU	C3E-C2E	6.89	1.51	1.31
3	L	612	EPU	C3E-C2E	6.87	1.51	1.31
3	G	607	EPU	C3E-C2E	6.74	1.51	1.31
3	D	604	EPU	C3E-C2E	6.69	1.51	1.31
3	C	603	EPU	C3E-C2E	6.37	1.50	1.31
3	H	608	EPU	C3E-C2E	6.37	1.50	1.31
3	F	606	EPU	C3E-C2E	6.20	1.49	1.31
3	C	603	EPU	O3-C3	-4.27	1.38	1.44
2	B	502	PO3	P-O1	4.23	1.51	1.46
2	H	508	PO3	P-O1	4.19	1.51	1.46
2	G	507	PO3	P-O1	4.19	1.51	1.46
2	E	504	PO3	P-O1	4.19	1.51	1.46
2	C	502	PO3	P-O1	4.18	1.51	1.46
2	L	512	PO3	P-O1	4.16	1.51	1.46
2	D	503	PO3	P-O1	4.14	1.51	1.46
2	A	501	PO3	P-O1	4.13	1.51	1.46
3	F	606	EPU	O3-C3	-4.12	1.38	1.44
3	B	602	EPU	O3-C3	-4.09	1.38	1.44
3	I	609	EPU	O3-C3	-3.54	1.39	1.44
3	E	605	EPU	O3-C3	-3.39	1.39	1.44
3	C	603	EPU	C4U-N3U	-3.29	1.31	1.37
3	I	609	EPU	PB-O1	-3.26	1.51	1.60
3	H	608	EPU	C2E-C1E	-3.26	1.46	1.49
3	D	604	EPU	PA-O3A	-3.25	1.54	1.59
3	A	601	EPU	C4U-N3U	-3.22	1.31	1.37
3	I	609	EPU	C4U-N3U	-3.17	1.31	1.37
3	E	605	EPU	C4U-N3U	-3.16	1.32	1.37
3	G	607	EPU	C4U-N3U	-3.15	1.32	1.37
3	D	604	EPU	O3-C3	-3.14	1.39	1.44
3	L	612	EPU	C3-C2	-3.13	1.47	1.53
3	A	601	EPU	O3-C3	-3.13	1.39	1.44
3	F	606	EPU	C2D-C1D	-3.12	1.49	1.53
3	J	610	EPU	O3-C3	-3.11	1.40	1.44
3	A	601	EPU	C6U-N1U	-3.10	1.30	1.35
3	D	604	EPU	C4U-N3U	-3.06	1.32	1.37
3	E	605	EPU	PA-O3A	-3.05	1.54	1.59
3	I	609	EPU	C6U-N1U	-3.04	1.30	1.35
3	B	602	EPU	C6U-N1U	-3.03	1.30	1.35
3	K	611	EPU	C6U-N1U	-3.02	1.30	1.35
3	C	603	EPU	C2E-C1E	-3.01	1.46	1.49
3	H	608	EPU	C4U-N3U	-2.99	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	612	EPU	O3-C3	-2.98	1.40	1.44
3	F	606	EPU	PB-O2B	-2.92	1.42	1.55
3	K	611	EPU	O3-C3	-2.92	1.40	1.44
3	J	610	EPU	C6U-N1U	-2.90	1.31	1.35
3	H	608	EPU	C2U-N3U	-2.86	1.31	1.37
3	A	601	EPU	PB-O1	-2.84	1.52	1.60
3	J	610	EPU	C3-C2	-2.79	1.48	1.53
3	C	603	EPU	C6U-N1U	-2.75	1.31	1.35
3	F	606	EPU	C6U-N1U	-2.73	1.31	1.35
3	I	609	EPU	O1-C1	-2.69	1.36	1.42
3	I	609	EPU	PA-O2A	-2.68	1.43	1.55
3	H	608	EPU	C6U-N1U	-2.68	1.31	1.35
3	J	610	EPU	C2D-C1D	-2.67	1.49	1.53
3	J	610	EPU	C4U-N3U	-2.67	1.32	1.37
3	L	612	EPU	C4U-N3U	-2.66	1.32	1.37
3	D	604	EPU	PB-O2B	-2.66	1.43	1.55
3	L	612	EPU	C6U-N1U	-2.65	1.31	1.35
3	C	603	EPU	PA-O3A	-2.59	1.55	1.59
3	D	604	EPU	C2U-N3U	-2.59	1.32	1.37
3	C	603	EPU	O2E-C1E	-2.59	1.22	1.30
3	E	605	EPU	C6U-N1U	-2.58	1.31	1.35
3	E	605	EPU	C2U-N3U	-2.57	1.32	1.37
3	A	601	EPU	O1-C1	-2.54	1.37	1.42
3	H	608	EPU	PB-O2B	-2.54	1.43	1.55
3	I	609	EPU	C2U-N3U	-2.53	1.32	1.37
3	D	604	EPU	PA-O2A	-2.51	1.43	1.55
3	C	603	EPU	PB-O2B	-2.50	1.43	1.55
3	F	606	EPU	O2E-C1E	-2.48	1.22	1.30
3	H	608	EPU	O3-C3	-2.48	1.40	1.44
3	C	603	EPU	C2U-N3U	-2.47	1.32	1.37
3	H	608	EPU	C2D-C1D	-2.46	1.50	1.53
3	F	606	EPU	C4U-N3U	-2.46	1.33	1.37
3	G	607	EPU	C6U-N1U	-2.45	1.31	1.35
3	D	604	EPU	O5-C5	-2.44	1.38	1.44
3	A	601	EPU	PA-O2A	-2.43	1.44	1.55
3	K	611	EPU	C3-C2	-2.41	1.48	1.53
3	A	601	EPU	PB-O2B	-2.40	1.44	1.55
3	F	606	EPU	O4D-C4D	-2.37	1.39	1.45
3	J	610	EPU	C2U-N3U	-2.36	1.32	1.37
3	A	601	EPU	C2U-N3U	-2.36	1.32	1.37
3	E	605	EPU	PB-O3A	-2.35	1.55	1.59
3	G	607	EPU	C2U-N3U	-2.35	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	609	EPU	PB-O2B	-2.34	1.44	1.55
3	G	607	EPU	PB-O2B	-2.34	1.44	1.55
3	E	605	EPU	PA-O2A	-2.34	1.44	1.55
3	F	606	EPU	PA-O2A	-2.33	1.44	1.55
3	C	603	EPU	PA-O2A	-2.33	1.44	1.55
3	E	605	EPU	C2D-C1D	-2.31	1.50	1.53
3	F	606	EPU	PB-O3A	-2.30	1.55	1.59
3	D	604	EPU	C6U-N1U	-2.30	1.32	1.35
3	K	611	EPU	C2E-C1E	-2.29	1.47	1.49
3	F	606	EPU	PB-O1	-2.29	1.54	1.60
3	F	606	EPU	PA-O3A	-2.29	1.55	1.59
3	L	612	EPU	C2D-C1D	-2.28	1.50	1.53
3	I	609	EPU	C2E-C1E	2.27	1.51	1.49
3	K	611	EPU	PA-O2A	-2.25	1.45	1.55
3	E	605	EPU	C3D-C2D	-2.24	1.47	1.53
3	D	604	EPU	PA-O1A	-2.24	1.42	1.51
3	B	602	EPU	O2E-C1E	-2.24	1.23	1.30
3	C	603	EPU	O7-C7	-2.24	1.18	1.23
2	J	510	PO3	P-O1	-2.23	1.44	1.46
3	A	601	EPU	C2D-C1D	-2.22	1.50	1.53
3	L	612	EPU	C2U-N3U	-2.22	1.33	1.37
3	K	611	EPU	PA-O3A	-2.21	1.55	1.59
3	K	611	EPU	PB-O2B	-2.21	1.45	1.55
3	H	608	EPU	PB-O1	-2.21	1.54	1.60
3	F	606	EPU	PB-O1B	-2.21	1.43	1.51
3	I	609	EPU	C2D-C1D	-2.20	1.50	1.53
3	C	603	EPU	C2D-C1D	-2.20	1.50	1.53
3	A	601	EPU	PA-O1A	-2.20	1.43	1.51
3	C	603	EPU	C3-C2	-2.19	1.49	1.53
3	K	611	EPU	O2E-C1E	-2.18	1.23	1.30
3	D	604	EPU	O7-C7	-2.17	1.18	1.23
3	F	606	EPU	C2U-N3U	-2.17	1.33	1.37
3	L	612	EPU	C3D-C2D	-2.16	1.47	1.53
3	G	607	EPU	PA-O3A	-2.16	1.56	1.59
3	A	601	EPU	O2E-C1E	-2.16	1.23	1.30
3	F	606	EPU	O7-C7	-2.15	1.18	1.23
3	I	609	EPU	C3-C2	-2.12	1.49	1.53
3	L	612	EPU	PA-O2A	-2.12	1.45	1.55
3	H	608	EPU	PA-O2A	-2.11	1.45	1.55
3	G	607	EPU	C2D-C1D	-2.10	1.50	1.53
3	I	609	EPU	O4D-C4D	-2.10	1.40	1.45
3	D	604	EPU	PB-O3A	-2.09	1.56	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	EPU	PA-O2A	-2.09	1.45	1.55
3	G	607	EPU	PA-O2A	-2.08	1.45	1.55
3	F	606	EPU	C1-C2	-2.08	1.49	1.53
3	E	605	EPU	O2E-C1E	-2.08	1.23	1.30
3	I	609	EPU	O7-C7	-2.08	1.18	1.23
3	B	602	EPU	C4U-N3U	-2.07	1.33	1.37
3	H	608	EPU	PB-O1B	-2.07	1.43	1.51
3	B	602	EPU	C2D-C1D	-2.07	1.50	1.53
3	G	607	EPU	O3-C2E	2.07	1.43	1.36
3	D	604	EPU	C2D-C1D	-2.05	1.50	1.53
3	K	611	EPU	PB-O1B	-2.05	1.43	1.51
3	F	606	EPU	C4-C5	-2.05	1.48	1.53
3	B	602	EPU	PB-O2B	-2.05	1.45	1.55
3	C	603	EPU	C4-C5	-2.04	1.48	1.53
3	G	607	EPU	PB-O3A	-2.03	1.56	1.59
3	J	610	EPU	O5-C5	-2.02	1.39	1.44
3	A	601	EPU	O7-C7	-2.02	1.18	1.23
3	K	611	EPU	C4U-N3U	-2.02	1.33	1.37
3	J	610	EPU	O2E-C1E	-2.02	1.23	1.30
3	J	610	EPU	O1-C1	-2.01	1.38	1.42
3	A	601	EPU	O4D-C4D	-2.01	1.40	1.45

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	EPU	C2U-N1U-C1D	9.99	124.47	118.21
3	H	608	EPU	C3E-C2E-C1E	-9.71	104.31	122.72
3	G	607	EPU	C3E-C2E-C1E	-9.37	104.96	122.72
3	D	604	EPU	C3E-C2E-C1E	-8.87	105.90	122.72
3	B	602	EPU	C3E-C2E-C1E	-8.49	106.63	122.72
3	A	601	EPU	N3U-C2U-N1U	8.16	122.78	115.97
3	L	612	EPU	C3E-C2E-C1E	-8.07	107.42	122.72
3	J	610	EPU	C3E-C2E-C1E	-7.93	107.67	122.72
3	I	609	EPU	N3U-C2U-N1U	7.79	122.47	115.97
3	E	605	EPU	N3U-C2U-N1U	7.51	122.24	115.97
3	G	607	EPU	N3U-C2U-N1U	7.44	122.19	115.97
3	K	611	EPU	C3E-C2E-C1E	-7.14	109.18	122.72
3	F	606	EPU	C3E-C2E-C1E	-7.06	109.34	122.72
3	D	604	EPU	N3U-C2U-N1U	7.05	121.86	115.97
3	E	605	EPU	C3E-C2E-C1E	-6.96	109.52	122.72
3	C	603	EPU	N3U-C2U-N1U	6.95	121.78	115.97
3	L	612	EPU	N3U-C2U-N1U	6.90	121.73	115.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	608	EPU	C3-O3-C2E	-6.89	102.41	121.91
3	B	602	EPU	N3U-C2U-N1U	6.55	121.44	115.97
3	H	608	EPU	C2U-N1U-C1D	6.52	122.30	118.21
3	C	603	EPU	C3E-C2E-C1E	-6.46	110.47	122.72
3	K	611	EPU	N3U-C2U-N1U	6.45	121.36	115.97
3	D	604	EPU	O5-C1-O1	-6.45	102.94	111.36
3	C	603	EPU	C3-C2-N2	-6.40	99.82	110.99
3	I	609	EPU	O5-C1-O1	-6.31	103.12	111.36
3	F	606	EPU	N3U-C2U-N1U	6.17	121.12	115.97
3	J	610	EPU	N3U-C2U-N1U	6.16	121.11	115.97
3	A	601	EPU	C3E-C2E-C1E	-6.11	111.13	122.72
3	I	609	EPU	C3E-C2E-C1E	-5.95	111.44	122.72
3	H	608	EPU	N3U-C2U-N1U	5.80	120.81	115.97
3	J	610	EPU	C4-C3-C2	-5.64	101.85	110.47
3	H	608	EPU	O1E-C1E-C2E	-5.58	113.19	121.81
3	J	610	EPU	O5-C1-O1	-5.52	104.15	111.36
3	A	601	EPU	C3-C2-N2	-5.28	101.78	110.99
3	F	606	EPU	C2U-N1U-C1D	5.23	121.48	118.21
3	I	609	EPU	C3-C2-N2	-5.16	101.98	110.99
3	J	610	EPU	C2U-N1U-C1D	5.14	121.43	118.21
3	J	610	EPU	C3-C2-N2	-5.03	102.21	110.99
3	A	601	EPU	O5-C1-O1	-4.95	104.90	111.36
3	C	603	EPU	C2U-N1U-C1D	4.94	121.31	118.21
3	L	612	EPU	C4-C3-C2	-4.85	103.05	110.47
3	C	603	EPU	C3-O3-C2E	-4.85	108.18	121.91
3	K	611	EPU	O5-C1-O1	-4.82	105.07	111.36
3	L	612	EPU	PB-O3A-PA	-4.80	117.61	131.68
3	L	612	EPU	C3-C2-N2	-4.51	103.13	110.99
3	K	611	EPU	C2U-N1U-C1D	4.42	120.98	118.21
3	J	610	EPU	C3-O3-C2E	-4.41	109.43	121.91
3	E	605	EPU	C3-O3-C2E	-4.35	109.60	121.91
3	G	607	EPU	C3-O3-C2E	-4.33	109.66	121.91
3	C	603	EPU	O3-C2E-C3E	-4.31	103.62	123.20
3	K	611	EPU	C4-C3-C2	-4.30	103.90	110.47
3	B	602	EPU	C3-O3-C2E	-4.29	109.78	121.91
3	L	612	EPU	C3-O3-C2E	-4.26	109.86	121.91
3	A	601	EPU	O2E-C1E-C2E	4.24	121.31	113.90
3	F	606	EPU	C3-O3-C2E	-4.21	109.99	121.91
3	H	608	EPU	O2E-C1E-C2E	4.18	121.21	113.90
3	F	606	EPU	C3-C2-N2	-4.14	103.77	110.99
3	D	604	EPU	C1-O5-C5	-4.11	105.74	113.73
3	G	607	EPU	C3-C2-N2	-4.09	103.85	110.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	609	EPU	C4-C3-C2	-4.07	104.24	110.47
3	K	611	EPU	C3-C2-N2	-4.06	103.90	110.99
3	I	609	EPU	O2E-C1E-C2E	4.03	120.95	113.90
3	F	606	EPU	O3-C2E-C3E	-4.03	104.93	123.20
3	L	612	EPU	O5-C1-O1	-4.02	106.11	111.36
3	K	611	EPU	O3-C2E-C1E	-3.82	101.87	113.60
3	D	604	EPU	O5-C1-C2	-3.70	102.82	110.78
3	C	603	EPU	O3-C2E-C1E	-3.65	102.39	113.60
3	J	610	EPU	C4D-O4D-C1D	3.61	113.67	109.75
3	E	605	EPU	C3-C2-N2	-3.58	104.75	110.99
3	L	612	EPU	O2E-C1E-C2E	3.53	120.06	113.90
3	J	610	EPU	O3-C2E-C3E	-3.51	107.28	123.20
3	L	612	EPU	O1E-C1E-C2E	-3.49	116.42	121.81
3	D	604	EPU	C3-C2-N2	-3.45	104.96	110.99
3	D	604	EPU	C3-O3-C2E	-3.44	112.18	121.91
3	B	602	EPU	C3D-C2D-C1D	3.43	106.27	100.91
3	L	612	EPU	O3D-C3D-C2D	-3.41	100.74	111.83
3	L	612	EPU	O3-C2E-C3E	-3.30	108.22	123.20
3	E	605	EPU	C4-C3-C2	-3.26	105.48	110.47
3	D	604	EPU	C4-C3-C2	-3.23	105.53	110.47
3	A	601	EPU	C3-O3-C2E	-3.22	112.80	121.91
3	B	602	EPU	O3-C2E-C3E	-3.20	108.67	123.20
3	I	609	EPU	C6-C5-C4	-3.17	105.33	113.00
3	I	609	EPU	O3-C2E-C3E	-3.16	108.87	123.20
3	D	604	EPU	C3-C4-C5	-3.14	102.53	109.64
3	A	601	EPU	C6-C5-C4	-3.09	105.53	113.00
3	D	604	EPU	O3-C2E-C3E	-3.08	109.25	123.20
3	H	608	EPU	O3-C2E-C3E	-3.04	109.39	123.20
3	A	601	EPU	C4-C3-C2	-3.03	105.83	110.47
3	F	606	EPU	O5-C1-C2	-3.02	104.28	110.78
3	A	601	EPU	O3-C2E-C3E	-3.02	109.51	123.20
3	I	609	EPU	O6-C6-C5	-2.99	101.07	111.36
3	J	610	EPU	O3D-C3D-C4D	-2.98	102.29	111.08
3	I	609	EPU	C5U-C6U-N1U	-2.97	117.85	121.21
3	E	605	EPU	O5-C1-C2	-2.95	104.43	110.78
3	D	604	EPU	C1-C2-N2	2.94	116.58	111.02
3	G	607	EPU	C3D-C2D-C1D	2.93	105.49	100.91
3	I	609	EPU	C3-O3-C2E	-2.93	113.62	121.91
3	J	610	EPU	O4D-C1D-C2D	-2.93	102.28	106.77
3	H	608	EPU	C3-C2-N2	-2.93	105.88	110.99
3	J	610	EPU	PB-O3A-PA	-2.90	123.19	131.68
3	C	603	EPU	C3D-C2D-C1D	2.89	105.43	100.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	611	EPU	O3-C2E-C3E	-2.83	110.35	123.20
3	C	603	EPU	O4-C4-C3	-2.83	103.26	109.85
3	K	611	EPU	C3D-C2D-C1D	2.82	105.32	100.91
3	L	612	EPU	C2D-C1D-N1U	-2.78	106.10	113.26
3	H	608	EPU	O3-C3-C2	2.78	113.36	108.19
3	E	605	EPU	O2E-C1E-C2E	2.75	118.70	113.90
3	B	602	EPU	C4D-O4D-C1D	2.75	112.73	109.75
3	K	611	EPU	C3-O3-C2E	-2.75	114.14	121.91
3	J	610	EPU	O6-C6-C5	-2.71	102.03	111.36
3	H	608	EPU	C3D-C2D-C1D	2.71	105.15	100.91
3	F	606	EPU	C4D-O4D-C1D	2.71	112.69	109.75
3	G	607	EPU	O5-C1-O1	-2.71	107.83	111.36
3	E	605	EPU	O3D-C3D-C2D	-2.70	103.06	111.83
3	J	610	EPU	O2E-C1E-C2E	2.69	118.61	113.90
3	E	605	EPU	C5U-C6U-N1U	-2.69	118.17	121.21
3	F	606	EPU	O5-C1-O1	-2.67	107.88	111.36
3	J	610	EPU	O1E-C1E-C2E	-2.67	117.69	121.81
3	J	610	EPU	C6-C5-C4	-2.65	106.60	113.00
3	E	605	EPU	O1-C1-C2	2.63	112.09	107.91
3	G	607	EPU	C5U-C6U-N1U	-2.63	118.24	121.21
3	D	604	EPU	O3-C2E-C1E	-2.61	105.59	113.60
3	L	612	EPU	C5U-C6U-N1U	-2.60	118.27	121.21
3	D	604	EPU	O3A-PA-O5D	-2.59	91.80	103.41
3	D	604	EPU	O1-C1-C2	2.58	112.02	107.91
3	C	603	EPU	O5-C1-C2	-2.58	105.23	110.78
3	K	611	EPU	C4D-O4D-C1D	2.56	112.53	109.75
3	K	611	EPU	O5-C1-C2	-2.56	105.28	110.78
3	F	606	EPU	C5U-C6U-N1U	-2.56	118.32	121.21
3	L	612	EPU	C6-C5-C4	-2.55	106.85	113.00
3	B	602	EPU	C3-C2-N2	-2.55	106.54	110.99
3	B	602	EPU	O1E-C1E-C2E	-2.53	117.90	121.81
3	C	603	EPU	C8-C7-N2	2.51	121.02	116.11
3	C	603	EPU	C2-N2-C7	-2.51	116.33	123.02
3	A	601	EPU	O6-C6-C5	-2.48	102.82	111.36
3	C	603	EPU	O1E-C1E-C2E	-2.48	117.98	121.81
3	A	601	EPU	C5U-C6U-N1U	-2.45	118.44	121.21
3	D	604	EPU	C2U-N1U-C1D	2.43	119.73	118.21
3	E	605	EPU	O1E-C1E-C2E	-2.42	118.07	121.81
3	F	606	EPU	C1-C2-C3	-2.41	105.42	109.92
3	E	605	EPU	O2D-C2D-C3D	-2.41	104.01	111.83
3	F	606	EPU	C3D-C2D-C1D	2.41	104.67	100.91
3	K	611	EPU	O2E-C1E-C2E	2.39	118.08	113.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	604	EPU	C3D-C2D-C1D	2.37	104.62	100.91
3	A	601	EPU	C3D-C2D-C1D	2.35	104.59	100.91
3	G	607	EPU	O3-C3-C2	2.34	112.53	108.19
3	H	608	EPU	C5U-C4U-N3U	2.33	121.10	116.70
3	H	608	EPU	C4D-O4D-C1D	2.32	112.27	109.75
3	L	612	EPU	C1-C2-N2	-2.32	106.63	111.02
3	E	605	EPU	O3-C2E-C3E	-2.32	112.67	123.20
3	H	608	EPU	C1-C2-N2	-2.31	106.65	111.02
3	J	610	EPU	O5D-PA-O1A	-2.31	100.34	109.37
3	F	606	EPU	O3D-C3D-C2D	-2.28	104.42	111.83
3	J	610	EPU	C2-N2-C7	-2.28	116.94	123.02
3	A	601	EPU	O4-C4-C3	-2.26	104.57	109.85
3	K	611	EPU	O2A-PA-O1A	2.25	124.79	112.21
3	G	607	EPU	C5U-C4U-N3U	2.23	120.90	116.70
3	G	607	EPU	C4-C3-C2	-2.22	107.06	110.47
3	L	612	EPU	C5U-C4U-N3U	2.22	120.89	116.70
3	C	603	EPU	O2E-C1E-C2E	2.20	117.75	113.90
3	D	604	EPU	O2D-C2D-C3D	-2.20	104.68	111.83
3	F	606	EPU	C2D-C3D-C4D	2.20	107.04	102.65
3	E	605	EPU	O2B-PB-O1B	2.20	124.48	112.21
3	H	608	EPU	O4-C4-C3	-2.19	104.75	109.85
3	B	602	EPU	O3-C2E-C1E	-2.19	106.89	113.60
3	G	607	EPU	O3A-PB-O1	-2.18	97.98	103.48
3	I	609	EPU	O3D-C3D-C2D	-2.17	104.77	111.83
3	B	602	EPU	PB-O3A-PA	-2.16	125.34	131.68
3	D	604	EPU	O6-C6-C5	-2.15	103.97	111.36
3	B	602	EPU	O3D-C3D-C2D	-2.14	104.87	111.83
3	L	612	EPU	O6-C6-C5	-2.14	104.00	111.36
3	B	602	EPU	O5-C1-O1	-2.14	108.57	111.36
3	I	609	EPU	O4-C4-C3	-2.13	104.88	109.85
3	E	605	EPU	O3A-PB-O1	-2.12	98.13	103.48
3	J	610	EPU	O1-C1-C2	2.11	111.27	107.91
3	E	605	EPU	PB-O3A-PA	-2.10	125.53	131.68
3	C	603	EPU	C5U-C4U-N3U	2.09	120.64	116.70
3	H	608	EPU	O5-C1-C2	-2.09	106.29	110.78
3	C	603	EPU	O5-C1-O1	-2.08	108.65	111.36
3	F	606	EPU	O3-C2E-C1E	-2.06	107.28	113.60
3	E	605	EPU	C2-N2-C7	-2.05	117.53	123.02
3	E	605	EPU	O5-C5-C6	2.05	111.38	106.34
3	E	605	EPU	O2A-PA-O1A	2.05	123.64	112.21
3	G	607	EPU	C1-C2-N2	-2.04	107.16	111.02
3	J	610	EPU	O3A-PB-O1	-2.04	98.32	103.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	605	EPU	C5U-C4U-N3U	2.03	120.52	116.70
3	B	602	EPU	C2-N2-C7	-2.03	117.61	123.02
3	G	607	EPU	O2D-C2D-C3D	-2.02	105.25	111.83
3	I	609	EPU	C1-O5-C5	-2.02	109.80	113.73
3	K	611	EPU	O4-C4-C5	2.01	114.57	109.28
3	F	606	EPU	C2D-C1D-N1U	-2.01	108.09	113.26
3	G	607	EPU	O1E-C1E-C2E	-2.00	118.72	121.81

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	609	EPU	O2E-C1E-C2E-C3E
3	A	601	EPU	O2E-C1E-C2E-C3E
3	G	607	EPU	C3-O3-C2E-C3E
3	L	612	EPU	O2E-C1E-C2E-C3E
3	E	605	EPU	O2E-C1E-C2E-C3E
3	C	603	EPU	O2E-C1E-C2E-C3E
3	J	610	EPU	O2E-C1E-C2E-C3E
3	A	601	EPU	O1E-C1E-C2E-C3E
3	I	609	EPU	O1E-C1E-C2E-C3E
3	B	602	EPU	O1E-C1E-C2E-C3E
3	B	602	EPU	O2E-C1E-C2E-C3E
3	E	605	EPU	O1E-C1E-C2E-C3E
3	L	612	EPU	O1E-C1E-C2E-C3E
3	C	603	EPU	O1E-C1E-C2E-C3E
3	F	606	EPU	C3-O3-C2E-C3E
3	D	604	EPU	C3-O3-C2E-C3E
3	I	609	EPU	C3-O3-C2E-C3E
3	A	601	EPU	C3-O3-C2E-C3E
3	K	611	EPU	O2E-C1E-C2E-C3E
3	L	612	EPU	C3-O3-C2E-C3E
3	K	611	EPU	C3-O3-C2E-C3E
3	K	611	EPU	O1E-C1E-C2E-C3E
3	H	608	EPU	O2E-C1E-C2E-C3E
3	B	602	EPU	C3-O3-C2E-C3E

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	418/418 (100%)	-0.08	4 (0%) 79 81	36, 55, 83, 120	0
1	B	418/418 (100%)	0.26	19 (4%) 32 33	37, 67, 100, 186	0
1	C	418/418 (100%)	-0.14	3 (0%) 84 86	26, 48, 71, 116	0
1	D	418/418 (100%)	-0.23	1 (0%) 93 94	30, 48, 72, 118	0
1	E	418/418 (100%)	-0.08	4 (0%) 79 81	32, 52, 77, 143	0
1	F	418/418 (100%)	0.03	6 (1%) 72 74	33, 55, 85, 127	0
1	G	418/418 (100%)	0.15	14 (3%) 44 45	34, 61, 98, 147	0
1	H	418/418 (100%)	-0.16	2 (0%) 88 90	32, 51, 69, 132	0
1	I	418/418 (100%)	0.43	40 (9%) 8 7	38, 71, 118, 170	0
1	J	418/418 (100%)	0.14	11 (2%) 53 55	34, 64, 97, 128	0
1	K	418/418 (100%)	0.02	6 (1%) 72 74	29, 53, 79, 169	0
1	L	418/418 (100%)	0.67	53 (12%) 4 4	42, 81, 129, 203	0
All	All	5016/5016 (100%)	0.08	163 (3%) 45 47	26, 57, 99, 203	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	418	GLY	9.4
1	I	215	ILE	6.8
1	L	215	ILE	6.5
1	L	221	LEU	5.8
1	K	418	GLY	5.8
1	L	222	GLY	5.6
1	L	39	VAL	5.3
1	B	418	GLY	5.2
1	I	216	GLU	5.1
1	I	136	ILE	5.1
1	I	177	GLU	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	81	CYS	4.8
1	D	418	GLY	4.7
1	E	418	GLY	4.7
1	I	99	PRO	4.1
1	L	197	PHE	4.0
1	I	152	LYS	4.0
1	I	181	ILE	4.0
1	J	12	LEU	3.9
1	L	277	GLU	3.9
1	J	72	ILE	3.9
1	J	273	ILE	3.8
1	L	12	LEU	3.7
1	I	134	ALA	3.7
1	J	201	LEU	3.6
1	B	47	LEU	3.6
1	I	171	CYS	3.6
1	L	37	GLU	3.6
1	G	59	GLN	3.5
1	L	213	ILE	3.5
1	F	225	VAL	3.5
1	G	56	LEU	3.4
1	I	132	LEU	3.4
1	G	418	GLY	3.4
1	I	147	VAL	3.3
1	L	30	PHE	3.3
1	L	279	TRP	3.3
1	L	282	LEU	3.2
1	I	151	LEU	3.2
1	L	205	ILE	3.2
1	K	330	ASN	3.2
1	G	401	ARG	3.2
1	L	175	LEU	3.1
1	L	41	ILE	3.1
1	L	26	LEU	3.1
1	B	395	ILE	3.0
1	H	115	CYS	3.0
1	I	148	ASP	3.0
1	B	273	ILE	3.0
1	I	349	SER	3.0
1	L	75	ARG	3.0
1	L	401	ARG	2.9
1	G	273	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	35	ALA	2.9
1	E	220	ARG	2.9
1	L	38	PRO	2.9
1	B	370	LEU	2.9
1	E	57	LEU	2.9
1	I	201	LEU	2.9
1	B	80	PHE	2.8
1	I	80	PHE	2.8
1	L	152	LYS	2.8
1	G	62	ALA	2.8
1	I	102	ALA	2.8
1	K	349	SER	2.8
1	L	248	LYS	2.8
1	K	412	ASN	2.7
1	G	12	LEU	2.7
1	L	63	LYS	2.7
1	L	117	ILE	2.7
1	K	248	LYS	2.7
1	E	330	ASN	2.6
1	I	137	LYS	2.6
1	F	115	CYS	2.6
1	I	129	LEU	2.6
1	L	199	ILE	2.6
1	I	42	GLN	2.6
1	B	358	GLU	2.6
1	J	359	LYS	2.6
1	L	64	VAL	2.6
1	G	1	MET	2.6
1	I	131	GLN	2.6
1	L	225	VAL	2.6
1	F	72	ILE	2.5
1	K	350	ASN	2.5
1	A	381	CYS	2.5
1	I	401	ARG	2.5
1	L	16	VAL	2.5
1	L	330	ASN	2.5
1	I	350	ASN	2.5
1	L	267	ARG	2.5
1	L	33	LEU	2.5
1	I	212	ARG	2.4
1	G	48	LYS	2.4
1	L	238	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	350	ASN	2.4
1	I	175	LEU	2.4
1	G	103	ARG	2.4
1	L	200	THR	2.4
1	I	86	LEU	2.4
1	L	151	LEU	2.4
1	B	63	LYS	2.4
1	L	351	THR	2.4
1	G	326	THR	2.4
1	I	57	LEU	2.4
1	L	216	GLU	2.4
1	F	347	ILE	2.3
1	J	330	ASN	2.3
1	L	274	GLU	2.3
1	L	326	THR	2.3
1	L	29	LEU	2.3
1	L	226	TYR	2.3
1	I	179	THR	2.3
1	I	60	LEU	2.3
1	L	44	VAL	2.3
1	L	318	GLU	2.2
1	B	286	GLY	2.2
1	J	74	ALA	2.2
1	L	171	CYS	2.2
1	B	146	SER	2.2
1	B	60	LEU	2.2
1	A	115	CYS	2.2
1	I	194	THR	2.2
1	I	34	LEU	2.2
1	L	100	LEU	2.2
1	B	219	GLU	2.2
1	J	116	THR	2.2
1	G	370	LEU	2.2
1	L	322	PHE	2.2
1	I	78	ASN	2.2
1	B	413	ILE	2.2
1	B	29	LEU	2.2
1	L	95	TRP	2.2
1	G	33	LEU	2.1
1	L	255	GLN	2.1
1	B	280	ILE	2.1
1	L	280	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	220	ARG	2.1
1	I	217	GLY	2.1
1	I	223	GLY	2.1
1	I	182	ILE	2.1
1	I	100	LEU	2.1
1	A	147	VAL	2.1
1	G	79	VAL	2.1
1	J	413	ILE	2.1
1	B	64	VAL	2.1
1	C	216	GLU	2.1
1	J	289	PRO	2.1
1	L	329	GLU	2.1
1	F	152	LYS	2.1
1	L	134	ALA	2.1
1	C	254	ALA	2.1
1	B	13	GLN	2.1
1	B	249	ILE	2.1
1	A	9	PRO	2.1
1	L	36	GLU	2.1
1	L	201	LEU	2.1
1	L	42	GLN	2.0
1	I	74	ALA	2.0
1	I	248	LYS	2.0
1	I	150	ARG	2.0
1	C	147	VAL	2.0
1	J	287	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	PO3	C	502	4/4	0.26	5.03	59,66,66,70	0
2	PO3	J	510	4/4	0.25	3.75	53,65,65,68	0
2	PO3	K	511	4/4	0.32	3.26	56,69,71,79	0
2	PO3	E	504	4/4	0.24	2.98	58,64,65,68	0
2	PO3	A	501	4/4	0.28	2.53	65,66,69,73	0
2	PO3	I	509	4/4	0.21	2.46	49,72,72,87	0
2	PO3	H	508	4/4	0.28	2.01	54,56,57,63	0
2	PO3	D	503	4/4	0.21	1.80	52,56,65,67	0
2	PO3	F	506	4/4	0.23	1.33	71,73,76,77	0
2	PO3	G	507	4/4	0.20	1.29	50,53,55,58	0
2	PO3	L	512	4/4	0.22	1.25	68,73,83,85	0
2	PO3	B	502	4/4	0.16	0.10	61,70,74,81	0
3	EPU	I	609	44/44	0.16	-0.12	55,65,70,74	0
3	EPU	C	603	44/44	0.14	-0.21	33,41,49,61	0
3	EPU	F	606	44/44	0.14	-0.30	33,41,52,67	0
3	EPU	G	607	44/44	0.16	-0.39	39,50,58,65	0
3	EPU	A	601	44/44	0.16	-0.44	38,51,59,63	0
3	EPU	H	608	44/44	0.14	-0.44	37,50,61,63	0
3	EPU	J	610	44/44	0.14	-0.46	42,48,54,61	0
3	EPU	B	602	44/44	0.14	-0.49	43,51,59,68	0
3	EPU	L	612	44/44	0.15	-0.57	56,64,70,77	0
3	EPU	D	604	44/44	0.12	-0.67	32,43,53,59	0
3	EPU	E	605	44/44	0.12	-0.81	34,42,56,62	0
3	EPU	K	611	44/44	0.12	-1.01	33,44,52,69	0

6.5 Other polymers ⓘ

There are no such residues in this entry.