



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2021 – 09:03 am BST

PDB ID : 7OMA
Title : Thosea asigna virus RdRP domain elongation complex
Authors : Ferrero, D.S.; Falqui, M.; Verdaguer, N.
Deposited on : 2021-05-21
Resolution : 3.10 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 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 : 2.22
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) : 2.22

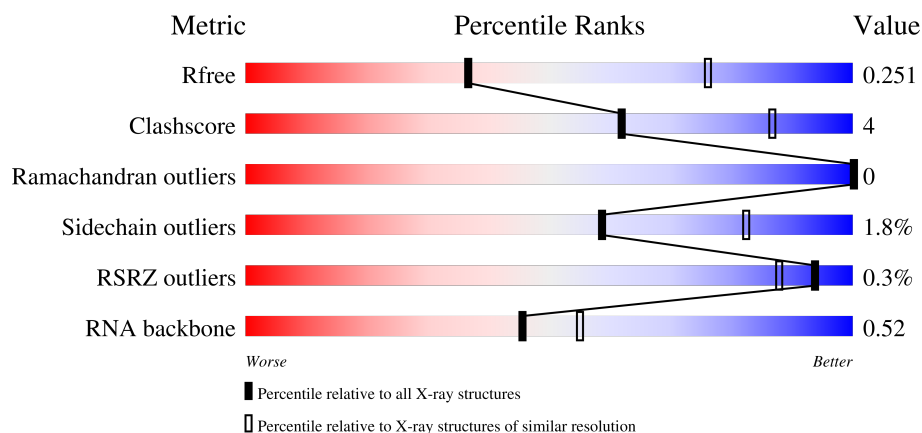
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



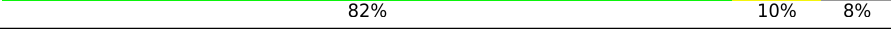
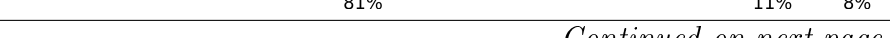
The reported resolution of this entry is 3.10 Å.

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.






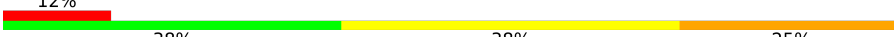
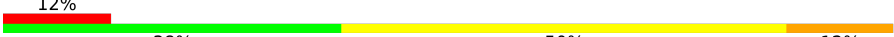
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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	684	
1	B	684	
1	C	684	
1	D	684	

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Mol	Chain	Length	Quality of chain
2	E	9	
2	G	9	
2	I	9	
2	L	9	
3	F	8	
3	H	8	
3	J	8	
3	K	8	

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	POP	B	701	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21230 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 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	628	Total	C	N	O	S	0	0	0
			4978	3156	863	933	26			
1	A	629	Total	C	N	O	S	0	0	0
			4986	3162	864	934	26			
1	C	629	Total	C	N	O	S	0	0	0
			4985	3160	864	935	26			
1	D	630	Total	C	N	O	S	0	0	0
			4993	3167	865	935	26			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	MET	-	initiating methionine	UNP Q6A562
B	-11	GLY	-	expression tag	UNP Q6A562
B	-10	SER	-	expression tag	UNP Q6A562
B	-9	SER	-	expression tag	UNP Q6A562
B	-8	HIS	-	expression tag	UNP Q6A562
B	-7	HIS	-	expression tag	UNP Q6A562
B	-6	HIS	-	expression tag	UNP Q6A562
B	-5	HIS	-	expression tag	UNP Q6A562
B	-4	HIS	-	expression tag	UNP Q6A562
B	-3	HIS	-	expression tag	UNP Q6A562
B	-2	SER	-	expression tag	UNP Q6A562
B	-1	GLN	-	expression tag	UNP Q6A562
B	0	ASP	-	expression tag	UNP Q6A562
B	1	LEU	-	expression tag	UNP Q6A562
B	2	GLU	-	expression tag	UNP Q6A562
B	3	ASN	-	expression tag	UNP Q6A562
B	4	LEU	-	expression tag	UNP Q6A562
B	5	TYR	-	expression tag	UNP Q6A562
B	6	PHE	-	expression tag	UNP Q6A562
B	7	GLN	-	expression tag	UNP Q6A562
B	8	GLY	-	expression tag	UNP Q6A562

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	GLY	-	expression tag	UNP Q6A562
B	10	SER	-	expression tag	UNP Q6A562
A	-12	MET	-	initiating methionine	UNP Q6A562
A	-11	GLY	-	expression tag	UNP Q6A562
A	-10	SER	-	expression tag	UNP Q6A562
A	-9	SER	-	expression tag	UNP Q6A562
A	-8	HIS	-	expression tag	UNP Q6A562
A	-7	HIS	-	expression tag	UNP Q6A562
A	-6	HIS	-	expression tag	UNP Q6A562
A	-5	HIS	-	expression tag	UNP Q6A562
A	-4	HIS	-	expression tag	UNP Q6A562
A	-3	HIS	-	expression tag	UNP Q6A562
A	-2	SER	-	expression tag	UNP Q6A562
A	-1	GLN	-	expression tag	UNP Q6A562
A	0	ASP	-	expression tag	UNP Q6A562
A	1	LEU	-	expression tag	UNP Q6A562
A	2	GLU	-	expression tag	UNP Q6A562
A	3	ASN	-	expression tag	UNP Q6A562
A	4	LEU	-	expression tag	UNP Q6A562
A	5	TYR	-	expression tag	UNP Q6A562
A	6	PHE	-	expression tag	UNP Q6A562
A	7	GLN	-	expression tag	UNP Q6A562
A	8	GLY	-	expression tag	UNP Q6A562
A	9	GLY	-	expression tag	UNP Q6A562
A	10	SER	-	expression tag	UNP Q6A562
C	-12	MET	-	initiating methionine	UNP Q6A562
C	-11	GLY	-	expression tag	UNP Q6A562
C	-10	SER	-	expression tag	UNP Q6A562
C	-9	SER	-	expression tag	UNP Q6A562
C	-8	HIS	-	expression tag	UNP Q6A562
C	-7	HIS	-	expression tag	UNP Q6A562
C	-6	HIS	-	expression tag	UNP Q6A562
C	-5	HIS	-	expression tag	UNP Q6A562
C	-4	HIS	-	expression tag	UNP Q6A562
C	-3	HIS	-	expression tag	UNP Q6A562
C	-2	SER	-	expression tag	UNP Q6A562
C	-1	GLN	-	expression tag	UNP Q6A562
C	0	ASP	-	expression tag	UNP Q6A562
C	1	LEU	-	expression tag	UNP Q6A562
C	2	GLU	-	expression tag	UNP Q6A562
C	3	ASN	-	expression tag	UNP Q6A562
C	4	LEU	-	expression tag	UNP Q6A562

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Chain	Residue	Modelled	Actual	Comment	Reference
C	5	TYR	-	expression tag	UNP Q6A562
C	6	PHE	-	expression tag	UNP Q6A562
C	7	GLN	-	expression tag	UNP Q6A562
C	8	GLY	-	expression tag	UNP Q6A562
C	9	GLY	-	expression tag	UNP Q6A562
C	10	SER	-	expression tag	UNP Q6A562
D	-12	MET	-	initiating methionine	UNP Q6A562
D	-11	GLY	-	expression tag	UNP Q6A562
D	-10	SER	-	expression tag	UNP Q6A562
D	-9	SER	-	expression tag	UNP Q6A562
D	-8	HIS	-	expression tag	UNP Q6A562
D	-7	HIS	-	expression tag	UNP Q6A562
D	-6	HIS	-	expression tag	UNP Q6A562
D	-5	HIS	-	expression tag	UNP Q6A562
D	-4	HIS	-	expression tag	UNP Q6A562
D	-3	HIS	-	expression tag	UNP Q6A562
D	-2	SER	-	expression tag	UNP Q6A562
D	-1	GLN	-	expression tag	UNP Q6A562
D	0	ASP	-	expression tag	UNP Q6A562
D	1	LEU	-	expression tag	UNP Q6A562
D	2	GLU	-	expression tag	UNP Q6A562
D	3	ASN	-	expression tag	UNP Q6A562
D	4	LEU	-	expression tag	UNP Q6A562
D	5	TYR	-	expression tag	UNP Q6A562
D	6	PHE	-	expression tag	UNP Q6A562
D	7	GLN	-	expression tag	UNP Q6A562
D	8	GLY	-	expression tag	UNP Q6A562
D	9	GLY	-	expression tag	UNP Q6A562
D	10	SER	-	expression tag	UNP Q6A562

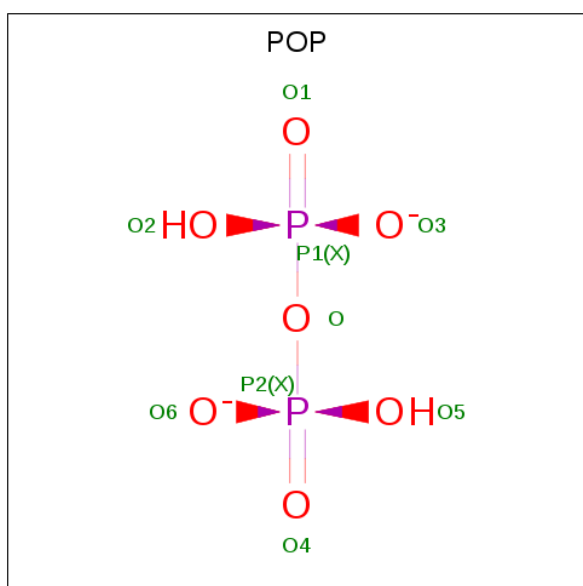
- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*AP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	7	Total 146	C 66	N 23	O 50	P 7	0	0	0
2	G	7	Total 146	C 66	N 23	O 50	P 7	0	0	0
2	I	7	Total 146	C 66	N 23	O 50	P 7	0	0	0
2	L	7	Total 146	C 66	N 23	O 50	P 7	0	0	0

- Molecule 3 is a RNA chain called RNA (5'-R(P*CP*AP*AP*AP*AP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	8	Total 168	C 76	N 29	O 55	P 8	0	0	0
3	H	8	Total 168	C 76	N 29	O 55	P 8	0	0	0
3	J	8	Total 168	C 76	N 29	O 55	P 8	0	0	0
3	K	8	Total 168	C 76	N 29	O 55	P 8	0	0	0

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O P	0	0
			9 7 2			
4	A	1	Total	O P	0	0
			9 7 2			
4	C	1	Total	O P	0	0
			9 7 2			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Mg	0	0
			2 2			
5	A	1	Total	Mg	0	0
			1 1			
5	D	1	Total	Mg	0	0
			1 1			

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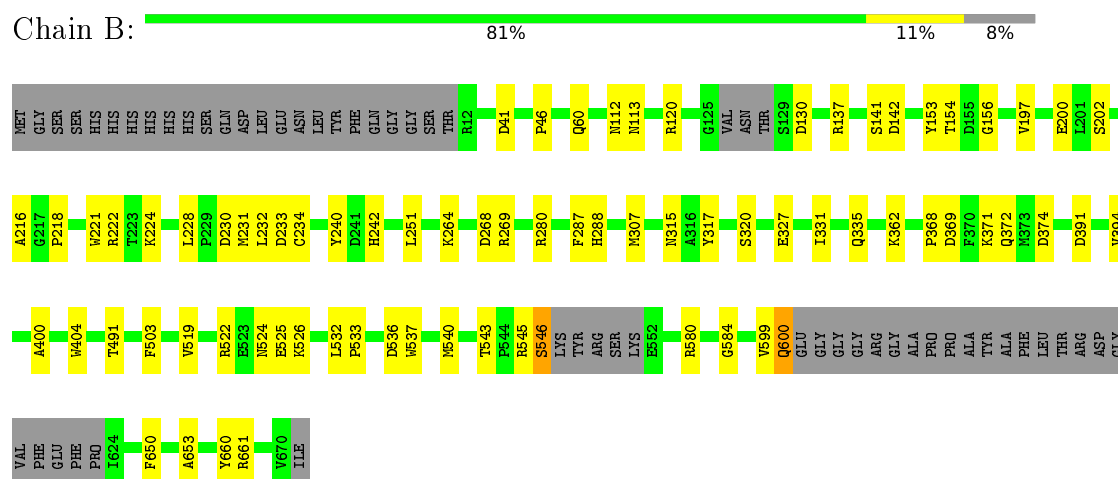
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total	Mg	0	0
			1	1		

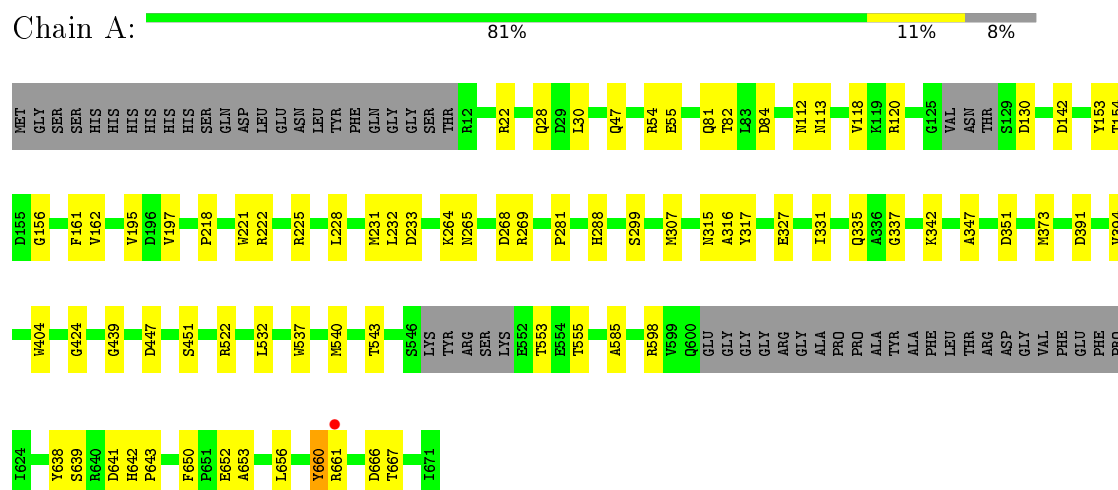
3 Residue-property plots

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.

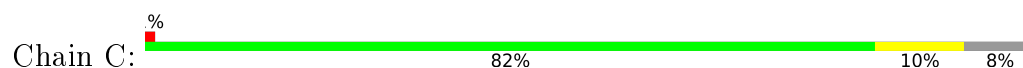
- Molecule 1: RNA-dependent RNA polymerase

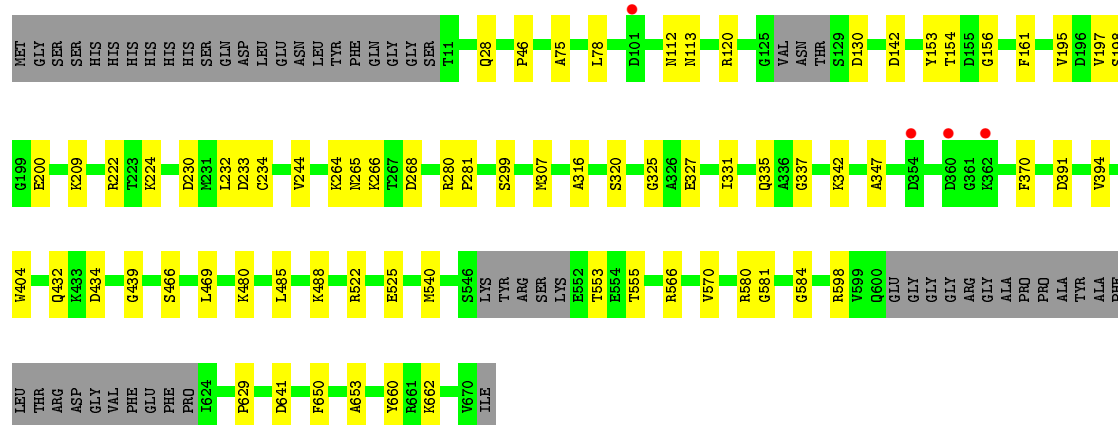


- Molecule 1: RNA-dependent RNA polymerase



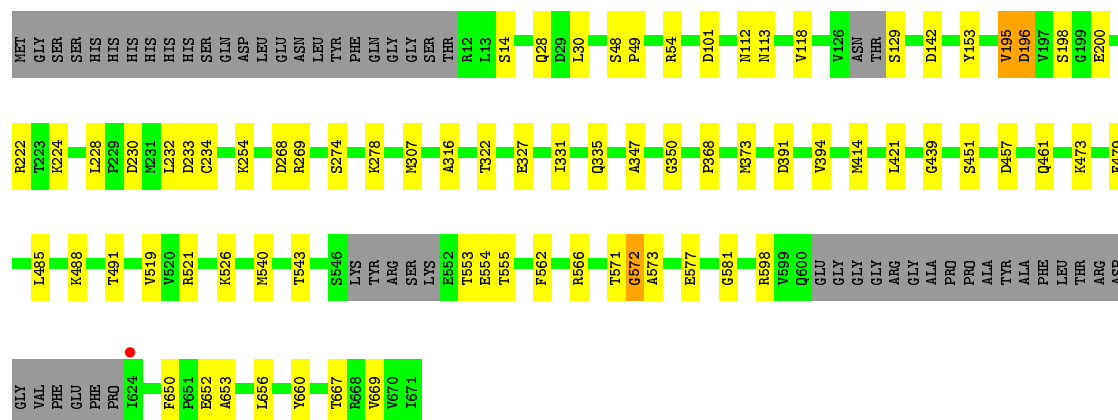
- Molecule 1: RNA-dependent RNA polymerase





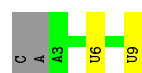
• Molecule 1: RNA-dependent RNA polymerase

Chain D: 81% 11% 8%



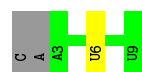
• Molecule 2: RNA (5'-R(P*AP*AP*AP*UP*UP*UP*U)-3')

Chain E: 56% 22% 22%



• Molecule 2: RNA (5'-R(P*AP*AP*AP*UP*UP*UP*U)-3')

Chain G: 67% 11% 22%

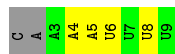
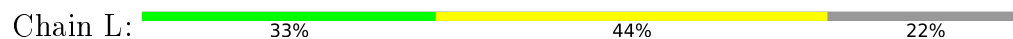


• Molecule 2: RNA (5'-R(P*AP*AP*AP*UP*UP*UP*U)-3')

Chain I: 56% 22% 22%



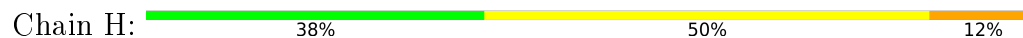
- Molecule 2: RNA (5'-R(P*AP*AP*AP*UP*UP*UP*U)-3')



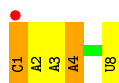
- Molecule 3: RNA (5'-R(P*CP*AP*AP*AP*AP*UP*UP*U)-3')



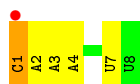
- Molecule 3: RNA (5'-R(P*CP*AP*AP*AP*AP*UP*UP*U)-3')



- Molecule 3: RNA (5'-R(P*CP*AP*AP*AP*AP*UP*UP*U)-3')



- Molecule 3: RNA (5'-R(P*CP*AP*AP*AP*AP*UP*UP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.79Å 207.31Å 115.98Å 90.00° 91.10° 90.00°	Depositor
Resolution (Å)	67.78 – 3.10 101.20 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (67.78-3.10) 99.9 (101.20-3.10)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.231 , 0.258 0.226 , 0.251	Depositor DCC
R_{free} test set	2836 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 23.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21230	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 3.07% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.36	2/5094 (0.0%)	0.56	1/6895 (0.0%)
1	B	0.29	0/5086	0.58	1/6884 (0.0%)
1	C	0.29	0/5093	0.57	1/6894 (0.0%)
1	D	0.44	4/5101 (0.1%)	0.59	5/6905 (0.1%)
2	E	0.29	0/162	0.84	0/249
2	G	0.29	0/162	0.79	0/249
2	I	0.30	0/162	0.79	0/249
2	L	0.28	0/162	0.70	0/249
3	F	0.34	0/187	1.09	2/288 (0.7%)
3	H	0.29	0/187	0.86	0/288
3	J	0.33	0/187	1.01	1/288 (0.3%)
3	K	0.33	0/187	0.96	2/288 (0.7%)
All	All	0.35	6/21770 (0.0%)	0.60	13/29726 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	660	TYR	C-N	14.89	1.68	1.34
1	D	571	THR	C-N	14.58	1.59	1.33
1	D	572	GLY	C-N	14.57	1.67	1.34
1	D	195	VAL	C-N	10.37	1.57	1.34
1	D	577	GLU	C-N	5.82	1.47	1.34
1	A	638	TYR	C-N	5.67	1.47	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	C	C2-N1-C1'	7.00	126.51	118.80
1	D	196	ASP	CB-CA-C	6.58	123.57	110.40
3	F	1	C	C6-N1-C1'	-6.50	113.00	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	196	ASP	N-CA-C	-6.34	93.89	111.00
3	J	1	C	C2-N1-C1'	6.02	125.42	118.80
3	K	1	C	C2-N1-C1'	5.75	125.13	118.80
1	D	571	THR	C-N-CA	-5.34	111.08	122.30
3	K	1	C	N1-C2-O2	5.27	122.06	118.90
1	B	142	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	142	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	473	LYS	CB-CA-C	-5.19	100.01	110.40
1	A	142	ASP	CB-CG-OD2	5.17	122.96	118.30
1	D	142	ASP	CB-CG-OD2	5.16	122.94	118.30

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	4986	0	4944	47	2
1	B	4978	0	4933	50	0
1	C	4985	0	4940	39	0
1	D	4993	0	4953	44	2
2	E	146	0	74	3	0
2	G	146	0	74	2	0
2	I	146	0	74	3	0
2	L	146	0	74	7	0
3	F	168	0	86	2	0
3	H	168	0	86	5	0
3	J	168	0	86	7	0
3	K	168	0	86	4	0
4	A	9	0	0	1	0
4	B	9	0	0	4	0
4	C	9	0	0	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	D	1	0	0	0	0
5	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21230	0	20410	180	2

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 (180) 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:D:572:GLY:C	1:D:573:ALA:N	1.67	1.46
1:A:660:TYR:C	1:A:661:ARG:N	1.68	1.45
1:A:54:ARG:NH1	1:A:55:GLU:OE1	2.02	0.91
1:A:269:ARG:NH2	2:E:6:U:OP1	2.11	0.84
1:A:269:ARG:NH1	1:A:543:THR:O	2.12	0.81
3:K:1:C:O2'	3:K:2:A:N7	2.16	0.78
1:D:269:ARG:NH1	1:D:543:THR:O	2.17	0.78
1:B:153:TYR:CE1	1:B:545:ARG:HG2	2.22	0.74
1:C:566:ARG:HG2	1:C:629:PRO:HD3	1.70	0.73
1:D:195:VAL:HG12	1:D:196:ASP:O	1.90	0.71
2:I:3:A:H61	3:J:8:U:H3	1.38	0.71
1:B:371:LYS:HA	4:B:701:POP:O2	1.91	0.70
1:B:660:TYR:HD1	1:A:233:ASP:HB3	1.59	0.68
1:A:373:MET:HE1	1:A:451:SER:HB2	1.75	0.67
1:A:28:GLN:HE21	1:A:598:ARG:HG2	1.60	0.65
1:C:120:ARG:HH22	1:C:264:LYS:HE3	1.62	0.65
1:D:540:MET:SD	2:L:6:U:H5''	2.38	0.63
1:C:660:TYR:HD1	1:D:233:ASP:HB3	1.63	0.63
1:A:195:VAL:HG23	1:A:299:SER:HB2	1.82	0.62
1:B:540:MET:SD	2:G:6:U:H5''	2.42	0.60
3:H:1:C:O2'	3:H:2:A:N7	2.33	0.60
1:C:112:ASN:OD1	1:C:113:ASN:N	2.35	0.59
1:C:327:GLU:O	1:C:331:ILE:HG23	2.02	0.59
3:J:1:C:H4'	3:J:1:C:OP1	2.01	0.59
1:A:650:PHE:HB2	1:A:653:ALA:HB2	1.85	0.59
1:D:112:ASN:OD1	1:D:113:ASN:N	2.35	0.58
1:A:112:ASN:OD1	1:A:113:ASN:N	2.34	0.58
1:D:650:PHE:HB2	1:D:653:ALA:HB2	1.86	0.58
1:A:327:GLU:O	1:A:331:ILE:HG23	2.03	0.57
1:B:320:SER:HB2	3:H:6:U:H4'	1.85	0.57
1:B:546:SER:O	1:B:546:SER:OG	2.22	0.57
1:D:572:GLY:CA	1:D:573:ALA:N	2.63	0.56
1:D:224:LYS:NZ	3:K:3:A:OP1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:652:GLU:HG2	1:D:656:LEU:HD23	1.86	0.56
1:B:153:TYR:CD1	1:B:545:ARG:HG2	2.40	0.56
1:B:112:ASN:OD1	1:B:113:ASN:N	2.37	0.55
1:C:316:ALA:HB2	1:C:347:ALA:HB1	1.87	0.55
1:B:327:GLU:O	1:B:331:ILE:HG23	2.07	0.55
1:D:327:GLU:O	1:D:331:ILE:HG23	2.05	0.55
1:B:545:ARG:NH2	2:G:6:U:OP2	2.40	0.55
1:C:153:TYR:CE1	1:C:268:ASP:HA	2.42	0.55
1:B:60:GLN:OE1	1:B:141:SER:OG	2.25	0.54
1:C:337:GLY:HA3	1:C:342:LYS:HB2	1.89	0.54
1:D:269:ARG:NH2	2:L:6:U:OP1	2.25	0.54
1:C:233:ASP:HB2	1:D:660:TYR:HD1	1.71	0.54
1:B:120:ARG:HH22	1:B:264:LYS:HE3	1.72	0.54
1:A:642:HIS:CD2	1:A:643:PRO:HD2	2.43	0.54
1:C:540:MET:SD	2:I:6:U:H5''	2.48	0.54
1:A:120:ARG:HH22	1:A:264:LYS:HE3	1.72	0.53
1:C:522:ARG:O	1:C:525:GLU:HG2	2.08	0.53
1:D:572:GLY:C	1:D:573:ALA:CA	2.71	0.53
1:B:197:VAL:HG22	1:B:404:TRP:CE2	2.43	0.53
1:B:224:LYS:NZ	3:H:3:A:OP1	2.41	0.52
1:D:350:GLY:HA3	2:L:8:U:O2'	2.10	0.52
1:B:153:TYR:CE1	1:B:268:ASP:HA	2.44	0.52
1:C:370:PHE:CZ	1:C:485:LEU:HD23	2.45	0.52
1:B:532:LEU:HD13	1:B:536:ASP:HB3	1.92	0.51
1:B:269:ARG:NE	1:B:543:THR:OG1	2.44	0.51
1:B:372:GLN:HA	4:B:701:POP:O5	2.10	0.51
1:C:553:THR:HG22	1:C:555:THR:H	1.76	0.51
1:D:153:TYR:CE1	1:D:268:ASP:HA	2.46	0.50
2:L:4:A:H2'	2:L:5:A:H8	1.75	0.50
1:B:200:GLU:OE1	1:B:202:SER:HB2	2.11	0.50
1:D:519:VAL:CG2	1:D:526:LYS:HB2	2.41	0.50
1:D:48:SER:OG	1:D:581:GLY:HA3	2.12	0.50
1:B:503:PHE:HE1	1:B:526:LYS:HG2	1.76	0.49
1:A:47:GLN:HG3	1:A:585:ALA:HB2	1.94	0.49
1:C:266:LYS:HD2	1:C:280:ARG:HD2	1.93	0.49
1:A:120:ARG:NH1	1:A:265:ASN:OD1	2.45	0.49
1:C:120:ARG:NH1	1:C:265:ASN:OD1	2.43	0.49
1:C:244:VAL:HG11	1:D:669:VAL:HG11	1.95	0.49
1:C:660:TYR:CD1	1:D:233:ASP:HB3	2.46	0.49
1:C:224:LYS:NZ	3:J:3:A:OP1	2.44	0.49
1:A:540:MET:SD	2:E:6:U:H5''	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:ASP:O	1:D:461:GLN:HG2	2.13	0.48
1:A:373:MET:CE	1:A:451:SER:HB2	2.42	0.48
1:B:372:GLN:HG3	1:B:374:ASP:OD1	2.14	0.48
2:L:4:A:H2'	2:L:5:A:C8	2.49	0.48
1:A:197:VAL:HG22	1:A:404:TRP:CE2	2.48	0.47
1:A:553:THR:HG22	1:A:555:THR:H	1.79	0.47
1:A:660:TYR:C	1:A:661:ARG:CA	2.72	0.47
1:D:322:THR:HG21	3:K:7:U:H4'	1.96	0.47
1:D:118:VAL:HG13	1:D:421:LEU:HD13	1.94	0.47
1:C:439:GLY:HA2	3:J:2:A:N3	2.30	0.47
1:D:479:PHE:HB3	1:D:485:LEU:HB2	1.97	0.47
1:B:400:ALA:HB1	1:A:667:THR:HG22	1.97	0.47
1:D:562:PHE:O	1:D:566:ARG:HG3	2.15	0.47
1:C:391:ASP:HA	1:C:394:VAL:HG22	1.96	0.47
1:C:650:PHE:HB2	1:C:653:ALA:HB2	1.96	0.47
1:A:373:MET:HE1	1:A:447:ASP:O	2.15	0.47
1:C:432:GLN:NE2	1:C:434:ASP:HB2	2.31	0.47
1:D:316:ALA:HB2	1:D:347:ALA:HB1	1.97	0.46
1:A:391:ASP:HA	1:A:394:VAL:HG22	1.96	0.46
1:B:660:TYR:CD1	1:A:233:ASP:HB3	2.45	0.46
1:A:118:VAL:O	1:A:424:GLY:N	2.30	0.46
1:B:233:ASP:HB3	1:A:660:TYR:HD1	1.81	0.46
1:A:82:THR:HG23	1:A:84:ASP:H	1.80	0.46
1:C:209:LYS:HA	1:D:14:SER:HA	1.96	0.46
1:B:218:PRO:HG3	1:B:221:TRP:CZ2	2.51	0.46
1:C:230:ASP:O	1:C:234:CYS:HB3	2.16	0.46
1:D:439:GLY:HA2	3:K:2:A:N3	2.31	0.46
1:B:46:PRO:O	1:B:584:GLY:HA3	2.16	0.45
1:D:230:ASP:O	1:D:234:CYS:HB3	2.16	0.45
1:A:161:PHE:CE1	1:A:281:PRO:HB3	2.51	0.45
3:H:3:A:H2'	3:H:4:A:O4'	2.16	0.45
3:J:2:A:H8	3:J:2:A:O5'	1.99	0.45
1:B:650:PHE:HB2	1:B:653:ALA:HB2	1.99	0.45
1:D:373:MET:CE	1:D:451:SER:HB2	2.46	0.45
1:A:652:GLU:HG2	1:A:656:LEU:HD13	1.99	0.45
1:B:280:ARG:NH2	4:B:701:POP:O6	2.50	0.44
1:A:337:GLY:HA3	1:A:342:LYS:HB2	1.98	0.44
1:D:28:GLN:HE21	1:D:598:ARG:HG2	1.82	0.44
3:F:3:A:H2'	3:F:4:A:O4'	2.16	0.44
1:A:153:TYR:CE1	1:A:268:ASP:HA	2.52	0.44
1:D:368:PRO:HA	1:D:491:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:PHE:CE1	1:C:281:PRO:HB3	2.53	0.44
1:D:48:SER:HA	1:D:49:PRO:HD3	1.72	0.44
1:B:130:ASP:OD1	1:B:130:ASP:N	2.44	0.44
1:C:46:PRO:O	1:C:584:GLY:HA3	2.18	0.44
2:L:5:A:H2'	2:L:6:U:C6	2.52	0.44
4:A:701:POP:O2	2:E:9:U:P	2.76	0.44
1:B:315:ASN:OD1	1:B:317:TYR:HB3	2.19	0.43
1:C:662:LYS:HE3	1:D:200:GLU:OE1	2.17	0.43
1:D:391:ASP:HA	1:D:394:VAL:HG22	1.99	0.43
1:B:519:VAL:CG1	1:B:526:LYS:HB3	2.48	0.43
1:C:154:THR:HG23	1:C:156:GLY:H	1.84	0.43
1:A:47:GLN:HG3	1:A:585:ALA:HA	2.01	0.43
1:C:198:SER:HA	1:D:667:THR:OG1	2.19	0.43
1:A:154:THR:HG23	1:A:156:GLY:H	1.83	0.43
1:A:218:PRO:HG3	1:A:221:TRP:CZ2	2.54	0.43
1:B:240:TYR:OH	1:A:666:ASP:O	2.20	0.43
1:B:532:LEU:HD22	1:B:533:PRO:HD2	2.00	0.43
1:A:315:ASN:OD1	1:A:317:TYR:HB3	2.19	0.43
1:A:641:ASP:N	1:A:641:ASP:OD1	2.52	0.43
1:B:371:LYS:HG3	4:B:701:POP:O2	2.19	0.42
1:A:47:GLN:HG3	1:A:585:ALA:CA	2.49	0.42
1:A:639:SER:HG	1:A:641:ASP:CG	2.23	0.42
1:C:197:VAL:HG22	1:C:404:TRP:CE2	2.54	0.42
1:A:652:GLU:HG2	1:A:652:GLU:O	2.19	0.42
1:C:75:ALA:HA	1:C:78:LEU:HD13	2.01	0.42
1:C:566:ARG:O	1:C:570:VAL:HG23	2.19	0.42
1:B:599:VAL:HG22	1:B:600:GLN:H	1.83	0.42
1:D:274:SER:HB3	1:D:278:LYS:HD2	2.02	0.42
1:B:41:ASP:OD1	1:C:581:GLY:HA3	2.20	0.42
1:D:196:ASP:OD1	1:D:198:SER:OG	2.33	0.42
1:C:28:GLN:HE21	1:C:598:ARG:HH11	1.66	0.42
1:D:652:GLU:O	1:D:656:LEU:HD23	2.20	0.42
1:B:362:LYS:HB2	1:B:362:LYS:HE3	1.92	0.42
1:B:545:ARG:HD2	3:H:1:C:N4	2.35	0.42
1:B:120:ARG:NH2	1:B:264:LYS:HG2	2.34	0.42
1:B:532:LEU:HB2	1:B:537:TRP:CE2	2.55	0.42
1:B:230:ASP:O	1:B:234:CYS:HB3	2.19	0.41
1:B:231:MET:HG2	1:B:288:HIS:HB3	2.02	0.41
1:A:228:LEU:O	1:A:232:LEU:HB2	2.21	0.41
1:A:231:MET:HG2	1:A:288:HIS:HB3	2.03	0.41
1:C:466:SER:HB3	1:C:469:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:VAL:HG23	1:C:299:SER:HB2	2.02	0.41
1:D:553:THR:HG22	1:D:555:THR:H	1.86	0.41
1:D:269:ARG:HH22	2:L:6:U:P	2.35	0.41
1:B:154:THR:HG23	1:B:156:GLY:H	1.86	0.41
1:B:532:LEU:HD23	1:B:532:LEU:HA	1.88	0.41
2:I:3:A:N6	3:J:8:U:H3	2.14	0.41
1:C:232:LEU:HD12	1:C:232:LEU:HA	1.95	0.41
1:C:641:ASP:OD1	1:C:641:ASP:N	2.53	0.41
1:D:228:LEU:O	1:D:232:LEU:HB2	2.21	0.41
1:D:554:GLU:H	1:D:554:GLU:HG2	1.69	0.41
1:B:228:LEU:O	1:B:232:LEU:HB2	2.20	0.41
1:B:242:HIS:ND1	1:B:251:LEU:HB2	2.36	0.41
1:B:391:ASP:HA	1:B:394:VAL:HG22	2.04	0.41
1:A:439:GLY:HA2	3:F:2:A:N3	2.36	0.41
1:A:532:LEU:HB2	1:A:537:TRP:CE2	2.56	0.41
3:J:3:A:H2'	3:J:4:A:O4'	2.21	0.41
1:B:368:PRO:HA	1:B:491:THR:HB	2.04	0.40
1:B:197:VAL:HG22	1:B:404:TRP:CZ2	2.56	0.40
1:A:81:GLN:O	1:A:162:VAL:HG11	2.22	0.40
1:A:316:ALA:HB2	1:A:347:ALA:HB1	2.03	0.40
1:A:351:ASP:HB3	1:A:373:MET:SD	2.62	0.40
1:C:320:SER:O	1:C:325:GLY:HA3	2.20	0.40
1:D:562:PHE:CZ	1:D:566:ARG:HD3	2.56	0.40
1:B:216:ALA:HB1	1:B:287:PHE:HB2	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ARG:NH1	1:D:49:PRO:CG[1_456]	1.89	0.31
1:A:661:ARG:NH1	1:D:49:PRO:CB[1_456]	2.11	0.09

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	621/684 (91%)	599 (96%)	22 (4%)	0	100	100
1	B	620/684 (91%)	597 (96%)	23 (4%)	0	100	100
1	C	621/684 (91%)	598 (96%)	23 (4%)	0	100	100
1	D	622/684 (91%)	602 (97%)	20 (3%)	0	100	100
All	All	2484/2736 (91%)	2396 (96%)	88 (4%)	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	536/581 (92%)	528 (98%)	8 (2%)	65	85
1	B	535/581 (92%)	523 (98%)	12 (2%)	52	78
1	C	536/581 (92%)	528 (98%)	8 (2%)	65	85
1	D	537/581 (92%)	526 (98%)	11 (2%)	55	80
All	All	2144/2324 (92%)	2105 (98%)	39 (2%)	59	82

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	137	ARG
1	B	222	ARG
1	B	307	MET
1	B	335	GLN
1	B	369	ASP
1	B	522	ARG
1	B	524	ASN
1	B	525	GLU
1	B	546	SER
1	B	580	ARG

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Mol	Chain	Res	Type
1	B	600	GLN
1	B	661	ARG
1	A	22	ARG
1	A	30	LEU
1	A	130	ASP
1	A	222	ARG
1	A	225	ARG
1	A	307	MET
1	A	335	GLN
1	A	522	ARG
1	C	130	ASP
1	C	200	GLU
1	C	222	ARG
1	C	307	MET
1	C	335	GLN
1	C	480	LYS
1	C	488	LYS
1	C	580	ARG
1	D	30	LEU
1	D	54	ARG
1	D	101	ASP
1	D	129	SER
1	D	222	ARG
1	D	254	LYS
1	D	307	MET
1	D	335	GLN
1	D	414	MET
1	D	488	LYS
1	D	521	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	28	GLN
1	B	58	GLN
1	B	113	ASN
1	B	253	ASN
1	B	402	GLN
1	B	432	GLN
1	A	28	GLN
1	A	88	GLN
1	A	253	ASN

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Mol	Chain	Res	Type
1	A	432	GLN
1	A	642	HIS
1	C	28	GLN
1	C	253	ASN
1	C	432	GLN
1	D	28	GLN
1	D	88	GLN
1	D	175	GLN
1	D	253	ASN
1	D	432	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	6/9 (66%)	0	0
2	G	6/9 (66%)	0	0
2	I	6/9 (66%)	0	0
2	L	6/9 (66%)	0	0
3	F	7/8 (87%)	1 (14%)	0
3	H	7/8 (87%)	1 (14%)	0
3	J	7/8 (87%)	1 (14%)	0
3	K	7/8 (87%)	1 (14%)	0
All	All	52/68 (76%)	4 (7%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	F	4	A
3	H	4	A
3	J	4	A
3	K	4	A

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

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
4	POP	A	701	5	6,8,8	0.73	0	13,13,13	1.36	1 (7%)
4	POP	C	701	5	6,8,8	0.76	0	13,13,13	1.45	1 (7%)
4	POP	B	701	5	6,8,8	0.80	0	13,13,13	1.23	1 (7%)

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
4	POP	A	701	5	-	0/6/6/6	-
4	POP	C	701	5	-	1/6/6/6	-
4	POP	B	701	5	-	1/6/6/6	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	C	701	POP	P2-O-P1	-4.10	118.77	132.83
4	A	701	POP	P2-O-P1	-3.90	119.45	132.83
4	B	701	POP	P2-O-P1	-3.53	120.71	132.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	701	POP	P2-O-P1-O2
4	B	701	POP	P2-O-P1-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	POP	1	0
4	B	701	POP	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	660:TYR	C	661:ARG	N	1.68
1	D	572:GLY	C	573:ALA	N	1.67

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	629/684 (91%)	-0.05	1 (0%) 95 90	25, 44, 63, 86	0
1	B	628/684 (91%)	-0.06	0 100 100	24, 42, 63, 81	0
1	C	629/684 (91%)	0.04	4 (0%) 89 78	28, 50, 75, 95	0
1	D	630/684 (92%)	0.08	1 (0%) 95 90	30, 57, 76, 109	0
2	E	7/9 (77%)	-0.37	0 100 100	28, 31, 37, 55	0
2	G	7/9 (77%)	-0.22	0 100 100	40, 43, 54, 66	0
2	I	7/9 (77%)	0.05	0 100 100	33, 41, 62, 66	0
2	L	7/9 (77%)	0.53	0 100 100	59, 61, 69, 85	0
3	F	8/8 (100%)	-0.08	0 100 100	26, 31, 41, 80	0
3	H	8/8 (100%)	0.25	0 100 100	35, 45, 55, 78	0
3	J	8/8 (100%)	0.03	1 (12%) 3 1	34, 37, 41, 78	0
3	K	8/8 (100%)	0.77	1 (12%) 3 1	51, 61, 69, 97	0
All	All	2576/2804 (91%)	0.01	8 (0%) 94 88	24, 49, 72, 109	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	624	ILE	3.3
1	C	360	ASP	3.1
1	C	362	LYS	3.0
1	A	661	ARG	2.6
3	K	1	C	2.6
3	J	1	C	2.5
1	C	354	ASP	2.2
1	C	101	ASP	2.1

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
5	MG	D	701	1/1	0.61	0.27	52,52,52,52	0
5	MG	B	703	1/1	0.73	0.13	48,48,48,48	0
5	MG	B	702	1/1	0.78	0.32	47,47,47,47	0
5	MG	I	101	1/1	0.80	0.12	89,89,89,89	0
4	POP	C	701	9/9	0.82	0.26	62,68,132,135	0
5	MG	A	702	1/1	0.83	0.14	45,45,45,45	0
4	POP	B	701	9/9	0.84	0.34	44,58,66,70	0
4	POP	A	701	9/9	0.89	0.20	44,55,73,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.