



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 07:06 PM BST

PDB ID : 6Z6B
Title : Structure of full-length La Crosse virus L protein (polymerase)
Authors : Cusack, S.; Gerlach, P.; Reguera, J.
Deposited on : 2020-05-28
Resolution : 3.96 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
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
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) : 2.13

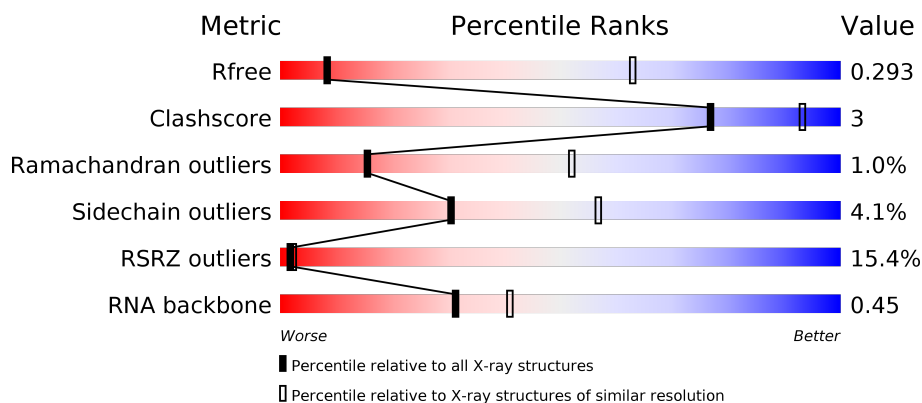
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.96 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	1025 (4.22-3.70)
Clashscore	141614	1085 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)
RSRZ outliers	127900	1013 (4.28-3.64)
RNA backbone	3102	1041 (4.84-3.00)

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 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	BBB	10	<div> <div>30%</div> <div>50%</div> <div>50%</div> </div>
1	UUU	10	<div> <div>60%</div> <div>40%</div> </div>
2	CCC	16	<div> <div>19%</div> <div>81%</div> <div>19%</div> </div>
2	HHH	16	<div> <div>13%</div> <div>75%</div> <div>19%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	DDD	8	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>13%88%13%</div>
3	XXX	8	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>25%75%25%</div>
4	EEE	2285	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>15%78%10% • 11%</div>
4	PPP	2285	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>12%79%10% • 11%</div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 34640 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 RNA chain called RNA (5'-R(P*AP*GP*UP*AP*GP*UP*GP*UP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BBB	10	Total	C	N	O	P	0	0	0
			216	96	39	71	10			
1	UUU	10	Total	C	N	O	P	0	0	0
			216	96	39	71	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CCC	16	Total	C	N	O	P	0	0	0
			336	151	56	113	16			
2	HHH	16	Total	C	N	O	P	0	0	0
			336	151	56	113	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	DDD	8	Total	C	N	O	P	0	0	0
			165	76	30	52	7			
3	XXX	8	Total	C	N	O	P	0	0	0
			165	76	30	52	7			

- Molecule 4 is a protein called RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	EEE	2031	Total	C	N	O	S	0	0	0
			16582	10626	2758	3090	108			
4	PPP	2036	Total	C	N	O	S	0	0	0
			16622	10651	2766	3096	109			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EEE	-21	MET	-	initiating methionine	UNP A5HC98
EEE	-20	GLY	-	expression tag	UNP A5HC98
EEE	-19	HIS	-	expression tag	UNP A5HC98
EEE	-18	HIS	-	expression tag	UNP A5HC98
EEE	-17	HIS	-	expression tag	UNP A5HC98
EEE	-16	HIS	-	expression tag	UNP A5HC98
EEE	-15	HIS	-	expression tag	UNP A5HC98
EEE	-14	HIS	-	expression tag	UNP A5HC98
EEE	-13	ASP	-	expression tag	UNP A5HC98
EEE	-12	TYR	-	expression tag	UNP A5HC98
EEE	-11	ASP	-	expression tag	UNP A5HC98
EEE	-10	ILE	-	expression tag	UNP A5HC98
EEE	-9	PRO	-	expression tag	UNP A5HC98
EEE	-8	THR	-	expression tag	UNP A5HC98
EEE	-7	THR	-	expression tag	UNP A5HC98
EEE	-6	GLU	-	expression tag	UNP A5HC98
EEE	-5	ASN	-	expression tag	UNP A5HC98
EEE	-4	LEU	-	expression tag	UNP A5HC98
EEE	-3	TYR	-	expression tag	UNP A5HC98
EEE	-2	PHE	-	expression tag	UNP A5HC98
EEE	-1	GLN	-	expression tag	UNP A5HC98
EEE	0	GLY	-	expression tag	UNP A5HC98
PPP	-21	MET	-	initiating methionine	UNP A5HC98
PPP	-20	GLY	-	expression tag	UNP A5HC98
PPP	-19	HIS	-	expression tag	UNP A5HC98
PPP	-18	HIS	-	expression tag	UNP A5HC98
PPP	-17	HIS	-	expression tag	UNP A5HC98
PPP	-16	HIS	-	expression tag	UNP A5HC98
PPP	-15	HIS	-	expression tag	UNP A5HC98
PPP	-14	HIS	-	expression tag	UNP A5HC98
PPP	-13	ASP	-	expression tag	UNP A5HC98
PPP	-12	TYR	-	expression tag	UNP A5HC98
PPP	-11	ASP	-	expression tag	UNP A5HC98
PPP	-10	ILE	-	expression tag	UNP A5HC98
PPP	-9	PRO	-	expression tag	UNP A5HC98
PPP	-8	THR	-	expression tag	UNP A5HC98
PPP	-7	THR	-	expression tag	UNP A5HC98
PPP	-6	GLU	-	expression tag	UNP A5HC98
PPP	-5	ASN	-	expression tag	UNP A5HC98
PPP	-4	LEU	-	expression tag	UNP A5HC98
PPP	-3	TYR	-	expression tag	UNP A5HC98
PPP	-2	PHE	-	expression tag	UNP A5HC98
PPP	-1	GLN	-	expression tag	UNP A5HC98

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Chain	Residue	Modelled	Actual	Comment	Reference
PPP	0	GLY	-	expression tag	UNP A5HC98

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

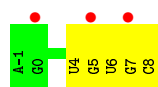
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	PPP	1	Total	Zn	0	0
			1	1		
5	EEE	1	Total	Zn	0	0
			1	1		

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.

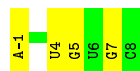
- Molecule 1: RNA (5'-R(P*AP*GP*UP*AP*GP*UP*GP*UP*GP*C)-3')

Chain BBB: 




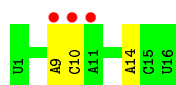
- Molecule 1: RNA (5'-R(P*AP*GP*UP*AP*GP*UP*GP*UP*GP*C)-3')

Chain UUU: 




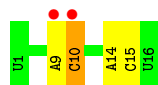
- Molecule 2: RNA (5'-R(P*UP*UP*AP*GP*UP*AP*GP*UP*AP*CP*AP*CP*UP*AP*CP*U)-3')

Chain CCC: 



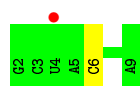
- Molecule 2: RNA (5'-R(P*UP*UP*AP*GP*UP*AP*GP*UP*AP*CP*AP*CP*UP*AP*CP*U)-3')

Chain HHH: 

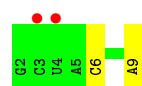
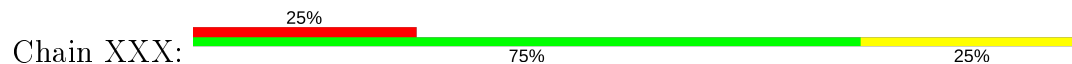


- Molecule 3: RNA (5'-R(*GP*CP*UP*AP*CP*UP*AP*A)-3')

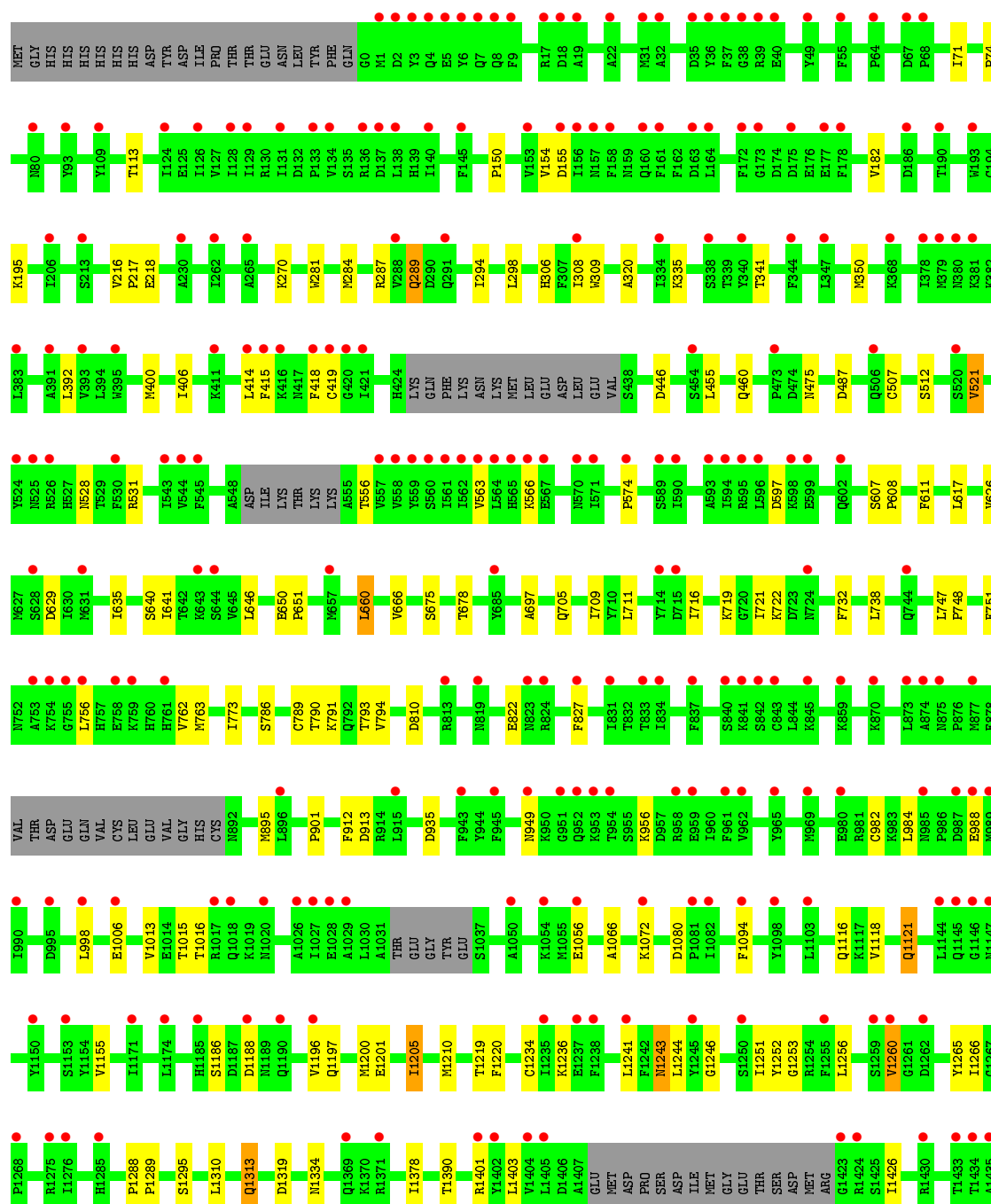
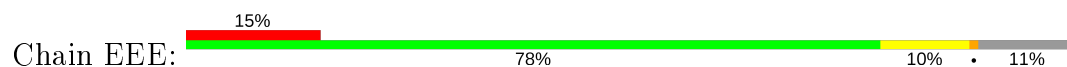
Chain DDD: 



- Molecule 3: RNA (5'-R(*GP*CP*UP*AP*CP*UP*AP*A)-3')



- Molecule 4: RNA-directed RNA polymerase L





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	371.19Å 145.32Å 234.19Å 90.00° 116.33° 90.00°	Depositor
Resolution (Å)	209.89 – 3.96 209.89 – 3.96	Depositor EDS
% Data completeness (in resolution range)	60.8 (209.89-3.96) 60.8 (209.89-3.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 4.02Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.264 , 0.299 0.261 , 0.293	Depositor DCC
R_{free} test set	1514 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å ²)	167.7	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 209.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	34640	wwPDB-VP
Average B, all atoms (Å ²)	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.77% 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: ZN

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	BBB	0.24	0/241	0.67	0/374
1	UUU	0.23	0/241	0.63	0/374
2	CCC	0.22	0/374	0.64	0/579
2	HHH	0.23	0/374	0.64	0/579
3	DDD	0.18	0/184	0.61	0/285
3	XXX	0.18	0/184	0.62	0/285
4	EEE	0.67	0/16918	0.70	0/22801
4	PPP	0.67	0/16960	0.70	0/22858
All	All	0.66	0/35476	0.70	0/48135

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BBB	216	0	108	0	0
1	UUU	216	0	108	1	0
2	CCC	336	0	171	0	0
2	HHH	336	0	171	2	0
3	DDD	165	0	85	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	XXX	165	0	85	0	0
4	EEE	16582	0	16651	104	0
4	PPP	16622	0	16692	105	0
5	EEE	1	0	0	0	0
5	PPP	1	0	0	0	0
All	All	34640	0	34071	203	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (203) 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)
4:EEE:716:ILE:HB	4:EEE:719:LYS:HE3	1.40	1.01
4:EEE:716:ILE:HB	4:EEE:719:LYS:CE	1.96	0.94
4:EEE:721:ILE:HG21	4:EEE:738:LEU:HD23	1.62	0.82
4:PPP:2152:ILE:HD11	4:PPP:2226:PHE:CZ	2.18	0.79
4:PPP:1522:SER:O	4:PPP:1526:ASP:HB2	1.85	0.76
4:PPP:1525:ARG:O	4:PPP:1529:ILE:HG13	1.92	0.69
4:EEE:716:ILE:CB	4:EEE:719:LYS:HE3	2.21	0.68
4:PPP:1739:HIS:NE2	4:PPP:2017:LYS:HG2	2.07	0.68
4:EEE:716:ILE:HD12	4:EEE:719:LYS:HE2	1.76	0.68
4:PPP:1310:LEU:HB2	4:PPP:1313:GLN:HG3	1.76	0.68
4:EEE:1310:LEU:HB2	4:EEE:1313:GLN:HG3	1.76	0.66
4:EEE:1403:LEU:HD11	4:EEE:1528:TYR:OH	1.97	0.65
4:PPP:2187:PRO:HB2	4:PPP:2189:CYS:SG	2.36	0.65
4:PPP:150:PRO:HB2	4:PPP:1751:ALA:HB2	1.78	0.65
4:PPP:2152:ILE:HD11	4:PPP:2226:PHE:HZ	1.60	0.65
4:PPP:2208:ILE:HD11	4:PPP:2234:ILE:CD1	2.28	0.64
4:EEE:721:ILE:HD12	4:EEE:1244:LEU:HB3	1.79	0.64
4:PPP:709:ILE:HG23	4:PPP:716:ILE:HG21	1.78	0.64
4:PPP:308:ILE:O	4:PPP:563:VAL:HG21	1.99	0.63
4:PPP:721:ILE:HG21	4:PPP:738:LEU:HD23	1.79	0.63
4:EEE:709:ILE:HG23	4:EEE:716:ILE:HG21	1.81	0.62
4:EEE:150:PRO:HB2	4:EEE:1751:ALA:HB2	1.82	0.61
4:EEE:308:ILE:O	4:EEE:563:VAL:HG21	1.99	0.61
4:PPP:1256:LEU:HD23	4:PPP:1295:SER:HB2	1.82	0.61
4:PPP:1197:GLN:HE21	4:PPP:1205:ILE:HD11	1.66	0.61
4:EEE:1256:LEU:HD23	4:EEE:1295:SER:HB2	1.82	0.61
4:EEE:1197:GLN:HE21	4:EEE:1205:ILE:HD11	1.65	0.61
4:EEE:2190:PHE:CZ	4:PPP:2247:PHE:CE2	2.90	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:PPP:1791:ILE:O	4:PPP:1795:PHE:HB2	2.01	0.60
4:EEE:1791:ILE:O	4:EEE:1795:PHE:HB2	2.02	0.59
4:PPP:2152:ILE:HD11	4:PPP:2226:PHE:CE1	2.36	0.59
4:EEE:982:CYS:HB3	4:EEE:988:GLU:HG2	1.85	0.58
4:EEE:1056:GLU:HG2	4:EEE:1236:LYS:HG2	1.85	0.58
4:PPP:1056:GLU:HG2	4:PPP:1236:LYS:HG2	1.85	0.58
4:EEE:721:ILE:HG21	4:EEE:738:LEU:CD2	2.34	0.57
4:PPP:1751:ALA:O	4:PPP:1755:HIS:HB3	2.05	0.57
4:PPP:982:CYS:HB3	4:PPP:988:GLU:HG2	1.85	0.57
4:PPP:2030:LEU:HA	4:PPP:2064:CYS:HA	1.86	0.56
4:PPP:153:VAL:HG22	4:PPP:1743:GLN:HE22	1.70	0.56
4:PPP:415:PHE:HA	4:PPP:419:CYS:HB2	1.88	0.55
4:EEE:415:PHE:HA	4:EEE:419:CYS:HB2	1.88	0.55
4:EEE:2030:LEU:HA	4:EEE:2064:CYS:HA	1.88	0.55
4:EEE:646:LEU:HD11	4:EEE:756:LEU:HD12	1.89	0.54
4:PPP:646:LEU:HD11	4:PPP:756:LEU:HD12	1.88	0.54
4:EEE:716:ILE:HB	4:EEE:719:LYS:HE2	1.85	0.54
4:EEE:2244:PHE:HA	4:PPP:2210:SER:HB2	1.88	0.54
4:PPP:721:ILE:HG21	4:PPP:738:LEU:CD2	2.38	0.54
4:EEE:2137:ILE:HG22	4:EEE:2138:SER:H	1.73	0.54
4:EEE:2055:LEU:HB2	4:EEE:2121:GLU:HB3	1.90	0.53
4:PPP:2055:LEU:HB2	4:PPP:2121:GLU:HB3	1.90	0.53
4:PPP:2137:ILE:HG22	4:PPP:2138:SER:H	1.73	0.53
4:PPP:660:LEU:HB3	4:PPP:697:ALA:HB1	1.91	0.52
4:EEE:660:LEU:HB3	4:EEE:697:ALA:HB1	1.91	0.52
4:EEE:822:GLU:HA	4:EEE:827:PHE:HB2	1.90	0.52
4:EEE:711:LEU:HD13	4:EEE:716:ILE:CG1	2.40	0.52
4:PPP:2151:LEU:HD11	4:PPP:2234:ILE:HD11	1.91	0.52
4:PPP:2190:PHE:CD1	4:PPP:2203:MET:HB3	2.45	0.52
4:PPP:822:GLU:HA	4:PPP:827:PHE:HB2	1.92	0.52
4:PPP:1739:HIS:NE2	4:PPP:2017:LYS:CG	2.73	0.51
4:PPP:2208:ILE:CD1	4:PPP:2234:ILE:CD1	2.88	0.51
4:EEE:650:GLU:HB3	4:EEE:651:PRO:HD3	1.93	0.51
4:PPP:1760:GLU:O	4:PPP:1763:ILE:HB	2.10	0.51
4:EEE:281:TRP:O	4:EEE:284:MET:HB3	2.12	0.50
4:PPP:626:VAL:HB	4:PPP:629:ASP:HB2	1.92	0.50
4:EEE:705:GLN:HB3	4:EEE:722:LYS:HD2	1.93	0.50
4:PPP:2189:CYS:SG	4:PPP:2190:PHE:N	2.85	0.50
4:EEE:1469:GLU:HG2	4:EEE:1628:ARG:HA	1.92	0.50
4:EEE:747:LEU:N	4:EEE:748:PRO:HD2	2.27	0.50
4:PPP:707:ARG:HA	4:PPP:722:LYS:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:EEE:216:VAL:HG12	4:EEE:217:PRO:HD3	1.94	0.50
4:PPP:1469:GLU:HG2	4:PPP:1628:ARG:HA	1.93	0.50
4:PPP:216:VAL:HG12	4:PPP:217:PRO:HD3	1.94	0.50
4:EEE:1072:LYS:HD2	4:EEE:1155:VAL:HG11	1.94	0.49
4:PPP:1072:LYS:HD2	4:PPP:1155:VAL:HG11	1.93	0.49
4:PPP:150:PRO:HB2	4:PPP:1751:ALA:CB	2.41	0.49
4:PPP:747:LEU:N	4:PPP:748:PRO:HD2	2.27	0.49
4:EEE:1760:GLU:O	4:EEE:1763:ILE:HB	2.12	0.49
4:EEE:626:VAL:HB	4:EEE:629:ASP:HB2	1.93	0.49
4:PPP:650:GLU:HB3	4:PPP:651:PRO:HD3	1.95	0.49
4:EEE:2203:MET:O	4:EEE:2206:GLU:HG3	2.13	0.49
4:PPP:281:TRP:O	4:PPP:284:MET:HB3	2.12	0.48
4:EEE:2207:PHE:CE1	4:PPP:2247:PHE:CE1	3.02	0.48
4:PPP:2203:MET:O	4:PPP:2206:GLU:HG3	2.13	0.48
4:EEE:2181:TYR:O	4:EEE:2184:PHE:HB2	2.14	0.47
4:PPP:1593:LEU:HD12	4:PPP:1744:ILE:HG22	1.96	0.47
4:EEE:150:PRO:CG	4:EEE:1751:ALA:HA	2.44	0.47
4:EEE:2130:THR:O	4:EEE:2141:ASN:ND2	2.47	0.47
4:PPP:1751:ALA:O	4:PPP:1755:HIS:CB	2.63	0.47
4:EEE:607:SER:N	4:EEE:608:PRO:CD	2.77	0.47
4:PPP:2208:ILE:CD1	4:PPP:2234:ILE:HD12	2.44	0.46
4:PPP:1718:THR:HG21	4:PPP:1745:LEU:HD21	1.97	0.46
4:EEE:1593:LEU:HD12	4:EEE:1744:ILE:HG22	1.97	0.46
4:EEE:1833:LEU:HD22	4:EEE:1982:ILE:HG21	1.98	0.46
4:PPP:607:SER:N	4:PPP:608:PRO:CD	2.78	0.46
4:PPP:1819:ILE:N	4:PPP:1820:PRO:HD2	2.31	0.46
4:EEE:2149:VAL:HA	4:EEE:2152:ILE:HD12	1.97	0.46
4:EEE:1819:ILE:N	4:EEE:1820:PRO:HD2	2.31	0.46
4:PPP:1819:ILE:HG22	4:PPP:2000:ILE:HD11	1.98	0.46
4:EEE:2077:LEU:HB2	4:EEE:2111:ARG:HG2	1.98	0.46
4:EEE:287:ARG:NH1	4:EEE:675:SER:OG	2.49	0.45
4:PPP:2148:VAL:O	4:PPP:2152:ILE:HG12	2.17	0.45
4:EEE:1730:ILE:HG22	4:EEE:1731:LYS:HG2	1.98	0.45
4:EEE:721:ILE:HD13	4:EEE:738:LEU:CD2	2.46	0.45
4:PPP:1121:GLN:HE21	4:PPP:1121:GLN:HA	1.81	0.45
4:EEE:2139:PRO:HA	4:EEE:2142:LEU:HB2	1.98	0.45
4:EEE:414:LEU:O	4:EEE:418:PHE:HB3	2.17	0.45
4:EEE:1819:ILE:HG22	4:EEE:2000:ILE:HD11	1.99	0.45
4:EEE:747:LEU:N	4:EEE:748:PRO:CD	2.80	0.45
4:PPP:1243:ASN:ND2	4:PPP:1244:LEU:O	2.50	0.45
4:PPP:2077:LEU:HB2	4:PPP:2111:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:EEE:2244:PHE:CD2	4:PPP:2210:SER:HA	2.52	0.45
4:PPP:287:ARG:NH1	4:PPP:675:SER:OG	2.49	0.45
4:PPP:747:LEU:N	4:PPP:748:PRO:CD	2.80	0.45
4:PPP:2169:HIS:O	4:PPP:2173:ILE:HG13	2.17	0.45
4:EEE:2169:HIS:O	4:EEE:2173:ILE:HG13	2.17	0.45
4:PPP:611:PHE:CE1	4:PPP:635:ILE:HG23	2.52	0.45
4:EEE:2173:ILE:HA	4:EEE:2178:ASP:HB2	1.99	0.44
4:PPP:1265:TYR:HB2	4:PPP:1506:LEU:HD22	1.99	0.44
4:EEE:216:VAL:N	4:EEE:217:PRO:CD	2.80	0.44
4:EEE:521:VAL:HG13	4:EEE:531:ARG:HD3	1.98	0.44
4:PPP:2139:PRO:HA	4:PPP:2142:LEU:HB2	1.98	0.44
4:PPP:521:VAL:HG13	4:PPP:531:ARG:HD3	1.99	0.44
4:EEE:74:PRO:HG3	4:EEE:113:THR:HA	2.00	0.44
4:PPP:1833:LEU:HD22	4:PPP:1982:ILE:HG21	1.98	0.44
4:PPP:216:VAL:N	4:PPP:217:PRO:CD	2.80	0.44
4:PPP:1289:PRO:HG3	4:PPP:1729:LEU:HA	2.00	0.44
4:PPP:1730:ILE:HG22	4:PPP:1731:LYS:HG2	1.99	0.44
4:PPP:1587:ILE:O	4:PPP:1590:THR:OG1	2.35	0.44
4:EEE:1587:ILE:O	4:EEE:1590:THR:OG1	2.35	0.44
4:EEE:611:PHE:CE1	4:EEE:635:ILE:HG23	2.53	0.44
4:EEE:2087:GLY:HA2	4:EEE:2098:ILE:O	2.18	0.44
4:PPP:1579:LEU:HD22	4:PPP:1749:HIS:HB3	1.99	0.44
4:EEE:2238:PHE:HB3	4:PPP:2202:VAL:HG21	1.99	0.44
4:PPP:773:ILE:HG21	4:PPP:1066:ALA:HB1	2.00	0.44
4:EEE:1121:GLN:HA	4:EEE:1121:GLN:HE21	1.82	0.43
4:EEE:150:PRO:HG3	4:EEE:1751:ALA:HA	1.99	0.43
4:EEE:2189:CYS:SG	4:EEE:2190:PHE:N	2.90	0.43
2:HHH:10:C:HO2'	4:PPP:395:TRP:HE1	1.66	0.43
4:EEE:1243:ASN:ND2	4:EEE:1244:LEU:O	2.50	0.43
4:EEE:1473:THR:HG21	4:EEE:1624:ALA:HB2	2.01	0.43
4:PPP:153:VAL:HG22	4:PPP:1743:GLN:NE2	2.32	0.43
2:HHH:15:C:C2	4:PPP:472:LYS:HG2	2.53	0.43
4:EEE:309:TRP:CD1	4:EEE:507:CYS:HA	2.54	0.43
4:PPP:2173:ILE:HA	4:PPP:2178:ASP:HB2	1.99	0.43
4:EEE:1265:TYR:HB2	4:EEE:1506:LEU:HD22	1.99	0.43
4:EEE:2155:LEU:HD21	4:EEE:2230:CYS:HA	2.00	0.43
4:EEE:773:ILE:HG21	4:EEE:1066:ALA:HB1	1.99	0.43
4:PPP:414:LEU:O	4:PPP:418:PHE:HB3	2.17	0.43
4:EEE:306:HIS:CE1	4:EEE:641:ILE:HG22	2.53	0.43
4:EEE:392:LEU:HB2	4:EEE:400:MET:HB2	2.01	0.43
4:PPP:998:LEU:HB2	4:PPP:1241:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:EEE:1244:LEU:O	4:EEE:1246:GLY:N	2.51	0.43
4:PPP:418:PHE:O	1:UUU:-1:A:H1'	2.19	0.43
4:PPP:350:MET:HE1	4:PPP:406:ILE:HD11	1.99	0.43
4:PPP:306:HIS:CE1	4:PPP:641:ILE:HG22	2.54	0.43
4:PPP:74:PRO:HG3	4:PPP:113:THR:HA	2.00	0.43
4:PPP:1610:MET:HG2	4:PPP:1611:PRO:HD2	2.01	0.42
4:EEE:719:LYS:NZ	4:EEE:1006:GLU:OE2	2.51	0.42
4:PPP:2087:GLY:HA2	4:PPP:2098:ILE:O	2.19	0.42
4:PPP:309:TRP:CD1	4:PPP:507:CYS:HA	2.54	0.42
4:EEE:1610:MET:HG2	4:EEE:1611:PRO:HD2	2.00	0.42
4:EEE:1579:LEU:HD22	4:EEE:1749:HIS:HB3	2.02	0.42
4:EEE:350:MET:HE1	4:EEE:406:ILE:HD11	2.01	0.42
4:PPP:1473:THR:HG21	4:PPP:1624:ALA:HB2	2.00	0.42
4:PPP:216:VAL:CG1	4:PPP:217:PRO:HD3	2.49	0.42
4:EEE:1016:THR:HG21	4:EEE:2090:ILE:O	2.20	0.42
4:EEE:216:VAL:CG1	4:EEE:217:PRO:HD3	2.48	0.42
4:PPP:1197:GLN:NE2	4:PPP:1200:MET:HG2	2.35	0.42
4:PPP:1784:ARG:NH2	4:PPP:1995:PHE:O	2.53	0.42
4:PPP:789:CYS:SG	4:PPP:1219:THR:HG23	2.60	0.42
4:PPP:711:LEU:HA	4:PPP:716:ILE:HG12	2.02	0.42
4:PPP:794:VAL:HG13	4:PPP:1220:PHE:HA	2.02	0.42
4:EEE:998:LEU:HB2	4:EEE:1241:LEU:HD23	2.02	0.42
4:EEE:1784:ARG:NH2	4:EEE:1995:PHE:O	2.53	0.42
4:EEE:2092:SER:OG	4:EEE:2094:PRO:HD2	2.20	0.42
4:EEE:789:CYS:SG	4:EEE:1219:THR:HG23	2.60	0.42
4:PPP:1244:LEU:O	4:PPP:1246:GLY:N	2.51	0.42
4:EEE:794:VAL:HG13	4:EEE:1220:PHE:HA	2.02	0.41
4:PPP:1197:GLN:HG3	4:PPP:1205:ILE:HD11	2.00	0.41
4:PPP:392:LEU:HB2	4:PPP:400:MET:HB2	2.01	0.41
4:PPP:762:VAL:HG11	4:PPP:949:ASN:HB2	2.02	0.41
4:EEE:1403:LEU:HD23	4:EEE:1527:LYS:HD2	2.02	0.41
4:EEE:289:GLN:HG2	4:EEE:294:ILE:HG13	2.02	0.41
4:PPP:218:GLU:N	4:PPP:218:GLU:OE1	2.54	0.41
4:EEE:1378:ILE:HG21	4:EEE:1579:LEU:HD11	2.03	0.41
4:EEE:1251:ILE:O	4:EEE:1253:GLY:N	2.54	0.41
4:EEE:308:ILE:HG13	4:EEE:308:ILE:O	2.20	0.41
4:PPP:748:PRO:HA	4:PPP:751:PHE:CE2	2.55	0.41
4:EEE:1013:VAL:HA	4:EEE:2090:ILE:HD11	2.03	0.41
4:EEE:2148:VAL:O	4:EEE:2152:ILE:HG13	2.20	0.41
4:EEE:748:PRO:HA	4:EEE:751:PHE:CE2	2.56	0.41
4:PPP:972:TYR:O	4:PPP:976:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:PPP:2092:SER:OG	4:PPP:2094:PRO:HD2	2.21	0.41
4:EEE:1288:PRO:HA	4:EEE:1289:PRO:HD3	1.97	0.41
4:PPP:308:ILE:HG13	4:PPP:308:ILE:O	2.20	0.41
4:EEE:2046:ASN:HA	4:EEE:2083:ASN:O	2.21	0.41
4:PPP:150:PRO:HG2	4:PPP:1751:ALA:HA	2.02	0.40
4:EEE:1289:PRO:HG3	4:EEE:1729:LEU:HA	2.02	0.40
4:EEE:2187:PRO:HB3	4:PPP:2251:MET:SD	2.62	0.40
4:EEE:762:VAL:HG11	4:EEE:949:ASN:HB2	2.02	0.40
4:EEE:218:GLU:N	4:EEE:218:GLU:OE1	2.54	0.40
4:EEE:721:ILE:HD12	4:EEE:1244:LEU:HD22	2.02	0.40
4:EEE:1015:THR:HB	4:EEE:1196:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	EEE	2009/2285 (88%)	1808 (90%)	180 (9%)	21 (1%)	15	52
4	PPP	2016/2285 (88%)	1812 (90%)	183 (9%)	21 (1%)	15	52
All	All	4025/4570 (88%)	3620 (90%)	363 (9%)	42 (1%)	15	52

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	EEE	1623	PRO
4	PPP	1623	PRO
4	EEE	270	LYS
4	EEE	678	THR
4	EEE	1234	CYS
4	EEE	1252	TYR
4	EEE	2155	LEU

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Mol	Chain	Res	Type
4	EEE	2159	GLU
4	EEE	2197	ARG
4	PPP	270	LYS
4	PPP	678	THR
4	PPP	1234	CYS
4	PPP	1252	TYR
4	PPP	2155	LEU
4	PPP	2159	GLU
4	PPP	2197	ARG
4	EEE	566	LYS
4	EEE	1186	SER
4	EEE	2180	MET
4	PPP	566	LYS
4	PPP	1186	SER
4	PPP	2180	MET
4	PPP	2239	GLU
4	EEE	1118	VAL
4	EEE	1334	ASN
4	EEE	2239	GLU
4	PPP	187	PHE
4	PPP	1118	VAL
4	PPP	1334	ASN
4	EEE	1260	VAL
4	EEE	1635	PRO
4	EEE	2011	LYS
4	EEE	2138	SER
4	PPP	714	TYR
4	PPP	1260	VAL
4	PPP	2011	LYS
4	PPP	2138	SER
4	EEE	320	ALA
4	EEE	1116	GLN
4	PPP	1116	GLN
4	EEE	901	PRO
4	PPP	901	PRO

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	
4	EEE	1873/2107 (89%)	1795 (96%)	78 (4%)	30	56
4	PPP	1877/2107 (89%)	1801 (96%)	76 (4%)	31	57
All	All	3750/4214 (89%)	3596 (96%)	154 (4%)	30	57

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	EEE	71	ILE
4	EEE	154	VAL
4	EEE	155	ASP
4	EEE	182	VAL
4	EEE	195	LYS
4	EEE	289	GLN
4	EEE	298	LEU
4	EEE	335	LYS
4	EEE	341	THR
4	EEE	446	ASP
4	EEE	455	LEU
4	EEE	460	GLN
4	EEE	475	ASN
4	EEE	487	ASP
4	EEE	512	SER
4	EEE	521	VAL
4	EEE	528	ASN
4	EEE	556	THR
4	EEE	574	PRO
4	EEE	597	ASP
4	EEE	617	LEU
4	EEE	640	SER
4	EEE	660	LEU
4	EEE	666	VAL
4	EEE	732	PHE
4	EEE	763	MET
4	EEE	786	SER
4	EEE	790	THR
4	EEE	791	LYS
4	EEE	793	THR
4	EEE	810	ASP
4	EEE	895	MET
4	EEE	912	PHE
4	EEE	913	ASP

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Mol	Chain	Res	Type
4	EEE	935	ASP
4	EEE	956	LYS
4	EEE	984	LEU
4	EEE	1080	ASP
4	EEE	1094	PHE
4	EEE	1121	GLN
4	EEE	1188	ASP
4	EEE	1200	MET
4	EEE	1201	GLU
4	EEE	1205	ILE
4	EEE	1210	MET
4	EEE	1243	ASN
4	EEE	1260	VAL
4	EEE	1266	ILE
4	EEE	1313	GLN
4	EEE	1319	ASP
4	EEE	1390	THR
4	EEE	1401	ARG
4	EEE	1426	ILE
4	EEE	1457	MET
4	EEE	1473	THR
4	EEE	1506	LEU
4	EEE	1571	GLN
4	EEE	1663	GLU
4	EEE	1679	ARG
4	EEE	1688	MET
4	EEE	1719	THR
4	EEE	1726	GLN
4	EEE	1732	ASP
4	EEE	1739	HIS
4	EEE	1776	ASP
4	EEE	1795	PHE
4	EEE	1835	LYS
4	EEE	2063	CYS
4	EEE	2064	CYS
4	EEE	2093	THR
4	EEE	2106	ARG
4	EEE	2117	LEU
4	EEE	2185	ASP
4	EEE	2204	PHE
4	EEE	2223	THR
4	EEE	2228	LYS

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Mol	Chain	Res	Type
4	EEE	2233	LEU
4	EEE	2240	THR
4	PPP	71	ILE
4	PPP	154	VAL
4	PPP	182	VAL
4	PPP	195	LYS
4	PPP	250	ASP
4	PPP	289	GLN
4	PPP	298	LEU
4	PPP	446	ASP
4	PPP	455	LEU
4	PPP	460	GLN
4	PPP	475	ASN
4	PPP	487	ASP
4	PPP	512	SER
4	PPP	521	VAL
4	PPP	528	ASN
4	PPP	556	THR
4	PPP	574	PRO
4	PPP	584	MET
4	PPP	597	ASP
4	PPP	617	LEU
4	PPP	640	SER
4	PPP	660	LEU
4	PPP	666	VAL
4	PPP	719	LYS
4	PPP	732	PHE
4	PPP	763	MET
4	PPP	786	SER
4	PPP	790	THR
4	PPP	791	LYS
4	PPP	793	THR
4	PPP	810	ASP
4	PPP	895	MET
4	PPP	912	PHE
4	PPP	913	ASP
4	PPP	935	ASP
4	PPP	984	LEU
4	PPP	1080	ASP
4	PPP	1094	PHE
4	PPP	1121	GLN
4	PPP	1188	ASP

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Mol	Chain	Res	Type
4	PPP	1201	GLU
4	PPP	1205	ILE
4	PPP	1210	MET
4	PPP	1243	ASN
4	PPP	1260	VAL
4	PPP	1266	ILE
4	PPP	1313	GLN
4	PPP	1390	THR
4	PPP	1401	ARG
4	PPP	1426	ILE
4	PPP	1457	MET
4	PPP	1473	THR
4	PPP	1506	LEU
4	PPP	1571	GLN
4	PPP	1663	GLU
4	PPP	1679	ARG
4	PPP	1688	MET
4	PPP	1719	THR
4	PPP	1726	GLN
4	PPP	1732	ASP
4	PPP	1739	HIS
4	PPP	1750	LYS
4	PPP	1776	ASP
4	PPP	1795	PHE
4	PPP	1835	LYS
4	PPP	2063	CYS
4	PPP	2064	CYS
4	PPP	2093	THR
4	PPP	2106	ARG
4	PPP	2117	LEU
4	PPP	2185	ASP
4	PPP	2204	PHE
4	PPP	2223	THR
4	PPP	2233	LEU
4	PPP	2238	PHE
4	PPP	2240	THR

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	BBB	9/10 (90%)	5 (55%)	1 (11%)
1	UUU	9/10 (90%)	3 (33%)	0
2	CCC	15/16 (93%)	3 (20%)	0
2	HHH	15/16 (93%)	3 (20%)	0
3	DDD	7/8 (87%)	1 (14%)	0
3	XXX	7/8 (87%)	2 (28%)	0
All	All	62/68 (91%)	17 (27%)	1 (1%)

All (17) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	BBB	4	U
1	BBB	5	G
1	BBB	6	U
1	BBB	7	G
1	BBB	8	C
2	CCC	9	A
2	CCC	10	C
2	CCC	14	A
3	DDD	6	C
2	HHH	9	A
2	HHH	10	C
2	HHH	14	A
1	UUU	4	U
1	UUU	5	G
1	UUU	7	G
3	XXX	6	C
3	XXX	9	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	BBB	5	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	BBB	10/10 (100%)	1.54	3 (30%) 0 0	153, 182, 218, 228	0
1	UUU	10/10 (100%)	1.19	0 100 100	122, 141, 171, 201	0
2	CCC	16/16 (100%)	1.11	3 (18%) 1 1	113, 200, 291, 292	0
2	HHH	16/16 (100%)	0.99	2 (12%) 3 5	93, 168, 206, 212	0
3	DDD	8/8 (100%)	0.46	1 (12%) 3 5	190, 224, 238, 244	0
3	XXX	8/8 (100%)	0.94	2 (25%) 0 0	145, 176, 201, 214	0
4	EEE	2031/2285 (88%)	0.96	346 (17%) 1 2	87, 211, 334, 415	0
4	PPP	2036/2285 (89%)	0.89	279 (13%) 3 3	80, 181, 312, 403	0
All	All	4135/4638 (89%)	0.93	636 (15%) 2 2	80, 193, 325, 415	0

All (636) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	EEE	1679	ARG	13.4
4	EEE	2188	LYS	9.2
4	EEE	1471	LEU	9.0
4	EEE	1501	GLN	9.0
4	EEE	157	ASN	8.7
4	EEE	958	ARG	8.7
4	EEE	2183	SER	8.6
4	EEE	959	GLU	8.4
4	PPP	1701	SER	8.4
4	EEE	1678	GLN	8.4
4	EEE	1472	VAL	8.1
4	EEE	3	TYR	7.8
4	PPP	1423	GLY	7.4
4	EEE	1262	ASP	7.3
4	PPP	2105	GLU	7.2
4	EEE	874	ALA	7.0

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Mol	Chain	Res	Type	RSRZ
4	EEE	1680	ASP	7.0
4	EEE	1701	SER	6.9
4	EEE	178	PHE	6.8
4	PPP	1981	ARG	6.7
4	PPP	73	ALA	6.6
4	EEE	133	PRO	6.6
4	PPP	1501	GLN	6.5
4	EEE	37	PHE	6.5
4	PPP	952	GLN	6.3
4	EEE	8	GLN	6.2
4	EEE	39	ARG	6.2
4	PPP	3	TYR	6.0
4	PPP	1702	THR	5.9
4	PPP	2000	ILE	5.9
4	PPP	1622	SER	5.9
4	EEE	129	ILE	5.8
4	PPP	178	PHE	5.7
4	PPP	2179	HIS	5.7
4	EEE	1699	VAL	5.7
4	EEE	1470	LEU	5.7
4	EEE	1692	TYR	5.6
4	EEE	175	ASP	5.6
4	EEE	593	ALA	5.6
4	EEE	419	CYS	5.5
4	EEE	1633	ASN	5.5
4	EEE	164	LEU	5.5
4	PPP	55	PHE	5.4
4	EEE	6	TYR	5.4
4	PPP	959	GLU	5.4
4	PPP	1997	LEU	5.4
4	EEE	1028	GLU	5.4
4	PPP	109	TYR	5.4
4	EEE	36	TYR	5.4
4	PPP	2002	VAL	5.2
4	EEE	834	ILE	5.2
4	EEE	2179	HIS	5.2
4	EEE	2105	GLU	5.1
4	EEE	1741	LEU	5.1
4	PPP	126	ILE	5.1
4	PPP	2155	LEU	5.1
4	EEE	953	LYS	5.1
4	EEE	40	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
4	EEE	1	MET	5.0
4	PPP	35	ASP	4.9
4	PPP	958	ARG	4.9
4	EEE	145	PHE	4.9
4	EEE	32	ALA	4.9
4	EEE	2082	MET	4.9
4	EEE	9	PHE	4.8
4	EEE	1369	GLN	4.8
4	EEE	1683	PHE	4.8
4	EEE	951	GLY	4.8
4	EEE	5	GLU	4.8
4	EEE	2002	VAL	4.7
4	EEE	1702	THR	4.7
4	EEE	35	ASP	4.6
4	EEE	840	SER	4.6
4	EEE	2192	GLY	4.6
4	PPP	1424	ARG	4.6
4	EEE	544	VAL	4.6
4	EEE	172	PHE	4.6
4	EEE	594	ILE	4.5
4	PPP	1262	ASP	4.5
4	PPP	76	ILE	4.5
4	PPP	953	LYS	4.5
4	EEE	1475	GLY	4.5
4	PPP	852	GLU	4.5
4	EEE	49	TYR	4.5
4	PPP	875	ASN	4.5
4	PPP	1995	PHE	4.4
2	CCC	9	A	4.4
4	EEE	714	TYR	4.4
4	PPP	1840	LYS	4.4
4	EEE	2047	TYR	4.4
4	PPP	1678	GLN	4.4
4	EEE	155	ASP	4.3
4	EEE	2079	ASP	4.3
4	EEE	843	CYS	4.3
4	PPP	2185	ASP	4.3
4	EEE	1498	LEU	4.3
4	EEE	1742	LYS	4.3
4	PPP	56	ILE	4.3
4	EEE	1698	TYR	4.2
4	EEE	952	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
4	EEE	128	ILE	4.2
4	EEE	2242	ARG	4.2
4	EEE	4	GLN	4.2
4	EEE	156	ILE	4.1
4	PPP	1259	SER	4.1
4	PPP	1	MET	4.1
4	PPP	1683	PHE	4.1
4	EEE	1684	GLU	4.1
4	EEE	873	LEU	4.1
4	EEE	2037	MET	4.1
4	EEE	1027	ILE	4.1
4	EEE	1819	ILE	4.1
4	EEE	1424	ARG	4.1
4	PPP	1473	THR	4.1
4	PPP	991	SER	4.0
4	EEE	158	PHE	4.0
4	EEE	595	ARG	4.0
4	PPP	141	ASN	4.0
4	EEE	1630	TYR	4.0
4	EEE	38	GLY	4.0
4	EEE	383	LEU	4.0
4	EEE	557	VAL	4.0
4	EEE	55	PHE	3.9
4	EEE	1245	TYR	3.9
4	EEE	1768	PHE	3.9
4	PPP	124	ILE	3.9
4	PPP	874	ALA	3.9
4	EEE	1238	PHE	3.9
4	EEE	193	TRP	3.9
4	PPP	164	LEU	3.9
4	EEE	2108	MET	3.9
4	PPP	142	SER	3.9
4	EEE	1627	LEU	3.9
4	EEE	1473	THR	3.9
4	EEE	754	LYS	3.9
4	EEE	80	ASN	3.8
4	EEE	2247	PHE	3.8
4	EEE	1423	GLY	3.8
4	PPP	2106	ARG	3.8
4	EEE	1145	GLN	3.8
4	EEE	561	ILE	3.8
4	EEE	545	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
4	EEE	965	TYR	3.8
4	EEE	18	ASP	3.8
4	EEE	380	ASN	3.8
4	EEE	759	LYS	3.8
4	EEE	875	ASN	3.8
4	EEE	859	LYS	3.8
4	EEE	378	ILE	3.7
4	PPP	1836	TYR	3.7
4	PPP	2144	CYS	3.7
4	PPP	1741	LEU	3.7
4	PPP	113	THR	3.7
4	EEE	1442	TYR	3.7
4	EEE	524	TYR	3.7
4	PPP	719	LYS	3.7
4	PPP	201	PHE	3.7
4	PPP	334	ILE	3.7
4	EEE	1260	VAL	3.7
4	PPP	1241	LEU	3.7
4	PPP	139	HIS	3.7
4	EEE	563	VAL	3.6
4	EEE	1029	ALA	3.6
4	EEE	93	TYR	3.6
4	EEE	1435	ALA	3.6
4	PPP	140	ILE	3.6
4	PPP	39	ARG	3.6
4	EEE	67	ASP	3.6
4	EEE	2106	ARG	3.6
4	EEE	344	PHE	3.6
4	EEE	334	ILE	3.6
4	EEE	379	MET	3.6
4	EEE	558	VAL	3.6
4	PPP	714	TYR	3.5
4	PPP	2	ASP	3.5
4	PPP	1283	ILE	3.5
4	EEE	308	ILE	3.5
4	PPP	160	GLN	3.5
4	EEE	2081	PRO	3.5
4	EEE	823	ASN	3.5
4	PPP	754	LYS	3.5
4	PPP	1627	LEU	3.5
4	PPP	68	PRO	3.5
4	PPP	2066	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
4	PPP	653	ARG	3.5
4	EEE	1474	LYS	3.5
4	EEE	1433	THR	3.5
4	PPP	419	CYS	3.4
4	PPP	2108	MET	3.4
4	EEE	1476	GLU	3.4
4	PPP	53	VAL	3.4
4	EEE	19	ALA	3.4
4	EEE	520	SER	3.4
4	PPP	1982	ILE	3.4
4	PPP	2188	LYS	3.4
4	EEE	1504	ALA	3.4
4	EEE	543	ILE	3.4
4	EEE	64	PRO	3.4
1	BBB	5	G	3.4
4	EEE	1840	LYS	3.4
4	PPP	51	ASN	3.4
2	CCC	10	C	3.4
4	EEE	915	LEU	3.4
4	EEE	1054	LYS	3.4
4	PPP	2237	LYS	3.3
4	EEE	340	TYR	3.3
4	EEE	2104	GLY	3.3
4	EEE	134	VAL	3.3
4	PPP	1470	LEU	3.3
4	EEE	368	LYS	3.3
4	EEE	177	GLU	3.3
4	PPP	985	ASN	3.3
4	PPP	1028	GLU	3.3
4	EEE	1771	ILE	3.3
4	EEE	1098	TYR	3.3
4	EEE	1674	ALA	3.3
4	PPP	1821	LEU	3.3
4	EEE	567	GLU	3.3
4	EEE	2015	PHE	3.3
2	HHH	9	A	3.3
4	PPP	89	TYR	3.2
4	PPP	658	ASN	3.2
4	EEE	7	GLN	3.2
4	EEE	1528	TYR	3.2
4	PPP	1447	TYR	3.2
4	PPP	1839	MET	3.2

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Mol	Chain	Res	Type	RSRZ
4	EEE	1241	LEU	3.2
4	PPP	760	HIS	3.2
4	PPP	2104	GLY	3.2
4	EEE	140	ILE	3.2
4	EEE	1687	GLU	3.2
4	EEE	824	ARG	3.2
4	PPP	1691	PHE	3.2
4	EEE	564	LEU	3.2
4	PPP	1514	SER	3.2
4	PPP	473	PRO	3.2
4	EEE	1797	TYR	3.2
4	PPP	127	VAL	3.2
4	PPP	1680	ASP	3.2
4	PPP	25	ILE	3.2
4	PPP	1248	PRO	3.2
4	PPP	1276	ILE	3.2
4	EEE	126	ILE	3.1
4	EEE	756	LEU	3.1
4	EEE	2080	ASP	3.1
4	PPP	1771	ILE	3.1
4	EEE	161	PHE	3.1
4	PPP	1472	VAL	3.1
4	PPP	1665	MET	3.1
4	PPP	2186	VAL	3.1
4	EEE	526	ARG	3.1
4	PPP	138	LEU	3.1
4	EEE	2000	ILE	3.1
4	EEE	136	ARG	3.1
4	PPP	67	ASP	3.1
4	EEE	1836	TYR	3.1
4	PPP	1050	ALA	3.1
4	EEE	421	ILE	3.1
4	EEE	418	PHE	3.1
4	EEE	393	VAL	3.1
4	PPP	2156	LYS	3.1
4	PPP	5	GLU	3.1
4	EEE	961	PHE	3.1
4	PPP	6	TYR	3.1
4	PPP	1679	ARG	3.1
4	EEE	989	MET	3.1
4	PPP	756	LEU	3.1
4	EEE	2017	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
4	PPP	998	LEU	3.0
4	EEE	560	SER	3.0
4	PPP	2010	ILE	3.0
4	EEE	877	MET	3.0
4	PPP	2151	LEU	3.0
4	PPP	172	PHE	3.0
4	PPP	1146	GLY	3.0
4	EEE	1285	HIS	3.0
4	EEE	949	ASN	3.0
4	EEE	2018	MET	3.0
4	EEE	715	ASP	3.0
4	PPP	2065	GLU	3.0
4	PPP	954	THR	3.0
4	EEE	414	LEU	3.0
4	EEE	995	ASP	3.0
4	EEE	411	LYS	3.0
4	PPP	988	GLU	3.0
4	PPP	1699	VAL	3.0
4	PPP	1991	ASN	3.0
4	EEE	137	ASP	3.0
4	EEE	1259	SER	3.0
4	EEE	1724	LEU	3.0
4	EEE	1691	PHE	3.0
4	PPP	2207	PHE	2.9
4	EEE	186	ASP	2.9
4	EEE	525	ASN	2.9
4	EEE	1188	ASP	2.9
4	EEE	506	GLN	2.9
4	EEE	631	MET	2.9
4	EEE	1404	VAL	2.9
4	PPP	945	PHE	2.9
4	PPP	965	TYR	2.9
4	EEE	570	ASN	2.9
4	PPP	1185	HIS	2.9
4	PPP	1526	ASP	2.9
4	EEE	1700	LYS	2.9
4	EEE	2001	LYS	2.9
4	PPP	1196	VAL	2.9
4	EEE	1072	LYS	2.9
4	EEE	1488	ARG	2.9
4	PPP	383	LEU	2.9
4	EEE	589	SER	2.9

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Mol	Chain	Res	Type	RSRZ
4	PPP	761	HIS	2.9
4	PPP	715	ASP	2.8
4	PPP	1145	GLN	2.8
4	EEE	1712	PRO	2.8
4	EEE	1816	THR	2.8
4	PPP	2001	LYS	2.8
4	EEE	1401	ARG	2.8
4	EEE	954	THR	2.8
4	EEE	1276	ILE	2.8
4	EEE	1507	PHE	2.8
4	PPP	2090	ILE	2.8
4	PPP	1443	SER	2.8
4	EEE	590	ILE	2.8
4	PPP	915	LEU	2.8
4	PPP	2234	ILE	2.8
4	EEE	758	GLU	2.8
4	EEE	1405	LEU	2.8
4	PPP	856	GLN	2.8
4	EEE	2003	GLY	2.8
4	EEE	896	LEU	2.8
4	EEE	990	ILE	2.8
4	PPP	590	ILE	2.8
4	PPP	74	PRO	2.8
4	PPP	1260	VAL	2.8
4	EEE	213	SER	2.8
4	PPP	1787	PHE	2.8
4	PPP	1476	GLU	2.8
4	PPP	1481	TYR	2.8
4	EEE	1235	ILE	2.7
4	EEE	138	LEU	2.7
4	EEE	1196	VAL	2.7
4	EEE	1006	GLU	2.7
4	PPP	525	ASN	2.7
4	EEE	2088	GLU	2.7
4	EEE	1758	THR	2.7
4	EEE	2033	LEU	2.7
4	PPP	943	PHE	2.7
4	PPP	2183	SER	2.7
4	PPP	1275	ARG	2.7
4	PPP	1748	GLY	2.7
4	EEE	1466	GLU	2.7
4	EEE	473	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
4	EEE	124	ILE	2.7
4	EEE	599	GLU	2.7
4	EEE	574	PRO	2.7
4	EEE	1026	ALA	2.7
4	EEE	1185	HIS	2.7
4	PPP	125	GLU	2.7
4	PPP	1693	GLN	2.7
4	EEE	1663	GLU	2.7
4	PPP	989	MET	2.7
4	EEE	1371	ARG	2.7
4	PPP	912	PHE	2.7
4	EEE	962	VAL	2.7
4	PPP	207	TYR	2.7
4	EEE	755	GLY	2.7
4	EEE	1081	PRO	2.7
4	PPP	1630	TYR	2.7
4	EEE	230	ALA	2.7
4	EEE	265	ALA	2.7
4	EEE	109	TYR	2.6
4	PPP	598	LYS	2.6
4	PPP	167	LEU	2.6
4	EEE	998	LEU	2.6
4	PPP	168	LEU	2.6
4	EEE	131	ILE	2.6
4	EEE	985	ASN	2.6
4	EEE	1481	TYR	2.6
4	PPP	1992	ASN	2.6
4	PPP	2003	GLY	2.6
4	PPP	1626	VAL	2.6
4	EEE	559	TYR	2.6
4	PPP	1349	LEU	2.6
4	PPP	381	LYS	2.6
4	PPP	763	MET	2.6
4	PPP	1692	TYR	2.6
4	PPP	570	ASN	2.6
4	EEE	381	LYS	2.6
4	EEE	347	LEU	2.6
4	EEE	291	GLN	2.6
4	EEE	1834	ASP	2.6
4	PPP	1465	LEU	2.6
4	EEE	598	LYS	2.6
4	PPP	230	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
4	PPP	2107	HIS	2.6
4	EEE	562	ILE	2.6
4	EEE	1514	SER	2.6
4	PPP	990	ILE	2.6
4	EEE	870	LYS	2.6
4	PPP	1504	ALA	2.6
4	EEE	1502	ASN	2.6
4	EEE	1614	ARG	2.6
4	EEE	17	ARG	2.6
4	EEE	2004	LEU	2.5
4	PPP	718	GLN	2.5
4	EEE	1430	ARG	2.5
4	PPP	1027	ILE	2.5
4	PPP	161	PHE	2.5
4	PPP	1256	LEU	2.5
4	EEE	1237	GLU	2.5
4	EEE	969	MET	2.5
4	EEE	1676	LYS	2.5
4	EEE	565	HIS	2.5
4	EEE	1020	ASN	2.5
4	PPP	995	ASP	2.5
4	PPP	1783	SER	2.5
4	EEE	2152	ILE	2.5
4	EEE	2021	PHE	2.5
4	PPP	1064	TRP	2.5
4	EEE	988	GLU	2.5
4	PPP	599	GLU	2.5
4	PPP	2047	TYR	2.5
4	PPP	1994	ILE	2.5
4	EEE	415	PHE	2.5
4	PPP	1527	LYS	2.5
4	PPP	630	ILE	2.5
4	PPP	1285	HIS	2.5
4	PPP	909	THR	2.5
4	EEE	1190	GLN	2.5
4	PPP	1513	PHE	2.5
4	EEE	571	ILE	2.5
4	PPP	496	MET	2.5
4	EEE	1171	ILE	2.5
4	PPP	36	TYR	2.5
4	EEE	2	ASP	2.4
4	PPP	9	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
4	PPP	2238	PHE	2.5
4	PPP	377	GLN	2.4
4	PPP	2081	PRO	2.4
4	EEE	1688	MET	2.4
4	PPP	657	MET	2.4
4	EEE	2195	ILE	2.4
4	EEE	420	GLY	2.4
4	EEE	827	PHE	2.4
4	EEE	153	VAL	2.4
4	PPP	1755	HIS	2.4
4	PPP	2148	VAL	2.4
4	PPP	90	ILE	2.4
4	EEE	1434	THR	2.4
4	EEE	980	GLU	2.4
4	PPP	93	TYR	2.4
4	PPP	841	LYS	2.4
4	PPP	2018	MET	2.4
4	EEE	744	GLN	2.4
4	PPP	961	PHE	2.4
4	EEE	1480	ASP	2.4
4	PPP	1988	ASP	2.4
4	PPP	980	GLU	2.4
4	PPP	2050	ILE	2.4
4	EEE	1487	PHE	2.4
4	PPP	924	LEU	2.4
4	PPP	1528	TYR	2.4
4	PPP	949	ASN	2.4
4	EEE	1483	GLU	2.4
4	EEE	31	MET	2.4
4	EEE	2251	MET	2.4
4	PPP	762	VAL	2.4
4	PPP	308	ILE	2.4
4	EEE	2187	PRO	2.4
4	EEE	1450	ARG	2.4
4	PPP	828	ARG	2.4
4	PPP	1250	SER	2.4
4	EEE	566	LYS	2.4
4	PPP	129	ILE	2.4
4	EEE	2240	THR	2.4
4	PPP	1524	ILE	2.4
4	PPP	1684	GLU	2.4
4	EEE	761	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
4	PPP	951	GLY	2.4
4	PPP	1742	LYS	2.4
4	PPP	1728	ASN	2.3
4	PPP	182	VAL	2.3
4	PPP	1471	LEU	2.3
4	EEE	1402	TYR	2.3
4	EEE	160	GLN	2.3
4	EEE	1050	ALA	2.3
4	PPP	58	ILE	2.3
4	EEE	1056	GLU	2.3
4	EEE	163	ASP	2.3
4	PPP	137	ASP	2.3
3	DDD	4	U	2.3
4	PPP	2152	ILE	2.3
4	EEE	987	ASP	2.3
4	EEE	1461	PHE	2.3
4	EEE	2155	LEU	2.3
4	EEE	391	ALA	2.3
4	EEE	628	SER	2.3
4	PPP	870	LYS	2.3
4	PPP	193	TRP	2.3
4	PPP	810	ASP	2.3
4	PPP	1054	LYS	2.3
4	EEE	1146	GLY	2.3
4	EEE	833	THR	2.3
4	PPP	833	THR	2.3
4	EEE	22	ALA	2.3
4	EEE	288	VAL	2.3
4	EEE	454	SER	2.3
4	PPP	834	ILE	2.3
4	PPP	1450	ARG	2.3
4	EEE	416	LYS	2.3
4	EEE	841	LYS	2.3
4	EEE	173	GLY	2.3
4	EEE	1465	LEU	2.3
4	EEE	1250	SER	2.3
1	BBB	7	G	2.3
4	PPP	2251	MET	2.3
4	EEE	845	LYS	2.3
4	EEE	1685	LEU	2.3
4	EEE	2249	LYS	2.3
4	PPP	401	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
4	EEE	602	GLN	2.3
4	EEE	644	SER	2.3
4	EEE	837	PHE	2.3
4	PPP	2187	PRO	2.3
4	PPP	916	TYR	2.3
4	EEE	945	PHE	2.3
4	EEE	2051	ARG	2.2
4	PPP	1238	PHE	2.3
4	PPP	1833	LEU	2.2
4	EEE	813	ARG	2.2
4	EEE	1174	LEU	2.2
4	PPP	565	HIS	2.2
4	EEE	1833	LEU	2.2
4	PPP	839	SER	2.2
4	EEE	1255	PHE	2.2
4	PPP	1112	ASN	2.2
4	PPP	2190	PHE	2.2
4	PPP	1228	LYS	2.2
4	PPP	911	VAL	2.2
4	EEE	1094	PHE	2.2
4	PPP	806	ASN	2.2
4	EEE	657	MET	2.2
4	EEE	1650	VAL	2.2
4	PPP	1578	ILE	2.2
4	PPP	1685	LEU	2.2
4	PPP	52	ASP	2.2
4	PPP	753	ALA	2.2
3	XXX	3	C	2.2
4	EEE	190	THR	2.2
4	EEE	530	PHE	2.2
4	EEE	2196	THR	2.2
4	EEE	262	ILE	2.2
4	PPP	31	MET	2.2
4	PPP	528	ASN	2.2
4	EEE	1746	SER	2.2
4	PPP	827	PHE	2.2
1	BBB	0	G	2.2
4	EEE	1082	ILE	2.2
4	PPP	2154	LEU	2.2
4	EEE	1275	ARG	2.2
4	PPP	1614	ARG	2.2
4	EEE	753	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
4	PPP	340	TYR	2.2
4	EEE	1018	GLN	2.2
4	EEE	2186	VAL	2.2
4	PPP	288	VAL	2.2
4	PPP	1018	GLN	2.2
4	EEE	1268	PRO	2.2
4	PPP	759	LYS	2.2
4	PPP	1456	GLY	2.2
4	PPP	1469	GLU	2.2
4	PPP	1730	ILE	2.2
4	EEE	685	TYR	2.2
4	PPP	1510	GLN	2.2
4	EEE	2234	ILE	2.2
4	PPP	54	PRO	2.2
4	PPP	330	SER	2.2
4	PPP	1495	LYS	2.2
4	EEE	842	SER	2.1
4	EEE	1144	LEU	2.1
4	PPP	414	LEU	2.1
4	PPP	116	ILE	2.1
4	PPP	1835	LYS	2.1
4	PPP	2194	PRO	2.1
2	HHH	10	C	2.1
3	XXX	4	U	2.1
4	EEE	395	TRP	2.1
4	PPP	840	SER	2.1
4	EEE	831	ILE	2.1
4	PPP	37	PHE	2.1
4	PPP	831	ILE	2.1
2	CCC	11	A	2.1
4	PPP	1698	TYR	2.1
4	PPP	1235	ILE	2.1
4	EEE	724	ASN	2.1
4	EEE	68	PRO	2.1
4	EEE	206	ILE	2.1
4	EEE	1150	TYR	2.1
4	PPP	235	ARG	2.1
4	EEE	1443	SER	2.1
4	EEE	2107	HIS	2.1
4	PPP	145	PHE	2.1
4	EEE	1017	ARG	2.1
4	EEE	643	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
4	PPP	843	CYS	2.1
4	PPP	557	VAL	2.1
4	PPP	561	ILE	2.1
4	EEE	596	LEU	2.1
4	EEE	1728	ASN	2.1
4	PPP	1507	PHE	2.1
4	PPP	1071	TYR	2.1
4	PPP	497	HIS	2.1
4	EEE	1103	LEU	2.1
4	EEE	1441	LEU	2.1
4	EEE	1995	PHE	2.1
4	PPP	1818	PHE	2.1
4	PPP	410	GLU	2.1
4	EEE	943	PHE	2.1
4	PPP	1487	PHE	2.1
4	EEE	1147	ASN	2.1
4	EEE	338	SER	2.1
4	EEE	1153	SER	2.1
4	PPP	781	ILE	2.1
4	PPP	1001	LEU	2.1
4	PPP	516	LYS	2.0
4	PPP	984	LEU	2.0
4	EEE	819	ASN	2.0
4	EEE	2238	PHE	2.0
4	EEE	1484	SER	2.0
4	PPP	1623	PRO	2.0
4	PPP	1266	ILE	2.0
4	EEE	1997	LEU	2.0
4	PPP	372	ARG	2.0
4	EEE	1813	TYR	2.0
4	PPP	544	VAL	2.0
4	PPP	1676	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 ⓘ

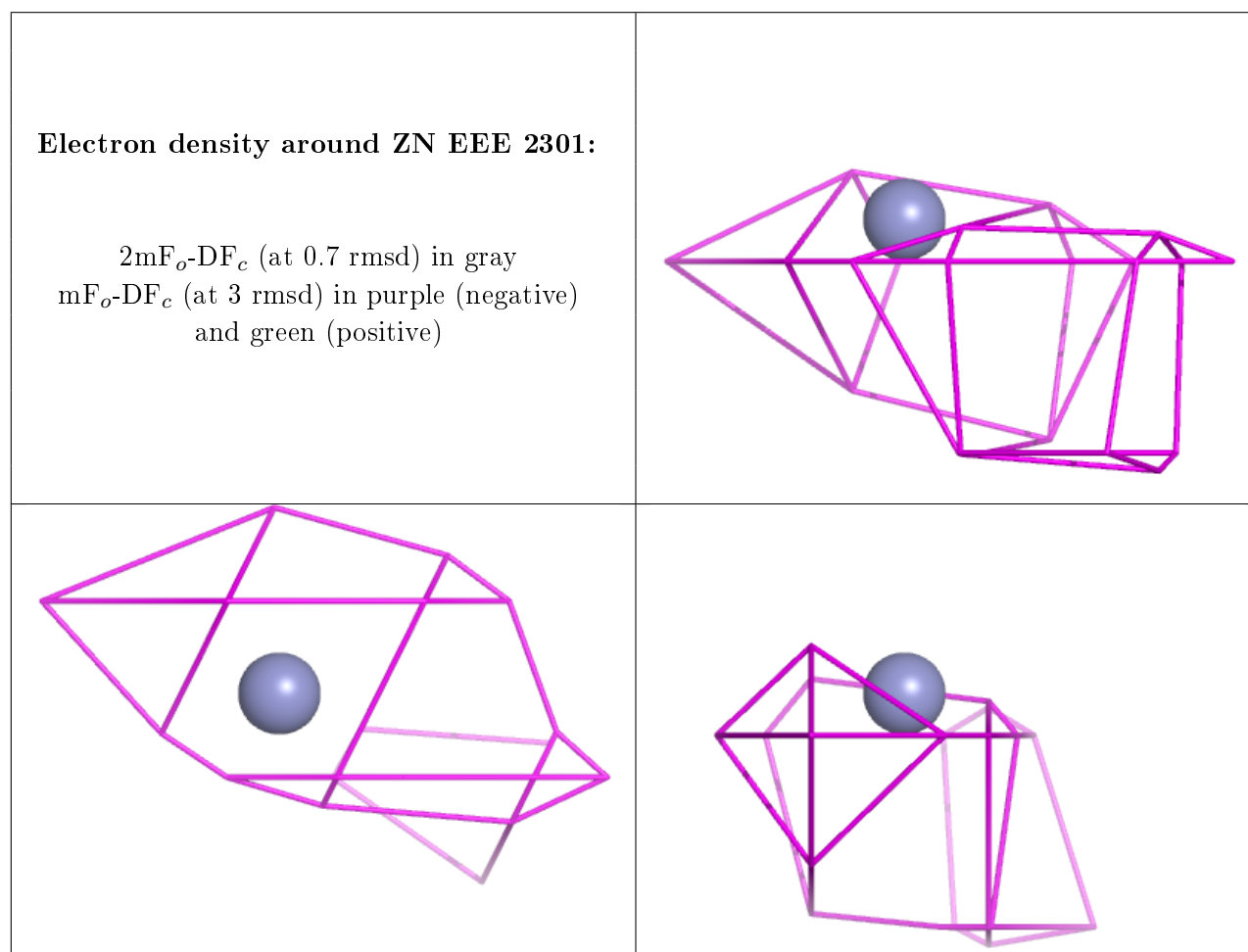
There are no monosaccharides in this entry.

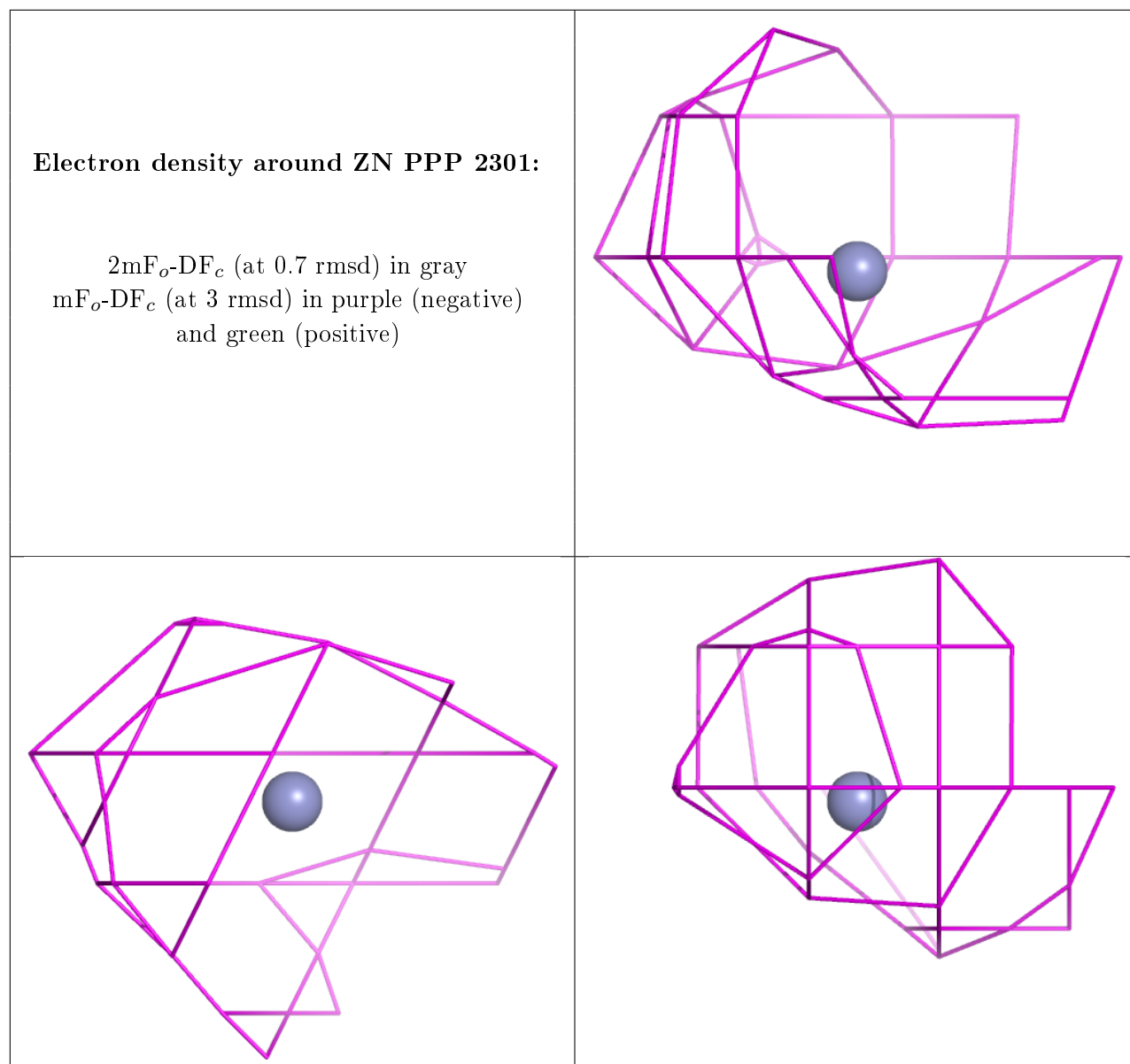
6.4 Ligands ⓘ

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. 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	ZN	EEE	2301	1/1	0.99	0.15	189,189,189,189	0
5	ZN	PPP	2301	1/1	0.99	0.23	117,117,117,117	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.