



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:55 PM UTC

PDB ID : 6Z6B / pdb_00006z6b
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

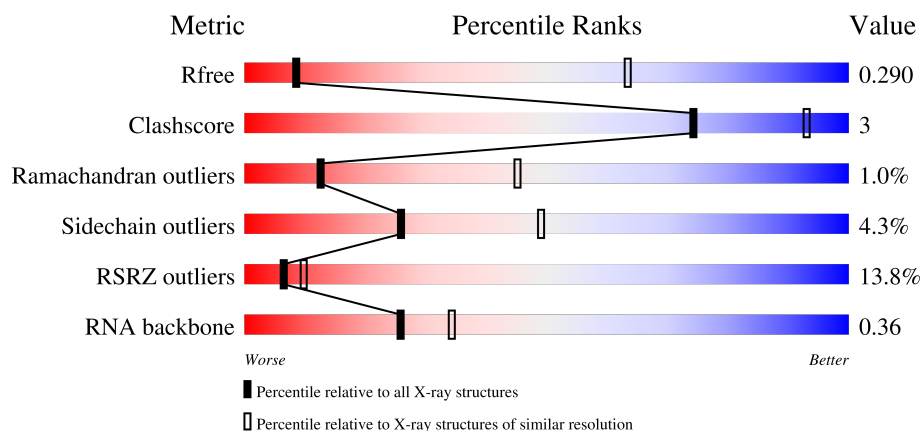
1 Overall quality at a glance

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}	180053	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)
RNA backbone	3983	1016 (4.80-3.10)

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	BBB	10	50% 50%
1	UUU	10	60% 40%
2	CCC	16	19% 81% 19%
2	HHH	16	6% 75% 25%

Continued on next page...

Continued from previous page...

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

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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

3 Residue-property plots [i](#)

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

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

Chain BBB: 



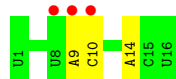
- Molecule 1: RNA (5'-R(P*AP*GP*UP*AP*GP*UP*GP*UP*GP*C)-3')

Chain UUU: 



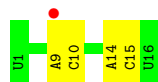
- Molecule 2: RNA (5'-R(P*UP*UP*AP*GP*UP*AP*GP*UP*AP*CP*AP*CP*UP*AP*CP*U)-3')

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: 



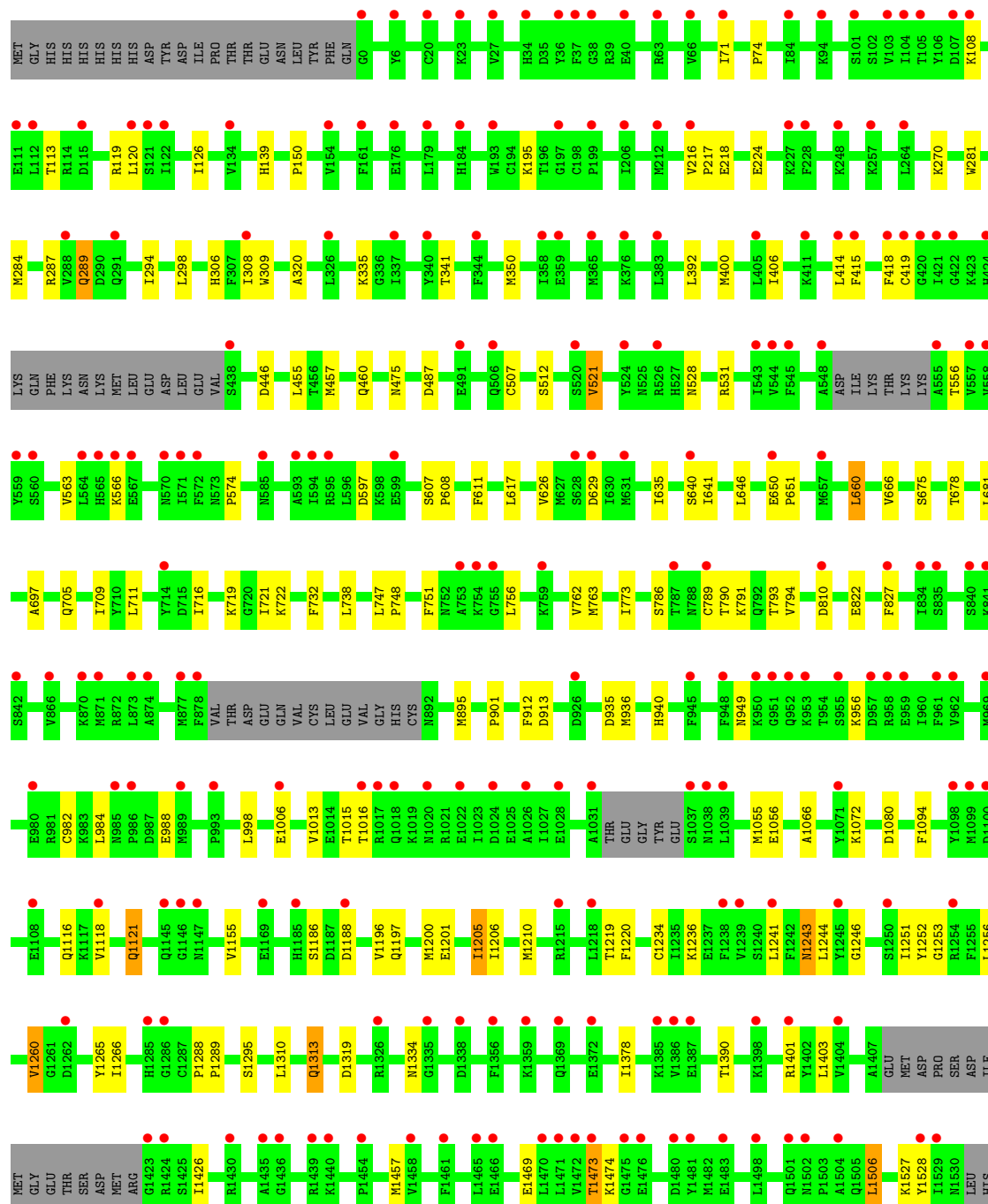
- Molecule 3: RNA (5'-R(*GP*CP*UP*AP*CP*UP*AP*A)-3')

Chain XXX:  75% 25%



- Molecule 4: RNA-directed RNA polymerase L

Chain EEE:  13% 78% 11% 11%





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 0.257 , 0.290	Depositor DCC
R_{free} test set	1514 reflections (1.52%)	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)	0.31 , 276.7	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	0.87	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	0.40	0/241	0.73	0/374
1	UUU	0.40	0/241	0.72	0/374
2	CCC	0.37	0/374	0.64	0/579
2	HHH	0.38	0/374	0.64	0/579
3	DDD	0.38	0/184	0.65	0/285
3	XXX	0.38	0/184	0.63	0/285
4	EEE	1.03	0/16918	1.47	2/22801 (0.0%)
4	PPP	1.02	0/16960	1.48	4/22858 (0.0%)
All	All	1.01	0/35476	1.45	6/48135 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	PPP	583	CYS	CA-C-N	6.21	128.85	120.65
4	PPP	583	CYS	C-N-CA	6.21	128.85	120.65
4	EEE	1474	LYS	CA-C-N	5.29	125.13	120.10
4	EEE	1474	LYS	C-N-CA	5.29	125.13	120.10
4	PPP	1474	LYS	CA-C-N	5.28	125.11	120.10
4	PPP	1474	LYS	C-N-CA	5.28	125.11	120.10

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	1	0
3	DDD	165	0	85	0	0
3	XXX	165	0	85	0	0
4	EEE	16582	0	16651	110	0
4	PPP	16622	0	16692	108	0
5	EEE	1	0	0	0	0
5	PPP	1	0	0	0	0
All	All	34640	0	34071	211	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 (211) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:EEE:1055:MET:HE1	4:EEE:1206:ILE:HA	1.91	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:PPP:1055:MET:HE1	4:PPP:1206:ILE:HA	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:747:LEU:N	4:EEE:748:PRO:HD2	2.27	0.50
4:EEE:1469:GLU:HG2	4:EEE:1628:ARG:HA	1.92	0.50
4:PPP:707:ARG:HA	4:PPP:722:LYS:HG3	1.93	0.50
4:EEE:216:VAL:HG12	4:EEE:217:PRO:HD3	1.94	0.50
4:PPP:216:VAL:HG12	4:PPP:217:PRO:HD3	1.94	0.50
4:PPP:1469:GLU:HG2	4:PPP:1628:ARG:HA	1.93	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:626:VAL:HB	4:EEE:629:ASP:HB2	1.93	0.49
4:EEE:1760:GLU:O	4:EEE:1763:ILE:HB	2.12	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:EEE:2251:MET:HE2	4:PPP:2187:PRO:HB3	1.96	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:PPP:2148:VAL:O	4:PPP:2152:ILE:HG12	2.17	0.45
4:EEE:721:ILE:HD13	4:EEE:738:LEU:CD2	2.46	0.45
4:EEE:1730:ILE:HG22	4:EEE:1731:LYS:HG2	1.98	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:747:LEU:N	4:EEE:748:PRO:CD	2.80	0.45
4:EEE:1819:ILE:HG22	4:EEE:2000:ILE:HD11	1.99	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
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:521:VAL:HG13	4:PPP:531:ARG:HD3	1.99	0.44
4:PPP:2139:PRO:HA	4:PPP:2142:LEU:HB2	1.98	0.44
4:EEE:74:PRO:HG3	4:EEE:113:THR:HA	2.00	0.44
4:PPP:216:VAL:N	4:PPP:217:PRO:CD	2.80	0.44
4:PPP:1833:LEU:HD22	4:PPP:1982:ILE:HG21	1.98	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:611:PHE:CE1	4:EEE:635:ILE:HG23	2.53	0.44
4:EEE:1587:ILE:O	4:EEE:1590:THR:OG1	2.35	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:457:MET:HE2	4:EEE:681:LEU:HB3	2.00	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:HE21	4:EEE:1121:GLN:HA	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:EEE:719:LYS:NZ	4:EEE:1006:GLU:CD	2.76	0.43
4:PPP:2173:ILE:HA	4:PPP:2178:ASP:HB2	1.99	0.43
4:EEE:773:ILE:HG21	4:EEE:1066:ALA:HB1	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:PPP:414:LEU:O	4:PPP:418:PHE:HB3	2.17	0.43
4:PPP:457:MET:HE2	4:PPP:681:LEU:HB3	2.01	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
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:74:PRO:HG3	4:PPP:113:THR:HA	2.00	0.43
4:PPP:306:HIS:CE1	4:PPP:641:ILE:HG22	2.54	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:309:TRP:CD1	4:PPP:507:CYS:HA	2.54	0.42
4:PPP:2087:GLY:HA2	4:PPP:2098:ILE:O	2.19	0.42
4:EEE:1579:LEU:HD22	4:EEE:1749:HIS:HB3	2.02	0.42
4:EEE:1610:MET:HG2	4:EEE:1611:PRO:HD2	2.00	0.42
4:PPP:216:VAL:CG1	4:PPP:217:PRO:HD3	2.49	0.42
4:PPP:1473:THR:HG21	4:PPP:1624:ALA:HB2	2.00	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:789:CYS:SG	4:PPP:1219:THR:HG23	2.60	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:EEE:719:LYS:HZ2	4:EEE:1006:GLU:CD	2.27	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:789:CYS:SG	4:EEE:1219:THR:HG23	2.60	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: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:392:LEU:HB2	4:PPP:400:MET:HB2	2.01	0.41
4:PPP:1197:GLN:HG3	4:PPP:1205:ILE:HD11	2.00	0.41
4:PPP:762:VAL:HG11	4:PPP:949:ASN:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:EEE:289:GLN:HG2	4:EEE:294:ILE:HG13	2.02	0.41
4:EEE:1403:LEU:HD23	4:EEE:1527:LYS:HD2	2.02	0.41
4:PPP:218:GLU:OE1	4:PPP:218:GLU:N	2.54	0.41
4:EEE:1378:ILE:HG21	4:EEE:1579:LEU:HD11	2.03	0.41
4:EEE:308:ILE:O	4:EEE:308:ILE:HG13	2.20	0.41
4:EEE:1251:ILE:O	4:EEE:1253:GLY:N	2.54	0.41
4:EEE:350:MET:HE1	4:EEE:406:ILE:HD11	2.02	0.41
4:PPP:748:PRO:HA	4:PPP:751:PHE:CE2	2.55	0.41
4:EEE:748:PRO:HA	4:EEE:751:PHE:CE2	2.56	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:PPP:936:MET:HE2	4:PPP:940:HIS:HB2	2.03	0.41
4:PPP:972:TYR:O	4:PPP:976:ARG:HB2	2.21	0.41
4:EEE:1288:PRO:HA	4:EEE:1289:PRO:HD3	1.97	0.41
4:PPP:308:ILE:O	4:PPP:308:ILE:HG13	2.20	0.41
4:PPP:350:MET:HE1	4:PPP:406:ILE:HD11	2.02	0.41
4:PPP:2092:SER:OG	4:PPP:2094:PRO:HD2	2.21	0.41
4:EEE:936:MET:HE2	4:EEE:940:HIS:HB2	2.03	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:762:VAL:HG11	4:EEE:949:ASN:HB2	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: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

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	
4	EEE	2009/2285 (88%)	1808 (90%)	180 (9%)	21 (1%)	12	45
4	PPP	2016/2285 (88%)	1812 (90%)	183 (9%)	21 (1%)	12	45
All	All	4025/4570 (88%)	3620 (90%)	363 (9%)	42 (1%)	12	45

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	1792 (96%)	81 (4%)	26	49
4	PPP	1877/2107 (89%)	1796 (96%)	81 (4%)	26	49
All	All	3750/4214 (89%)	3588 (96%)	162 (4%)	26	49

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	EEE	71	ILE
4	EEE	108	LYS
4	EEE	119	ARG
4	EEE	120	LEU
4	EEE	126	ILE
4	EEE	139	HIS
4	EEE	195	LYS
4	EEE	224	GLU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
4	EEE	2233	LEU
4	EEE	2240	THR
4	PPP	71	ILE
4	PPP	108	LYS
4	PPP	119	ARG
4	PPP	120	LEU
4	PPP	126	ILE
4	PPP	139	HIS
4	PPP	175	ASP
4	PPP	195	LYS
4	PPP	224	GLU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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

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

5.3.3 RNA [i](#)

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	BBB	10/10 (100%)	0.55	0	100	100	153, 182, 218, 228	0
1	UUU	10/10 (100%)	0.05	0	100	100	122, 141, 171, 201	0
2	CCC	16/16 (100%)	0.93	3 (18%)	3	6	113, 200, 291, 292	0
2	HHH	16/16 (100%)	-0.08	1 (6%)	26	22	93, 168, 206, 212	0
3	DDD	8/8 (100%)	0.49	0	100	100	190, 224, 238, 244	0
3	XXX	8/8 (100%)	0.32	0	100	100	145, 176, 200, 214	0
4	EEE	2031/2285 (88%)	0.82	293 (14%)	6	9	87, 211, 334, 414	0
4	PPP	2036/2285 (89%)	0.75	275 (13%)	7	10	80, 181, 312, 403	0
All	All	4135/4638 (89%)	0.78	572 (13%)	6	10	80, 193, 325, 414	0

All (572) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	PPP	2179	HIS	14.4
4	PPP	2183	SER	9.7
4	PPP	2185	ASP	9.7
4	EEE	1679	ARG	9.6
4	PPP	2144	CYS	8.8
4	PPP	1693	GLN	7.9
4	EEE	419	CYS	7.8
4	EEE	567	GLU	7.1
4	PPP	952	GLN	7.1
4	PPP	754	LYS	7.0
4	EEE	1692	TYR	6.4
4	EEE	548	ALA	6.4
4	EEE	1098	TYR	6.4
4	PPP	1472	VAL	6.3
4	PPP	1269	TYR	6.2
4	EEE	1472	VAL	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	PPP	1701	SER	6.1
4	EEE	874	ALA	5.9
4	PPP	1836	TYR	5.9
4	PPP	1483	GLU	5.6
4	EEE	873	LEU	5.6
4	PPP	1682	VAL	5.5
4	EEE	1471	LEU	5.4
2	CCC	9	A	5.3
4	PPP	874	ALA	5.3
4	PPP	2105	GLU	5.2
4	PPP	1702	THR	5.2
4	EEE	1693	GLN	5.1
4	PPP	958	ARG	5.1
4	PPP	2	ASP	5.1
4	PPP	873	LEU	5.1
4	EEE	557	VAL	5.1
4	EEE	291	GLN	5.0
4	PPP	1430	ARG	5.0
4	EEE	421	ILE	4.9
4	PPP	1526	ASP	4.9
4	EEE	985	ASN	4.9
4	EEE	2188	LYS	4.9
4	PPP	567	GLU	4.8
4	EEE	840	SER	4.8
4	PPP	1749	HIS	4.8
4	PPP	2155	LEU	4.8
4	PPP	1018	GLN	4.8
4	EEE	1239	VAL	4.8
4	PPP	1840	LYS	4.8
4	PPP	870	LYS	4.8
4	PPP	438	SER	4.7
4	EEE	545	PHE	4.7
4	PPP	1270	GLU	4.7
4	EEE	193	TRP	4.7
4	EEE	570	ASN	4.6
4	PPP	548	ALA	4.6
4	EEE	1238	PHE	4.6
4	EEE	877	MET	4.6
4	PPP	1752	ILE	4.6
4	PPP	2002	VAL	4.5
4	EEE	1018	GLN	4.5
4	EEE	1747	GLY	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	PPP	1014	GLU	4.5
4	EEE	134	VAL	4.5
4	EEE	1501	GLN	4.5
4	PPP	1981	ARG	4.5
4	EEE	1684	GLU	4.5
4	PPP	953	LYS	4.4
4	EEE	1262	ASP	4.4
4	EEE	962	VAL	4.3
4	EEE	593	ALA	4.3
4	PPP	1679	ARG	4.2
4	EEE	544	VAL	4.2
4	EEE	383	LEU	4.2
4	PPP	2188	LYS	4.2
4	PPP	570	ASN	4.2
4	EEE	566	LYS	4.2
4	PPP	1028	GLU	4.2
4	EEE	101	SER	4.2
4	PPP	841	LYS	4.2
4	EEE	0	GLY	4.1
4	EEE	438	SER	4.1
4	EEE	558	VAL	4.1
4	PPP	419	CYS	4.1
4	EEE	199	PRO	4.1
4	EEE	841	LYS	4.1
4	EEE	524	TYR	4.0
4	PPP	1273	ALA	4.0
4	EEE	1039	LEU	4.0
4	PPP	1239	VAL	4.0
4	EEE	526	ARG	4.0
4	PPP	714	TYR	4.0
4	PPP	956	LYS	4.0
4	EEE	1749	HIS	4.0
4	EEE	1006	GLU	4.0
4	PPP	823	ASN	4.0
4	PPP	813	ARG	4.0
4	PPP	2156	LYS	3.9
4	EEE	959	GLU	3.9
4	PPP	1837	ASP	3.9
4	PPP	2151	LEU	3.9
4	EEE	1470	LEU	3.9
4	PPP	1367	VAL	3.8
4	PPP	94	LYS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	PPP	1262	ASP	3.8
4	PPP	959	GLU	3.8
4	PPP	2233	LEU	3.7
4	EEE	104	ILE	3.7
4	PPP	153	VAL	3.7
4	PPP	1250	SER	3.7
4	EEE	424	HIS	3.7
4	EEE	1473	THR	3.7
4	EEE	559	TYR	3.7
4	PPP	1241	LEU	3.7
4	PPP	1435	ALA	3.7
4	EEE	414	LEU	3.7
4	PPP	1185	HIS	3.7
4	PPP	39	ARG	3.6
4	EEE	629	ASP	3.6
4	PPP	1276	ILE	3.6
4	EEE	1100	ASP	3.6
4	PPP	1493	ARG	3.6
4	EEE	40	GLU	3.6
4	EEE	94	LYS	3.6
4	EEE	1458	VAL	3.5
4	EEE	1678	GLN	3.5
4	PPP	1465	LEU	3.5
4	PPP	2180	MET	3.5
4	EEE	1544	LEU	3.5
4	PPP	2212	PRO	3.5
4	EEE	1071	TYR	3.5
4	EEE	754	LYS	3.5
4	EEE	2183	SER	3.5
4	PPP	1480	ASP	3.5
4	PPP	2236	SER	3.5
4	PPP	985	ASN	3.5
4	EEE	1435	ALA	3.4
4	PPP	1255	PHE	3.4
4	EEE	1024	ASP	3.4
4	EEE	1241	LEU	3.4
4	EEE	108	LYS	3.4
4	EEE	1984	ILE	3.4
4	PPP	1529	ILE	3.4
4	PPP	965	TYR	3.4
4	PPP	177	GLU	3.4
4	EEE	2161	SER	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	PPP	1638	GLN	3.4
4	PPP	2104	GLY	3.4
4	PPP	1460	LEU	3.3
4	EEE	1017	ARG	3.3
4	PPP	104	ILE	3.3
4	EEE	415	PHE	3.3
4	EEE	1633	ASN	3.3
4	PPP	1692	TYR	3.3
4	PPP	569	GLU	3.3
4	EEE	365	MET	3.3
4	EEE	1768	PHE	3.3
4	PPP	1691	PHE	3.3
4	EEE	951	GLY	3.3
4	EEE	1483	GLU	3.3
4	EEE	958	ARG	3.3
4	PPP	2137	ILE	3.3
4	EEE	628	SER	3.3
4	EEE	2251	MET	3.3
4	PPP	626	VAL	3.2
4	EEE	115	ASP	3.2
4	EEE	66	VAL	3.2
4	EEE	1028	GLU	3.2
4	PPP	856	GLN	3.2
4	EEE	1756	ASN	3.2
4	EEE	2192	GLY	3.2
4	EEE	789	CYS	3.2
4	EEE	1145	GLN	3.2
4	EEE	1680	ASP	3.2
4	EEE	288	VAL	3.2
4	EEE	755	GLY	3.2
4	EEE	948	PHE	3.2
4	PPP	2238	PHE	3.2
4	EEE	585	ASN	3.2
4	EEE	1038	ASN	3.2
4	PPP	1450	ARG	3.2
4	PPP	335	LYS	3.2
4	EEE	571	ILE	3.1
4	EEE	1146	GLY	3.1
4	PPP	1424	ARG	3.1
4	EEE	1836	TYR	3.1
4	EEE	1760	GLU	3.1
4	PPP	599	GLU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	PPP	2221	VAL	3.1
4	EEE	1498	LEU	3.1
4	EEE	337	ILE	3.1
4	EEE	1819	ILE	3.1
4	EEE	1423	GLY	3.1
4	EEE	870	LYS	3.1
4	PPP	2027	LYS	3.1
4	EEE	2047	TYR	3.1
4	EEE	1480	ASP	3.1
4	PPP	993	PRO	3.1
4	EEE	422	GLY	3.1
4	PPP	989	MET	3.1
4	PPP	390	ASN	3.1
4	PPP	852	GLU	3.1
4	PPP	2232	ALA	3.1
4	EEE	411	LYS	3.1
4	EEE	1440	LYS	3.1
4	EEE	1099	MET	3.1
4	PPP	1747	GLY	3.1
4	EEE	2250	LEU	3.1
4	PPP	1379	ALA	3.1
4	PPP	1622	SER	3.1
4	EEE	834	ILE	3.1
4	EEE	63	ARG	3.1
4	EEE	1782	LEU	3.1
4	EEE	111	GLU	3.0
4	PPP	657	MET	3.0
4	EEE	1627	LEU	3.0
4	PPP	35	ASP	3.0
4	PPP	1423	GLY	3.0
4	PPP	867	GLN	3.0
4	PPP	1471	LEU	3.0
4	EEE	1816	THR	3.0
4	EEE	878	PHE	3.0
4	PPP	1741	LEU	3.0
4	PPP	986	PRO	3.0
4	PPP	1266	ILE	3.0
4	EEE	120	LEU	3.0
4	EEE	1372	GLU	3.0
4	EEE	36	TYR	3.0
4	PPP	6	TYR	3.0
4	EEE	2139	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	EEE	759	LYS	3.0
4	PPP	598	LYS	2.9
4	PPP	193	TRP	2.9
4	PPP	878	PHE	2.9
4	PPP	1461	PHE	2.9
4	PPP	1683	PHE	2.9
4	PPP	2207	PHE	2.9
4	PPP	101	SER	2.9
4	PPP	408	LYS	2.9
4	EEE	1529	ILE	2.9
4	EEE	866	VAL	2.9
4	EEE	1386	VAL	2.9
4	PPP	1699	VAL	2.9
4	PPP	1785	SER	2.9
4	EEE	599	GLU	2.9
4	PPP	810	ASP	2.9
4	EEE	953	LYS	2.9
4	PPP	954	THR	2.9
4	EEE	714	TYR	2.9
4	PPP	629	ASP	2.8
4	PPP	2087	GLY	2.8
4	PPP	2148	VAL	2.8
4	EEE	506	GLN	2.8
4	PPP	1501	GLN	2.8
4	EEE	2019	VAL	2.8
4	EEE	2193	ASN	2.8
4	PPP	2158	ASN	2.8
4	EEE	2185	ASP	2.8
4	PPP	115	ASP	2.8
4	PPP	2066	GLY	2.8
4	EEE	257	LYS	2.8
4	EEE	1801	LYS	2.8
4	EEE	6	TYR	2.8
4	PPP	1544	LEU	2.8
4	EEE	20	CYS	2.8
4	EEE	969	MET	2.8
4	EEE	23	LYS	2.8
4	PPP	381	LYS	2.8
4	EEE	1454	PRO	2.8
4	EEE	2195	ILE	2.8
4	PPP	199	PRO	2.8
4	PPP	1470	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	PPP	1771	ILE	2.8
4	EEE	1108	GLU	2.8
4	PPP	875	ASN	2.8
4	PPP	1476	GLU	2.8
4	PPP	1658	ASN	2.8
4	EEE	27	VAL	2.8
4	EEE	1037	SER	2.8
4	EEE	340	TYR	2.8
4	EEE	1245	TYR	2.8
4	PPP	1279	ALA	2.8
4	PPP	2229	LYS	2.8
4	PPP	163	ASP	2.8
4	PPP	566	LYS	2.7
4	PPP	1473	THR	2.7
4	EEE	112	LEU	2.7
4	EEE	2124	ILE	2.7
4	EEE	1404	VAL	2.7
4	PPP	991	SER	2.7
4	EEE	1630	TYR	2.7
4	PPP	2139	PRO	2.7
4	EEE	2004	LEU	2.7
4	EEE	1147	ASN	2.7
4	PPP	2234	ILE	2.7
4	EEE	376	LYS	2.7
4	PPP	195	LYS	2.7
4	PPP	1591	HIS	2.7
4	EEE	1356	PHE	2.7
4	EEE	103	VAL	2.7
4	EEE	993	PRO	2.7
4	PPP	107	ASP	2.7
4	PPP	1010	ARG	2.7
4	PPP	2128	ALA	2.7
4	EEE	2158	ASN	2.7
4	EEE	657	MET	2.7
4	PPP	1238	PHE	2.7
4	PPP	154	VAL	2.6
4	EEE	206	ILE	2.6
4	PPP	2005	ASP	2.6
4	EEE	2214	THR	2.6
4	EEE	1436	GLY	2.6
2	CCC	10	C	2.6
4	EEE	594	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	EEE	2217	PRO	2.6
4	PPP	389	ASN	2.6
4	EEE	950	LYS	2.6
4	EEE	1385	LYS	2.6
4	PPP	1743	GLN	2.6
4	PPP	197	GLY	2.6
4	PPP	1099	MET	2.6
4	EEE	418	PHE	2.6
4	PPP	228	PHE	2.6
4	PPP	1680	ASP	2.6
4	PPP	1762	ASN	2.6
4	EEE	1430	ARG	2.6
4	EEE	248	LYS	2.6
4	PPP	227	LYS	2.6
4	PPP	1750	LYS	2.6
4	EEE	1828	LEU	2.6
4	EEE	2082	MET	2.6
4	EEE	197	GLY	2.6
4	EEE	827	PHE	2.6
4	EEE	105	THR	2.6
4	PPP	1259	SER	2.6
4	EEE	1614	ARG	2.6
4	PPP	871	MET	2.6
4	EEE	2089	ALA	2.6
4	EEE	1285	HIS	2.5
4	PPP	424	HIS	2.5
4	PPP	781	ILE	2.5
4	PPP	780	ASN	2.5
4	EEE	564	LEU	2.5
4	EEE	212	MET	2.5
4	EEE	945	PHE	2.5
4	EEE	1031	ALA	2.5
4	PPP	84	ILE	2.5
4	EEE	1359	LYS	2.5
4	PPP	1576	TYR	2.5
4	PPP	1614	ARG	2.5
4	EEE	176	GLU	2.5
4	EEE	1650	VAL	2.5
4	EEE	810	ASP	2.5
4	PPP	1275	ARG	2.5
4	EEE	650	GLU	2.5
4	EEE	1466	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	PPP	21	VAL	2.5
4	EEE	107	ASP	2.5
4	PPP	1686	LYS	2.5
4	EEE	787	THR	2.5
4	EEE	2242	ARG	2.5
4	PPP	1351	SER	2.5
4	PPP	1787	PHE	2.5
4	EEE	122	ILE	2.5
4	EEE	1757	ALA	2.5
4	EEE	2095	ILE	2.5
4	EEE	1215	ARG	2.5
4	PPP	235	ARG	2.5
4	PPP	1285	HIS	2.5
4	EEE	2044	ASN	2.5
4	EEE	405	LEU	2.5
4	EEE	565	HIS	2.4
4	EEE	2247	PHE	2.4
4	PPP	415	PHE	2.4
4	PPP	988	GLU	2.4
4	PPP	73	ALA	2.4
4	EEE	1475	GLY	2.4
4	EEE	560	SER	2.4
2	HHH	9	A	2.4
4	EEE	1398	LYS	2.4
4	EEE	1528	TYR	2.4
4	PPP	3	TYR	2.4
4	PPP	948	PHE	2.4
4	PPP	1447	TYR	2.4
4	EEE	1476	GLU	2.4
4	EEE	1424	ARG	2.4
4	EEE	216	VAL	2.4
4	PPP	103	VAL	2.4
4	EEE	184	HIS	2.4
4	PPP	2250	LEU	2.4
4	PPP	496	MET	2.4
4	PPP	1839	MET	2.4
4	EEE	227	LYS	2.4
4	PPP	1349	LEU	2.4
4	EEE	1657	GLU	2.4
4	EEE	1504	ALA	2.4
4	EEE	1020	ASN	2.4
4	EEE	2104	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	PPP	463	LYS	2.4
4	PPP	955	SER	2.4
4	PPP	983	LYS	2.4
4	PPP	1452	SER	2.4
4	PPP	2009	THR	2.4
4	EEE	1286	GLY	2.4
4	EEE	1635	PRO	2.4
4	PPP	68	PRO	2.4
4	EEE	37	PHE	2.4
4	PPP	180	LEU	2.4
4	EEE	1188	ASP	2.4
4	PPP	17	ARG	2.4
4	EEE	2180	MET	2.4
4	EEE	1022	GLU	2.4
4	PPP	1145	GLN	2.3
4	PPP	1222	CYS	2.3
4	PPP	1990	LEU	2.3
4	PPP	238	THR	2.3
4	PPP	1386	VAL	2.3
4	PPP	1428	THR	2.3
4	PPP	1742	LYS	2.3
4	PPP	822	GLU	2.3
4	EEE	71	ILE	2.3
4	PPP	34	HIS	2.3
4	EEE	842	SER	2.3
4	EEE	2016	SER	2.3
4	EEE	154	VAL	2.3
4	EEE	1118	VAL	2.3
4	PPP	787	THR	2.3
4	EEE	1026	ALA	2.3
4	PPP	2239	GLU	2.3
4	EEE	228	PHE	2.3
4	EEE	1701	SER	2.3
4	PPP	354	GLY	2.3
4	PPP	840	SER	2.3
4	PPP	2016	SER	2.3
4	EEE	1698	TYR	2.3
4	PPP	69	LEU	2.3
4	PPP	961	PHE	2.3
4	EEE	640	SER	2.3
4	PPP	201	PHE	2.3
4	PPP	2147	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	EEE	986	PRO	2.3
4	EEE	1699	VAL	2.3
4	PPP	473	PRO	2.3
4	PPP	2108	MET	2.3
4	PPP	1039	LEU	2.3
4	EEE	344	PHE	2.3
4	EEE	1831	ALA	2.3
4	EEE	1369	GLN	2.3
4	EEE	2159	GLU	2.3
4	PPP	288	VAL	2.3
4	EEE	1401	ARG	2.3
4	PPP	1507	PHE	2.2
4	PPP	1681	ILE	2.2
4	EEE	1622	SER	2.2
4	EEE	1387	GLU	2.2
4	PPP	980	GLU	2.2
4	EEE	38	GLY	2.2
4	EEE	2120	ARG	2.2
4	PPP	2194	PRO	2.2
4	EEE	1465	LEU	2.2
4	EEE	1702	THR	2.2
4	PPP	196	THR	2.2
4	EEE	961	PHE	2.2
4	EEE	1461	PHE	2.2
4	EEE	2160	TRP	2.2
4	PPP	1801	LYS	2.2
4	EEE	835	SER	2.2
4	EEE	2088	GLU	2.2
4	PPP	1196	VAL	2.2
4	EEE	1741	LEU	2.2
4	PPP	1218	LEU	2.2
4	PPP	1685	LEU	2.2
4	PPP	837	PHE	2.2
4	PPP	1398	LYS	2.2
4	PPP	2047	TYR	2.2
4	EEE	1254	ARG	2.2
4	PPP	63	ARG	2.2
4	EEE	491	GLU	2.2
4	PPP	2213	GLY	2.2
4	EEE	1695	CYS	2.2
4	EEE	1326	ARG	2.2
4	EEE	1989	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	EEE	420	GLY	2.2
4	EEE	2024	PRO	2.2
4	EEE	2194	PRO	2.2
4	PPP	0	GLY	2.2
4	PPP	642	THR	2.2
4	PPP	1204	LYS	2.2
4	PPP	159	ASN	2.2
4	EEE	871	MET	2.2
4	PPP	1688	MET	2.2
4	EEE	520	SER	2.2
4	PPP	383	LEU	2.2
4	PPP	2201	TRP	2.2
4	EEE	308	ILE	2.2
4	PPP	1382	LYS	2.2
4	PPP	2214	THR	2.2
4	EEE	631	MET	2.2
4	EEE	957	ASP	2.1
4	EEE	1250	SER	2.1
4	EEE	1439	ARG	2.1
4	PPP	1280	GLN	2.1
4	PPP	1596	TYR	2.1
4	PPP	1696	TYR	2.1
4	PPP	2019	VAL	2.1
4	EEE	161	PHE	2.1
4	PPP	732	PHE	2.1
4	PPP	1487	PHE	2.1
4	EEE	980	GLU	2.1
4	PPP	1623	PRO	2.1
4	PPP	1733	LYS	2.1
4	EEE	179	LEU	2.1
4	EEE	1218	LEU	2.1
4	EEE	2128	ALA	2.1
2	CCC	8	U	2.1
4	EEE	989	MET	2.1
4	EEE	34	HIS	2.1
4	EEE	1625	LEU	2.1
4	PPP	1782	LEU	2.1
4	PPP	1671	MET	2.1
4	EEE	555	ALA	2.1
4	EEE	1502	ASN	2.1
4	EEE	1752	ILE	2.1
4	PPP	1453	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	PPP	2237	LYS	2.1
4	EEE	1691	PHE	2.1
4	EEE	1185	HIS	2.1
4	EEE	1338	ASP	2.1
4	PPP	998	LEU	2.1
4	PPP	1793	ASP	2.1
4	PPP	2143	GLY	2.1
4	EEE	359	GLU	2.1
4	PPP	1684	GLU	2.1
4	PPP	1689	THR	2.1
4	EEE	1602	ARG	2.1
4	EEE	84	ILE	2.1
4	EEE	543	ILE	2.1
4	PPP	1504	ALA	2.1
4	PPP	1814	ASN	2.1
4	EEE	1566	THR	2.1
4	PPP	824	ARG	2.1
4	PPP	789	CYS	2.1
4	EEE	121	SER	2.1
4	PPP	984	LEU	2.1
4	PPP	1047	LEU	2.1
4	EEE	1481	TYR	2.0
4	PPP	64	PRO	2.0
4	EEE	595	ARG	2.0
4	EEE	926	ASP	2.0
4	PPP	1319	ASP	2.0
4	EEE	358	ILE	2.0
4	EEE	1169	GLU	2.0
4	EEE	1697	GLU	2.0
4	PPP	1037	SER	2.0
4	PPP	1249	PHE	2.0
4	EEE	264	LEU	2.0
4	EEE	952	GLN	2.0
4	PPP	1983	LEU	2.0
4	PPP	1490	ASN	2.0
4	EEE	2218	PRO	2.0
4	PPP	833	THR	2.0
4	EEE	572	PHE	2.0
4	EEE	955	SER	2.0
4	EEE	2045	LEU	2.0
4	PPP	809	ALA	2.0
4	PPP	1333	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	EEE	1335	GLY	2.0
4	PPP	1439	ARG	2.0
4	PPP	2228	LYS	2.0
4	EEE	1681	ILE	2.0
4	PPP	2216	ILE	2.0
4	EEE	1016	THR	2.0
4	EEE	326	LEU	2.0
4	EEE	753	ALA	2.0
4	PPP	1271	ASP	2.0
4	PPP	1631	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

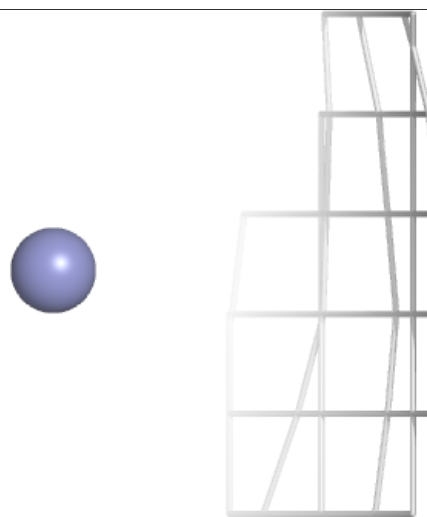
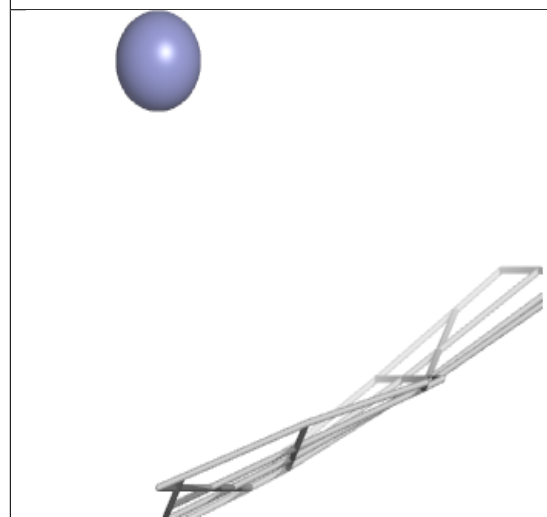
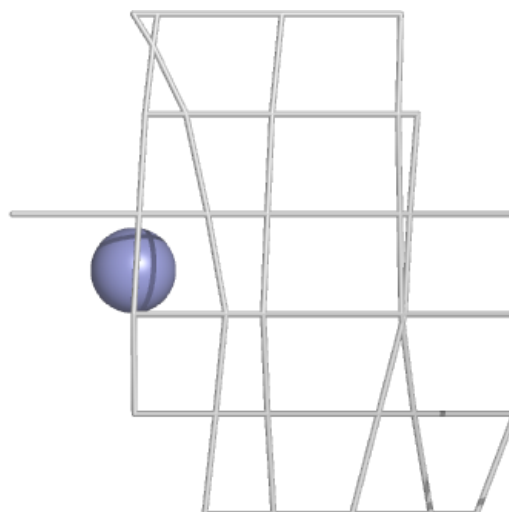
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

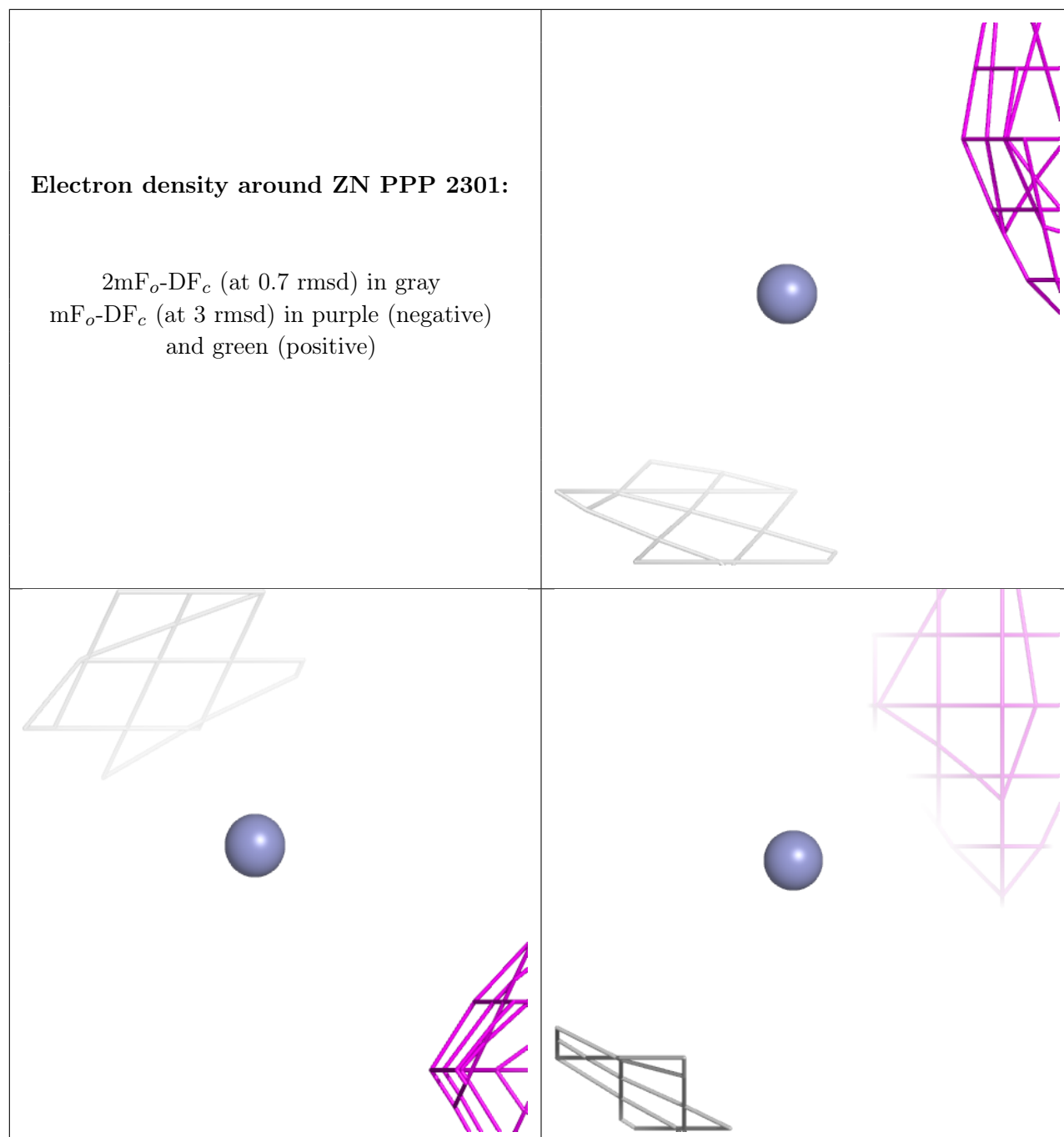
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	EEE	2301	1/1	0.99	0.04	189,189,189,189	0
5	ZN	PPP	2301	1/1	1.00	0.06	117,117,117,117	0

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.

Electron density around ZN EEE 2301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.