



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:43 PM GMT

PDB ID : 3U9F
Title : Structure of CATI in complex with chloramphenicol
Authors : Biswas, T.; Garneau-Tsodikova, S.; Tsodikov, O.V.
Deposited on : 2011-10-18
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

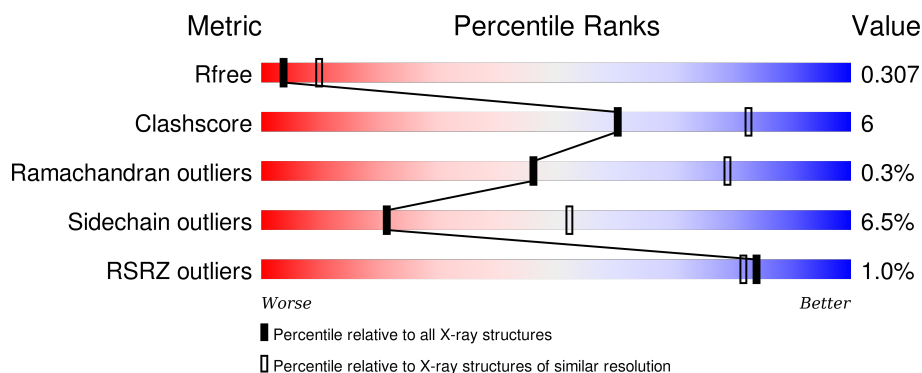
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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	219	<div> <div></div> <div>82%15% ..</div> </div>
1	B	219	<div> <div>%</div> <div>82%14% ..</div> </div>
1	C	219	<div> <div></div> <div>79%16% ..</div> </div>
1	D	219	<div> <div>%</div> <div>79%16% ..</div> </div>
1	E	219	<div> <div></div> <div>79%12% . 5%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	219	
1	G	219	
1	H	219	
1	I	219	
1	J	219	
1	K	219	
1	L	219	
1	M	219	
1	N	219	
1	O	219	
1	P	219	
1	R	219	
1	S	219	

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
2	CLM	E	221	-	-	-	X
2	CLM	P	221	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32549 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 Chloramphenicol acetyltransferase.

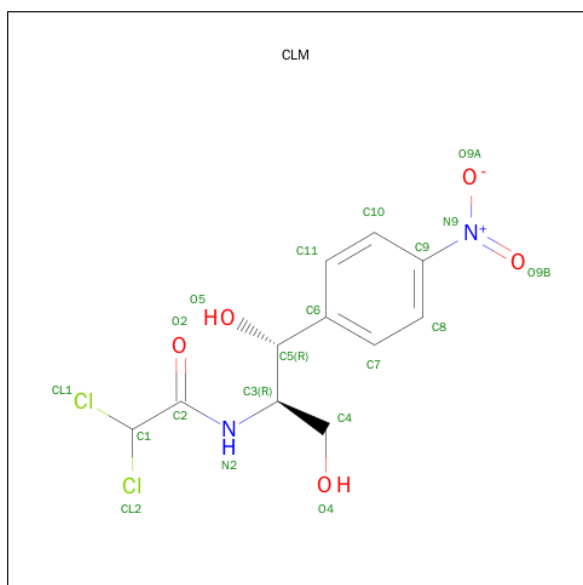
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1780	1157	292	318	13			
1	B	215	Total	C	N	O	S	0	0	0
			1786	1161	294	318	13			
1	C	216	Total	C	N	O	S	0	0	0
			1784	1159	293	319	13			
1	D	211	Total	C	N	O	S	0	0	0
			1752	1138	288	313	13			
1	E	207	Total	C	N	O	S	0	0	0
			1716	1116	279	308	13			
1	F	211	Total	C	N	O	S	0	0	0
			1752	1138	288	313	13			
1	G	214	Total	C	N	O	S	0	0	0
			1774	1153	291	317	13			
1	H	213	Total	C	N	O	S	0	0	0
			1767	1148	290	316	13			
1	I	213	Total	C	N	O	S	0	0	0
			1767	1148	290	316	13			
1	J	216	Total	C	N	O	S	0	0	0
			1788	1161	293	321	13			
1	K	216	Total	C	N	O	S	0	0	0
			1788	1161	293	321	13			
1	L	216	Total	C	N	O	S	0	0	0
			1784	1159	293	319	13			
1	M	211	Total	C	N	O	S	0	0	0
			1752	1138	288	313	13			
1	N	212	Total	C	N	O	S	0	0	0
			1759	1142	289	315	13			
1	O	211	Total	C	N	O	S	0	0	0
			1752	1138	288	313	13			
1	P	215	Total	C	N	O	S	0	0	0
			1780	1157	292	318	13			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	214	Total	C	N	O	S	0	0	0
			1770	1151	291	315	13			
1	S	214	Total	C	N	O	S	0	0	0
			1774	1153	291	317	13			

- Molecule 2 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		
2	B	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		
2	C	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		
2	D	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		
2	E	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		
2	F	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		
2	G	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		
2	H	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		
2	I	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	J	1	Total 20	C 11	Cl 2	N 2	O 5	0	0
2	K	1	Total 20	C 11	Cl 2	N 2	O 5	0	0
2	L	1	Total 20	C 11	Cl 2	N 2	O 5	0	0
2	M	1	Total 20	C 11	Cl 2	N 2	O 5	0	0
2	N	1	Total 20	C 11	Cl 2	N 2	O 5	0	0
2	O	1	Total 20	C 11	Cl 2	N 2	O 5	0	0
2	P	1	Total 20	C 11	Cl 2	N 2	O 5	0	0
2	R	1	Total 20	C 11	Cl 2	N 2	O 5	0	0
2	S	1	Total 20	C 11	Cl 2	N 2	O 5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total 24	O 24	0	0
3	B	24	Total 24	O 24	0	0
3	C	18	Total 18	O 18	0	0
3	D	19	Total 19	O 19	0	0
3	E	16	Total 16	O 16	0	0
3	F	28	Total 28	O 28	0	0
3	G	23	Total 23	O 23	0	0
3	H	19	Total 19	O 19	0	0
3	I	21	Total 21	O 21	0	0
3	J	25	Total 25	O 25	0	0

Continued on next page...

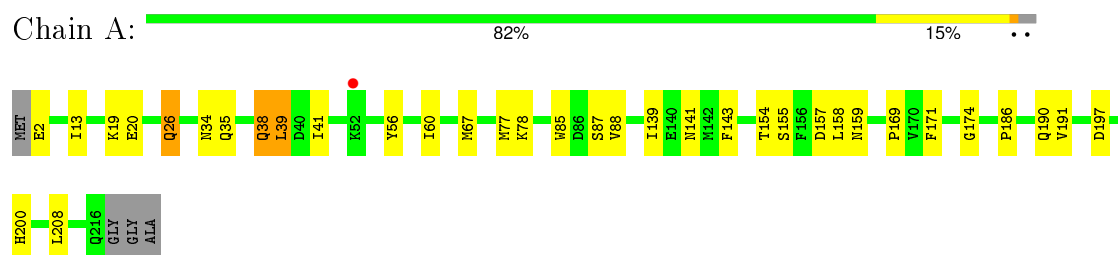
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	24	Total 24	O 24	0	0
3	L	25	Total 25	O 25	0	0
3	M	16	Total 16	O 16	0	0
3	N	19	Total 19	O 19	0	0
3	O	14	Total 14	O 14	0	0
3	P	14	Total 14	O 14	0	0
3	R	13	Total 13	O 13	0	0
3	S	22	Total 22	O 22	0	0

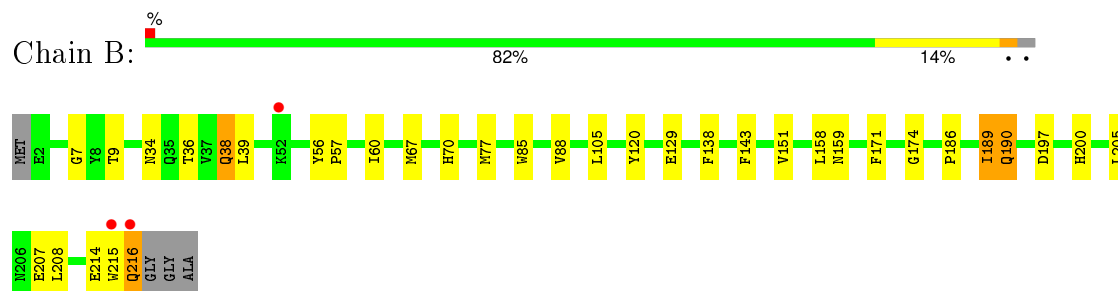
3 Residue-property plots [i](#)

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

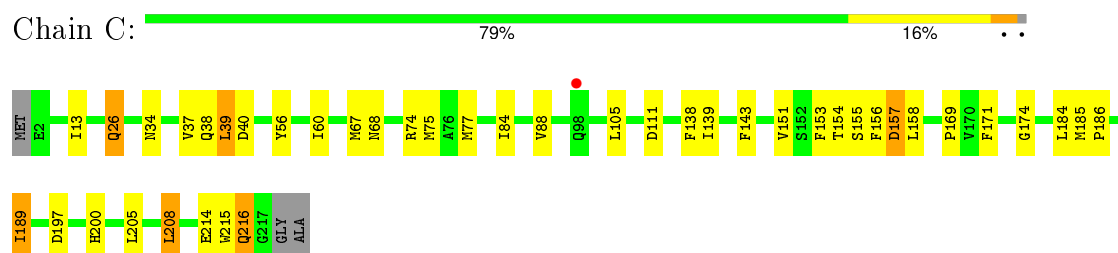
• Molecule 1: Chloramphenicol acetyltransferase



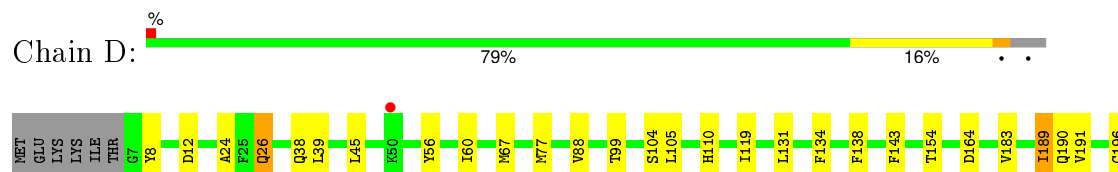
• Molecule 1: Chloramphenicol acetyltransferase

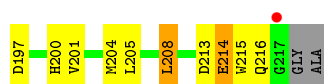


• Molecule 1: Chloramphenicol acetyltransferase



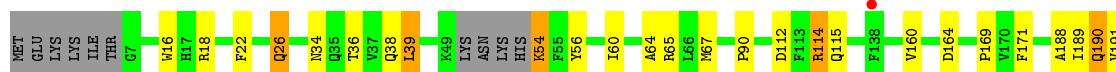
• Molecule 1: Chloramphenicol acetyltransferase





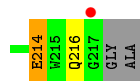
- Molecule 1: Chloramphenicol acetyltransferase

Chain E: 79% 12% 5%



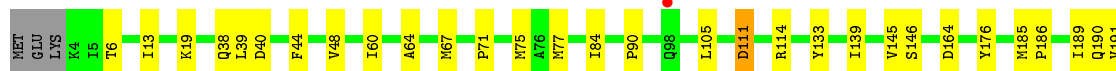
- Molecule 1: Chloramphenicol acetyltransferase

Chain F: 84% 10% 2%



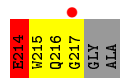
- Molecule 1: Chloramphenicol acetyltransferase

Chain G: 81% 15% 1%



- Molecule 1: Chloramphenicol acetyltransferase

Chain H: 81% 15% 1%



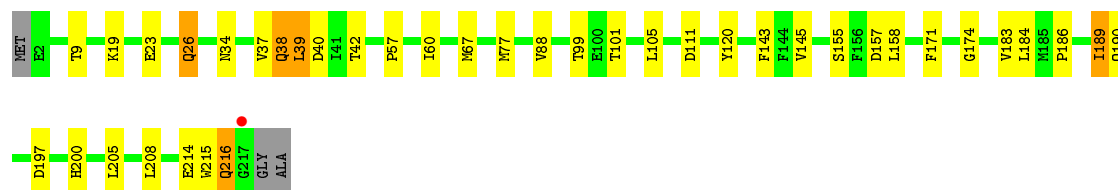
- Molecule 1: Chloramphenicol acetyltransferase

Chain I: 82% 14% 2%



- Molecule 1: Chloramphenicol acetyltransferase

Chain J: 81% 16% ..



- Molecule 1: Chloramphenicol acetyltransferase

Chain K: 79% 17% ..



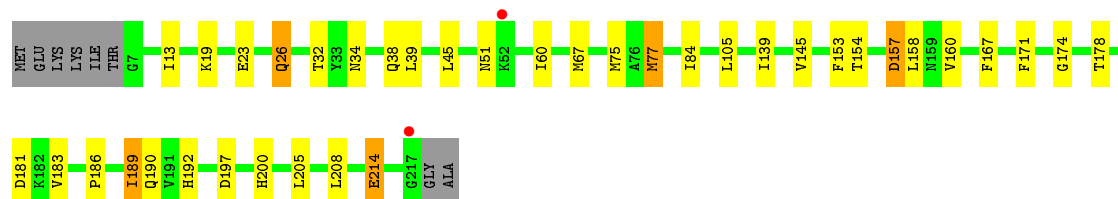
- Molecule 1: Chloramphenicol acetyltransferase

Chain L: 81% 16% ..



- Molecule 1: Chloramphenicol acetyltransferase

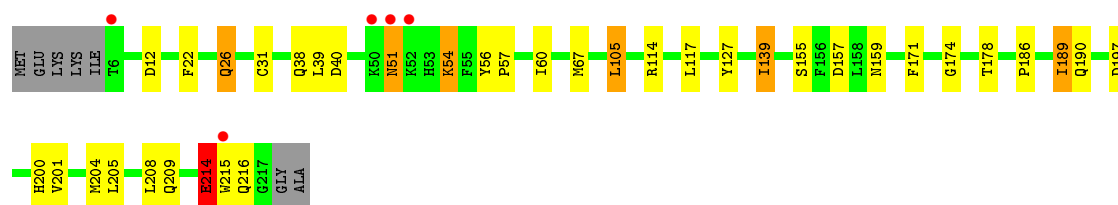
Chain M: 79% 15% ..



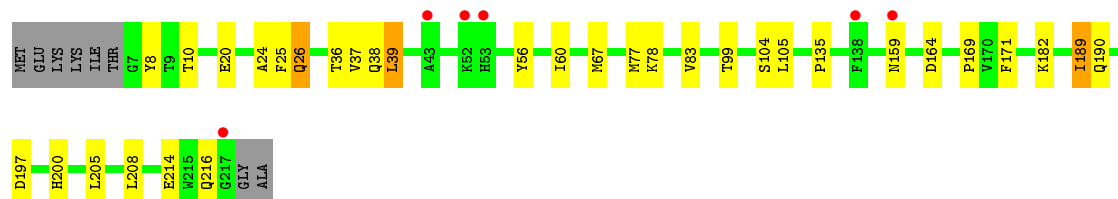
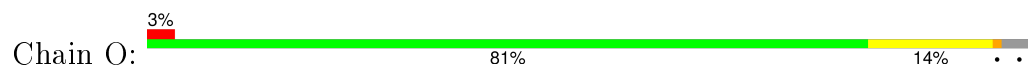
- Molecule 1: Chloramphenicol acetyltransferase

Chain N: 80% 14% ..

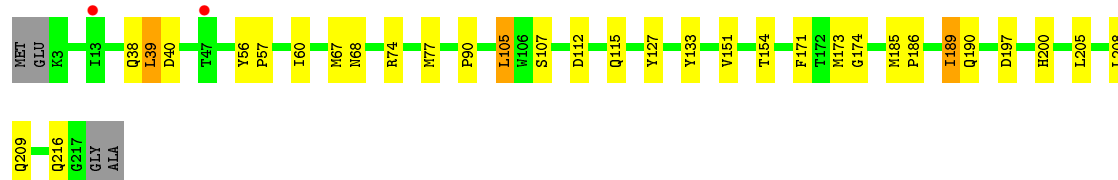
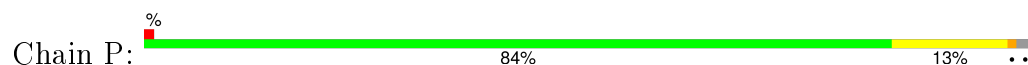




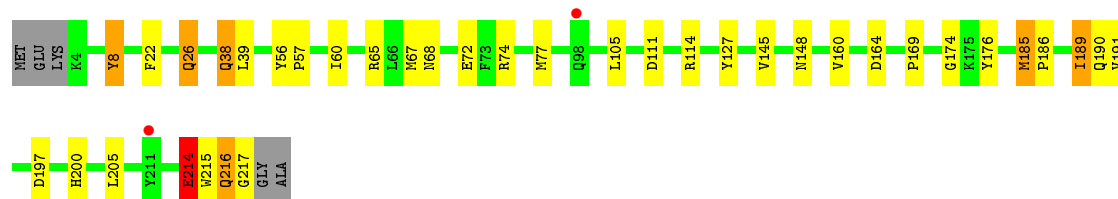
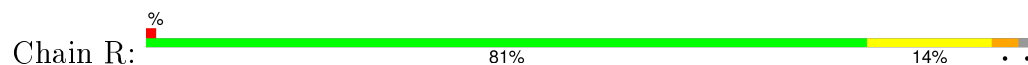
• Molecule 1: Chloramphenicol acetyltransferase



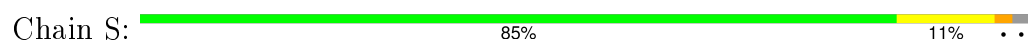
• Molecule 1: Chloramphenicol acetyltransferase



• Molecule 1: Chloramphenicol acetyltransferase



• Molecule 1: Chloramphenicol acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	107.34Å 114.43Å 114.37Å 119.97° 97.83° 98.64°	Depositor
Resolution (Å)	35.00 – 2.90 41.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	86.8 (35.00-2.90) 69.1 (41.29-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.236 , 0.309 0.235 , 0.307	Depositor DCC
R_{free} test set	4369 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.929	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 35.6	EDS
Estimated twinning fraction	0.055 for -h,-l,-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 95102 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32549	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0/1839	0.49	0/2497
1	B	0.36	0/1845	0.50	0/2503
1	C	0.35	0/1843	0.50	0/2502
1	D	0.36	0/1811	0.50	1/2458 (0.0%)
1	E	0.36	0/1773	0.48	0/2407
1	F	0.35	0/1811	0.48	1/2458 (0.0%)
1	G	0.36	0/1833	0.48	1/2488 (0.0%)
1	H	0.35	0/1826	0.49	0/2479
1	I	0.35	0/1826	0.49	1/2479 (0.0%)
1	J	0.36	0/1847	0.50	0/2507
1	K	0.36	0/1847	0.48	0/2507
1	L	0.35	0/1843	0.49	0/2502
1	M	0.36	0/1811	0.48	0/2458
1	N	0.36	0/1818	0.50	0/2468
1	O	0.36	0/1811	0.50	0/2458
1	P	0.35	0/1839	0.47	0/2496
1	R	0.35	0/1829	0.51	0/2483
1	S	0.35	0/1833	0.50	1/2488 (0.0%)
All	All	0.35	0/32885	0.49	5/44638 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	R	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	208	LEU	CA-CB-CG	6.11	129.35	115.30
1	G	208	LEU	CA-CB-CG	6.06	129.24	115.30
1	S	208	LEU	CA-CB-CG	5.33	127.56	115.30
1	D	208	LEU	CA-CB-CG	5.12	127.06	115.30
1	F	208	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	8	TYR	Peptide

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	1780	0	1662	25	0
1	B	1786	0	1680	20	0
1	C	1784	0	1665	27	0
1	D	1752	0	1637	16	0
1	E	1716	0	1597	24	0
1	F	1752	0	1637	17	0
1	G	1774	0	1661	15	0
1	H	1767	0	1655	18	0
1	I	1767	0	1655	18	0
1	J	1788	0	1669	27	0
1	K	1788	0	1669	23	0
1	L	1784	0	1665	21	0
1	M	1752	0	1637	23	0
1	N	1759	0	1644	28	0
1	O	1752	0	1637	20	0
1	P	1780	0	1665	16	0
1	R	1770	0	1657	20	0
1	S	1774	0	1661	13	0
2	A	20	0	11	0	0
2	B	20	0	11	0	0
2	C	20	0	11	0	0
2	D	20	0	11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	20	0	11	0	0
2	F	20	0	11	0	0
2	G	20	0	11	1	0
2	H	20	0	11	0	0
2	I	20	0	11	0	0
2	J	20	0	11	0	0
2	K	20	0	11	0	0
2	L	20	0	11	0	0
2	M	20	0	11	0	0
2	N	20	0	11	0	0
2	O	20	0	11	0	0
2	P	20	0	11	0	0
2	R	20	0	11	0	0
2	S	20	0	11	0	0
3	A	24	0	0	1	0
3	B	24	0	0	0	0
3	C	18	0	0	0	0
3	D	19	0	0	1	0
3	E	16	0	0	1	0
3	F	28	0	0	0	0
3	G	23	0	0	0	0
3	H	19	0	0	1	0
3	I	21	0	0	4	0
3	J	25	0	0	1	0
3	K	24	0	0	0	0
3	L	25	0	0	1	0
3	M	16	0	0	0	0
3	N	19	0	0	1	0
3	O	14	0	0	0	0
3	P	14	0	0	0	0
3	R	13	0	0	0	0
3	S	22	0	0	0	0
All	All	32549	0	29951	346	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 6.

All (346) 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:S:5:ILE:HG23	1:S:6:THR:H	1.00	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:5:ILE:HG23	1:S:6:THR:N	1.76	0.97
1:M:197:ASP:H	1:M:200:HIS:HD2	1.14	0.96
1:R:197:ASP:H	1:R:200:HIS:HD2	1.12	0.96
1:S:5:ILE:CG2	1:S:6:THR:H	1.78	0.96
1:H:197:ASP:H	1:H:200:HIS:HD2	1.17	0.93
1:J:215:TRP:HB3	3:J:807:HOH:O	1.77	0.85
1:C:197:ASP:H	1:C:200:HIS:HD2	1.25	0.84
1:L:197:ASP:H	1:L:200:HIS:HD2	1.25	0.81
1:A:197:ASP:H	1:A:200:HIS:HD2	1.27	0.81
1:O:56:TYR:O	1:O:60:ILE:HG12	1.82	0.80
1:B:197:ASP:H	1:B:200:HIS:HD2	1.27	0.79
1:F:56:TYR:O	1:F:60:ILE:HG12	1.82	0.78
1:P:197:ASP:H	1:P:200:HIS:HD2	1.28	0.77
1:C:67:MET:HE2	1:C:171:PHE:HE1	1.49	0.77
1:E:197:ASP:H	1:E:200:HIS:HD2	1.34	0.75
1:R:197:ASP:H	1:R:200:HIS:CD2	2.02	0.75
1:K:129:GLU:HB3	1:O:8:TYR:HB3	1.67	0.75
1:I:135:PRO:HD3	3:I:762:HOH:O	1.88	0.74
1:B:174:GLY:HA3	1:B:186:PRO:HG2	1.69	0.74
1:N:26:GLN:HE21	1:N:26:GLN:HA	1.52	0.73
1:J:67:MET:HE2	1:J:171:PHE:HE1	1.54	0.72
1:D:213:ASP:HB3	3:D:1075:HOH:O	1.89	0.72
1:L:39:LEU:HD11	1:L:208:LEU:HD11	1.71	0.72
1:O:197:ASP:H	1:O:200:HIS:HD2	1.36	0.71
1:B:56:TYR:O	1:B:60:ILE:HG12	1.90	0.71
1:N:56:TYR:O	1:N:60:ILE:HG12	1.90	0.71
1:M:197:ASP:H	1:M:200:HIS:CD2	2.04	0.71
1:E:26:GLN:HA	1:E:26:GLN:HE21	1.56	0.71
1:J:174:GLY:HA3	1:J:186:PRO:HG2	1.72	0.70
1:F:26:GLN:HA	1:F:26:GLN:HE21	1.58	0.69
1:R:67:MET:HE3	1:R:169:PRO:HG2	1.75	0.69
1:C:56:TYR:O	1:C:60:ILE:HG12	1.92	0.69
1:I:197:ASP:H	1:I:200:HIS:HD2	1.41	0.69
1:J:67:MET:HE2	1:J:171:PHE:CE1	2.28	0.68
1:K:56:TYR:O	1:K:60:ILE:HG12	1.95	0.66
1:L:56:TYR:O	1:L:60:ILE:HG12	1.95	0.66
1:K:197:ASP:H	1:K:200:HIS:HD2	1.43	0.66
1:A:67:MET:CE	1:A:171:PHE:HE1	2.09	0.66
1:A:56:TYR:O	1:A:60:ILE:HG12	1.96	0.65
1:F:197:ASP:H	1:F:200:HIS:HD2	1.44	0.64
1:D:56:TYR:O	1:D:60:ILE:HG12	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:67:MET:HE2	1:O:171:PHE:HE1	1.63	0.63
1:P:39:LEU:HD11	1:P:208:LEU:HD11	1.81	0.62
1:I:56:TYR:O	1:I:60:ILE:HG12	2.00	0.62
1:C:67:MET:HE2	1:C:171:PHE:CE1	2.34	0.62
1:A:26:GLN:HA	1:A:26:GLN:HE21	1.64	0.62
1:H:64:ALA:HB2	1:H:90:PRO:HG3	1.82	0.62
1:C:67:MET:CE	1:C:171:PHE:HE1	2.13	0.61
1:S:197:ASP:H	1:S:200:HIS:HD2	1.48	0.61
1:B:197:ASP:H	1:B:200:HIS:CD2	2.16	0.60
1:L:39:LEU:HD11	1:L:208:LEU:CD1	2.31	0.60
1:A:67:MET:HE1	1:A:171:PHE:HE1	1.65	0.60
1:O:37:VAL:HG21	1:O:205:LEU:HD13	1.82	0.60
1:K:26:GLN:HA	1:K:26:GLN:HE21	1.66	0.60
1:J:189:ILE:HD11	1:J:205:LEU:HD11	1.83	0.60
1:F:39:LEU:HD11	1:F:208:LEU:HD11	1.84	0.59
1:F:189:ILE:HD11	1:F:205:LEU:HD21	1.84	0.59
1:G:197:ASP:H	1:G:200:HIS:CD2	2.21	0.59
1:P:174:GLY:HA3	1:P:186:PRO:HG2	1.83	0.59
1:H:197:ASP:H	1:H:200:HIS:CD2	2.08	0.59
1:J:88:VAL:HG12	1:J:143:PHE:HD1	1.67	0.58
1:K:174:GLY:HA3	1:K:186:PRO:HG2	1.85	0.58
1:F:197:ASP:H	1:F:200:HIS:CD2	2.21	0.58
1:S:197:ASP:H	1:S:200:HIS:CD2	2.21	0.58
1:L:197:ASP:H	1:L:200:HIS:CD2	2.15	0.57
1:R:56:TYR:O	1:R:60:ILE:HG12	2.03	0.57
1:F:174:GLY:HA3	1:F:186:PRO:HG2	1.86	0.57
1:M:174:GLY:HA3	1:M:186:PRO:HG2	1.84	0.57
1:K:189:ILE:HD11	1:K:205:LEU:HD11	1.85	0.57
1:H:7:GLY:O	1:H:85:TRP:HA	2.05	0.57
1:B:189:ILE:HD11	1:B:205:LEU:HD21	1.85	0.57
1:I:189:ILE:HD11	1:I:205:LEU:HD21	1.87	0.56
1:P:197:ASP:H	1:P:200:HIS:CD2	2.17	0.56
1:A:67:MET:HE1	1:A:171:PHE:CE1	2.39	0.56
1:N:67:MET:CE	1:N:171:PHE:HE1	2.18	0.56
1:C:174:GLY:HA3	1:C:186:PRO:HG2	1.88	0.56
1:D:197:ASP:HB2	1:D:200:HIS:HD2	1.71	0.56
1:M:60:ILE:HD13	1:M:145:VAL:HG11	1.87	0.56
1:S:67:MET:HE2	1:S:171:PHE:HE1	1.71	0.56
1:A:38:GLN:NE2	1:C:154:THR:HG21	2.22	0.55
1:F:60:ILE:HD12	1:F:145:VAL:HG11	1.89	0.55
1:J:67:MET:CE	1:J:171:PHE:HE1	2.19	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ASN:ND2	1:B:158:LEU:H	2.05	0.55
1:A:197:ASP:H	1:A:200:HIS:CD2	2.16	0.55
1:O:189:ILE:HD11	1:O:205:LEU:HD21	1.89	0.55
1:I:34:ASN:ND2	1:I:190:GLN:HB3	2.22	0.54
1:J:39:LEU:HD11	1:J:208:LEU:HD11	1.90	0.54
1:H:65:ARG:HH12	1:H:217:GLY:HA2	1.72	0.54
1:A:67:MET:CE	1:A:171:PHE:CE1	2.89	0.54
1:E:112:ASP:HB3	1:E:115:GLN:HB2	1.90	0.54
1:G:64:ALA:HB2	1:G:90:PRO:HG3	1.89	0.54
1:C:67:MET:HE3	1:C:169:PRO:HG2	1.88	0.54
1:D:45:LEU:HD12	1:D:183:VAL:HG11	1.90	0.54
1:N:155:SER:HB3	1:O:36:THR:HB	1.89	0.54
1:P:173:MET:HB2	1:P:185:MET:CE	2.39	0.53
1:S:67:MET:CE	1:S:171:PHE:HE1	2.21	0.53
1:L:96:HIS:HB2	1:L:99:THR:HG22	1.91	0.53
1:A:154:THR:HG21	1:B:38:GLN:NE2	2.24	0.53
1:G:111:ASP:HB2	1:J:111:ASP:HB3	1.90	0.53
1:J:34:ASN:ND2	1:J:158:LEU:H	2.07	0.53
1:L:88:VAL:HG12	1:L:143:PHE:HD1	1.73	0.53
1:K:155:SER:HB3	1:L:36:THR:HB	1.90	0.53
1:M:26:GLN:HA	1:M:26:GLN:HE21	1.73	0.53
1:P:56:TYR:O	1:P:60:ILE:HG12	2.09	0.53
1:A:88:VAL:HG12	1:A:143:PHE:HD1	1.74	0.53
1:H:56:TYR:O	1:H:60:ILE:HG12	2.09	0.52
1:O:67:MET:CE	1:O:171:PHE:HE1	2.22	0.52
1:N:67:MET:HE1	1:N:171:PHE:HE1	1.73	0.52
1:S:56:TYR:O	1:S:60:ILE:HG12	2.10	0.52
1:P:112:ASP:HB3	1:P:115:GLN:HB2	1.92	0.52
1:N:174:GLY:HA3	1:N:186:PRO:HG2	1.91	0.52
1:D:110:HIS:CE1	1:D:119:ILE:HG13	2.44	0.52
1:R:65:ARG:HH12	1:R:217:GLY:HA2	1.74	0.52
1:A:159:ASN:HD21	1:B:159:ASN:CG	2.13	0.52
1:C:88:VAL:HG12	1:C:143:PHE:HD1	1.74	0.52
1:E:160:VAL:HA	1:F:31:CYS:HB3	1.90	0.52
1:M:75:MET:HG2	1:M:84:ILE:HG12	1.92	0.52
1:M:67:MET:HE2	1:M:171:PHE:HE1	1.75	0.52
1:J:39:LEU:HD11	1:J:208:LEU:CD1	2.40	0.52
1:E:56:TYR:O	1:E:60:ILE:HG12	2.09	0.51
1:J:26:GLN:HE21	1:J:26:GLN:HA	1.75	0.51
1:N:54:LYS:HB3	1:N:57:PRO:CG	2.39	0.51
1:A:174:GLY:HA3	1:A:186:PRO:HG2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:197:ASP:H	1:G:200:HIS:HD2	1.56	0.51
1:A:154:THR:HG21	1:B:38:GLN:HE21	1.75	0.51
1:N:40:ASP:HB3	1:N:209:GLN:HE22	1.76	0.51
1:G:75:MET:HG2	1:G:84:ILE:HG12	1.93	0.51
1:H:99:THR:HG21	1:H:131:LEU:HD22	1.92	0.51
1:N:26:GLN:HE21	1:N:26:GLN:CA	2.21	0.51
1:B:88:VAL:HG12	1:B:143:PHE:HD1	1.75	0.51
1:B:129:GLU:HG2	1:F:8:TYR:CE2	2.46	0.51
1:C:34:ASN:ND2	1:C:158:LEU:H	2.08	0.50
1:J:60:ILE:HD13	1:J:145:VAL:HG11	1.94	0.50
1:N:26:GLN:NE2	1:N:26:GLN:HA	2.25	0.50
1:P:173:MET:HB2	1:P:185:MET:HE2	1.93	0.50
1:G:71:PRO:HB2	1:G:84:ILE:HD13	1.94	0.50
1:N:197:ASP:H	1:N:200:HIS:HD2	1.59	0.50
1:C:67:MET:CE	1:C:171:PHE:CE1	2.92	0.50
1:D:197:ASP:H	1:D:200:HIS:CD2	2.30	0.50
1:H:26:GLN:HE21	1:H:26:GLN:HA	1.77	0.50
1:O:26:GLN:HA	1:O:26:GLN:HE21	1.77	0.50
1:R:105:LEU:HD13	1:R:127:TYR:HB2	1.92	0.50
1:C:189:ILE:HD11	1:C:205:LEU:HD11	1.94	0.50
1:J:42:THR:HG23	1:J:183:VAL:HG23	1.93	0.50
1:I:76:ALA:HA	1:I:167:PHE:HD2	1.76	0.49
1:A:155:SER:HB3	1:B:36:THR:HB	1.92	0.49
1:M:67:MET:CE	1:M:171:PHE:HE1	2.25	0.49
1:M:34:ASN:ND2	1:M:158:LEU:H	2.10	0.49
1:D:197:ASP:HB2	1:D:200:HIS:CD2	2.48	0.49
1:K:75:MET:HG2	1:K:84:ILE:HG12	1.94	0.49
1:E:26:GLN:CA	1:E:26:GLN:HE21	2.24	0.49
1:J:67:MET:CE	1:J:171:PHE:CE1	2.94	0.48
1:L:88:VAL:CG1	1:L:143:PHE:HD1	2.26	0.48
1:G:60:ILE:CD1	1:G:145:VAL:HG11	2.43	0.48
1:L:45:LEU:HD12	1:L:183:VAL:HG11	1.95	0.48
1:D:201:VAL:O	1:D:204:MET:HG3	2.14	0.48
1:R:56:TYR:HB3	1:R:57:PRO:CD	2.43	0.48
1:H:34:ASN:HB2	1:H:157:ASP:OD2	2.14	0.48
1:C:68:ASN:HA	1:C:74:ARG:HD3	1.95	0.48
1:I:197:ASP:H	1:I:200:HIS:CD2	2.28	0.48
1:I:99:THR:HG21	1:I:131:LEU:HD22	1.96	0.48
1:C:157:ASP:N	1:C:157:ASP:OD2	2.46	0.48
1:S:67:MET:HE2	1:S:171:PHE:CE1	2.48	0.48
1:K:45:LEU:HD22	1:K:49:LYS:HD2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:39:LEU:CD1	1:L:208:LEU:HD11	2.43	0.48
1:L:75:MET:HG2	1:L:84:ILE:HG12	1.96	0.48
1:E:22:PHE:O	1:E:26:GLN:HB2	2.14	0.48
1:N:201:VAL:O	1:N:204:MET:HG3	2.13	0.47
1:F:70:HIS:HE1	1:F:207:GLU:OE1	1.97	0.47
1:H:75:MET:HG2	1:H:84:ILE:HG12	1.95	0.47
1:G:176:TYR:HB3	1:G:185:MET:HG3	1.96	0.47
1:C:75:MET:HG2	1:C:84:ILE:HG12	1.97	0.47
1:E:65:ARG:HG3	3:E:224:HOH:O	2.15	0.47
1:C:37:VAL:HG21	1:C:205:LEU:HD13	1.96	0.47
1:I:26:GLN:HE22	1:I:165:ASN:ND2	2.13	0.47
1:R:68:ASN:HA	1:R:74:ARG:HH11	1.80	0.47
1:H:22:PHE:O	1:H:26:GLN:HB2	2.15	0.47
1:J:40:ASP:HA	1:J:184:LEU:HD23	1.97	0.47
1:A:67:MET:HE2	1:A:171:PHE:HE1	1.80	0.47
1:M:77:MET:HE3	1:M:167:PHE:HE2	1.80	0.47
1:E:54:LYS:HE2	1:E:54:LYS:HA	1.97	0.47
1:K:34:ASN:ND2	1:K:158:LEU:H	2.13	0.47
1:S:158:LEU:HD23	1:S:190:GLN:HG2	1.96	0.46
1:N:139:ILE:HA	1:N:139:ILE:HD13	1.86	0.46
1:E:197:ASP:H	1:E:200:HIS:CD2	2.23	0.46
1:O:67:MET:HE3	1:O:169:PRO:HG2	1.96	0.46
1:K:157:ASP:HB2	1:L:157:ASP:OD2	2.15	0.46
1:J:77:MET:HA	1:J:77:MET:HE2	1.97	0.46
1:O:67:MET:CE	1:O:171:PHE:CE1	2.98	0.46
1:F:158:LEU:HD23	1:F:190:GLN:HG2	1.97	0.46
1:L:58:ALA:O	1:L:62:ILE:HG12	2.15	0.46
1:R:176:TYR:HB3	1:R:185:MET:HG3	1.97	0.46
1:K:129:GLU:HB3	1:O:8:TYR:CB	2.41	0.46
1:N:197:ASP:H	1:N:200:HIS:CD2	2.33	0.46
1:A:157:ASP:HB2	1:C:157:ASP:OD1	2.15	0.46
1:K:37:VAL:HG21	1:K:205:LEU:HD13	1.97	0.46
1:H:214:GLU:HB3	1:H:215:TRP:H	1.60	0.46
1:F:56:TYR:CE1	1:F:60:ILE:HD11	2.51	0.46
1:D:214:GLU:HB3	1:D:215:TRP:H	1.57	0.46
1:H:154:THR:HG21	1:I:38:GLN:NE2	2.31	0.46
1:J:155:SER:HB3	1:K:36:THR:HB	1.98	0.46
1:H:34:ASN:HA	1:H:189:ILE:O	2.16	0.46
1:N:189:ILE:HD11	1:N:205:LEU:HD21	1.98	0.46
1:I:132:ALA:O	3:I:762:HOH:O	2.21	0.45
1:J:197:ASP:H	1:J:200:HIS:HD2	1.62	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:ASN:ND2	1:E:190:GLN:HB3	2.31	0.45
1:N:214:GLU:HB3	1:N:215:TRP:H	1.60	0.45
1:F:19:LYS:O	1:F:23:GLU:HB2	2.16	0.45
1:H:76:ALA:HB2	3:H:538:HOH:O	2.15	0.45
1:D:104:SER:HB2	1:D:134:PHE:CE1	2.52	0.45
1:L:67:MET:HE2	1:L:171:PHE:HE1	1.81	0.45
1:D:154:THR:HG21	1:E:38:GLN:NE2	2.32	0.45
1:P:68:ASN:HA	1:P:74:ARG:HH11	1.81	0.45
1:O:8:TYR:OH	1:O:78:LYS:HG2	2.17	0.45
1:P:154:THR:HG21	1:R:38:GLN:NE2	2.32	0.45
1:I:67:MET:CE	1:I:171:PHE:HE1	2.30	0.45
1:R:148:ASN:O	1:R:174:GLY:HA2	2.17	0.45
1:E:67:MET:CE	1:E:171:PHE:HE1	2.30	0.45
1:M:157:ASP:HB2	1:N:157:ASP:OD2	2.16	0.45
1:C:197:ASP:H	1:C:200:HIS:CD2	2.17	0.45
1:A:169:PRO:HB3	1:A:191:VAL:HG12	1.98	0.45
1:J:216:GLN:HE21	1:J:216:GLN:H	1.64	0.45
1:N:54:LYS:CE	1:N:54:LYS:HA	2.47	0.45
1:E:64:ALA:HB2	1:E:90:PRO:HG3	1.98	0.45
1:K:197:ASP:H	1:K:200:HIS:CD2	2.31	0.44
1:O:67:MET:HE2	1:O:171:PHE:CE1	2.49	0.44
1:D:197:ASP:H	1:D:200:HIS:HD2	1.65	0.44
1:N:215:TRP:HB3	3:N:227:HOH:O	2.16	0.44
1:A:35:GLN:HA	1:C:155:SER:O	2.18	0.44
1:B:70:HIS:HE1	1:B:207:GLU:OE1	1.99	0.44
1:A:34:ASN:ND2	1:A:158:LEU:H	2.15	0.44
1:R:72:GLU:HG3	1:R:200:HIS:HB3	1.99	0.44
1:J:37:VAL:HG21	1:J:205:LEU:HD13	1.98	0.44
1:I:174:GLY:HA3	1:I:186:PRO:HG2	1.98	0.44
1:B:57:PRO:HB3	1:B:120:TYR:CE2	2.53	0.44
1:G:146:SER:HB2	2:G:221:CLM:O5	2.18	0.44
1:R:56:TYR:HB3	1:R:57:PRO:HD3	2.00	0.44
1:C:215:TRP:HB3	1:C:216:GLN:NE2	2.32	0.44
1:F:22:PHE:O	1:F:26:GLN:HB2	2.18	0.44
1:E:39:LEU:HD11	1:E:208:LEU:HD11	1.98	0.44
1:M:189:ILE:HD11	1:M:205:LEU:HD11	1.99	0.44
1:L:22:PHE:O	1:L:26:GLN:HB2	2.18	0.44
1:G:114:ARG:HH12	1:G:216:GLN:HE21	1.66	0.44
1:R:189:ILE:HD11	1:R:205:LEU:HD21	2.00	0.44
1:E:214:GLU:HB3	1:E:215:TRP:H	1.59	0.43
1:L:215:TRP:HB3	3:L:225:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:51:ASN:N	1:N:51:ASN:OD1	2.51	0.43
1:K:56:TYR:CE1	1:K:147:ALA:HB2	2.53	0.43
1:J:34:ASN:HD21	1:J:158:LEU:H	1.66	0.43
1:E:16:TRP:CE2	1:E:18:ARG:HB2	2.54	0.43
1:N:22:PHE:O	1:N:26:GLN:HB2	2.17	0.43
1:P:67:MET:HE2	1:P:171:PHE:HE1	1.82	0.43
1:O:24:ALA:C	1:O:26:GLN:H	2.21	0.43
1:E:67:MET:HE2	1:E:171:PHE:HE1	1.83	0.43
1:S:72:GLU:HG3	1:S:200:HIS:HB3	2.00	0.43
1:J:197:ASP:H	1:J:200:HIS:CD2	2.37	0.43
1:A:13:ILE:O	1:A:19:LYS:HB3	2.18	0.43
1:K:10:THR:HA	1:K:83:VAL:HG12	2.01	0.43
1:R:26:GLN:HA	1:R:26:GLN:HE21	1.84	0.43
1:C:67:MET:HE3	1:C:169:PRO:CG	2.49	0.43
1:M:67:MET:CE	1:M:171:PHE:CE1	3.01	0.43
1:B:67:MET:HE2	1:B:171:PHE:CE1	2.54	0.43
1:G:44:PHE:O	1:G:48:VAL:HG23	2.18	0.43
1:O:10:THR:HA	1:O:83:VAL:HG12	2.01	0.43
1:A:39:LEU:HD13	1:A:41:ILE:HG23	2.00	0.43
1:A:139:ILE:HA	1:A:139:ILE:HD13	1.91	0.43
1:C:13:ILE:HG13	1:C:13:ILE:H	1.67	0.43
1:P:40:ASP:HB3	1:P:209:GLN:HE22	1.84	0.43
1:N:54:LYS:HE3	1:N:54:LYS:HA	2.00	0.42
1:S:70:HIS:HE1	1:S:207:GLU:OE1	2.00	0.42
1:N:54:LYS:HB3	1:N:57:PRO:HG2	2.01	0.42
1:R:185:MET:HA	1:R:186:PRO:HD2	1.94	0.42
1:G:216:GLN:CD	1:G:216:GLN:H	2.22	0.42
1:M:154:THR:HG21	1:N:38:GLN:NE2	2.34	0.42
1:J:19:LYS:O	1:J:23:GLU:HB2	2.18	0.42
1:C:151:VAL:HG13	1:C:153:PHE:HD2	1.84	0.42
1:P:189:ILE:HD11	1:P:205:LEU:HD21	2.01	0.42
1:I:26:GLN:HE22	1:I:165:ASN:HD22	1.67	0.42
1:M:32:THR:HG22	1:M:192:HIS:HA	2.01	0.42
1:P:105:LEU:HD13	1:P:127:TYR:HB2	2.01	0.42
1:O:104:SER:O	1:O:135:PRO:HD2	2.20	0.42
1:F:56:TYR:N	1:F:57:PRO:HD2	2.34	0.42
1:M:67:MET:HE2	1:M:171:PHE:CE1	2.54	0.42
1:B:57:PRO:HB3	1:B:120:TYR:CD2	2.55	0.42
1:C:153:PHE:CE1	1:C:156:PHE:HB2	2.55	0.42
1:B:190:GLN:HG3	1:B:190:GLN:O	2.19	0.42
1:B:7:GLY:O	1:B:85:TRP:HE3	2.03	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ASN:HD21	1:B:158:LEU:H	1.68	0.42
1:D:88:VAL:HG12	1:D:143:PHE:HD1	1.85	0.42
1:P:90:PRO:HD2	1:P:107:SER:O	2.20	0.42
1:H:160:VAL:HA	1:I:31:CYS:HB3	2.01	0.42
1:B:215:TRP:HB3	1:B:216:GLN:OE1	2.19	0.42
1:R:114:ARG:HH22	1:R:216:GLN:NE2	2.16	0.42
1:E:169:PRO:HB3	1:E:191:VAL:HG12	2.02	0.42
1:E:26:GLN:HA	1:E:26:GLN:NE2	2.27	0.41
1:H:6:THR:HG22	1:H:7:GLY:H	1.85	0.41
1:K:88:VAL:HG12	1:K:143:PHE:HD1	1.85	0.41
1:I:168:ALA:HA	1:I:169:PRO:HD2	1.94	0.41
1:G:13:ILE:O	1:G:19:LYS:HB3	2.20	0.41
1:E:39:LEU:HD11	1:E:208:LEU:CD1	2.50	0.41
1:H:174:GLY:HA3	1:H:186:PRO:HG2	2.02	0.41
1:O:39:LEU:HD11	1:O:208:LEU:CD1	2.49	0.41
1:M:13:ILE:HG13	1:M:13:ILE:H	1.70	0.41
1:D:24:ALA:C	1:D:26:GLN:H	2.24	0.41
1:K:96:HIS:HB2	1:K:99:THR:HG22	2.01	0.41
1:E:36:THR:HG23	1:E:188:ALA:HB2	2.01	0.41
1:O:67:MET:HE3	1:O:169:PRO:CG	2.51	0.41
1:M:139:ILE:HA	1:M:139:ILE:HD13	1.95	0.41
1:J:99:THR:HG23	1:J:101:THR:H	1.85	0.41
1:R:214:GLU:HB3	1:R:215:TRP:H	1.57	0.41
1:M:160:VAL:HA	1:N:31:CYS:HB3	2.02	0.41
1:C:26:GLN:HA	1:C:26:GLN:HE21	1.86	0.41
1:F:204:MET:O	1:F:208:LEU:HB2	2.20	0.41
1:N:67:MET:HE1	1:N:171:PHE:CE1	2.53	0.41
1:M:34:ASN:ND2	1:M:190:GLN:HB3	2.35	0.41
1:M:19:LYS:O	1:M:23:GLU:HB2	2.20	0.41
1:C:39:LEU:HD11	1:C:208:LEU:HD11	2.03	0.41
1:S:148:ASN:HD21	1:S:151:VAL:HG13	1.86	0.41
1:I:103:SER:HB3	3:I:762:HOH:O	2.20	0.41
1:R:60:ILE:CD1	1:R:145:VAL:HG11	2.51	0.41
1:M:153:PHE:CE1	1:M:186:PRO:HB2	2.56	0.41
1:R:22:PHE:O	1:R:26:GLN:HB2	2.21	0.41
1:G:40:ASP:HB3	1:G:209:GLN:HE22	1.85	0.41
1:K:39:LEU:O	1:K:184:LEU:HA	2.21	0.41
1:P:56:TYR:HB3	1:P:57:PRO:HD3	2.02	0.41
1:G:185:MET:HA	1:G:186:PRO:HD2	1.92	0.41
1:D:99:THR:HG21	1:D:131:LEU:HD22	2.02	0.41
1:A:2:GLU:N	3:A:308:HOH:O	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:45:LEU:HD22	1:L:49:LYS:HD2	2.02	0.40
1:E:65:ARG:HH12	1:E:217:GLY:HA2	1.85	0.40
1:K:89:HIS:HA	1:K:90:PRO:HD3	1.97	0.40
1:E:114:ARG:H	1:E:114:ARG:HG2	1.67	0.40
1:I:103:SER:CB	3:I:762:HOH:O	2.68	0.40
1:L:19:LYS:HG3	1:L:20:GLU:N	2.36	0.40
1:C:40:ASP:HA	1:C:184:LEU:HD23	2.03	0.40
1:N:159:ASN:HD21	1:O:159:ASN:CG	2.25	0.40
1:K:51:ASN:ND2	1:K:216:GLN:HE21	2.19	0.40
1:N:105:LEU:HD13	1:N:127:TYR:HB2	2.03	0.40
1:D:189:ILE:HD11	1:D:205:LEU:HD21	2.03	0.40
1:K:158:LEU:HD22	1:K:170:VAL:HG11	2.03	0.40
1:L:214:GLU:HB3	1:L:215:TRP:H	1.62	0.40
1:M:45:LEU:HD12	1:M:183:VAL:HG11	2.03	0.40
1:A:85:TRP:CD2	1:A:141:ASN:HB3	2.57	0.40
1:J:38:GLN:NE2	1:L:154:THR:HG21	2.36	0.40
1:J:57:PRO:HB3	1:J:120:TYR:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/219 (97%)	201 (94%)	11 (5%)	1 (0%)	34	71
1	B	213/219 (97%)	206 (97%)	7 (3%)	0	100	100
1	C	214/219 (98%)	204 (95%)	10 (5%)	0	100	100
1	D	209/219 (95%)	199 (95%)	10 (5%)	0	100	100
1	E	203/219 (93%)	194 (96%)	9 (4%)	0	100	100
1	F	209/219 (95%)	201 (96%)	7 (3%)	1 (0%)	34	71
1	G	212/219 (97%)	207 (98%)	5 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	211/219 (96%)	202 (96%)	8 (4%)	1 (0%)	34	71
1	I	211/219 (96%)	200 (95%)	11 (5%)	0	100	100
1	J	214/219 (98%)	209 (98%)	5 (2%)	0	100	100
1	K	214/219 (98%)	201 (94%)	12 (6%)	1 (0%)	34	71
1	L	214/219 (98%)	202 (94%)	11 (5%)	1 (0%)	34	71
1	M	209/219 (95%)	201 (96%)	7 (3%)	1 (0%)	34	71
1	N	210/219 (96%)	200 (95%)	9 (4%)	1 (0%)	34	71
1	O	209/219 (95%)	200 (96%)	8 (4%)	1 (0%)	34	71
1	P	213/219 (97%)	202 (95%)	11 (5%)	0	100	100
1	R	212/219 (97%)	202 (95%)	9 (4%)	1 (0%)	34	71
1	S	212/219 (97%)	203 (96%)	7 (3%)	2 (1%)	21	57
All	All	3802/3942 (96%)	3634 (96%)	157 (4%)	11 (0%)	46	79

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	LYS
1	F	214	GLU
1	L	78	LYS
1	S	5	ILE
1	H	214	GLU
1	R	214	GLU
1	M	214	GLU
1	N	214	GLU
1	O	25	PHE
1	K	3	LYS
1	S	27	SER

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	190/194 (98%)	182 (96%)	8 (4%)	36	73
1	B	192/194 (99%)	180 (94%)	12 (6%)	22	54
1	C	190/194 (98%)	176 (93%)	14 (7%)	17	44
1	D	188/194 (97%)	171 (91%)	17 (9%)	12	34
1	E	184/194 (95%)	175 (95%)	9 (5%)	31	67
1	F	188/194 (97%)	178 (95%)	10 (5%)	28	63
1	G	190/194 (98%)	174 (92%)	16 (8%)	14	37
1	H	190/194 (98%)	177 (93%)	13 (7%)	20	49
1	I	190/194 (98%)	180 (95%)	10 (5%)	28	63
1	J	191/194 (98%)	181 (95%)	10 (5%)	29	64
1	K	191/194 (98%)	180 (94%)	11 (6%)	25	58
1	L	190/194 (98%)	177 (93%)	13 (7%)	20	49
1	M	188/194 (97%)	176 (94%)	12 (6%)	22	53
1	N	189/194 (97%)	174 (92%)	15 (8%)	15	41
1	O	188/194 (97%)	175 (93%)	13 (7%)	19	48
1	P	190/194 (98%)	181 (95%)	9 (5%)	32	68
1	R	189/194 (97%)	175 (93%)	14 (7%)	17	44
1	S	190/194 (98%)	176 (93%)	14 (7%)	17	44
All	All	3408/3492 (98%)	3188 (94%)	220 (6%)	21	52

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	26	GLN
1	A	38	GLN
1	A	39	LEU
1	A	77	MET
1	A	87	SER
1	A	190	GLN
1	A	208	LEU
1	B	9	THR
1	B	38	GLN
1	B	39	LEU
1	B	77	MET
1	B	105	LEU
1	B	138	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	151	VAL
1	B	189	ILE
1	B	190	GLN
1	B	208	LEU
1	B	214	GLU
1	B	216	GLN
1	C	26	GLN
1	C	38	GLN
1	C	39	LEU
1	C	77	MET
1	C	105	LEU
1	C	111	ASP
1	C	138	PHE
1	C	139	ILE
1	C	157	ASP
1	C	185	MET
1	C	189	ILE
1	C	208	LEU
1	C	214	GLU
1	C	216	GLN
1	D	8	TYR
1	D	12	ASP
1	D	26	GLN
1	D	38	GLN
1	D	39	LEU
1	D	67	MET
1	D	77	MET
1	D	105	LEU
1	D	138	PHE
1	D	164	ASP
1	D	189	ILE
1	D	190	GLN
1	D	191	VAL
1	D	196	CYS
1	D	208	LEU
1	D	214	GLU
1	D	216	GLN
1	E	26	GLN
1	E	39	LEU
1	E	54	LYS
1	E	114	ARG
1	E	164	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	189	ILE
1	E	190	GLN
1	E	214	GLU
1	E	216	GLN
1	F	26	GLN
1	F	39	LEU
1	F	67	MET
1	F	105	LEU
1	F	138	PHE
1	F	189	ILE
1	F	190	GLN
1	F	204	MET
1	F	214	GLU
1	F	216	GLN
1	G	6	THR
1	G	38	GLN
1	G	39	LEU
1	G	67	MET
1	G	77	MET
1	G	105	LEU
1	G	111	ASP
1	G	133	TYR
1	G	139	ILE
1	G	164	ASP
1	G	189	ILE
1	G	190	GLN
1	G	191	VAL
1	G	208	LEU
1	G	214	GLU
1	G	216	GLN
1	H	5	ILE
1	H	6	THR
1	H	12	ASP
1	H	26	GLN
1	H	38	GLN
1	H	39	LEU
1	H	77	MET
1	H	150	TRP
1	H	151	VAL
1	H	189	ILE
1	H	190	GLN
1	H	214	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	216	GLN
1	I	6	THR
1	I	9	THR
1	I	38	GLN
1	I	39	LEU
1	I	45	LEU
1	I	77	MET
1	I	189	ILE
1	I	208	LEU
1	I	214	GLU
1	I	216	GLN
1	J	9	THR
1	J	26	GLN
1	J	38	GLN
1	J	39	LEU
1	J	105	LEU
1	J	157	ASP
1	J	189	ILE
1	J	190	GLN
1	J	214	GLU
1	J	216	GLN
1	K	26	GLN
1	K	38	GLN
1	K	39	LEU
1	K	77	MET
1	K	97	GLU
1	K	105	LEU
1	K	189	ILE
1	K	190	GLN
1	K	208	LEU
1	K	214	GLU
1	K	216	GLN
1	L	9	THR
1	L	38	GLN
1	L	39	LEU
1	L	77	MET
1	L	105	LEU
1	L	133	TYR
1	L	157	ASP
1	L	179	GLN
1	L	181	ASP
1	L	189	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	190	GLN
1	L	214	GLU
1	L	216	GLN
1	M	26	GLN
1	M	38	GLN
1	M	39	LEU
1	M	51	ASN
1	M	77	MET
1	M	105	LEU
1	M	157	ASP
1	M	178	THR
1	M	181	ASP
1	M	189	ILE
1	M	208	LEU
1	M	214	GLU
1	N	12	ASP
1	N	26	GLN
1	N	39	LEU
1	N	51	ASN
1	N	54	LYS
1	N	105	LEU
1	N	114	ARG
1	N	117	LEU
1	N	139	ILE
1	N	178	THR
1	N	189	ILE
1	N	190	GLN
1	N	208	LEU
1	N	214	GLU
1	N	216	GLN
1	O	20	GLU
1	O	26	GLN
1	O	38	GLN
1	O	39	LEU
1	O	77	MET
1	O	99	THR
1	O	105	LEU
1	O	164	ASP
1	O	182	LYS
1	O	189	ILE
1	O	190	GLN
1	O	214	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	216	GLN
1	P	38	GLN
1	P	39	LEU
1	P	77	MET
1	P	105	LEU
1	P	133	TYR
1	P	151	VAL
1	P	189	ILE
1	P	190	GLN
1	P	216	GLN
1	R	8	TYR
1	R	26	GLN
1	R	38	GLN
1	R	39	LEU
1	R	77	MET
1	R	111	ASP
1	R	160	VAL
1	R	164	ASP
1	R	185	MET
1	R	189	ILE
1	R	190	GLN
1	R	191	VAL
1	R	214	GLU
1	R	216	GLN
1	S	9	THR
1	S	12	ASP
1	S	39	LEU
1	S	77	MET
1	S	104	SER
1	S	138	PHE
1	S	151	VAL
1	S	164	ASP
1	S	181	ASP
1	S	189	ILE
1	S	190	GLN
1	S	208	LEU
1	S	214	GLU
1	S	216	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	38	GLN
1	A	61	HIS
1	A	70	HIS
1	A	159	ASN
1	A	165	ASN
1	A	200	HIS
1	B	34	ASN
1	B	38	GLN
1	B	70	HIS
1	B	118	HIS
1	B	165	ASN
1	B	200	HIS
1	C	34	ASN
1	C	38	GLN
1	C	70	HIS
1	C	162	ASN
1	C	165	ASN
1	C	200	HIS
1	D	26	GLN
1	D	38	GLN
1	D	110	HIS
1	D	165	ASN
1	D	200	HIS
1	D	209	GLN
1	E	26	GLN
1	E	34	ASN
1	E	38	GLN
1	E	61	HIS
1	E	70	HIS
1	E	159	ASN
1	E	162	ASN
1	E	165	ASN
1	E	200	HIS
1	F	17	HIS
1	F	26	GLN
1	F	34	ASN
1	F	70	HIS
1	F	165	ASN
1	F	200	HIS
1	G	34	ASN
1	G	115	GLN
1	G	200	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	216	GLN
1	H	26	GLN
1	H	34	ASN
1	H	51	ASN
1	H	70	HIS
1	H	115	GLN
1	H	165	ASN
1	H	200	HIS
1	I	34	ASN
1	I	70	HIS
1	I	159	ASN
1	I	165	ASN
1	I	200	HIS
1	J	26	GLN
1	J	34	ASN
1	J	38	GLN
1	J	61	HIS
1	J	70	HIS
1	J	200	HIS
1	K	34	ASN
1	K	38	GLN
1	K	51	ASN
1	K	61	HIS
1	K	70	HIS
1	K	159	ASN
1	K	165	ASN
1	K	200	HIS
1	L	30	GLN
1	L	34	ASN
1	L	38	GLN
1	L	61	HIS
1	L	70	HIS
1	L	165	ASN
1	L	200	HIS
1	M	26	GLN
1	M	34	ASN
1	M	38	GLN
1	M	70	HIS
1	M	159	ASN
1	M	165	ASN
1	M	200	HIS
1	N	26	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	61	HIS
1	N	70	HIS
1	N	159	ASN
1	N	200	HIS
1	N	209	GLN
1	O	70	HIS
1	O	110	HIS
1	O	159	ASN
1	O	165	ASN
1	O	190	GLN
1	O	200	HIS
1	P	26	GLN
1	P	30	GLN
1	P	34	ASN
1	P	35	GLN
1	P	159	ASN
1	P	165	ASN
1	P	200	HIS
1	R	38	GLN
1	R	53	HIS
1	R	70	HIS
1	R	159	ASN
1	R	200	HIS
1	S	34	ASN
1	S	38	GLN
1	S	70	HIS
1	S	115	GLN
1	S	148	ASN
1	S	165	ASN
1	S	200	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	CLM	A	221	-	18,20,20	0.85	0	22,27,27	0.70	0
2	CLM	B	221	-	18,20,20	0.84	0	22,27,27	0.57	0
2	CLM	C	221	-	18,20,20	0.85	0	22,27,27	0.62	0
2	CLM	D	221	-	18,20,20	0.91	1 (5%)	22,27,27	0.88	0
2	CLM	E	221	-	18,20,20	0.83	1 (5%)	22,27,27	0.99	0
2	CLM	F	221	-	18,20,20	0.85	0	22,27,27	0.69	0
2	CLM	G	221	-	18,20,20	0.88	1 (5%)	22,27,27	0.74	0
2	CLM	H	221	-	18,20,20	0.85	0	22,27,27	0.74	0
2	CLM	I	221	-	18,20,20	0.88	0	22,27,27	0.80	0
2	CLM	J	221	-	18,20,20	0.85	0	22,27,27	0.87	0
2	CLM	K	221	-	18,20,20	0.87	0	22,27,27	0.78	0
2	CLM	L	221	-	18,20,20	0.88	0	22,27,27	0.62	0
2	CLM	M	221	-	18,20,20	0.83	0	22,27,27	0.73	0
2	CLM	N	221	-	18,20,20	0.88	1 (5%)	22,27,27	0.72	0
2	CLM	O	221	-	18,20,20	0.88	1 (5%)	22,27,27	0.77	0
2	CLM	P	221	-	18,20,20	0.89	1 (5%)	22,27,27	0.93	0
2	CLM	R	221	-	18,20,20	0.86	0	22,27,27	0.79	0
2	CLM	S	221	-	18,20,20	0.86	0	22,27,27	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CLM	A	221	-	-	0/22/22/22	0/1/1/1
2	CLM	B	221	-	-	0/22/22/22	0/1/1/1
2	CLM	C	221	-	-	0/22/22/22	0/1/1/1
2	CLM	D	221	-	-	0/22/22/22	0/1/1/1
2	CLM	E	221	-	-	0/22/22/22	0/1/1/1
2	CLM	F	221	-	-	0/22/22/22	0/1/1/1
2	CLM	G	221	-	-	0/22/22/22	0/1/1/1
2	CLM	H	221	-	-	0/22/22/22	0/1/1/1
2	CLM	I	221	-	-	0/22/22/22	0/1/1/1
2	CLM	J	221	-	-	0/22/22/22	0/1/1/1
2	CLM	K	221	-	-	0/22/22/22	0/1/1/1
2	CLM	L	221	-	-	0/22/22/22	0/1/1/1
2	CLM	M	221	-	-	0/22/22/22	0/1/1/1
2	CLM	N	221	-	-	0/22/22/22	0/1/1/1
2	CLM	O	221	-	-	2/22/22/22	0/1/1/1
2	CLM	P	221	-	-	2/22/22/22	0/1/1/1
2	CLM	R	221	-	-	0/22/22/22	0/1/1/1
2	CLM	S	221	-	-	0/22/22/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	221	CLM	C1-C2	-2.38	1.49	1.53
2	O	221	CLM	C6-C5	-2.17	1.48	1.51
2	G	221	CLM	C6-C5	-2.05	1.48	1.51
2	E	221	CLM	C6-C5	-2.04	1.48	1.51
2	P	221	CLM	C6-C5	-2.03	1.48	1.51
2	N	221	CLM	C1-C2	-2.02	1.49	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	221	CLM	C8-C9-N9-O9B
2	O	221	CLM	C10-C9-N9-O9B
2	P	221	CLM	C10-C9-N9-O9B
2	P	221	CLM	C8-C9-N9-O9B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	221	CLM	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	215/219 (98%)	-0.31	1 (0%) 91 90	47, 65, 90, 107	0
1	B	215/219 (98%)	-0.21	3 (1%) 78 76	44, 64, 89, 103	0
1	C	216/219 (98%)	-0.31	1 (0%) 91 90	44, 61, 85, 99	0
1	D	211/219 (96%)	-0.12	2 (0%) 85 84	48, 71, 102, 116	0
1	E	207/219 (94%)	-0.28	1 (0%) 91 90	47, 64, 91, 110	0
1	F	211/219 (96%)	-0.11	5 (2%) 62 57	52, 72, 100, 114	0
1	G	214/219 (97%)	-0.11	2 (0%) 85 84	60, 77, 99, 111	0
1	H	213/219 (97%)	-0.12	2 (0%) 85 84	62, 80, 101, 110	0
1	I	213/219 (97%)	-0.16	1 (0%) 91 90	60, 77, 94, 104	0
1	J	216/219 (98%)	-0.29	1 (0%) 91 90	43, 59, 81, 94	0
1	K	216/219 (98%)	-0.17	1 (0%) 91 90	43, 68, 92, 105	0
1	L	216/219 (98%)	-0.38	1 (0%) 91 90	43, 63, 91, 101	0
1	M	211/219 (96%)	-0.26	2 (0%) 85 84	49, 67, 96, 110	0
1	N	212/219 (96%)	-0.24	5 (2%) 62 57	42, 63, 91, 111	0
1	O	211/219 (96%)	-0.01	6 (2%) 56 50	53, 75, 107, 121	0
1	P	215/219 (98%)	-0.09	2 (0%) 85 84	62, 77, 98, 109	0
1	R	214/219 (97%)	-0.19	2 (0%) 85 84	58, 74, 95, 105	0
1	S	214/219 (97%)	-0.11	0 100 100	60, 75, 93, 104	0
All	All	3840/3942 (97%)	-0.19	38 (0%) 84 82	42, 70, 96, 121	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	217	GLY	5.5
1	N	51	ASN	5.2
1	D	217	GLY	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	217	GLY	4.8
1	O	217	GLY	4.7
1	N	52	LYS	4.6
1	R	98	GLN	3.8
1	O	52	LYS	3.1
1	M	217	GLY	3.0
1	P	47	THR	3.0
1	R	211	TYR	2.9
1	B	215	TRP	2.9
1	O	138	PHE	2.9
1	L	217	GLY	2.8
1	P	13	ILE	2.8
1	J	217	GLY	2.8
1	G	217	GLY	2.8
1	F	52	LYS	2.5
1	I	50	LYS	2.5
1	N	6	THR	2.5
1	A	52	LYS	2.5
1	H	217	GLY	2.5
1	N	50	LYS	2.4
1	O	159	ASN	2.4
1	G	98	GLN	2.4
1	N	215	TRP	2.4
1	O	43	ALA	2.3
1	M	52	LYS	2.3
1	O	53	HIS	2.2
1	B	216	GLN	2.2
1	F	98	GLN	2.2
1	B	52	LYS	2.1
1	E	138	PHE	2.1
1	D	50	LYS	2.1
1	F	49	LYS	2.1
1	C	98	GLN	2.1
1	H	98	GLN	2.0
1	F	157	ASP	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 [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CLM	P	221	20/20	0.81	0.26	2.37	65,67,74,76	0
2	CLM	E	221	20/20	0.91	0.24	2.17	54,56,65,67	0
2	CLM	N	221	20/20	0.90	0.22	1.79	56,58,65,67	0
2	CLM	H	221	20/20	0.89	0.23	1.56	66,67,75,77	0
2	CLM	S	221	20/20	0.89	0.26	1.38	62,63,71,74	0
2	CLM	J	221	20/20	0.92	0.20	1.24	59,62,65,68	0
2	CLM	C	221	20/20	0.90	0.20	1.18	62,64,70,73	0
2	CLM	M	221	20/20	0.94	0.19	1.17	57,59,66,67	0
2	CLM	A	221	20/20	0.92	0.19	0.88	66,68,71,74	0
2	CLM	G	221	20/20	0.89	0.21	0.86	62,65,69,73	0
2	CLM	I	221	20/20	0.90	0.20	0.83	62,64,70,72	0
2	CLM	O	221	20/20	0.90	0.19	-0.03	58,60,71,71	0
2	CLM	D	221	20/20	0.91	0.16	-0.07	53,56,64,65	0
2	CLM	K	221	20/20	0.92	0.17	-0.18	61,64,70,73	0
2	CLM	R	221	20/20	0.91	0.16	-0.19	57,59,64,67	0
2	CLM	F	221	20/20	0.93	0.15	-0.51	58,60,67,69	0
2	CLM	L	221	20/20	0.95	0.13	-0.57	53,54,57,60	0
2	CLM	B	221	20/20	0.95	0.13	-0.62	52,55,59,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.