



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:08 PM UTC

PDB ID : 6MX2 / pdb\_00006mx2  
Title : Crystal Structure of ClpP1 from Clostridium difficile 630.  
Authors : Lavey, N.P.; Thomas, L.M.; Duerfeldt, A.S.  
Deposited on : 2018-10-30  
Resolution : 2.50 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

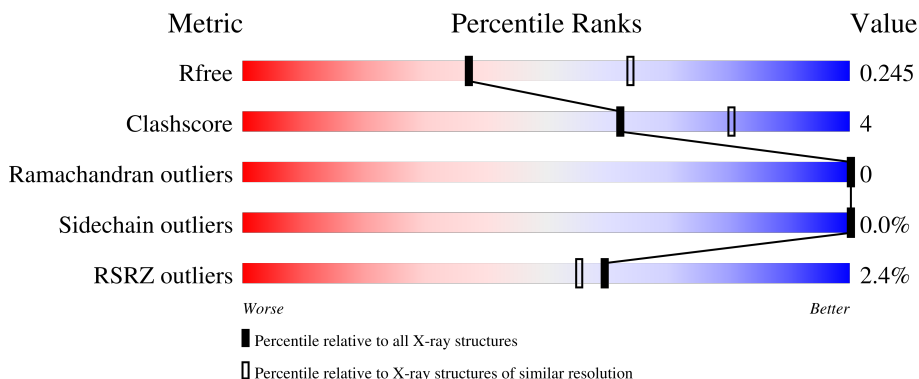
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	194	 2% 87% 7% 6%
1	B	194	 2% 82% 13% 5%
1	C	194	 4% 83% 10% 7%
1	D	194	 % 83% 10% 7%
1	E	194	 % 88% 6% 6%

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Mol	Chain	Length	Quality of chain
1	F	194	<p>3% 82% 12% 6%</p>
1	G	194	<p>3% 81% 13% 6%</p>
1	H	194	<p>% 87% 6% 7%</p>
1	I	194	<p>3% 82% 11% 7%</p>
1	J	194	<p>4% 87% 10% .</p>
1	K	194	<p>% 80% 13% 6%</p>
1	L	194	<p>3% 90% 5% 6%</p>
1	M	194	<p>3% 85% 8% 7%</p>
1	N	194	<p>3% 83% 10% 7%</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 20432 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	182	Total 1403	C 891	N 236	O 268	S 8	0	0	0
1	B	185	Total 1425	C 905	N 239	O 273	S 8	0	0	0
1	C	181	Total 1395	C 888	N 232	O 267	S 8	0	0	0
1	D	181	Total 1393	C 887	N 232	O 266	S 8	0	0	0
1	E	182	Total 1399	C 890	N 233	O 268	S 8	0	0	0
1	F	183	Total 1407	C 896	N 234	O 269	S 8	0	0	0
1	G	183	Total 1408	C 896	N 234	O 270	S 8	0	0	0
1	H	181	Total 1394	C 888	N 232	O 266	S 8	0	0	0
1	I	180	Total 1385	C 881	N 231	O 265	S 8	0	0	0
1	J	187	Total 1441	C 915	N 242	O 276	S 8	0	0	0
1	K	182	Total 1400	C 890	N 233	O 269	S 8	0	0	0
1	L	183	Total 1407	C 896	N 234	O 269	S 8	0	0	0
1	M	181	Total 1392	C 885	N 232	O 267	S 8	0	0	0
1	N	180	Total 1378	C 877	N 227	O 266	S 8	0	0	0

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0
2	G	2	Total Na 2 2	0	0
2	H	1	Total Na 1 1	0	0
2	I	2	Total Na 2 2	0	0
2	J	1	Total Na 1 1	0	0
2	K	1	Total Na 1 1	0	0
2	L	2	Total Na 2 2	0	0
2	M	1	Total Na 1 1	0	0
2	N	1	Total Na 1 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total C O 6 3 3	0	0
3	N	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	55	Total O 55 55	0	0
4	B	47	Total O 47 47	0	0
4	C	62	Total O 62 62	0	0
4	D	60	Total O 60 60	0	0
4	E	70	Total O 70 70	0	0
4	F	53	Total O 53 53	0	0
4	G	52	Total O 52 52	0	0
4	H	57	Total O 57 57	0	0
4	I	57	Total O 57 57	0	0
4	J	50	Total O 50 50	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	K	76	Total O 76 76	0	0
4	L	47	Total O 47 47	0	0
4	M	41	Total O 41 41	0	0
4	N	49	Total O 49 49	0	0

### 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: ATP-dependent Clp protease proteolytic subunit

Chain A: 




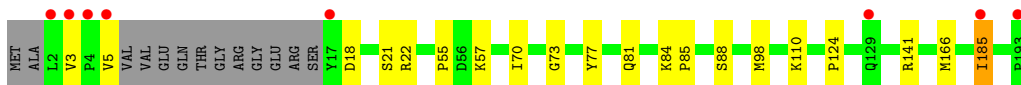
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B: 




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C: 




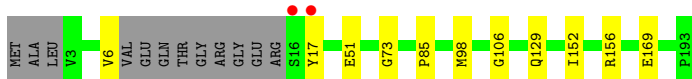
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D: 

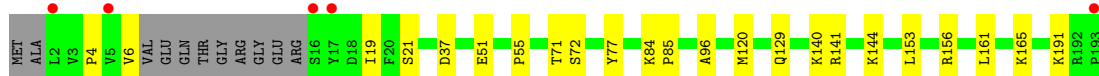
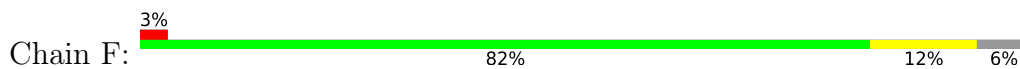


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

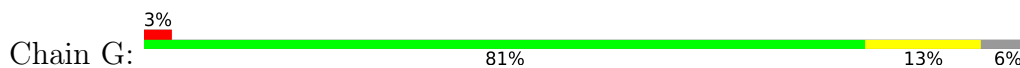
Chain E: 



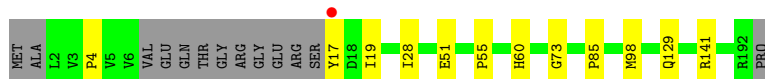
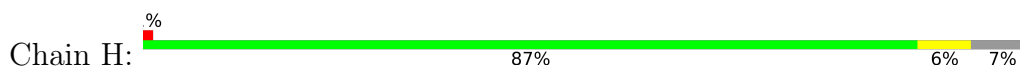
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



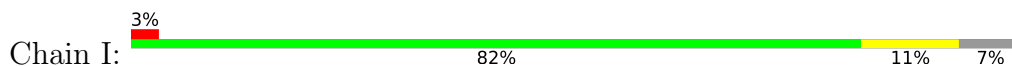
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



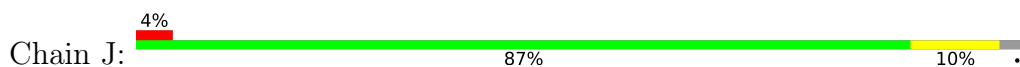
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



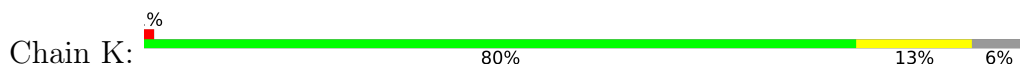
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



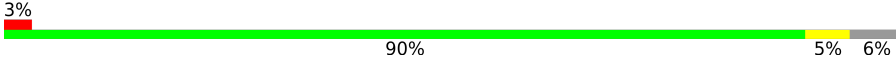
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:  3% 90% 5% 6%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:  3% 85% 8% 7%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:  3% 83% 10% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.33Å 97.37Å 106.49Å 113.15° 104.56° 103.21°	Depositor
Resolution (Å)	34.90 – 2.50 34.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (34.90-2.50) 98.2 (34.90-2.50)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.193 , 0.244 0.194 , 0.245	Depositor DCC
$R_{free}$ test set	5438 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtrriage
Anisotropy	0.011	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	20432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NA, GOL

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	0.09	0/1422	0.26	0/1915
1	B	0.09	0/1444	0.27	0/1945
1	C	0.10	0/1415	0.26	0/1906
1	D	0.09	0/1413	0.26	0/1905
1	E	0.09	0/1419	0.25	0/1913
1	F	0.10	0/1427	0.27	0/1924
1	G	0.09	0/1428	0.26	0/1924
1	H	0.08	0/1413	0.25	0/1904
1	I	0.10	0/1404	0.27	0/1891
1	J	0.09	0/1460	0.26	0/1967
1	K	0.09	0/1420	0.26	0/1913
1	L	0.09	0/1426	0.26	0/1922
1	M	0.10	0/1411	0.26	0/1901
1	N	0.10	0/1397	0.28	0/1884
All	All	0.09	0/19899	0.26	0/26814

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1403	0	1437	17	0
1	B	1425	0	1462	17	0
1	C	1395	0	1428	15	0
1	D	1393	0	1426	12	0
1	E	1399	0	1431	7	0
1	F	1407	0	1442	16	0
1	G	1408	0	1442	20	0
1	H	1394	0	1430	9	0
1	I	1385	0	1420	16	0
1	J	1441	0	1479	13	0
1	K	1400	0	1431	15	0
1	L	1407	0	1444	6	0
1	M	1392	0	1424	12	0
1	N	1378	0	1408	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	2	0	0	0	0
2	H	1	0	0	0	0
2	I	2	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	2	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
3	M	6	0	8	1	0
3	N	6	0	8	0	0
4	A	55	0	0	1	0
4	B	47	0	0	2	0
4	C	62	0	0	1	0
4	D	60	0	0	1	0
4	E	70	0	0	0	0
4	F	53	0	0	1	0
4	G	52	0	0	1	0
4	H	57	0	0	1	0
4	I	57	0	0	2	0
4	J	50	0	0	1	0
4	K	76	0	0	0	0
4	L	47	0	0	0	0
4	M	41	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	49	0	0	0	0
All	All	20432	0	20120	162	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 4.

All (162) 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:A:161:LEU:HD11	1:A:165:LYS:HE3	1.45	0.95
1:A:161:LEU:CD1	1:A:165:LYS:HE3	2.01	0.89
1:I:21:SER:HB2	1:J:4:PRO:HD2	1.62	0.81
1:I:76:ILE:HG22	1:I:80:MET:HE2	1.72	0.72
1:A:161:LEU:HG	1:A:165:LYS:NZ	2.05	0.72
1:K:18:ASP:OD1	1:K:21:SER:OG	2.07	0.71
1:G:112:LEU:HD23	1:G:187:GLU:HB2	1.72	0.71
1:A:73:GLY:HA3	1:A:98:MET:HE2	1.73	0.71
1:M:73:GLY:HA3	1:M:98:MET:HE2	1.72	0.70
1:A:161:LEU:O	1:A:165:LYS:HD3	1.92	0.69
1:C:73:GLY:HA3	1:C:98:MET:HE2	1.75	0.69
1:E:73:GLY:HA3	1:E:98:MET:HE2	1.75	0.69
1:I:73:GLY:HA3	1:I:98:MET:HE2	1.73	0.68
1:J:73:GLY:HA3	1:J:98:MET:HE2	1.75	0.68
1:N:73:GLY:HA3	1:N:98:MET:HE2	1.75	0.67
1:D:73:GLY:HA3	1:D:98:MET:HE2	1.76	0.66
1:F:141:ARG:NH1	1:G:118:GLU:OE2	2.27	0.66
1:L:73:GLY:HA3	1:L:98:MET:HE2	1.77	0.66
1:K:37:ASP:OD1	1:K:72:SER:OG	2.14	0.65
1:H:73:GLY:HA3	1:H:98:MET:HE2	1.77	0.65
1:K:73:GLY:HA3	1:K:98:MET:HE2	1.79	0.65
1:G:6:VAL:N	1:G:17:TYR:O	2.32	0.63
1:K:141:ARG:NH1	1:L:118:GLU:OE2	2.34	0.60
1:G:22:ARG:NH2	4:G:302:HOH:O	2.33	0.60
1:B:55:PRO:HB2	1:B:84:LYS:HD3	1.83	0.59
1:D:37:ASP:OD1	1:D:72:SER:OG	2.21	0.59
1:K:5:VAL:HA	1:K:18:ASP:HA	1.85	0.58
1:L:51:GLU:OE1	1:M:192:ARG:NH1	2.35	0.58
1:E:106:GLY:O	1:E:156:ARG:NH2	2.36	0.58
1:F:140:LYS:O	1:F:144:LYS:HG3	2.05	0.57
1:B:1:ALA:N	4:B:301:HOH:O	2.30	0.57
1:I:77:TYR:HA	1:I:80:MET:HE3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLY:HA3	1:B:98:MET:HE2	1.87	0.56
1:F:55:PRO:HB2	1:F:84:LYS:HD3	1.87	0.56
1:B:3:VAL:HG23	1:B:19:ILE:HB	1.85	0.56
1:A:118:GLU:OE2	1:G:141:ARG:NH1	2.40	0.55
1:B:4:PRO:HA	1:B:18:ASP:HA	1.88	0.54
1:B:21:SER:HB2	1:C:5:VAL:H	1.73	0.54
1:F:77:TYR:OH	1:F:156:ARG:NH1	2.40	0.54
1:N:4:PRO:HA	1:N:18:ASP:HA	1.89	0.54
1:N:113:ALA:HB3	1:N:185:ILE:HD13	1.90	0.54
1:J:140:LYS:O	1:J:144:LYS:HG3	2.08	0.54
1:F:71:THR:HG21	1:G:94:MET:HE2	1.89	0.53
1:I:17:TYR:N	4:I:306:HOH:O	2.42	0.53
1:B:90:ILE:HG23	1:B:112:LEU:HD22	1.90	0.52
1:A:15:ARG:NH1	4:A:305:HOH:O	2.40	0.52
1:N:185:ILE:HD12	1:N:187:GLU:O	2.09	0.52
1:H:51:GLU:HG3	1:H:85:PRO:HD3	1.91	0.51
1:C:55:PRO:HB2	1:C:84:LYS:HD3	1.91	0.51
1:I:192:ARG:NH2	4:I:303:HOH:O	2.38	0.51
1:M:161:LEU:HG	1:M:165:LYS:HE3	1.93	0.51
1:G:152:ILE:O	1:G:156:ARG:HG2	2.10	0.51
1:C:141:ARG:NE	1:D:118:GLU:OE2	2.43	0.50
1:I:17:TYR:OH	1:I:25:LYS:HE3	2.10	0.50
1:A:173:PHE:CG	1:G:141:ARG:HG3	2.47	0.50
1:H:17:TYR:N	4:H:303:HOH:O	2.43	0.50
1:H:141:ARG:NH2	1:I:118:GLU:OE2	2.45	0.50
1:M:78:ASP:HB3	1:N:114:LEU:HD23	1.91	0.50
1:F:161:LEU:HG	1:F:165:LYS:HE3	1.92	0.50
1:J:74:MET:HE1	1:J:101:PHE:CE2	2.47	0.50
1:L:6:VAL:HG21	1:L:22:ARG:HB2	1.94	0.50
1:M:163:LYS:NZ	1:M:167:ASP:OD2	2.41	0.49
1:M:71:THR:HG21	1:N:94:MET:HE2	1.93	0.49
1:E:152:ILE:O	1:E:156:ARG:HG2	2.13	0.49
1:G:129:GLN:OE1	1:H:129:GLN:NE2	2.45	0.49
1:N:37:ASP:OD2	1:N:72:SER:OG	2.28	0.49
1:L:6:VAL:HG23	1:L:17:TYR:HB2	1.94	0.49
1:F:4:PRO:HD2	1:F:19:ILE:HG21	1.95	0.49
1:A:51:GLU:OE1	1:B:192:ARG:NH1	2.47	0.48
1:B:161:LEU:HG	1:B:165:LYS:HE3	1.95	0.48
1:I:2:LEU:O	1:I:4:PRO:HD3	2.14	0.47
1:F:21:SER:HB3	1:G:5:VAL:O	2.14	0.47
1:J:2:LEU:H	1:J:2:LEU:HD23	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:97:SER:HG	1:N:122:HIS:CE1	2.33	0.47
1:B:106:GLY:O	1:B:156:ARG:NH2	2.48	0.47
1:E:51:GLU:HG3	1:E:85:PRO:HD3	1.97	0.47
1:G:124:PRO:HG3	1:G:149:LEU:HD12	1.97	0.47
1:K:97:SER:OG	1:K:122:HIS:NE2	2.47	0.47
1:G:16:SER:O	1:G:16:SER:OG	2.29	0.47
1:G:97:SER:HG	1:G:122:HIS:CE1	2.30	0.47
1:G:112:LEU:CD2	1:G:187:GLU:HB2	2.44	0.46
1:J:144:LYS:NZ	4:J:306:HOH:O	2.48	0.46
1:K:124:PRO:HG3	1:K:149:LEU:HD12	1.97	0.46
1:M:21:SER:HG	1:N:4:PRO:HD2	1.80	0.46
1:J:141:ARG:HD2	1:K:173:PHE:CD1	2.51	0.46
1:M:122:HIS:O	3:M:201:GOL:H2	2.16	0.46
1:C:88:SER:HB2	1:C:110:LYS:HB3	1.98	0.46
1:C:22:ARG:HH11	1:C:22:ARG:HG3	1.81	0.45
1:K:94:MET:HG3	1:K:118:GLU:HB3	1.98	0.45
1:D:70:ILE:HD11	1:D:124:PRO:HB3	1.98	0.45
1:A:18:ASP:OD2	1:A:21:SER:OG	2.29	0.45
1:G:18:ASP:OD1	1:G:21:SER:OG	2.30	0.45
1:K:29:ILE:HD11	1:K:50:LEU:HD12	1.98	0.45
1:M:42:LEU:HD21	1:N:2:LEU:HD12	1.97	0.45
1:D:64:ASN:HB2	1:D:92:ILE:HG13	1.99	0.45
1:E:129:GLN:HG2	1:J:127:GLY:HA3	1.98	0.45
1:H:4:PRO:HD2	1:H:19:ILE:HG21	1.99	0.45
1:D:153:LEU:HD23	1:D:153:LEU:HA	1.85	0.44
1:I:70:ILE:HD13	1:I:149:LEU:HD11	2.00	0.44
1:F:51:GLU:HG3	1:F:85:PRO:HD3	1.98	0.44
1:N:70:ILE:HD11	1:N:124:PRO:HB3	2.00	0.44
1:J:3:VAL:HB	1:J:19:ILE:HB	2.00	0.44
1:L:57:LYS:O	1:L:85:PRO:HB3	2.18	0.44
1:B:27:ARG:HG2	1:B:50:LEU:HD22	2.00	0.44
1:A:51:GLU:HG3	1:A:85:PRO:HD3	1.99	0.44
1:J:77:TYR:O	1:J:81:GLN:HG2	2.18	0.44
1:K:176:ALA:O	1:K:185:ILE:HD11	2.17	0.44
1:E:169:GLU:HG3	1:K:170:ARG:HH21	1.83	0.43
1:F:129:GLN:CD	1:I:127:GLY:HA3	2.43	0.43
1:M:21:SER:OG	1:N:4:PRO:HD2	2.18	0.43
1:F:141:ARG:HG3	1:G:173:PHE:CG	2.53	0.43
1:F:191:LYS:HE3	1:F:191:LYS:HB3	1.88	0.43
1:A:161:LEU:HG	1:A:165:LYS:CE	2.48	0.43
1:D:3:VAL:HA	1:D:4:PRO:HD3	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:SER:HG	1:D:122:HIS:CE1	2.37	0.43
1:F:37:ASP:OD1	1:F:72:SER:OG	2.36	0.43
1:G:55:PRO:HB2	1:G:84:LYS:HD3	1.99	0.43
1:F:153:LEU:HD23	1:F:153:LEU:HA	1.86	0.43
1:H:28:ILE:HD13	1:H:60:HIS:HB2	2.01	0.43
1:B:94:MET:HE2	1:B:94:MET:HB3	1.92	0.43
1:C:70:ILE:HD11	1:C:124:PRO:HB3	2.01	0.43
1:C:166:MET:HE3	1:C:166:MET:HB2	1.88	0.43
1:I:191:LYS:HE3	1:I:191:LYS:HB3	1.92	0.43
1:B:113:ALA:HB3	1:B:185:ILE:HD13	2.02	0.42
1:B:140:LYS:NZ	4:B:307:HOH:O	2.52	0.42
1:B:88:SER:OG	1:B:110:LYS:O	2.29	0.42
1:C:141:ARG:NH1	4:C:309:HOH:O	2.52	0.42
1:G:106:GLY:O	1:G:156:ARG:NH2	2.51	0.42
1:J:115:PRO:HG2	1:J:190:THR:HB	2.02	0.42
1:A:25:LYS:HE2	1:A:25:LYS:HB3	1.89	0.42
1:M:3:VAL:HA	1:M:4:PRO:HD3	1.78	0.42
1:C:185:ILE:HD13	1:C:185:ILE:HA	1.77	0.42
1:G:88:SER:OG	1:G:110:LYS:O	2.34	0.42
1:I:22:ARG:O	1:I:25:LYS:HB2	2.20	0.42
1:G:58:ASP:OD2	1:G:110:LYS:NZ	2.50	0.42
1:J:97:SER:HG	1:J:122:HIS:CE1	2.36	0.42
1:K:39:THR:O	1:K:43:ILE:HG12	2.19	0.42
1:E:6:VAL:N	1:E:17:TYR:O	2.29	0.41
1:F:6:VAL:O	4:F:301:HOH:O	2.21	0.41
1:A:21:SER:OG	1:B:4:PRO:HD2	2.20	0.41
1:K:64:ASN:HB2	1:K:92:ILE:HG13	2.02	0.41
1:D:141:ARG:NH1	4:D:306:HOH:O	2.48	0.41
1:C:77:TYR:O	1:C:81:GLN:HG2	2.21	0.41
1:I:162:GLU:H	1:I:162:GLU:CD	2.28	0.41
1:C:3:VAL:HG22	1:C:18:ASP:HB2	2.01	0.41
1:H:141:ARG:HD2	1:I:173:PHE:CD1	2.56	0.41
1:N:55:PRO:HA	1:N:85:PRO:HG3	2.03	0.41
1:A:161:LEU:HG	1:A:165:LYS:HZ2	1.79	0.41
1:I:37:ASP:OD2	1:I:72:SER:OG	2.38	0.41
1:M:55:PRO:HA	1:M:85:PRO:HG3	2.02	0.41
1:N:124:PRO:HG3	1:N:149:LEU:HD12	2.02	0.41
1:C:57:LYS:O	1:C:85:PRO:HB3	2.20	0.41
1:D:51:GLU:HG3	1:D:85:PRO:HD3	2.02	0.41
1:C:22:ARG:HG3	1:C:22:ARG:NH1	2.36	0.40
1:A:141:ARG:HD2	1:B:173:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:94:MET:HE2	1:J:94:MET:HB3	1.89	0.40
1:A:161:LEU:CG	1:A:165:LYS:HE3	2.48	0.40
1:D:18:ASP:OD1	1:D:21:SER:OG	2.27	0.40
1:K:77:TYR:O	1:K:81:GLN:HG2	2.21	0.40
1:C:21:SER:HB3	1:D:5:VAL:O	2.21	0.40
1:F:96:ALA:HB1	1:F:120:MET:HE3	2.03	0.40
1:H:55:PRO:HA	1:H:85:PRO:HG3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	178/194 (92%)	173 (97%)	5 (3%)	0	100	100
1	B	181/194 (93%)	177 (98%)	4 (2%)	0	100	100
1	C	177/194 (91%)	170 (96%)	7 (4%)	0	100	100
1	D	177/194 (91%)	174 (98%)	3 (2%)	0	100	100
1	E	178/194 (92%)	173 (97%)	5 (3%)	0	100	100
1	F	179/194 (92%)	172 (96%)	7 (4%)	0	100	100
1	G	179/194 (92%)	174 (97%)	5 (3%)	0	100	100
1	H	177/194 (91%)	170 (96%)	7 (4%)	0	100	100
1	I	176/194 (91%)	169 (96%)	7 (4%)	0	100	100
1	J	183/194 (94%)	179 (98%)	4 (2%)	0	100	100
1	K	178/194 (92%)	174 (98%)	4 (2%)	0	100	100
1	L	179/194 (92%)	173 (97%)	6 (3%)	0	100	100
1	M	177/194 (91%)	171 (97%)	6 (3%)	0	100	100
1	N	176/194 (91%)	170 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2495/2716 (92%)	2419 (97%)	76 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	151/160 (94%)	151 (100%)	0	100	100
1	B	153/160 (96%)	153 (100%)	0	100	100
1	C	150/160 (94%)	149 (99%)	1 (1%)	76	89
1	D	150/160 (94%)	150 (100%)	0	100	100
1	E	151/160 (94%)	151 (100%)	0	100	100
1	F	152/160 (95%)	152 (100%)	0	100	100
1	G	152/160 (95%)	152 (100%)	0	100	100
1	H	150/160 (94%)	150 (100%)	0	100	100
1	I	148/160 (92%)	148 (100%)	0	100	100
1	J	155/160 (97%)	155 (100%)	0	100	100
1	K	151/160 (94%)	151 (100%)	0	100	100
1	L	152/160 (95%)	152 (100%)	0	100	100
1	M	150/160 (94%)	150 (100%)	0	100	100
1	N	148/160 (92%)	148 (100%)	0	100	100
All	All	2113/2240 (94%)	2112 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	185	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	129	GLN
1	N	81	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 19 ligands modelled in this entry, 17 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	M	201	-	5,5,5	0.93	0	5,5,5	1.08	0
3	GOL	N	201	-	5,5,5	0.96	0	5,5,5	1.13	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
3	GOL	M	201	-	-	4/4/4/4	-
3	GOL	N	201	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	201	GOL	O1-C1-C2-C3
3	M	201	GOL	C1-C2-C3-O3
3	M	201	GOL	O1-C1-C2-O2
3	M	201	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	201	GOL	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	182/194 (93%)	-0.16	3 (1%) 70 67	20, 28, 44, 64	0
1	B	185/194 (95%)	0.05	4 (2%) 62 58	20, 29, 48, 60	0
1	C	181/194 (93%)	-0.07	8 (4%) 39 34	20, 27, 43, 67	0
1	D	181/194 (93%)	-0.19	1 (0%) 85 83	19, 26, 42, 62	0
1	E	182/194 (93%)	-0.20	2 (1%) 78 75	17, 26, 41, 63	0
1	F	183/194 (94%)	-0.05	5 (2%) 56 51	20, 28, 46, 65	0
1	G	183/194 (94%)	-0.16	5 (2%) 56 51	18, 27, 44, 70	0
1	H	181/194 (93%)	-0.06	1 (0%) 85 83	21, 30, 46, 62	0
1	I	180/194 (92%)	-0.01	6 (3%) 49 45	19, 28, 47, 61	0
1	J	187/194 (96%)	-0.07	7 (3%) 45 40	19, 28, 51, 64	0
1	K	182/194 (93%)	-0.21	2 (1%) 78 75	14, 25, 41, 65	0
1	L	183/194 (94%)	-0.20	6 (3%) 49 45	17, 24, 42, 59	0
1	M	181/194 (93%)	0.02	5 (2%) 55 50	21, 29, 45, 71	0
1	N	180/194 (92%)	-0.04	6 (3%) 49 45	21, 29, 47, 72	0
All	All	2551/2716 (93%)	-0.10	61 (2%) 59 55	14, 28, 46, 72	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	VAL	5.0
1	N	17	TYR	4.9
1	H	17	TYR	4.3
1	D	17	TYR	4.3
1	G	17	TYR	3.9
1	L	7	VAL	3.8
1	I	17	TYR	3.7
1	G	5	VAL	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	N	5	VAL	3.7
1	F	17	TYR	3.7
1	K	17	TYR	3.7
1	M	17	TYR	3.6
1	I	2	LEU	3.5
1	C	3	VAL	3.5
1	E	16	SER	3.5
1	L	2	LEU	3.3
1	I	1	ALA	3.2
1	M	3	VAL	3.2
1	G	16	SER	3.2
1	M	6	VAL	3.1
1	F	2	LEU	3.1
1	J	2	LEU	3.0
1	J	15	ARG	3.0
1	K	16	SER	3.0
1	I	3	VAL	2.9
1	J	190	THR	2.8
1	C	193	PRO	2.8
1	E	17	TYR	2.8
1	F	16	SER	2.8
1	N	16	SER	2.8
1	M	56	ASP	2.7
1	G	6	VAL	2.7
1	J	16	SER	2.7
1	B	2	LEU	2.7
1	F	193	PRO	2.7
1	C	2	LEU	2.7
1	B	6	VAL	2.6
1	L	6	VAL	2.6
1	C	4	PRO	2.6
1	C	17	TYR	2.6
1	B	14	GLU	2.6
1	F	5	VAL	2.6
1	A	17	TYR	2.5
1	J	4	PRO	2.5
1	J	7	VAL	2.4
1	L	5	VAL	2.4
1	N	1	ALA	2.4
1	C	185	ILE	2.4
1	L	17	TYR	2.4
1	J	191	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	16	SER	2.3
1	G	193	PRO	2.3
1	N	4	PRO	2.3
1	I	4	PRO	2.3
1	M	5	VAL	2.2
1	N	3	VAL	2.1
1	C	129	GLN	2.1
1	B	4	PRO	2.1
1	A	3	VAL	2.1
1	I	162	GLU	2.1
1	A	16	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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	GOL	M	201	6/6	0.84	0.13	26,29,41,42	0
3	GOL	N	201	6/6	0.85	0.16	28,35,40,45	0
2	NA	M	202	1/1	0.90	0.07	34,34,34,34	0
2	NA	G	202	1/1	0.90	0.07	28,28,28,28	0
2	NA	L	202	1/1	0.90	0.10	28,28,28,28	0
2	NA	I	201	1/1	0.94	0.05	31,31,31,31	0
2	NA	A	201	1/1	0.95	0.05	32,32,32,32	0
2	NA	E	201	1/1	0.95	0.05	25,25,25,25	0
2	NA	C	201	1/1	0.96	0.04	21,21,21,21	0
2	NA	N	202	1/1	0.96	0.04	31,31,31,31	0
2	NA	I	202	1/1	0.97	0.05	29,29,29,29	0
2	NA	D	201	1/1	0.97	0.09	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NA	F	201	1/1	0.97	0.04	29,29,29,29	0
2	NA	G	201	1/1	0.98	0.03	17,17,17,17	0
2	NA	H	201	1/1	0.98	0.03	28,28,28,28	0
2	NA	J	201	1/1	0.98	0.03	24,24,24,24	0
2	NA	K	201	1/1	0.98	0.03	20,20,20,20	0
2	NA	L	201	1/1	0.98	0.04	21,21,21,21	0
2	NA	B	201	1/1	0.99	0.03	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.