Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 03:09 AM EDT

PDB ID	:	1YG6
Title	:	ClpP
Authors	:	Bewley, M.C.; Graziano, V.; Griffin, K.; Flanagan, J.M.
Deposited on	:	2005-01-04
Resolution	:	1.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

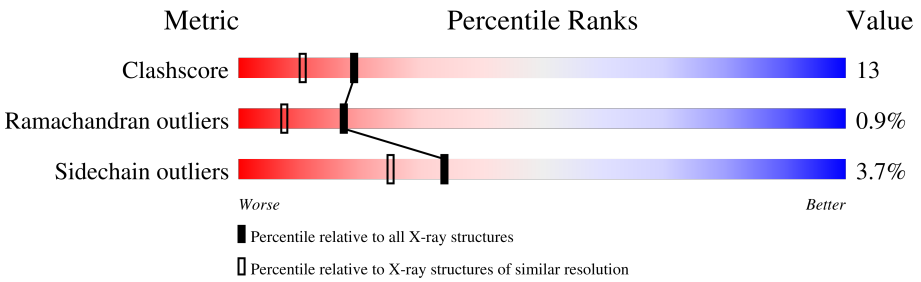
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	193	79% 18% •
1	B	193	79% 17% • ••
1	C	193	77% 20% ••
1	D	193	75% 24% •
1	E	193	76% 22% •
1	F	193	78% 19% ••
1	G	193	77% 19% •••
1	H	193	74% 19% •• •

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Mol	Chain	Length	Quality of chain
1	I	193	75% 19% • 5%
1	J	193	75% 19% • 5%
1	K	193	75% 15% • 8%
1	L	193	81% 12% •• 6%
1	M	193	79% 14% • 6%
1	N	193	74% 17% • 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPD	B	194	-	X	-	-

2 Entry composition (i)

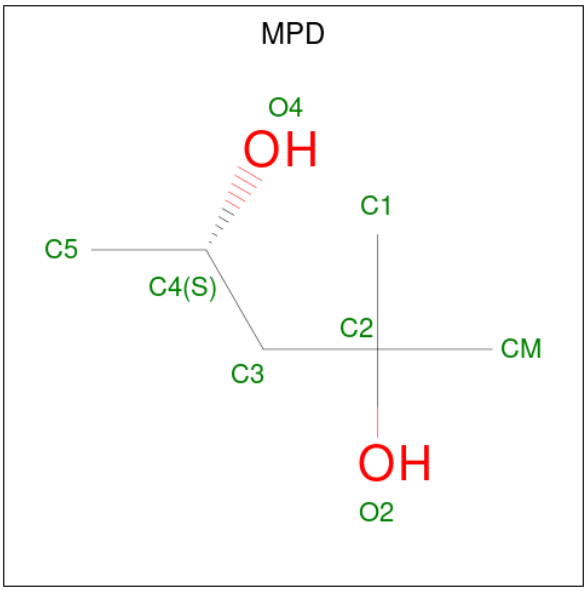
There are 3 unique types of molecules in this entry. The entry contains 21540 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	193	1507	950	262	283	12	0	0	0
1	B	192	1502	947	261	282	12	0	0	0
1	C	189	1480	931	258	279	12	0	0	0
1	D	193	1507	950	262	283	12	0	0	0
1	E	193	1507	950	262	283	12	0	0	0
1	F	193	1507	950	262	283	12	0	0	0
1	G	192	1502	947	261	282	12	0	0	0
1	H	186	1457	915	255	276	11	0	0	0
1	I	184	1439	905	252	271	11	0	0	0
1	J	184	1439	905	252	271	11	0	0	0
1	K	178	1391	879	240	261	11	0	0	0
1	L	182	1426	898	250	267	11	0	0	0
1	M	182	1426	898	250	267	11	0	0	0
1	N	177	1385	876	239	259	11	0	0	0

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	8	6	2	0	0
2	B	1	8	6	2	0	0
2	C	1	8	6	2	0	0
2	D	1	8	6	2	0	0
2	E	1	8	6	2	0	0
2	F	1	8	6	2	0	0
2	G	1	8	6	2	0	0
2	H	1	8	6	2	0	0
2	I	1	8	6	2	0	0
2	J	1	8	6	2	0	0
2	K	1	8	6	2	0	0
2	L	1	8	6	2	0	0
2	M	1	8	6	2	0	0
2	N	1	8	6	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	75	Total O 75 75	0	0
3	B	62	Total O 62 62	0	0
3	C	53	Total O 53 53	0	0
3	D	33	Total O 33 33	0	0
3	E	65	Total O 65 65	0	0
3	F	69	Total O 69 69	0	0
3	G	89	Total O 89 89	0	0
3	H	60	Total O 60 60	0	0
3	I	61	Total O 61 61	0	0
3	J	52	Total O 52 52	0	0
3	K	61	Total O 61 61	0	0
3	L	102	Total O 102 102	0	0
3	M	104	Total O 104 104	0	0
3	N	67	Total O 67 67	0	0

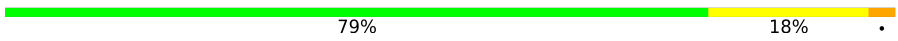
3 Residue-property plots (i)

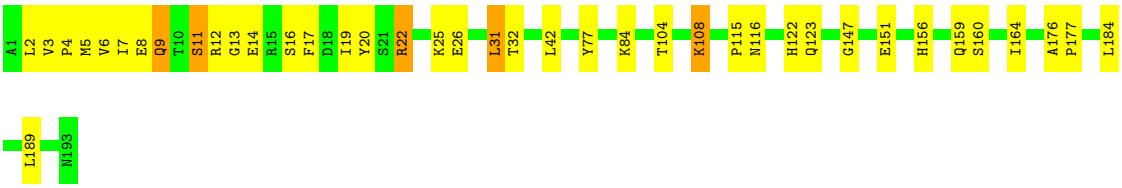
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



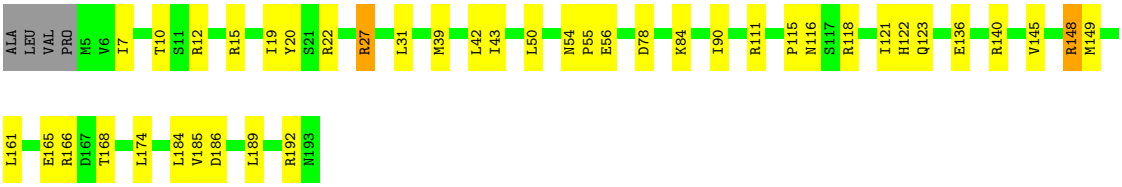


• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:

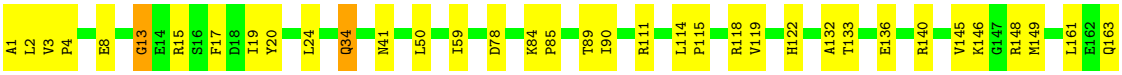
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

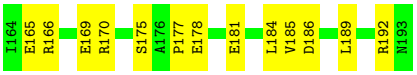
Chain C:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

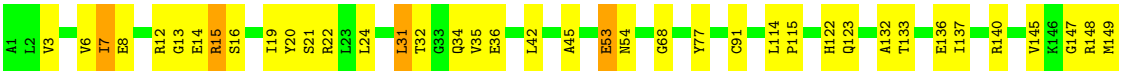
Chain D:

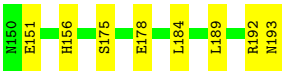




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

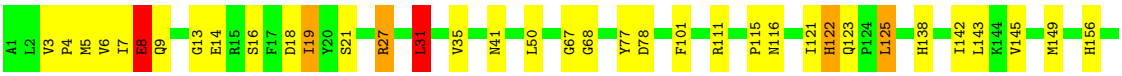
Chain E:





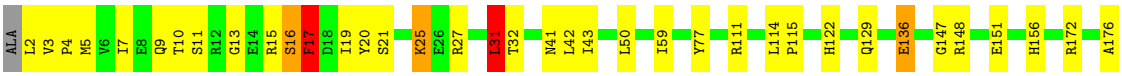
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

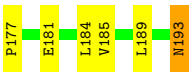
Chain F:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

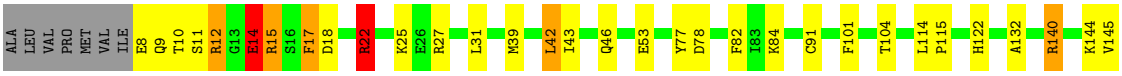
Chain G:





• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H:

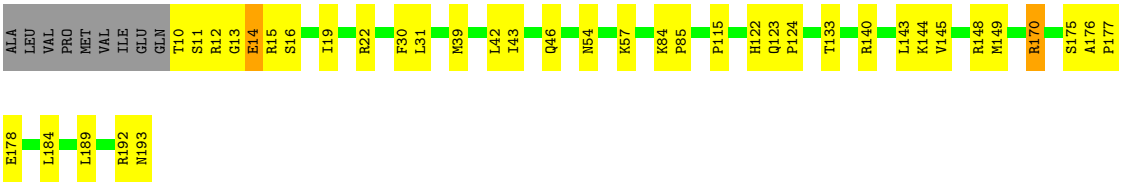


• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I:

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:

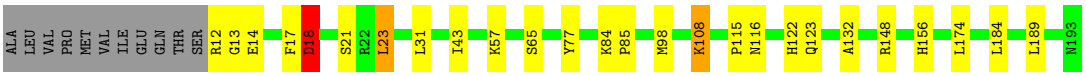


• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:

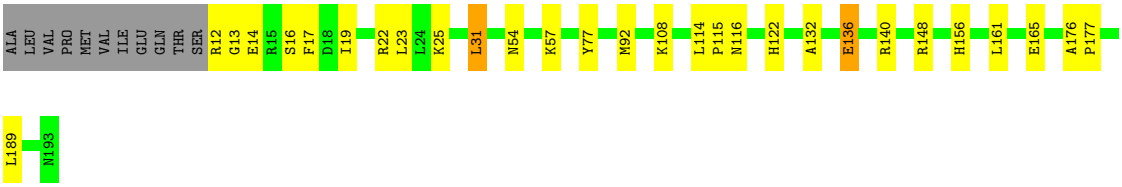
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:



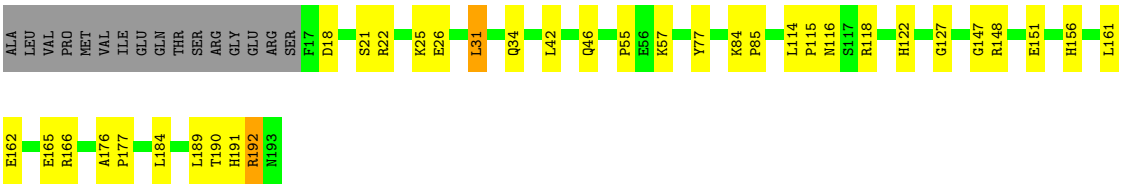
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	192.50Å 103.30Å 159.00Å 90.00° 98.40° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.90)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21540	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

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: MPD

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	0.51	0/1531	0.66	1/2064 (0.0%)
1	B	0.46	0/1526	0.65	1/2057 (0.0%)
1	C	0.43	0/1503	0.62	0/2024
1	D	0.43	0/1531	0.61	0/2064
1	E	0.49	0/1531	0.65	0/2064
1	F	0.55	0/1531	0.67	1/2064 (0.0%)
1	G	0.58	0/1526	0.70	1/2057 (0.0%)
1	H	0.51	1/1480 (0.1%)	0.87	3/1993 (0.2%)
1	I	0.47	0/1462	0.69	1/1969 (0.1%)
1	J	0.44	0/1462	0.62	0/1969
1	K	0.48	0/1414	0.66	1/1906 (0.1%)
1	L	0.59	0/1449	0.71	1/1951 (0.1%)
1	M	0.61	1/1449 (0.1%)	0.70	1/1951 (0.1%)
1	N	0.51	0/1408	0.66	1/1898 (0.1%)
All	All	0.51	2/20803 (0.0%)	0.68	12/28031 (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	H	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	14	GLU	CD-OE2	6.89	1.33	1.25
1	M	14	GLU	CD-OE2	6.86	1.33	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	22	ARG	CG-CD-NE	23.98	162.17	111.80
1	H	22	ARG	CB-CG-CD	7.88	132.09	111.60
1	L	12	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	I	15	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	A	31	LEU	CA-CB-CG	6.37	129.95	115.30
1	G	31	LEU	CA-CB-CG	5.83	128.70	115.30
1	M	31	LEU	CA-CB-CG	5.72	128.45	115.30
1	N	31	LEU	CA-CB-CG	5.71	128.43	115.30
1	B	31	LEU	CA-CB-CG	5.70	128.42	115.30
1	H	22	ARG	CD-NE-CZ	5.55	131.37	123.60
1	F	31	LEU	CA-CB-CG	5.38	127.67	115.30
1	K	31	LEU	CA-CB-CG	5.19	127.24	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	22	ARG	Sidechain

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	1507	0	1521	50	0
1	B	1502	0	1513	55	0
1	C	1480	0	1486	37	0
1	D	1507	0	1521	50	0
1	E	1507	0	1521	38	0
1	F	1507	0	1521	44	0
1	G	1502	0	1513	39	0
1	H	1457	0	1455	70	0
1	I	1439	0	1441	98	0
1	J	1439	0	1443	67	0
1	K	1391	0	1396	38	0
1	L	1426	0	1431	24	0
1	M	1426	0	1431	31	0
1	N	1385	0	1391	34	0
2	A	8	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8	0	13	1	0
2	C	8	0	14	1	0
2	D	8	0	14	1	0
2	E	8	0	14	2	0
2	F	8	0	14	3	0
2	G	8	0	14	1	0
2	H	8	0	14	1	0
2	I	8	0	14	1	0
2	J	8	0	14	0	0
2	K	8	0	14	2	0
2	L	8	0	14	1	0
2	M	8	0	14	2	0
2	N	8	0	14	1	0
3	A	75	0	0	2	0
3	B	62	0	0	0	0
3	C	53	0	0	0	0
3	D	33	0	0	0	0
3	E	65	0	0	0	0
3	F	69	0	0	1	0
3	G	89	0	0	3	0
3	H	60	0	0	11	0
3	I	61	0	0	0	0
3	J	52	0	0	0	0
3	K	61	0	0	1	0
3	L	102	0	0	3	0
3	M	104	0	0	1	0
3	N	67	0	0	0	0
All	All	21540	0	20779	538	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 13.

All (538) 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:I:15:ARG:CZ	1:I:20:TYR:HE2	1.34	1.37
1:I:15:ARG:HG3	1:J:42:LEU:CD1	1.58	1.33
1:I:15:ARG:CG	1:J:42:LEU:HD11	1.59	1.32
1:H:8:GLU:CD	1:I:29:ILE:HG22	1.52	1.29
1:I:13:GLY:O	1:I:14:GLU:HG3	1.35	1.20
1:I:15:ARG:CZ	1:I:20:TYR:CE2	2.27	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:31:LEU:HD13	1:I:43:ILE:CD1	1.79	1.12
2:B:194:MPD:H13	2:B:194:MPD:O4	1.47	1.10
1:I:14:GLU:CD	1:J:46:GLN:HE22	1.55	1.08
1:H:9:GLN:N	3:H:237:HOH:O	1.83	1.08
1:A:17:PHE:CE2	1:B:10:THR:CG2	2.37	1.07
1:N:192:ARG:HB2	1:N:192:ARG:HH11	1.16	1.06
1:I:15:ARG:CG	1:J:42:LEU:CD1	2.25	1.05
1:K:172:ARG:HB2	1:K:172:ARG:HH11	1.23	1.03
1:I:15:ARG:NE	1:I:20:TYR:HE2	1.55	1.03
1:I:15:ARG:NE	1:I:20:TYR:CE2	2.29	1.01
1:H:8:GLU:CD	1:I:29:ILE:CG2	2.29	1.01
1:A:17:PHE:CZ	1:B:10:THR:HG23	1.95	1.00
1:B:8:GLU:OE2	1:B:11:SER:OG	1.78	1.00
1:H:8:GLU:OE1	1:I:29:ILE:CG2	2.13	0.97
1:A:159:GLN:HB2	1:A:164:ILE:HD11	1.48	0.96
1:H:8:GLU:OE2	1:I:30:PHE:C	1.77	0.95
1:I:15:ARG:NE	1:J:42:LEU:HD13	1.80	0.95
1:I:18:ASP:HB2	1:I:21:SER:HB2	1.48	0.94
1:I:13:GLY:O	1:I:14:GLU:CG	2.17	0.93
2:G:194:MPD:H13	2:G:194:MPD:O4	1.70	0.91
1:I:15:ARG:HE	1:J:42:LEU:HD13	1.34	0.91
2:F:194:MPD:O4	2:F:194:MPD:H13	1.71	0.91
2:A:194:MPD:O4	2:A:194:MPD:H13	1.70	0.91
2:I:194:MPD:H13	2:I:194:MPD:O4	1.70	0.91
1:A:17:PHE:HE2	1:B:10:THR:CG2	1.76	0.91
2:M:194:MPD:O4	2:M:194:MPD:H13	1.70	0.90
2:C:194:MPD:O4	2:C:194:MPD:H13	1.70	0.90
1:A:17:PHE:CZ	1:B:10:THR:CG2	2.55	0.89
2:N:194:MPD:H13	2:N:194:MPD:O4	1.70	0.89
2:E:194:MPD:H13	2:E:194:MPD:O4	1.70	0.89
2:H:194:MPD:O4	2:H:194:MPD:H13	1.70	0.88
1:C:31:LEU:HD13	1:C:43:ILE:CD1	2.04	0.88
1:I:192:ARG:O	1:I:193:ASN:HB2	1.74	0.88
1:L:31:LEU:HD13	1:L:43:ILE:CD1	2.02	0.88
2:D:194:MPD:H13	2:D:194:MPD:O4	1.70	0.88
1:A:17:PHE:HE2	1:B:10:THR:HG21	1.38	0.87
2:K:194:MPD:O4	2:K:194:MPD:H13	1.70	0.87
1:G:7:ILE:HG22	1:G:9:GLN:H	1.37	0.87
1:A:17:PHE:HZ	1:B:10:THR:HG23	1.39	0.86
1:H:8:GLU:HG3	1:I:43:ILE:HG12	1.57	0.85
1:H:31:LEU:HD13	1:H:43:ILE:CD1	2.05	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:15:ARG:NH2	1:I:20:TYR:CE2	2.45	0.84
1:A:160:SER:O	1:A:164:ILE:HD13	1.76	0.84
1:D:118:ARG:HG3	1:D:118:ARG:HH11	1.42	0.84
1:N:192:ARG:HH11	1:N:192:ARG:CB	1.91	0.83
1:H:140:ARG:NE	1:H:144:LYS:HE3	1.92	0.83
1:D:15:ARG:HG3	1:E:8:GLU:HG3	1.59	0.83
1:A:11:SER:HA	1:B:10:THR:OG1	1.78	0.83
1:J:31:LEU:HD13	1:J:43:ILE:CD1	2.09	0.82
1:H:8:GLU:HB2	1:I:46:GLN:HE22	1.44	0.82
1:I:15:ARG:HG2	1:I:19:ILE:CG2	2.09	0.82
1:C:12:ARG:HH21	1:C:19:ILE:HB	1.44	0.81
1:I:14:GLU:HB2	1:J:42:LEU:HD21	1.61	0.81
1:I:14:GLU:OE1	1:J:46:GLN:NE2	2.13	0.81
1:I:31:LEU:HD13	1:I:43:ILE:HD12	1.63	0.81
1:I:14:GLU:CD	1:J:46:GLN:NE2	2.32	0.80
1:E:24:LEU:HD23	1:F:6:VAL:HG11	1.63	0.79
1:L:108:LYS:HZ2	1:L:108:LYS:HA	1.48	0.79
1:I:10:THR:HG23	1:I:11:SER:H	1.47	0.78
1:A:84:LYS:HE3	1:B:192:ARG:HG3	1.64	0.78
1:H:17:PHE:HE2	1:H:25:LYS:HD2	1.48	0.78
1:B:3:VAL:H	1:B:4:PRO:HD2	1.48	0.78
1:I:14:GLU:HB2	1:J:42:LEU:CD2	2.14	0.78
1:B:27:ARG:NH1	1:B:58:ASP:O	2.16	0.78
1:A:17:PHE:CE2	1:B:10:THR:HG21	2.17	0.77
1:F:35:VAL:HG13	1:F:68:GLY:HA3	1.66	0.77
1:I:15:ARG:HG3	1:J:42:LEU:HD11	0.82	0.77
1:D:111:ARG:O	1:D:185:VAL:HG13	1.85	0.76
1:F:111:ARG:O	1:F:185:VAL:HG13	1.86	0.76
1:B:84:LYS:NZ	1:B:84:LYS:HB3	2.00	0.76
1:H:12:ARG:HG3	1:H:15:ARG:HA	1.68	0.76
1:H:8:GLU:O	1:H:10:THR:HG23	1.85	0.76
1:L:31:LEU:HD13	1:L:43:ILE:HD11	1.68	0.75
1:C:121:ILE:HG22	1:C:168:THR:HG22	1.69	0.75
1:I:15:ARG:HE	1:J:42:LEU:CD1	1.99	0.75
1:I:15:ARG:HG2	1:I:19:ILE:HG21	1.69	0.74
1:I:31:LEU:HD12	1:I:39:MET:HE2	1.67	0.74
1:J:31:LEU:HD13	1:J:43:ILE:HD13	1.69	0.74
1:A:84:LYS:HE3	1:B:192:ARG:CG	2.18	0.74
1:I:31:LEU:CD1	1:I:43:ILE:CD1	2.65	0.73
1:J:54:ASN:ND2	1:J:57:LYS:HE3	2.02	0.73
1:G:50:LEU:HD13	1:G:59:ILE:HD12	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:ARG:HH12	1:J:170:ARG:CZ	2.01	0.72
1:C:42:LEU:HD11	1:D:4:PRO:HD2	1.72	0.72
1:B:36:GLU:OE2	1:B:38:HIS:N	2.23	0.71
1:E:6:VAL:HG12	1:E:7:ILE:HG13	1.72	0.71
1:K:140:ARG:NH1	1:K:144:LYS:HZ1	1.88	0.71
1:I:31:LEU:HD11	1:I:39:MET:HE1	1.70	0.71
1:I:31:LEU:CD1	1:I:39:MET:CE	2.69	0.71
1:I:108:LYS:HE2	1:I:108:LYS:HA	1.71	0.71
1:H:8:GLU:OE2	1:I:29:ILE:HG22	1.91	0.71
1:D:170:ARG:HH12	1:J:170:ARG:NE	1.88	0.70
1:H:84:LYS:HE2	1:N:192:ARG:HG3	1.73	0.70
1:D:89:THR:C	1:D:90:ILE:HD12	2.13	0.69
1:F:35:VAL:CG1	1:F:68:GLY:HA3	2.22	0.69
1:D:170:ARG:HG3	1:D:170:ARG:HH11	1.56	0.69
1:M:12:ARG:HB2	1:N:42:LEU:HD11	1.75	0.69
1:J:10:THR:OG1	1:K:18:ASP:OD1	2.09	0.69
1:H:8:GLU:OE1	1:I:29:ILE:HG22	1.82	0.69
1:C:136:GLU:HG2	1:C:140:ARG:HH21	1.58	0.69
1:M:12:ARG:HH11	1:N:46:GLN:HE22	1.41	0.68
1:A:11:SER:CA	1:B:10:THR:OG1	2.41	0.68
1:F:19:ILE:HD13	1:F:19:ILE:O	1.94	0.68
1:G:3:VAL:N	1:G:4:PRO:HD2	2.09	0.68
1:H:31:LEU:HD13	1:H:43:ILE:HD11	1.74	0.68
1:G:177:PRO:O	1:G:181:GLU:HG3	1.94	0.68
1:L:65:SER:HB2	3:L:282:HOH:O	1.93	0.68
1:I:31:LEU:HD11	1:I:39:MET:CE	2.24	0.67
1:E:35:VAL:HG22	1:E:68:GLY:HA3	1.76	0.67
1:N:192:ARG:HB2	1:N:192:ARG:NH1	2.01	0.67
1:E:45:ALA:HB1	1:F:19:ILE:HD12	1.76	0.67
1:J:192:ARG:HG2	1:K:84:LYS:HE3	1.76	0.66
1:I:15:ARG:NE	1:J:42:LEU:CD1	2.58	0.66
1:H:8:GLU:CB	1:I:46:GLN:HE22	2.08	0.66
1:J:15:ARG:CG	1:J:22:ARG:HE	2.08	0.66
1:B:8:GLU:HG2	1:B:9:GLN:H	1.59	0.66
1:E:136:GLU:OE2	1:E:140:ARG:NH1	2.29	0.66
1:I:31:LEU:HD13	1:I:43:ILE:HD13	1.77	0.66
1:A:17:PHE:CE2	1:B:10:THR:HG22	2.32	0.65
1:C:121:ILE:CG2	1:C:168:THR:HG22	2.25	0.65
1:H:8:GLU:OE1	1:I:29:ILE:HG23	1.97	0.65
1:K:140:ARG:CZ	1:K:144:LYS:HZ3	2.09	0.65
1:F:27:ARG:NH2	1:F:50:LEU:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:115:PRO:HD3	1:H:189:LEU:O	1.96	0.65
1:G:136:GLU:HG2	3:G:205:HOH:O	1.96	0.64
1:I:25:LYS:NZ	1:I:25:LYS:HB3	2.12	0.64
1:I:15:ARG:HG2	1:I:19:ILE:HG22	1.79	0.64
1:D:169:GLU:OE1	1:K:133:THR:HG21	1.98	0.64
1:M:19:ILE:O	1:M:23:LEU:HD23	1.96	0.64
2:F:194:MPD:H13	2:F:194:MPD:HO4	1.62	0.64
1:A:108:LYS:HD2	1:A:108:LYS:O	1.97	0.64
1:H:176:ALA:HB3	1:H:177:PRO:HD3	1.80	0.64
1:B:17:PHE:HB2	1:B:21:SER:OG	1.97	0.64
1:H:8:GLU:N	1:I:46:GLN:HE22	1.96	0.64
1:J:175:SER:OG	1:J:178:GLU:HG3	1.98	0.64
1:M:13:GLY:HA3	1:N:21:SER:OG	1.98	0.63
1:C:115:PRO:HD3	1:C:189:LEU:O	1.97	0.63
1:I:31:LEU:HD13	1:I:43:ILE:HD11	1.79	0.63
1:K:140:ARG:NH1	1:K:144:LYS:NZ	2.46	0.63
1:N:25:LYS:NZ	1:N:25:LYS:HB3	2.12	0.63
1:B:176:ALA:HB3	1:B:177:PRO:HD3	1.81	0.63
1:E:115:PRO:HD3	1:E:189:LEU:O	1.97	0.63
1:N:190:THR:HG22	1:N:191:HIS:ND1	2.14	0.63
1:L:108:LYS:HZ2	1:L:108:LYS:CA	2.11	0.63
1:G:50:LEU:CD1	1:G:59:ILE:HD12	2.29	0.62
1:J:12:ARG:NH1	1:K:17:PHE:HA	2.14	0.62
1:G:3:VAL:H	1:G:4:PRO:HD2	1.64	0.62
1:M:12:ARG:HD2	1:N:42:LEU:HD21	1.80	0.62
1:I:15:ARG:CD	1:J:42:LEU:HD13	2.30	0.62
1:M:176:ALA:HB3	1:M:177:PRO:HD3	1.81	0.62
1:B:115:PRO:HD3	1:B:189:LEU:O	1.99	0.62
1:J:31:LEU:HD13	1:J:43:ILE:HD11	1.82	0.61
1:M:115:PRO:HD3	1:M:189:LEU:O	1.99	0.61
1:D:118:ARG:HG3	1:D:118:ARG:NH1	2.14	0.61
1:H:8:GLU:OE2	1:I:31:LEU:N	2.33	0.61
1:H:10:THR:HG21	1:I:46:GLN:CD	2.21	0.61
1:F:125:LEU:H	1:F:125:LEU:HD23	1.64	0.61
1:J:10:THR:OG1	1:K:18:ASP:CG	2.39	0.61
1:C:78:ASP:HB3	1:D:114:LEU:HD23	1.82	0.61
1:H:8:GLU:N	1:I:46:GLN:NE2	2.48	0.61
2:K:194:MPD:H13	2:K:194:MPD:HO4	1.65	0.60
1:I:14:GLU:HB3	1:J:46:GLN:NE2	2.16	0.60
1:I:15:ARG:CG	1:J:42:LEU:HD13	2.28	0.60
1:B:84:LYS:HB3	1:B:84:LYS:HZ2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:12:ARG:NH1	1:N:46:GLN:HE22	2.00	0.60
1:I:31:LEU:HD12	1:I:39:MET:CE	2.31	0.60
1:B:15:ARG:HH21	1:D:13:GLY:H	1.49	0.60
1:E:193:ASN:N	1:E:193:ASN:HD22	1.99	0.60
1:G:111:ARG:O	1:G:185:VAL:HG22	2.02	0.60
1:M:12:ARG:HD3	1:N:46:GLN:NE2	2.16	0.60
1:N:176:ALA:HB3	1:N:177:PRO:HD3	1.83	0.59
1:E:13:GLY:HA2	1:E:15:ARG:NH1	2.18	0.59
1:F:78:ASP:HB3	1:G:114:LEU:HD13	1.84	0.59
1:K:176:ALA:HB3	1:K:177:PRO:HD3	1.85	0.59
1:H:8:GLU:HB2	1:I:46:GLN:NE2	2.17	0.59
1:H:140:ARG:CD	1:H:144:LYS:HE3	2.33	0.59
1:A:11:SER:C	1:B:10:THR:OG1	2.41	0.59
1:D:175:SER:OG	1:D:178:GLU:HG3	2.02	0.59
1:H:140:ARG:O	1:H:140:ARG:HD3	2.02	0.59
1:D:50:LEU:HD13	1:D:59:ILE:HD12	1.83	0.59
1:D:84:LYS:HB2	1:D:85:PRO:HD3	1.85	0.59
1:F:5:MET:HB3	1:F:16:SER:HB2	1.85	0.59
1:M:161:LEU:O	1:M:165:GLU:HG3	2.03	0.59
1:G:193:ASN:N	1:G:193:ASN:HD22	2.00	0.59
1:F:77:TYR:OH	1:F:156:HIS:HE1	1.85	0.59
1:C:31:LEU:HD13	1:C:43:ILE:HD11	1.84	0.58
1:G:193:ASN:HD22	1:G:193:ASN:H	1.51	0.58
1:A:159:GLN:CB	1:A:164:ILE:HD11	2.28	0.58
1:H:8:GLU:CA	1:I:46:GLN:HE22	2.16	0.58
1:N:161:LEU:O	1:N:165:GLU:HG3	2.03	0.58
1:D:119:VAL:HG11	1:D:184:LEU:CD2	2.33	0.58
1:I:15:ARG:HG2	1:J:42:LEU:HD11	1.75	0.58
1:H:140:ARG:HD3	1:H:140:ARG:C	2.23	0.58
1:L:156:HIS:HD2	3:L:203:HOH:O	1.85	0.58
1:D:41:ASN:ND2	1:E:32:THR:HG21	2.17	0.58
1:H:91:CYS:O	1:H:114:LEU:HD13	2.04	0.58
1:J:176:ALA:HB3	1:J:177:PRO:HD3	1.85	0.58
1:F:125:LEU:HD23	1:F:125:LEU:N	2.19	0.58
1:H:140:ARG:HE	1:H:144:LYS:HE3	1.68	0.58
1:M:12:ARG:HD2	1:N:42:LEU:CD2	2.34	0.58
1:H:190:THR:HG22	1:H:191:HIS:ND1	2.19	0.58
1:F:35:VAL:HG13	1:F:68:GLY:CA	2.32	0.57
1:N:55:PRO:HB2	1:N:84:LYS:HD2	1.84	0.57
1:I:31:LEU:CD1	1:I:39:MET:HE2	2.33	0.57
1:G:31:LEU:HD22	1:G:43:ILE:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:172:ARG:HH11	1:K:172:ARG:CB	2.08	0.57
1:C:174:LEU:HD22	1:C:184:LEU:HD12	1.86	0.57
1:E:53:GLU:HG3	1:E:54:ASN:N	2.18	0.57
1:K:172:ARG:HB2	1:K:172:ARG:NH1	2.07	0.57
1:A:32:THR:OG1	1:G:41:ASN:ND2	2.38	0.57
1:C:12:ARG:NH2	1:C:19:ILE:HB	2.18	0.57
1:D:115:PRO:HD3	1:D:189:LEU:O	2.05	0.57
1:A:176:ALA:HB3	1:A:177:PRO:HD3	1.85	0.56
1:H:8:GLU:N	3:H:203:HOH:O	2.39	0.56
1:G:25:LYS:HE3	1:G:25:LYS:HA	1.86	0.56
1:I:31:LEU:CD1	1:I:39:MET:HE1	2.34	0.56
1:C:111:ARG:O	1:C:185:VAL:HG22	2.05	0.56
1:I:31:LEU:CD1	1:I:43:ILE:HD11	2.35	0.56
1:B:123:GLN:HE21	1:I:132:ALA:HB3	1.70	0.56
1:C:161:LEU:O	1:C:165:GLU:HG3	2.06	0.56
1:I:176:ALA:HB3	1:I:177:PRO:HD3	1.87	0.56
1:J:10:THR:O	1:J:11:SER:HB2	2.06	0.56
1:F:35:VAL:HG12	1:F:67:GLY:C	2.25	0.56
1:A:14:GLU:H	1:B:10:THR:HB	1.71	0.56
1:H:42:LEU:HD12	1:H:46:GLN:NE2	2.20	0.56
1:K:140:ARG:CZ	1:K:144:LYS:NZ	2.69	0.56
1:C:27:ARG:NH2	1:C:50:LEU:O	2.38	0.56
1:G:2:LEU:HD23	1:G:2:LEU:O	2.06	0.56
1:I:15:ARG:CD	1:J:42:LEU:CD1	2.84	0.56
1:G:77:TYR:OH	1:G:156:HIS:HE1	1.88	0.56
1:M:54:ASN:ND2	1:M:57:LYS:HE3	2.20	0.55
1:B:21:SER:HB3	1:C:12:ARG:HB3	1.88	0.55
1:J:115:PRO:HD3	1:J:189:LEU:O	2.06	0.55
1:D:170:ARG:HH22	1:J:170:ARG:HD2	1.70	0.55
1:G:3:VAL:N	1:G:4:PRO:CD	2.69	0.55
1:H:27:ARG:NH1	3:H:254:HOH:O	2.39	0.55
1:F:35:VAL:CG1	1:F:68:GLY:CA	2.85	0.55
1:H:170:ARG:HH21	1:I:134:ASP:CG	2.10	0.55
1:D:119:VAL:HG11	1:D:184:LEU:HD23	1.89	0.55
1:H:12:ARG:HA	1:H:18:ASP:HA	1.90	0.54
1:I:15:ARG:HG2	1:J:42:LEU:CD1	2.30	0.54
1:M:140:ARG:HB2	1:M:140:ARG:NH1	2.22	0.54
1:D:146:LYS:NZ	1:K:133:THR:HG23	2.22	0.54
1:E:34:GLN:O	1:E:34:GLN:HG3	2.07	0.54
1:J:193:ASN:OD1	1:K:84:LYS:HE2	2.06	0.54
1:B:161:LEU:O	1:B:165:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:ARG:C	1:F:185:VAL:HG13	2.27	0.54
1:G:19:ILE:HG23	1:G:20:TYR:N	2.23	0.54
1:H:8:GLU:HA	3:H:203:HOH:O	2.07	0.54
1:H:12:ARG:NE	1:I:18:ASP:HB3	2.22	0.54
1:M:140:ARG:HB2	1:M:140:ARG:HH11	1.72	0.54
1:E:15:ARG:NH2	1:F:13:GLY:H	2.06	0.54
1:H:8:GLU:HG3	1:I:43:ILE:CG1	2.35	0.54
1:J:15:ARG:HE	1:J:22:ARG:HE	1.54	0.54
1:H:148:ARG:HH11	1:N:116:ASN:ND2	2.06	0.54
1:J:84:LYS:HB2	1:J:85:PRO:HD3	1.89	0.54
1:I:14:GLU:CG	1:J:46:GLN:HE22	2.21	0.53
1:J:192:ARG:O	1:J:193:ASN:HB2	2.06	0.53
1:N:192:ARG:HH11	1:N:192:ARG:CG	2.22	0.53
1:E:35:VAL:HG22	1:E:68:GLY:CA	2.39	0.53
1:M:12:ARG:HD3	1:N:46:GLN:CD	2.29	0.53
1:B:8:GLU:HG2	1:B:9:GLN:N	2.22	0.53
1:D:170:ARG:HG3	1:D:170:ARG:NH1	2.23	0.53
1:I:15:ARG:HG3	1:J:42:LEU:HD13	1.77	0.53
1:M:156:HIS:HD2	3:M:207:HOH:O	1.91	0.52
1:E:147:GLY:O	1:E:151:GLU:HG3	2.09	0.52
1:G:3:VAL:H	1:G:4:PRO:CD	2.23	0.52
1:I:12:ARG:HD3	3:K:231:HOH:O	2.09	0.52
1:L:116:ASN:ND2	1:M:148:ARG:HH11	2.07	0.52
1:D:2:LEU:HD12	1:D:2:LEU:N	2.25	0.52
1:J:15:ARG:HG2	1:J:22:ARG:HE	1.74	0.52
1:C:31:LEU:HD13	1:C:43:ILE:HD12	1.89	0.52
1:D:90:ILE:HD12	1:D:90:ILE:N	2.25	0.52
1:I:13:GLY:C	1:I:14:GLU:HG3	2.22	0.52
1:E:31:LEU:C	1:E:31:LEU:HD12	2.30	0.52
1:I:161:LEU:O	1:I:165:GLU:HG3	2.10	0.52
1:J:170:ARG:HH22	1:K:131:GLN:NE2	2.07	0.52
1:N:115:PRO:HD3	1:N:189:LEU:O	2.10	0.52
1:A:104:THR:HG23	1:A:184:LEU:O	2.10	0.52
1:D:148:ARG:HG2	1:D:148:ARG:HH11	1.75	0.52
1:E:77:TYR:OH	1:E:156:HIS:HE1	1.93	0.52
1:G:172:ARG:HB2	3:G:275:HOH:O	2.09	0.52
1:H:53:GLU:HB3	3:H:254:HOH:O	2.10	0.52
1:J:13:GLY:O	1:J:15:ARG:N	2.43	0.51
1:E:148:ARG:HH11	1:F:116:ASN:HD22	1.57	0.51
1:H:82:PHE:CE2	1:N:192:ARG:NH1	2.79	0.51
1:C:111:ARG:C	1:C:185:VAL:HG23	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:176:ALA:HB1	1:K:188:ILE:HD12	1.92	0.51
1:H:8:GLU:HB3	3:H:200:HOH:O	2.09	0.51
1:A:116:ASN:HD22	1:G:148:ARG:HD2	1.76	0.51
1:A:8:GLU:HG3	1:G:15:ARG:CZ	2.41	0.51
1:I:116:ASN:ND2	1:J:148:ARG:HH11	2.09	0.51
1:D:185:VAL:CG1	1:D:186:ASP:N	2.73	0.51
1:D:185:VAL:HG12	1:D:186:ASP:N	2.25	0.51
1:E:192:ARG:HH11	1:E:192:ARG:HG2	1.76	0.51
1:N:77:TYR:OH	1:N:156:HIS:HE1	1.94	0.51
1:D:132:ALA:HB3	1:K:123:GLN:HE21	1.76	0.51
1:B:17:PHE:CE1	1:B:22:ARG:HD2	2.46	0.50
1:I:115:PRO:HD3	1:I:189:LEU:O	2.10	0.50
1:A:22:ARG:O	1:A:26:GLU:OE1	2.30	0.50
1:M:77:TYR:OH	1:M:156:HIS:HE1	1.94	0.50
1:A:13:GLY:HA3	1:B:10:THR:O	2.11	0.50
1:B:84:LYS:HB2	1:B:85:PRO:HD3	1.92	0.50
1:C:111:ARG:O	1:C:185:VAL:CG2	2.60	0.50
1:L:116:ASN:HD22	1:M:148:ARG:HH11	1.60	0.50
1:B:9:GLN:O	1:B:10:THR:OG1	2.24	0.50
1:D:19:ILE:HG23	1:D:20:TYR:N	2.27	0.50
1:F:35:VAL:HG12	1:F:67:GLY:O	2.12	0.50
1:H:17:PHE:CE2	1:H:25:LYS:HD2	2.37	0.50
1:H:10:THR:HG21	1:I:46:GLN:CG	2.42	0.49
1:J:11:SER:HB3	1:J:19:ILE:HB	1.93	0.49
1:A:164:ILE:HG13	3:A:269:HOH:O	2.12	0.49
1:C:145:VAL:O	1:C:149:MET:HG2	2.12	0.49
1:I:14:GLU:HB3	1:J:46:GLN:CD	2.32	0.49
1:I:192:ARG:O	1:I:193:ASN:CB	2.55	0.49
1:J:15:ARG:HG2	1:J:22:ARG:NE	2.27	0.49
1:F:185:VAL:HG12	1:F:186:ASP:N	2.28	0.49
1:H:10:THR:CG2	1:I:46:GLN:CD	2.81	0.49
1:N:162:GLU:O	1:N:166:ARG:HG2	2.12	0.49
1:B:31:LEU:HD22	1:B:43:ILE:HD13	1.95	0.49
1:J:192:ARG:CG	1:K:84:LYS:HE3	2.41	0.49
1:A:22:ARG:NH2	1:A:25:LYS:HD2	2.28	0.49
1:I:116:ASN:HD22	1:J:148:ARG:HH11	1.59	0.49
1:A:11:SER:O	1:B:10:THR:OG1	2.31	0.49
1:A:123:GLN:HE21	1:H:132:ALA:HB3	1.78	0.49
1:D:50:LEU:CD1	1:D:59:ILE:HD12	2.43	0.49
1:E:42:LEU:HD11	1:F:4:PRO:HD2	1.94	0.49
1:C:42:LEU:HD11	1:D:4:PRO:CD	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:77:TYR:OH	1:I:156:HIS:HE1	1.95	0.49
1:M:92:MET:HB3	1:M:114:LEU:HD12	1.94	0.49
1:N:25:LYS:HB3	1:N:25:LYS:HZ2	1.76	0.49
1:F:115:PRO:HD3	1:F:189:LEU:O	2.12	0.48
1:I:12:ARG:HD2	1:K:38:HIS:HB3	1.95	0.48
1:M:25:LYS:HB3	1:M:25:LYS:NZ	2.28	0.48
1:C:84:LYS:HG2	1:D:192:ARG:HG2	1.94	0.48
1:I:12:ARG:CD	1:K:38:HIS:HB3	2.43	0.48
1:K:77:TYR:OH	1:K:156:HIS:HE1	1.96	0.48
1:B:2:LEU:HD23	1:B:2:LEU:N	2.28	0.48
1:E:7:ILE:O	1:E:16:SER:HA	2.13	0.48
1:M:22:ARG:O	1:M:22:ARG:HD3	2.14	0.48
1:B:123:GLN:NE2	1:I:132:ALA:HB3	2.27	0.48
1:H:77:TYR:OH	1:H:156:HIS:HE1	1.97	0.48
1:J:10:THR:HG1	1:K:18:ASP:CG	2.17	0.48
1:G:5:MET:HA	1:G:17:PHE:O	2.13	0.48
1:I:15:ARG:NH2	1:I:20:TYR:CZ	2.82	0.48
1:J:14:GLU:N	1:J:14:GLU:OE1	2.47	0.48
1:H:8:GLU:CG	1:I:29:ILE:HG22	2.41	0.47
1:D:170:ARG:HH12	1:J:170:ARG:NH2	2.12	0.47
1:F:161:LEU:O	1:F:165:GLU:HG3	2.14	0.47
1:K:118:ARG:HG3	1:K:118:ARG:HH11	1.79	0.47
1:D:177:PRO:O	1:D:181:GLU:HG3	2.14	0.47
1:F:7:ILE:HG23	1:F:9:GLN:HE21	1.78	0.47
1:G:31:LEU:HD22	1:G:43:ILE:CD1	2.43	0.47
1:G:59:ILE:HG13	3:G:281:HOH:O	2.15	0.47
1:H:8:GLU:N	1:I:43:ILE:HG13	2.29	0.47
1:J:15:ARG:CG	1:J:22:ARG:NE	2.76	0.47
1:A:77:TYR:OH	1:A:156:HIS:HE1	1.98	0.47
1:E:192:ARG:HD3	1:E:193:ASN:H	1.80	0.47
1:A:159:GLN:HB2	1:A:164:ILE:CD1	2.33	0.47
1:G:27:ARG:NH2	1:G:59:ILE:HD11	2.29	0.47
1:A:3:VAL:HG23	1:A:3:VAL:O	2.15	0.47
1:F:8:GLU:N	1:F:8:GLU:OE1	2.47	0.47
1:G:115:PRO:HD3	1:G:189:LEU:O	2.15	0.47
1:H:8:GLU:HB3	3:H:237:HOH:O	2.14	0.47
1:J:140:ARG:NH1	1:J:144:LYS:HG3	2.30	0.47
1:B:148:ARG:HH11	1:C:116:ASN:ND2	2.13	0.46
1:H:8:GLU:CA	3:H:203:HOH:O	2.62	0.46
1:H:12:ARG:C	1:H:14:GLU:H	2.19	0.46
1:M:136:GLU:OE1	1:M:140:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:ILE:O	1:F:122:HIS:HB3	2.15	0.46
1:I:25:LYS:HB3	1:I:25:LYS:HZ3	1.78	0.46
1:I:145:VAL:O	1:I:149:MET:HG2	2.14	0.46
1:A:6:VAL:HG23	1:A:6:VAL:O	2.15	0.46
1:A:4:PRO:HD2	1:G:42:LEU:HD11	1.97	0.46
1:A:7:ILE:HG12	1:A:17:PHE:HB2	1.98	0.46
1:B:148:ARG:HH11	1:C:116:ASN:HD22	1.63	0.46
1:D:118:ARG:NH1	1:D:118:ARG:CG	2.74	0.46
1:G:5:MET:HG3	1:G:17:PHE:HA	1.97	0.46
1:J:140:ARG:HG3	1:J:144:LYS:NZ	2.31	0.46
1:K:116:ASN:HD22	1:L:148:ARG:HH11	1.64	0.46
1:A:8:GLU:HG2	1:A:9:GLN:N	2.31	0.46
1:E:193:ASN:N	1:E:193:ASN:ND2	2.64	0.46
1:F:31:LEU:HD12	1:F:31:LEU:C	2.36	0.46
1:H:8:GLU:C	3:H:237:HOH:O	2.33	0.46
1:D:1:ALA:HB3	1:D:3:VAL:HG12	1.98	0.46
1:D:148:ARG:CZ	1:D:148:ARG:HB3	2.46	0.46
1:E:42:LEU:HD21	1:F:4:PRO:HD3	1.98	0.46
1:K:43:ILE:HG22	1:K:47:MET:CE	2.46	0.46
1:L:57:LYS:O	1:L:85:PRO:HB3	2.16	0.46
1:A:164:ILE:N	1:A:164:ILE:HD12	2.30	0.45
1:A:19:ILE:HG23	1:A:20:TYR:N	2.31	0.45
1:E:137:ILE:HD13	1:E:140:ARG:HH22	1.81	0.45
1:B:84:LYS:HB3	1:B:84:LYS:HZ3	1.76	0.45
1:K:115:PRO:HD3	1:K:189:LEU:O	2.17	0.45
1:K:161:LEU:O	1:K:165:GLU:HG3	2.17	0.45
1:N:84:LYS:HB2	1:N:85:PRO:HD3	1.97	0.45
1:D:78:ASP:HB3	1:E:114:LEU:HD23	1.99	0.45
1:G:147:GLY:O	1:G:151:GLU:HG3	2.16	0.45
1:H:161:LEU:O	1:H:165:GLU:HG3	2.16	0.45
1:L:77:TYR:OH	1:L:156:HIS:HE1	1.99	0.45
1:A:84:LYS:HG3	1:B:192:ARG:HG2	1.99	0.45
1:B:51:GLU:OE2	1:B:84:LYS:HG2	2.17	0.45
1:G:7:ILE:HA	1:G:16:SER:CB	2.46	0.45
1:G:176:ALA:HB3	1:G:177:PRO:HD3	1.98	0.45
1:L:13:GLY:O	1:L:14:GLU:HB2	2.17	0.45
1:F:14:GLU:HB2	1:G:7:ILE:HD11	1.98	0.45
1:F:145:VAL:O	1:F:149:MET:HG2	2.16	0.45
1:F:185:VAL:CG1	1:F:186:ASP:N	2.79	0.45
1:H:11:SER:O	1:H:12:ARG:HB3	2.17	0.45
1:A:84:LYS:HE3	1:B:192:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:PHE:HE1	1:B:22:ARG:HD2	1.82	0.44
1:E:133:THR:H	1:L:123:GLN:HE22	1.64	0.44
1:G:4:PRO:HG2	1:G:19:ILE:HB	1.99	0.44
1:I:15:ARG:O	1:I:17:PHE:N	2.50	0.44
1:K:55:PRO:HB2	1:K:84:LYS:HD2	1.99	0.44
1:B:3:VAL:N	1:B:4:PRO:HD2	2.25	0.44
1:D:161:LEU:O	1:D:165:GLU:HG3	2.17	0.44
1:L:115:PRO:HD3	1:L:189:LEU:O	2.16	0.44
1:A:156:HIS:HD2	3:A:204:HOH:O	2.00	0.44
1:H:8:GLU:CB	3:H:200:HOH:O	2.65	0.44
1:E:123:GLN:HE21	1:L:132:ALA:HB3	1.82	0.44
1:L:174:LEU:HD22	1:L:184:LEU:HD12	1.98	0.44
1:A:147:GLY:O	1:A:151:GLU:HG3	2.17	0.44
1:B:77:TYR:OH	1:B:156:HIS:HE1	2.00	0.44
1:B:123:GLN:HE22	1:I:133:THR:H	1.65	0.44
1:K:116:ASN:ND2	1:L:148:ARG:HH11	2.15	0.44
1:F:122:HIS:C	1:F:122:HIS:CD2	2.91	0.44
1:H:31:LEU:CD1	1:H:39:MET:CE	2.96	0.44
1:N:18:ASP:O	1:N:22:ARG:HG3	2.17	0.44
1:N:57:LYS:O	1:N:85:PRO:HB3	2.18	0.44
1:A:164:ILE:CD1	1:A:164:ILE:N	2.80	0.44
1:H:9:GLN:CA	3:H:237:HOH:O	2.50	0.44
1:J:145:VAL:O	1:J:149:MET:HG2	2.18	0.44
1:D:163:GLN:NE2	1:D:166:ARG:NH2	2.66	0.44
1:E:15:ARG:HD2	1:E:15:ARG:N	2.33	0.44
1:M:116:ASN:HD21	1:N:148:ARG:NH2	2.16	0.44
1:N:192:ARG:NH1	1:N:192:ARG:CG	2.81	0.44
1:D:111:ARG:C	1:D:185:VAL:HG13	2.39	0.43
1:D:146:LYS:NZ	1:K:133:THR:CG2	2.80	0.43
1:F:21:SER:HB3	1:G:5:MET:O	2.18	0.43
1:H:78:ASP:HB3	1:N:114:LEU:HD23	2.00	0.43
1:E:12:ARG:HG3	1:E:12:ARG:HH11	1.82	0.43
1:D:133:THR:H	1:K:123:GLN:HE22	1.66	0.43
1:J:123:GLN:HB2	1:J:124:PRO:CD	2.48	0.43
1:L:18:ASP:HB3	1:L:21:SER:HB2	1.99	0.43
1:A:22:ARG:HH21	1:A:25:LYS:HB3	1.83	0.43
1:F:41:ASN:ND2	1:G:32:THR:OG1	2.52	0.43
1:I:10:THR:HG23	1:I:11:SER:N	2.26	0.43
1:C:90:ILE:N	1:C:90:ILE:HD12	2.33	0.43
1:H:11:SER:OG	1:H:12:ARG:HD3	2.18	0.43
2:M:194:MPD:H13	2:M:194:MPD:HO4	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ASP:CB	1:D:114:LEU:HD23	2.48	0.43
1:A:17:PHE:CE2	1:B:10:THR:HG23	2.24	0.43
1:D:119:VAL:HG11	1:D:184:LEU:HD21	2.01	0.43
1:B:84:LYS:HD3	1:C:192:ARG:HG2	2.01	0.43
1:C:15:ARG:HG2	1:C:15:ARG:HH11	1.84	0.43
1:C:31:LEU:HD12	1:C:39:MET:CE	2.49	0.43
1:D:132:ALA:HB3	1:K:123:GLN:NE2	2.34	0.43
1:H:31:LEU:CD1	1:H:39:MET:HE3	2.49	0.43
1:C:148:ARG:HG3	1:C:148:ARG:HH11	1.84	0.42
1:F:138:HIS:O	1:F:142:ILE:HG12	2.19	0.42
1:F:166:ARG:NH1	1:F:166:ARG:HB2	2.34	0.42
1:I:12:ARG:HG2	1:I:12:ARG:HH11	1.83	0.42
1:J:22:ARG:HH11	1:J:22:ARG:HG3	1.83	0.42
1:E:145:VAL:O	1:E:149:MET:HG2	2.19	0.42
1:H:42:LEU:HD13	1:H:42:LEU:O	2.20	0.42
1:K:84:LYS:N	1:K:85:PRO:HD2	2.34	0.42
1:A:115:PRO:HD3	1:A:189:LEU:O	2.19	0.42
1:H:114:LEU:N	1:H:114:LEU:HD12	2.34	0.42
1:D:170:ARG:HH22	1:J:170:ARG:CD	2.32	0.42
1:E:91:CYS:O	1:E:114:LEU:HD13	2.19	0.42
1:F:143:LEU:HD11	1:M:136:GLU:HG3	2.01	0.42
2:E:194:MPD:H13	2:E:194:MPD:HO4	1.81	0.42
1:B:41:ASN:ND2	1:C:20:TYR:OH	2.52	0.42
1:E:3:VAL:HG23	1:E:3:VAL:O	2.20	0.42
1:C:31:LEU:HD12	1:C:39:MET:HE2	2.01	0.42
1:J:15:ARG:NE	1:J:22:ARG:HE	2.18	0.42
1:F:101:PHE:HB2	2:F:194:MPD:H13	2.01	0.42
1:H:31:LEU:HD13	1:H:43:ILE:HD13	1.96	0.42
1:A:108:LYS:HD2	1:A:108:LYS:C	2.41	0.42
1:C:7:ILE:O	1:C:7:ILE:HG23	2.20	0.41
1:E:132:ALA:HB3	1:L:123:GLN:HE21	1.85	0.41
1:F:3:VAL:HG11	1:F:18:ASP:HB2	2.01	0.41
1:H:163:GLN:OE1	1:H:163:GLN:HA	2.20	0.41
1:K:47:MET:HE1	1:K:76:ILE:HG23	2.01	0.41
1:K:145:VAL:O	1:K:149:MET:HG2	2.20	0.41
1:M:12:ARG:HH11	1:N:46:GLN:NE2	2.13	0.41
1:M:140:ARG:HH11	1:M:140:ARG:CB	2.32	0.41
1:D:34:GLN:HE21	1:D:34:GLN:HB3	1.58	0.41
1:K:43:ILE:HG22	1:K:47:MET:HE1	2.01	0.41
1:M:16:SER:O	1:M:17:PHE:HB2	2.19	0.41
1:E:137:ILE:CD1	1:E:140:ARG:HH22	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:GLU:OE2	1:J:30:PHE:O	2.38	0.41
1:L:31:LEU:HG	3:L:282:HOH:O	2.20	0.41
1:C:166:ARG:HH11	1:C:166:ARG:HG3	1.85	0.41
1:E:175:SER:OG	1:E:178:GLU:HG3	2.21	0.41
1:F:156:HIS:HD2	3:F:204:HOH:O	2.04	0.41
1:M:116:ASN:ND2	1:N:148:ARG:CZ	2.83	0.41
1:D:146:LYS:HZ2	1:K:133:THR:HG23	1.84	0.41
1:F:123:GLN:NE2	1:M:132:ALA:HB3	2.35	0.41
1:N:147:GLY:O	1:N:151:GLU:HG3	2.21	0.41
1:A:9:GLN:NE2	1:A:9:GLN:HA	2.36	0.41
1:B:177:PRO:O	1:B:181:GLU:HG3	2.20	0.41
1:E:21:SER:HB3	1:F:6:VAL:HG12	2.02	0.41
1:L:17:PHE:CD2	1:M:17:PHE:HD1	2.37	0.41
1:L:23:LEU:HD12	1:L:23:LEU:HA	1.92	0.41
1:B:27:ARG:HH12	1:B:59:ILE:HG13	1.85	0.41
1:D:145:VAL:O	1:D:149:MET:HG2	2.21	0.41
1:I:11:SER:HB3	1:J:39:MET:HB2	2.03	0.41
1:I:14:GLU:CB	1:J:46:GLN:NE2	2.84	0.41
1:J:57:LYS:O	1:J:85:PRO:HB3	2.21	0.41
1:L:84:LYS:HB3	1:L:85:PRO:HD3	2.03	0.41
1:C:123:GLN:HE22	1:J:133:THR:H	1.67	0.41
1:F:35:VAL:HG12	1:F:68:GLY:HA3	2.02	0.41
1:B:31:LEU:HD22	1:B:43:ILE:CD1	2.52	0.40
1:G:10:THR:OG1	1:G:11:SER:N	2.54	0.40
1:G:129:GLN:HG2	1:N:127:GLY:HA3	2.03	0.40
1:A:2:LEU:HG	1:A:3:VAL:HG13	2.03	0.40
1:A:5:MET:O	1:G:21:SER:HB3	2.22	0.40
1:C:54:ASN:HA	1:C:55:PRO:HD2	1.96	0.40
1:F:166:ARG:HB2	1:F:166:ARG:CZ	2.51	0.40
1:L:98:MET:HE1	2:L:194:MPD:HM1	2.03	0.40
1:B:3:VAL:H	1:B:4:PRO:CD	2.26	0.40
1:B:122:HIS:C	1:B:122:HIS:CD2	2.95	0.40
1:C:111:ARG:C	1:C:185:VAL:CG2	2.89	0.40
1:C:185:VAL:HG22	1:C:186:ASP:N	2.37	0.40
1:E:19:ILE:HG23	1:E:20:TYR:N	2.35	0.40
1:H:42:LEU:HD12	1:H:46:GLN:HE21	1.87	0.40
1:H:145:VAL:O	1:H:149:MET:HG2	2.21	0.40
1:H:101:PHE:O	1:H:104:THR:HG22	2.21	0.40
1:I:14:GLU:CG	1:J:46:GLN:NE2	2.82	0.40
1:I:25:LYS:HB3	1:I:25:LYS:HZ2	1.86	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	191/193 (99%)	178 (93%)	9 (5%)	4 (2%)	7 1
1	B	190/193 (98%)	177 (93%)	10 (5%)	3 (2%)	9 2
1	C	187/193 (97%)	177 (95%)	9 (5%)	1 (0%)	29 18
1	D	191/193 (99%)	179 (94%)	10 (5%)	2 (1%)	15 6
1	E	191/193 (99%)	181 (95%)	7 (4%)	3 (2%)	9 2
1	F	191/193 (99%)	181 (95%)	9 (5%)	1 (0%)	29 18
1	G	190/193 (98%)	179 (94%)	8 (4%)	3 (2%)	9 2
1	H	184/193 (95%)	176 (96%)	6 (3%)	2 (1%)	14 5
1	I	182/193 (94%)	170 (93%)	10 (6%)	2 (1%)	14 5
1	J	182/193 (94%)	170 (93%)	10 (6%)	2 (1%)	14 5
1	K	176/193 (91%)	172 (98%)	4 (2%)	0	100 100
1	L	180/193 (93%)	172 (96%)	7 (4%)	1 (1%)	25 15
1	M	180/193 (93%)	172 (96%)	8 (4%)	0	100 100
1	N	175/193 (91%)	171 (98%)	4 (2%)	0	100 100
All	All	2590/2702 (96%)	2455 (95%)	111 (4%)	24 (1%)	17 7

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	14	GLU
1	D	8	GLU
1	H	15	ARG
1	I	14	GLU
1	I	16	SER
1	B	192	ARG
1	E	15	ARG
1	F	8	GLU
1	G	13	GLY

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Mol	Chain	Res	Type
1	G	16	SER
1	J	14	GLU
1	J	16	SER
1	A	11	SER
1	A	16	SER
1	B	12	ARG
1	C	10	THR
1	E	14	GLU
1	G	17	PHE
1	L	18	ASP
1	A	9	GLN
1	A	12	ARG
1	B	3	VAL
1	E	7	ILE
1	D	13	GLY

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	163/163 (100%)	158 (97%)	5 (3%)	40	32
1	B	163/163 (100%)	155 (95%)	8 (5%)	25	15
1	C	160/163 (98%)	154 (96%)	6 (4%)	33	24
1	D	163/163 (100%)	157 (96%)	6 (4%)	34	25
1	E	163/163 (100%)	157 (96%)	6 (4%)	34	25
1	F	163/163 (100%)	156 (96%)	7 (4%)	29	19
1	G	163/163 (100%)	156 (96%)	7 (4%)	29	19
1	H	157/163 (96%)	151 (96%)	6 (4%)	33	24
1	I	155/163 (95%)	151 (97%)	4 (3%)	46	39
1	J	155/163 (95%)	151 (97%)	4 (3%)	46	39
1	K	150/163 (92%)	142 (95%)	8 (5%)	22	13
1	L	153/163 (94%)	149 (97%)	4 (3%)	46	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	153/163 (94%)	149 (97%)	4 (3%)	46	39
1	N	149/163 (91%)	142 (95%)	7 (5%)	26	16
All	All	2210/2282 (97%)	2128 (96%)	82 (4%)	34	25

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	31	LEU
1	A	42	LEU
1	A	108	LYS
1	A	122	HIS
1	B	22	ARG
1	B	31	LEU
1	B	34	GLN
1	B	36	GLU
1	B	84	LYS
1	B	122	HIS
1	B	160	SER
1	B	172	ARG
1	C	22	ARG
1	C	27	ARG
1	C	56	GLU
1	C	118	ARG
1	C	122	HIS
1	C	148	ARG
1	D	17	PHE
1	D	24	LEU
1	D	34	GLN
1	D	122	HIS
1	D	136	GLU
1	D	140	ARG
1	E	22	ARG
1	E	31	LEU
1	E	36	GLU
1	E	53	GLU
1	E	122	HIS
1	E	184	LEU
1	F	8	GLU
1	F	19	ILE
1	F	27	ARG

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Mol	Chain	Res	Type
1	F	31	LEU
1	F	122	HIS
1	F	125	LEU
1	F	170	ARG
1	G	17	PHE
1	G	25	LYS
1	G	31	LEU
1	G	122	HIS
1	G	136	GLU
1	G	184	LEU
1	G	193	ASN
1	H	12	ARG
1	H	17	PHE
1	H	22	ARG
1	H	42	LEU
1	H	122	HIS
1	H	140	ARG
1	I	108	LYS
1	I	122	HIS
1	I	129	GLN
1	I	148	ARG
1	J	122	HIS
1	J	143	LEU
1	J	170	ARG
1	J	184	LEU
1	K	17	PHE
1	K	22	ARG
1	K	31	LEU
1	K	118	ARG
1	K	122	HIS
1	K	148	ARG
1	K	172	ARG
1	K	184	LEU
1	L	18	ASP
1	L	23	LEU
1	L	108	LYS
1	L	122	HIS
1	M	31	LEU
1	M	108	LYS
1	M	122	HIS
1	M	136	GLU
1	N	26	GLU

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Mol	Chain	Res	Type
1	N	31	LEU
1	N	34	GLN
1	N	118	ARG
1	N	122	HIS
1	N	184	LEU
1	N	192	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	41	ASN
1	A	116	ASN
1	A	123	GLN
1	A	156	HIS
1	A	163	GLN
1	B	41	ASN
1	B	94	GLN
1	B	116	ASN
1	B	123	GLN
1	B	129	GLN
1	B	156	HIS
1	B	163	GLN
1	C	41	ASN
1	C	116	ASN
1	C	123	GLN
1	D	9	GLN
1	D	34	GLN
1	D	41	ASN
1	D	116	ASN
1	D	163	GLN
1	E	41	ASN
1	E	122	HIS
1	E	123	GLN
1	E	156	HIS
1	E	193	ASN
1	F	9	GLN
1	F	41	ASN
1	F	116	ASN
1	F	123	GLN
1	F	156	HIS
1	G	41	ASN

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Mol	Chain	Res	Type
1	G	116	ASN
1	G	123	GLN
1	G	156	HIS
1	G	163	GLN
1	G	193	ASN
1	H	41	ASN
1	H	46	GLN
1	H	123	GLN
1	H	156	HIS
1	I	34	GLN
1	I	46	GLN
1	I	116	ASN
1	I	123	GLN
1	I	129	GLN
1	I	156	HIS
1	I	163	GLN
1	I	191	HIS
1	J	41	ASN
1	J	46	GLN
1	J	116	ASN
1	J	156	HIS
1	J	163	GLN
1	J	191	HIS
1	K	116	ASN
1	K	123	GLN
1	K	131	GLN
1	K	156	HIS
1	L	116	ASN
1	L	122	HIS
1	L	123	GLN
1	L	129	GLN
1	L	156	HIS
1	M	116	ASN
1	M	123	GLN
1	M	156	HIS
1	N	34	GLN
1	N	38	HIS
1	N	46	GLN
1	N	116	ASN
1	N	123	GLN
1	N	156	HIS
1	N	193	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	MPD	B	194	-	7,7,7	2.06	3 (42%)	9,10,10	3.69	6 (66%)
2	MPD	I	194	-	7,7,7	1.52	2 (28%)	9,10,10	3.66	6 (66%)
2	MPD	A	194	-	7,7,7	1.52	2 (28%)	9,10,10	3.66	6 (66%)
2	MPD	E	194	-	7,7,7	1.51	2 (28%)	9,10,10	3.65	6 (66%)
2	MPD	J	194	-	7,7,7	1.21	1 (14%)	9,10,10	0.92	1 (11%)
2	MPD	L	194	-	7,7,7	1.20	1 (14%)	9,10,10	0.92	1 (11%)
2	MPD	M	194	-	7,7,7	1.49	2 (28%)	9,10,10	3.66	6 (66%)
2	MPD	N	194	-	7,7,7	1.51	2 (28%)	9,10,10	3.65	6 (66%)
2	MPD	F	194	-	7,7,7	1.51	2 (28%)	9,10,10	3.66	6 (66%)
2	MPD	G	194	-	7,7,7	1.50	2 (28%)	9,10,10	3.65	6 (66%)
2	MPD	K	194	-	7,7,7	1.51	2 (28%)	9,10,10	3.66	6 (66%)
2	MPD	C	194	-	7,7,7	1.51	2 (28%)	9,10,10	3.66	6 (66%)
2	MPD	D	194	-	7,7,7	1.51	2 (28%)	9,10,10	3.66	6 (66%)
2	MPD	H	194	-	7,7,7	1.51	2 (28%)	9,10,10	3.65	6 (66%)

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	MPD	B	194	-	-	0/5/5/5	-
2	MPD	I	194	-	-	0/5/5/5	-
2	MPD	A	194	-	-	0/5/5/5	-
2	MPD	E	194	-	-	0/5/5/5	-
2	MPD	J	194	-	-	0/5/5/5	-
2	MPD	L	194	-	-	0/5/5/5	-
2	MPD	M	194	-	-	0/5/5/5	-
2	MPD	N	194	-	-	0/5/5/5	-
2	MPD	F	194	-	-	0/5/5/5	-
2	MPD	G	194	-	-	0/5/5/5	-
2	MPD	K	194	-	-	0/5/5/5	-
2	MPD	C	194	-	-	0/5/5/5	-
2	MPD	D	194	-	-	0/5/5/5	-
2	MPD	H	194	-	-	0/5/5/5	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	194	MPD	O4-C4	-4.03	1.25	1.43
2	G	194	MPD	C3-C2	2.90	1.61	1.53
2	E	194	MPD	C3-C2	2.89	1.61	1.53
2	D	194	MPD	C3-C2	2.88	1.61	1.53
2	C	194	MPD	C3-C2	2.87	1.61	1.53
2	N	194	MPD	C3-C2	2.87	1.61	1.53
2	I	194	MPD	C3-C2	2.87	1.61	1.53
2	A	194	MPD	C3-C2	2.86	1.61	1.53
2	K	194	MPD	C3-C2	2.86	1.61	1.53
2	F	194	MPD	C3-C2	2.86	1.61	1.53
2	H	194	MPD	C3-C2	2.85	1.61	1.53
2	M	194	MPD	C3-C2	2.83	1.61	1.53
2	B	194	MPD	O2-C2	2.74	1.51	1.44
2	A	194	MPD	O2-C2	2.67	1.51	1.44
2	H	194	MPD	O2-C2	2.66	1.51	1.44
2	I	194	MPD	O2-C2	2.66	1.51	1.44
2	J	194	MPD	O2-C2	2.66	1.51	1.44
2	N	194	MPD	O2-C2	2.64	1.51	1.44
2	C	194	MPD	O2-C2	2.64	1.51	1.44
2	L	194	MPD	O2-C2	2.64	1.51	1.44
2	F	194	MPD	O2-C2	2.63	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	194	MPD	O2-C2	2.63	1.51	1.44
2	D	194	MPD	O2-C2	2.62	1.51	1.44
2	E	194	MPD	O2-C2	2.62	1.51	1.44
2	M	194	MPD	O2-C2	2.60	1.51	1.44
2	G	194	MPD	O2-C2	2.57	1.51	1.44
2	B	194	MPD	C3-C2	2.23	1.59	1.53

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	194	MPD	O2-C2-C3	-6.15	86.70	109.80
2	A	194	MPD	O2-C2-C3	-6.12	86.82	109.80
2	I	194	MPD	O2-C2-C3	-6.11	86.83	109.80
2	D	194	MPD	O2-C2-C3	-6.11	86.85	109.80
2	G	194	MPD	O2-C2-C3	-6.11	86.86	109.80
2	M	194	MPD	O2-C2-C3	-6.11	86.86	109.80
2	N	194	MPD	O2-C2-C3	-6.10	86.88	109.80
2	H	194	MPD	O2-C2-C3	-6.10	86.89	109.80
2	K	194	MPD	O2-C2-C3	-6.09	86.90	109.80
2	E	194	MPD	O2-C2-C3	-6.09	86.91	109.80
2	F	194	MPD	O2-C2-C3	-6.09	86.92	109.80
2	B	194	MPD	O2-C2-C3	-5.73	88.28	109.80
2	F	194	MPD	CM-C2-C3	-5.06	86.40	109.96
2	K	194	MPD	CM-C2-C3	-5.05	86.45	109.96
2	M	194	MPD	CM-C2-C3	-5.04	86.49	109.96
2	A	194	MPD	CM-C2-C3	-5.04	86.50	109.96
2	E	194	MPD	CM-C2-C3	-5.04	86.50	109.96
2	I	194	MPD	CM-C2-C3	-5.04	86.51	109.96
2	D	194	MPD	CM-C2-C3	-5.04	86.51	109.96
2	H	194	MPD	CM-C2-C3	-5.04	86.51	109.96
2	C	194	MPD	CM-C2-C3	-5.02	86.57	109.96
2	N	194	MPD	CM-C2-C3	-5.02	86.60	109.96
2	G	194	MPD	CM-C2-C3	-5.01	86.65	109.96
2	B	194	MPD	CM-C2-C3	-4.84	87.42	109.96
2	F	194	MPD	O2-C2-CM	4.63	122.92	108.08
2	A	194	MPD	O2-C2-CM	4.61	122.88	108.08
2	M	194	MPD	O2-C2-CM	4.59	122.81	108.08
2	D	194	MPD	O2-C2-CM	4.59	122.80	108.08
2	H	194	MPD	O2-C2-CM	4.58	122.79	108.08
2	K	194	MPD	O2-C2-CM	4.58	122.78	108.08
2	I	194	MPD	O2-C2-CM	4.58	122.76	108.08
2	C	194	MPD	O2-C2-CM	4.56	122.72	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	194	MPD	O2-C2-CM	4.53	122.61	108.08
2	E	194	MPD	O2-C2-CM	4.52	122.59	108.08
2	N	194	MPD	O2-C2-CM	4.52	122.57	108.08
2	B	194	MPD	O2-C2-C1	4.21	121.58	108.08
2	C	194	MPD	O2-C2-C1	4.16	121.42	108.08
2	G	194	MPD	O2-C2-C1	4.15	121.40	108.08
2	N	194	MPD	O2-C2-C1	4.15	121.39	108.08
2	E	194	MPD	O2-C2-C1	4.12	121.30	108.08
2	I	194	MPD	O2-C2-C1	4.11	121.28	108.08
2	M	194	MPD	O2-C2-C1	4.10	121.23	108.08
2	D	194	MPD	O2-C2-C1	4.10	121.22	108.08
2	K	194	MPD	O2-C2-C1	4.09	121.21	108.08
2	A	194	MPD	O2-C2-C1	4.09	121.20	108.08
2	H	194	MPD	O2-C2-C1	4.09	121.19	108.08
2	F	194	MPD	O2-C2-C1	4.07	121.13	108.08
2	B	194	MPD	C1-C2-C3	-4.00	91.36	109.96
2	B	194	MPD	O2-C2-CM	3.88	120.52	108.08
2	B	194	MPD	CM-C2-C1	3.48	117.82	110.57
2	G	194	MPD	C1-C2-C3	-3.24	94.87	109.96
2	N	194	MPD	C1-C2-C3	-3.22	94.96	109.96
2	E	194	MPD	C1-C2-C3	-3.22	94.97	109.96
2	M	194	MPD	C1-C2-C3	-3.21	95.01	109.96
2	C	194	MPD	C1-C2-C3	-3.21	95.01	109.96
2	A	194	MPD	C1-C2-C3	-3.21	95.02	109.96
2	D	194	MPD	C1-C2-C3	-3.21	95.02	109.96
2	I	194	MPD	C1-C2-C3	-3.21	95.03	109.96
2	H	194	MPD	C1-C2-C3	-3.21	95.03	109.96
2	K	194	MPD	C1-C2-C3	-3.20	95.04	109.96
2	F	194	MPD	C1-C2-C3	-3.19	95.09	109.96
2	E	194	MPD	CM-C2-C1	2.64	116.08	110.57
2	N	194	MPD	CM-C2-C1	2.61	116.00	110.57
2	H	194	MPD	CM-C2-C1	2.60	115.99	110.57
2	K	194	MPD	CM-C2-C1	2.59	115.98	110.57
2	G	194	MPD	CM-C2-C1	2.59	115.96	110.57
2	D	194	MPD	CM-C2-C1	2.58	115.94	110.57
2	I	194	MPD	CM-C2-C1	2.57	115.92	110.57
2	M	194	MPD	CM-C2-C1	2.57	115.92	110.57
2	F	194	MPD	CM-C2-C1	2.56	115.91	110.57
2	A	194	MPD	CM-C2-C1	2.55	115.88	110.57
2	C	194	MPD	CM-C2-C1	2.52	115.83	110.57
2	J	194	MPD	O4-C4-C3	-2.35	101.87	111.36
2	L	194	MPD	O4-C4-C3	-2.33	101.94	111.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	194	MPD	1	0
2	I	194	MPD	1	0
2	A	194	MPD	1	0
2	E	194	MPD	2	0
2	L	194	MPD	1	0
2	M	194	MPD	2	0
2	N	194	MPD	1	0
2	F	194	MPD	3	0
2	G	194	MPD	1	0
2	K	194	MPD	2	0
2	C	194	MPD	1	0
2	D	194	MPD	1	0
2	H	194	MPD	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.