



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:52 PM UTC

PDB ID : 1YG6 / pdb_00001yg6
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

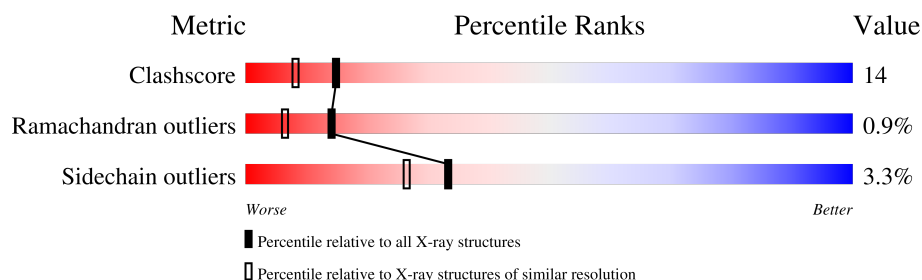
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	193	77% 19% .
1	B	193	77% 20% ..
1	C	193	73% 24% ...
1	D	193	70% 27% .
1	E	193	71% 25% .
1	F	193	74% 22% ..
1	G	193	75% 21% ...
1	H	193	72% 21% ...

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Mol	Chain	Length	Quality of chain
1	I	193	 72%22%• 5%
1	J	193	 72%22%•• 5%
1	K	193	 73%18%• 8%
1	L	193	 77%15%•• 6%
1	M	193	 77%15%• 6%
1	N	193	 72%19%• 8%

2 Entry composition

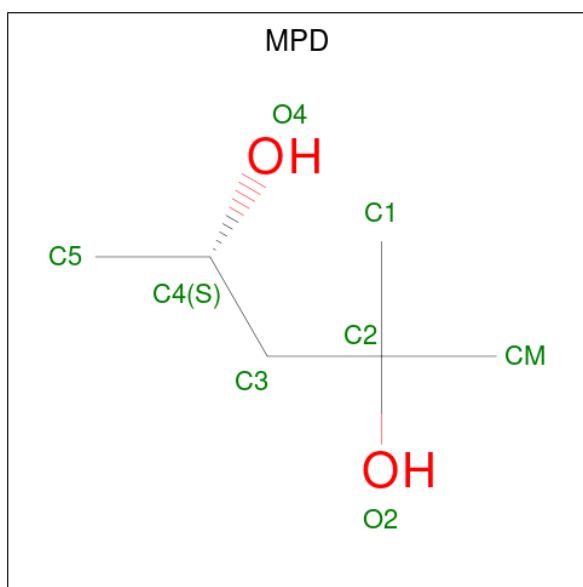
There are 3 unique types of molecules in this entry. The entry contains 21540 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 3 is water.

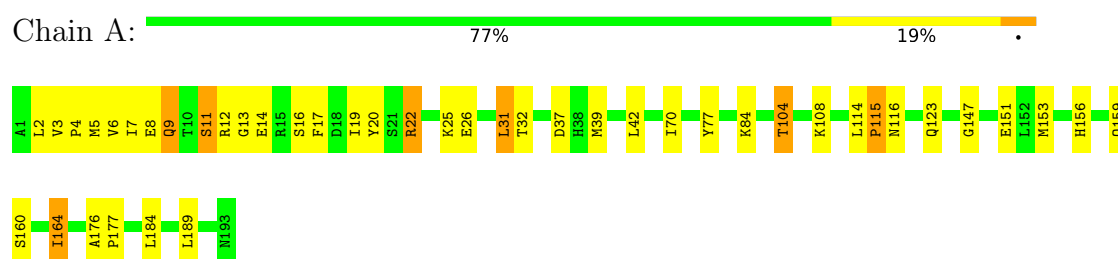
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total 75	O 75	0	0
3	B	62	Total 62	O 62	0	0
3	C	53	Total 53	O 53	0	0
3	D	33	Total 33	O 33	0	0
3	E	65	Total 65	O 65	0	0
3	F	69	Total 69	O 69	0	0
3	G	89	Total 89	O 89	0	0
3	H	60	Total 60	O 60	0	0
3	I	61	Total 61	O 61	0	0
3	J	52	Total 52	O 52	0	0
3	K	61	Total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

3 Residue-property plots

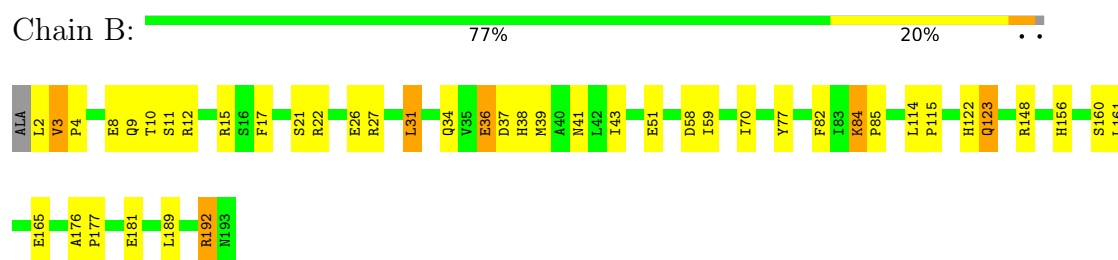
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

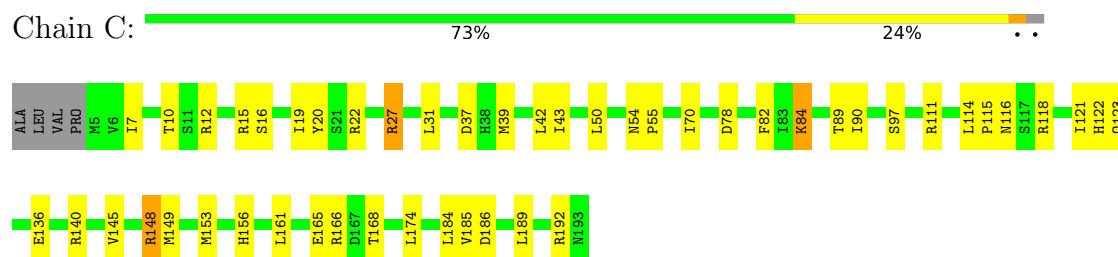
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



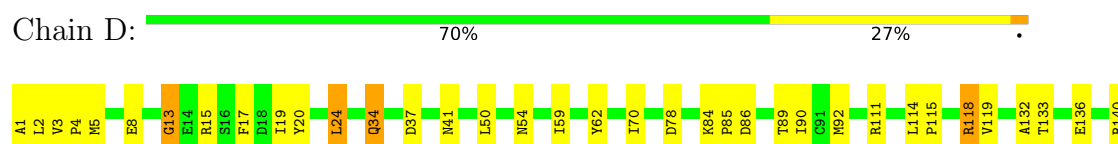
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

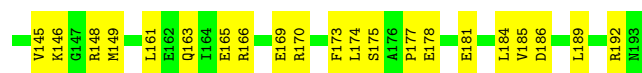


• Molecule 1: ATP-dependent Clp protease proteolytic subunit



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

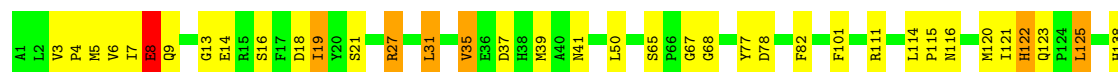




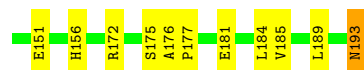
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



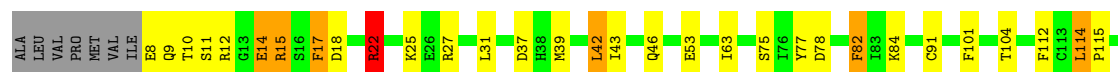
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



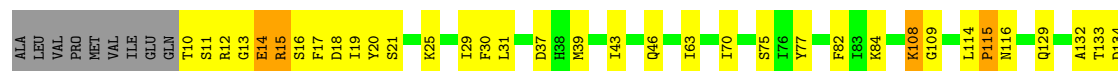
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



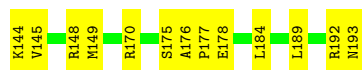
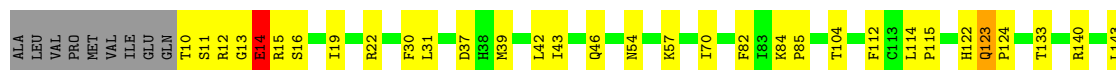
- Molecule 1: ATP-dependent Clp protease proteolytic subunit





- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J: 72% 22% 5%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K: 73% 18% 8%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L: 77% 15% 6%



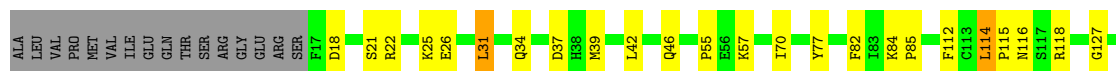
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M: 77% 15% 6%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N: 72% 19% 8%



G147	R148	E151	H156	L161	E162	E165	R166	A176	P177	L184	L189	T190	H191	R192	N193
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4 Data and refinement statistics

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

5.1 Standard geometry

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	0.65	0/1531	0.95	4/2064 (0.2%)
1	B	0.58	0/1526	0.95	7/2057 (0.3%)
1	C	0.54	0/1503	0.95	8/2024 (0.4%)
1	D	0.54	0/1531	0.93	6/2064 (0.3%)
1	E	0.63	0/1531	0.94	7/2064 (0.3%)
1	F	0.70	0/1531	0.96	4/2064 (0.2%)
1	G	0.76	0/1526	0.96	5/2057 (0.2%)
1	H	0.57	0/1480	1.11	8/1993 (0.4%)
1	I	0.58	0/1462	0.98	8/1969 (0.4%)
1	J	0.57	0/1462	0.94	7/1969 (0.4%)
1	K	0.63	0/1414	0.91	4/1906 (0.2%)
1	L	0.74	0/1449	0.94	7/1951 (0.4%)
1	M	0.74	0/1449	0.94	5/1951 (0.3%)
1	N	0.66	0/1408	0.95	5/1898 (0.3%)
All	All	0.64	0/20803	0.96	85/28031 (0.3%)

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

There are no bond length outliers.

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	22	ARG	CG-CD-NE	22.80	162.17	112.00
1	A	37	ASP	N-CA-C	9.25	122.21	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	22	ARG	CB-CG-CD	9.04	132.09	111.30
1	E	37	ASP	N-CA-C	8.57	121.39	111.11
1	I	37	ASP	N-CA-C	7.97	120.67	111.11
1	N	37	ASP	N-CA-C	7.93	120.62	111.11
1	B	37	ASP	N-CA-C	7.70	120.35	111.11
1	M	37	ASP	N-CA-C	7.62	120.25	111.11
1	K	37	ASP	N-CA-C	7.53	120.15	111.11
1	J	37	ASP	N-CA-C	7.30	119.87	111.11
1	H	37	ASP	N-CA-C	7.16	119.70	111.11
1	C	70	ILE	N-CA-C	6.93	117.07	110.42
1	G	37	ASP	N-CA-C	6.92	119.42	111.11
1	F	37	ASP	N-CA-C	6.89	119.38	111.11
1	B	70	ILE	N-CA-C	6.66	116.81	110.42
1	H	82	PHE	N-CA-C	6.62	118.57	111.36
1	E	70	ILE	N-CA-C	6.60	116.76	110.42
1	N	114	LEU	N-CA-C	-6.38	100.83	110.39
1	E	114	LEU	N-CA-C	-6.32	101.89	110.36
1	D	70	ILE	N-CA-C	6.31	116.47	110.42
1	G	114	LEU	N-CA-C	-6.06	101.30	110.39
1	L	114	LEU	N-CA-C	-6.05	101.32	110.39
1	M	82	PHE	N-CA-C	6.04	117.67	111.14
1	L	115	PRO	N-CA-C	6.04	122.74	113.75
1	J	114	LEU	N-CA-C	-5.95	102.38	110.36
1	A	114	LEU	N-CA-C	-5.93	101.49	110.39
1	B	114	LEU	N-CA-C	-5.92	101.51	110.39
1	J	82	PHE	N-CA-C	5.89	117.50	111.14
1	M	115	PRO	N-CA-C	5.87	122.50	113.75
1	L	19	ILE	N-CA-C	-5.85	103.77	111.09
1	E	82	PHE	N-CA-C	5.80	117.41	111.14
1	I	63	ILE	N-CA-C	5.79	116.34	107.77
1	E	55	PRO	N-CA-C	5.77	121.13	114.03
1	I	114	LEU	N-CA-C	-5.74	101.78	110.39
1	I	70	ILE	N-CA-C	5.68	115.87	110.42
1	N	70	ILE	N-CA-C	5.68	115.87	110.42
1	F	114	LEU	N-CA-C	-5.65	101.91	110.39
1	A	115	PRO	N-CA-C	5.63	122.14	113.75
1	H	75	SER	N-CA-C	-5.63	105.29	111.82
1	K	82	PHE	N-CA-C	5.61	117.07	111.07
1	G	70	ILE	N-CA-C	5.60	115.80	110.42
1	L	70	ILE	N-CA-C	5.59	115.79	110.42
1	H	114	LEU	N-CA-C	-5.57	102.03	110.39
1	E	63	ILE	N-CA-C	5.54	115.87	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	24	LEU	N-CA-C	-5.53	105.40	111.82
1	M	114	LEU	N-CA-C	-5.52	102.11	110.39
1	N	112	PHE	N-CA-C	5.51	118.06	109.52
1	I	115	PRO	N-CA-C	5.50	121.95	113.75
1	J	70	ILE	N-CA-C	5.50	115.70	110.42
1	C	156	HIS	N-CA-C	5.49	118.19	111.82
1	D	54	ASN	CA-C-N	5.48	125.19	119.82
1	D	54	ASN	C-N-CA	5.48	125.19	119.82
1	K	70	ILE	N-CA-C	5.45	115.65	110.42
1	N	82	PHE	N-CA-C	5.45	117.30	111.36
1	C	37	ASP	N-CA-C	5.44	120.35	111.37
1	B	82	PHE	N-CA-C	5.41	118.35	111.69
1	K	65	SER	N-CA-C	5.41	116.99	108.23
1	B	123	GLN	CA-C-N	5.40	125.33	119.76
1	B	123	GLN	C-N-CA	5.40	125.33	119.76
1	D	37	ASP	N-CA-C	5.38	120.25	111.37
1	G	175	SER	N-CA-C	-5.37	103.61	110.53
1	H	112	PHE	N-CA-C	5.36	117.83	109.52
1	F	82	PHE	N-CA-C	5.36	116.92	111.14
1	I	75	SER	N-CA-C	-5.35	105.61	111.82
1	L	12	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	A	70	ILE	N-CA-C	5.31	115.52	110.42
1	C	84	LYS	CA-C-N	-5.30	114.78	120.03
1	C	84	LYS	C-N-CA	-5.30	114.78	120.03
1	I	82	PHE	N-CA-C	5.30	117.13	111.36
1	C	114	LEU	N-CA-C	-5.28	102.47	110.39
1	I	15	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	L	38	HIS	N-CA-C	5.24	117.07	111.36
1	J	123	GLN	CA-C-N	5.23	125.14	119.76
1	J	123	GLN	C-N-CA	5.23	125.14	119.76
1	L	37	ASP	N-CA-C	5.22	119.99	111.37
1	M	63	ILE	N-CA-C	5.20	115.35	107.75
1	C	82	PHE	N-CA-C	5.18	117.01	111.36
1	D	86	ASP	N-CA-C	-5.16	102.05	110.20
1	H	63	ILE	N-CA-C	5.15	115.26	107.75
1	J	112	PHE	N-CA-C	5.09	117.42	109.52
1	E	97	SER	CB-CA-C	-5.09	110.69	116.54
1	C	97	SER	CB-CA-C	-5.05	110.73	116.54
1	B	26	GLU	N-CA-C	-5.04	106.97	113.02
1	G	63	ILE	N-CA-C	5.04	115.17	108.11
1	F	65	SER	N-CA-C	5.04	116.39	108.23

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

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	52	0
1	B	1502	0	1513	58	0
1	C	1480	0	1486	42	0
1	D	1507	0	1521	52	0
1	E	1507	0	1521	44	0
1	F	1507	0	1521	47	0
1	G	1502	0	1513	42	0
1	H	1457	0	1455	69	0
1	I	1439	0	1441	95	0
1	J	1439	0	1443	71	0
1	K	1391	0	1396	38	0
1	L	1426	0	1431	29	0
1	M	1426	0	1431	34	0
1	N	1385	0	1391	35	0
2	A	8	0	14	2	0
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	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	572	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 14.

All (572) 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:H:8:GLU:CD	1:I:29:ILE:HG22	1.52	1.34
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: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
1:I:14:GLU:CD	1:J:46:GLN:HE22	1.55	1.13
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:H:9:GLN:N	3:H:237:HOH:O	1.83	1.08
1:I:31:LEU:CD1	1:I:39:MET:HE1	1.84	1.07
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:H:8:GLU:CD	1:I:29:ILE:CG2	2.29	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:31:LEU:HD11	1:I:39:MET:HE1	1.36	1.02
1:I:15:ARG:NE	1:I:20:TYR:CE2	2.29	1.01
1:A:17:PHE:CZ	1:B:10:THR:HG23	1.95	1.00
1:H:8:GLU:OE2	1:I:30:PHE:C	1.77	1.00
1:B:8:GLU:OE2	1:B:11:SER:OG	1.78	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:K:43:ILE:HG22	1:K:47:MET:HE2	1.54	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:H:31:LEU:CD1	1:H:39:MET:HE1	2.04	0.87
1:G:7:ILE:HG22	1:G:9:GLN:H	1.37	0.87
1:I:14:GLU:CD	1:J:46:GLN:NE2	2.32	0.86
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:24:LEU:HD23	1:F:6:VAL:HG11	1.63	0.79
1:L:108:LYS:HZ2	1:L:108:LYS:HA	1.47	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:C:31:LEU:HD12	1:C:39:MET:HE1	1.64	0.78
1:I:31:LEU:HD12	1:I:39:MET:HE1	1.65	0.77
1:H:31:LEU:HD12	1:H:39:MET:HE1	1.65	0.77
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:C:31:LEU:CD1	1:C:39:MET:HE1	2.15	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:L:31:LEU:CD1	1:L:39:MET:HE1	2.15	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:J:31:LEU:CD1	1:J:39:MET:HE1	2.17	0.74
1:I:15:ARG:HG2	1:I:19:ILE:HG21	1.69	0.74
1:K:140:ARG:NH1	1:K:144:LYS:HZ1	1.85	0.74
1:D:89:THR:C	1:D:90:ILE:HD12	2.13	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
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:N:31:LEU:HD13	1:N:39:MET:HE1	1.71	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:HD13	1:B:39:MET:HE1	1.73	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:F:120:MET:HE2	1:F:173:PHE:CE1	2.26	0.70
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:31:LEU:HD12	1:J:39:MET:HE1	1.75	0.69
1:J:10:THR:OG1	1:K:18:ASP:OD1	2.09	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:L:31:LEU:HD12	1:L:39:MET:HE1	1.74	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:E:31:LEU:HD13	1:E:39:MET:HE1	1.76	0.66
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:I:31:LEU:CD1	1:I:39:MET:CE	2.69	0.66
1:E:136:GLU:OE2	1:E:140:ARG:NH1	2.29	0.66
1:H:10:THR:HG21	1:I:46:GLN:CD	2.21	0.66
1:I:31:LEU:HD13	1:I:43:ILE:HD13	1.77	0.66
1:J:10:THR:OG1	1:K:18:ASP:CG	2.39	0.66
2:F:194:MPD:H13	2:F:194:MPD:HO4	1.60	0.65
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:F:27:ARG:NH2	1:F:50:LEU:O	2.30	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:108:LYS:HZ2	1:L:108:LYS:CA	2.11	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
1:A:11:SER:C	1:B:10:THR:OG1	2.41	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:H:140:ARG:HD3	1:H:140:ARG:C	2.23	0.64
1:J:175:SER:OG	1:J:178:GLU:HG3	1.98	0.64
1:F:31:LEU:HD13	1:F:39:MET:HE1	1.80	0.63
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:I:13:GLY:C	1:I:14:GLU:HG3	2.22	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:G:50:LEU:CD1	1:G:59:ILE:HD12	2.29	0.62
1:K:31:LEU:HD13	1:K:39:MET:HE1	1.81	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:H:8:GLU:C	3:H:237:HOH:O	2.33	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
2:K:194:MPD:H13	2:K:194:MPD:HO4	1.64	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:K:140:ARG:CZ	1:K:144:LYS:HZ3	2.12	0.61
1:H:8:GLU:OE2	1:I:31:LEU:N	2.33	0.61
1:F:125:LEU:H	1:F:125:LEU:HD23	1.64	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
1:F:35:VAL:HG12	1:F:67:GLY:C	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H:170:ARG:HH21	1:I:134:ASP:CG	2.10	0.59
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:F:111:ARG:C	1:F:185:VAL:HG13	2.27	0.59
1:E:120:MET:HE2	1:E:173:PHE:CE2	2.37	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:D:175:SER:OG	1:D:178:GLU:HG3	2.02	0.59
1:H:140:ARG:HD3	1:H:140:ARG:O	2.02	0.59
1:K:44:VAL:HA	1:K:47:MET:HE3	1.83	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:12:ARG:HD3	1:N:46:GLN:CD	2.29	0.57
1:N:55:PRO:HB2	1:N:84:LYS:HD2	1.84	0.57
1:G:31:LEU:HD22	1:G:43:ILE:HD13	1.86	0.57
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:31:LEU:HD13	1:A:39:MET:HE1	1.87	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:E:31:LEU:C	1:E:31:LEU:HD12	2.30	0.57
1:A:176:ALA:HB3	1:A:177:PRO:HD3	1.85	0.56
1:J:31:LEU:HD11	1:J:39:MET:HE1	1.86	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:J:10:THR:HG1	1:K:18:ASP:CG	2.13	0.56
1:M:31:LEU:HD13	1:M:39:MET:HE1	1.85	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: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:N:25:LYS:HB3	1:N:25:LYS:HZ3	1.70	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:C:111:ARG:C	1:C:185:VAL:HG23	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:VAL:CG1	1:F:68:GLY:CA	2.85	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:14:GLU:HB3	1:J:46:GLN:CD	2.32	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
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:H:10:THR:CG2	1:I:46:GLN:CD	2.81	0.54
1:J:15:ARG:HE	1:J:22:ARG:HE	1.54	0.54
1:H:31:LEU:HD11	1:H:39:MET:HE1	1.85	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:L:31:LEU:HD11	1:L:39:MET:HE1	1.90	0.53
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: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:25:LYS:HB3	1:I:25:LYS:HZ3	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:12:ARG:C	1:H:14:GLU:H	2.19	0.51
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:I:31:LEU:HD11	1:I:39:MET:CE	2.24	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:F:120:MET:HE2	1:F:173:PHE:HE1	1.73	0.50
1:I:115:PRO:HD3	1:I:189:LEU:O	2.10	0.50
1:L:98:MET:HE2	2:L:194:MPD:HM1	1.94	0.50
1:A:22:ARG:O	1:A:26:GLU:OE1	2.30	0.50
1:C:121:ILE:HD13	1:C:153:MET:HE2	1.94	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:C:31:LEU:HD11	1:C:39:MET:HE1	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:192:ARG:O	1:I:193:ASN:CB	2.55	0.49
1:F:31:LEU:HD12	1:F:31:LEU:C	2.36	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: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:E:31:LEU:CD1	1:E:39:MET:HE1	2.40	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
2:E:194:MPD:H13	2:E:194:MPD:HO4	1.73	0.49
1:F:122:HIS:C	1:F:122:HIS:CD2	2.91	0.49
1:C:42:LEU:HD11	1:D:4:PRO:CD	2.39	0.49
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: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:D:111:ARG:C	1:D:185:VAL:HG13	2.39	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:136:GLU:OE1	1:M:140:ARG:NH1	2.48	0.46
1:A:108:LYS:HD2	1:A:108:LYS:C	2.41	0.46
1:F:121:ILE:O	1:F:122:HIS:HB3	2.15	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: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: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:E:137:ILE:HD13	1:E:140:ARG:HH22	1.81	0.45
1:A:153:MET:HE2	2:A:194:MPD:HM2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:77:TYR:OH	1:L:156:HIS:HE1	1.99	0.45
1:A:19:ILE:HG23	1:A:20:TYR:N	2.31	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:B:122:HIS:C	1:B:122:HIS:CD2	2.95	0.45
1:C:111:ARG:C	1:C:185:VAL:CG2	2.89	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:E:136:GLU:CD	1:E:140:ARG:NH1	2.74	0.45
1:I:108:LYS:HZ3	1:I:109:GLY:N	2.14	0.45
1:E:136:GLU:CD	1:E:140:ARG:HH12	2.25	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
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:B:27:ARG:NH1	1:B:58:ASP:C	2.75	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: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:D:62:TYR:HB3	1:D:92:MET:HE2	1.99	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:K:31:LEU:HD12	1:K:31:LEU:C	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:HIS:C	1:C:122:HIS:CD2	2.96	0.44
1:L:15:ARG:C	1:L:17:PHE:N	2.75	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:C:16:SER:HB3	1:D:5:MET:HE2	2.00	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:C:89:THR:C	1:C:90:ILE:HD12	2.43	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:M:136:GLU:CD	1:M:140:ARG:HH12	2.26	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:G:2:LEU:HD23	1:G:2:LEU:C	2.44	0.43
1:G:111:ARG:C	1:G:185:VAL:HG22	2.43	0.43
1:I:10:THR:HG23	1:I:11:SER:N	2.26	0.43
1:C:90:ILE:HD12	1:C:90:ILE:N	2.33	0.43
1:H:11:SER:OG	1:H:12:ARG:HD3	2.18	0.43
1:C:78:ASP:CB	1:D:114:LEU:HD23	2.48	0.43
1:J:122:HIS:C	1:J:122:HIS:CD2	2.96	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:D:132:ALA:HB3	1:K:123:GLN:NE2	2.34	0.43
1:L:122:HIS:CD2	1:L:122:HIS:C	2.97	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:M:162:GLU:CD	1:M:162:GLU:H	2.26	0.42
1:E:122:HIS:C	1:E:122:HIS:CD2	2.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:41:ASN:ND2	1:C:20:TYR:OH	2.52	0.42
1:D:173:PHE:C	1:D:174:LEU:HD12	2.45	0.42
1:E:3:VAL:HG23	1:E:3:VAL:O	2.20	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: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:G:31:LEU:HD13	1:G:39:MET:HE1	2.02	0.41
1:H:163:GLN:OE1	1:H:163:GLN:HA	2.20	0.41
1:B:8:GLU:C	1:B:10:THR:H	2.27	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:3:VAL:H	1:B:4:PRO:CD	2.26	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

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	191/193 (99%)	178 (93%)	9 (5%)	4 (2%)	5	1
1	B	190/193 (98%)	177 (93%)	10 (5%)	3 (2%)	7	2
1	C	187/193 (97%)	177 (95%)	9 (5%)	1 (0%)	24	16
1	D	191/193 (99%)	179 (94%)	10 (5%)	2 (1%)	12	5
1	E	191/193 (99%)	181 (95%)	7 (4%)	3 (2%)	7	2
1	F	191/193 (99%)	181 (95%)	9 (5%)	1 (0%)	24	16
1	G	190/193 (98%)	179 (94%)	8 (4%)	3 (2%)	7	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	184/193 (95%)	176 (96%)	6 (3%)	2 (1%)	11	4
1	I	182/193 (94%)	170 (93%)	10 (6%)	2 (1%)	11	4
1	J	182/193 (94%)	170 (93%)	10 (6%)	2 (1%)	11	4
1	K	176/193 (91%)	172 (98%)	4 (2%)	0	100	100
1	L	180/193 (93%)	172 (96%)	7 (4%)	1 (1%)	21	13
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%)	14	6

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
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 ⓘ

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%)	35	29
1	B	163/163 (100%)	158 (97%)	5 (3%)	35	29
1	C	160/163 (98%)	156 (98%)	4 (2%)	42	37
1	D	163/163 (100%)	157 (96%)	6 (4%)	30	22
1	E	163/163 (100%)	156 (96%)	7 (4%)	26	18
1	F	163/163 (100%)	155 (95%)	8 (5%)	22	14
1	G	163/163 (100%)	156 (96%)	7 (4%)	26	18
1	H	157/163 (96%)	154 (98%)	3 (2%)	50	47
1	I	155/163 (95%)	151 (97%)	4 (3%)	40	35
1	J	155/163 (95%)	151 (97%)	4 (3%)	40	35
1	K	150/163 (92%)	143 (95%)	7 (5%)	23	15
1	L	153/163 (94%)	149 (97%)	4 (3%)	40	35
1	M	153/163 (94%)	149 (97%)	4 (3%)	40	35
1	N	149/163 (91%)	143 (96%)	6 (4%)	28	20
All	All	2210/2282 (97%)	2136 (97%)	74 (3%)	33	26

All (74) 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	104	THR
1	A	164	ILE
1	B	31	LEU
1	B	34	GLN
1	B	36	GLU
1	B	84	LYS
1	B	160	SER
1	C	22	ARG

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Mol	Chain	Res	Type
1	C	27	ARG
1	C	118	ARG
1	C	148	ARG
1	D	17	PHE
1	D	24	LEU
1	D	34	GLN
1	D	118	ARG
1	D	136	GLU
1	D	140	ARG
1	E	22	ARG
1	E	31	LEU
1	E	34	GLN
1	E	36	GLU
1	E	53	GLU
1	E	184	LEU
1	E	193	ASN
1	F	8	GLU
1	F	19	ILE
1	F	27	ARG
1	F	31	LEU
1	F	35	VAL
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	35	VAL
1	G	136	GLU
1	G	184	LEU
1	G	193	ASN
1	H	17	PHE
1	H	22	ARG
1	H	42	LEU
1	I	84	LYS
1	I	108	LYS
1	I	129	GLN
1	I	148	ARG
1	J	14	GLU
1	J	104	THR
1	J	143	LEU
1	J	184	LEU

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Mol	Chain	Res	Type
1	K	17	PHE
1	K	22	ARG
1	K	31	LEU
1	K	36	GLU
1	K	148	ARG
1	K	172	ARG
1	K	184	LEU
1	L	18	ASP
1	L	19	ILE
1	L	23	LEU
1	L	108	LYS
1	M	31	LEU
1	M	84	LYS
1	M	108	LYS
1	M	136	GLU
1	N	26	GLU
1	N	31	LEU
1	N	34	GLN
1	N	118	ARG
1	N	184	LEU
1	N	192	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) 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	38	HIS
1	B	41	ASN
1	B	94	GLN
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	C	193	ASN

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Mol	Chain	Res	Type
1	D	9	GLN
1	D	34	GLN
1	D	41	ASN
1	D	123	GLN
1	D	163	GLN
1	E	38	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
1	G	116	ASN
1	G	123	GLN
1	G	156	HIS
1	G	193	ASN
1	H	41	ASN
1	H	46	GLN
1	H	123	GLN
1	H	156	HIS
1	H	193	ASN
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	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

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Mol	Chain	Res	Type
1	L	123	GLN
1	L	129	GLN
1	L	156	HIS
1	L	163	GLN
1	M	116	ASN
1	M	123	GLN
1	M	156	HIS
1	M	193	ASN
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	163	GLN
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 oligosaccharides 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	C	194	-	7,7,7	1.44	2 (28%)	9,10,10	3.77	6 (66%)
2	MPD	G	194	-	7,7,7	1.43	2 (28%)	9,10,10	3.76	6 (66%)
2	MPD	H	194	-	7,7,7	1.44	2 (28%)	9,10,10	3.76	6 (66%)
2	MPD	L	194	-	7,7,7	1.19	1 (14%)	9,10,10	0.93	1 (11%)
2	MPD	F	194	-	7,7,7	1.43	2 (28%)	9,10,10	3.77	6 (66%)
2	MPD	D	194	-	7,7,7	1.44	2 (28%)	9,10,10	3.77	6 (66%)
2	MPD	B	194	-	7,7,7	2.09	2 (28%)	9,10,10	3.80	6 (66%)
2	MPD	K	194	-	7,7,7	1.43	2 (28%)	9,10,10	3.76	6 (66%)
2	MPD	N	194	-	7,7,7	1.44	2 (28%)	9,10,10	3.76	6 (66%)
2	MPD	J	194	-	7,7,7	1.20	1 (14%)	9,10,10	0.94	1 (11%)
2	MPD	M	194	-	7,7,7	1.42	2 (28%)	9,10,10	3.77	6 (66%)
2	MPD	I	194	-	7,7,7	1.44	2 (28%)	9,10,10	3.77	6 (66%)
2	MPD	E	194	-	7,7,7	1.44	2 (28%)	9,10,10	3.76	6 (66%)
2	MPD	A	194	-	7,7,7	1.44	2 (28%)	9,10,10	3.77	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	C	194	-	-	0/5/5/5	-
2	MPD	G	194	-	-	0/5/5/5	-
2	MPD	H	194	-	-	0/5/5/5	-
2	MPD	L	194	-	-	0/5/5/5	-
2	MPD	F	194	-	-	0/5/5/5	-
2	MPD	D	194	-	-	0/5/5/5	-
2	MPD	B	194	-	-	0/5/5/5	-
2	MPD	K	194	-	-	0/5/5/5	-
2	MPD	N	194	-	-	0/5/5/5	-
2	MPD	J	194	-	-	0/5/5/5	-
2	MPD	M	194	-	-	0/5/5/5	-
2	MPD	I	194	-	-	0/5/5/5	-
2	MPD	E	194	-	-	0/5/5/5	-
2	MPD	A	194	-	-	0/5/5/5	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	194	MPD	O4-C4	-4.24	1.25	1.43
2	B	194	MPD	O2-C2	2.82	1.51	1.44
2	A	194	MPD	O2-C2	2.75	1.51	1.44
2	H	194	MPD	O2-C2	2.74	1.51	1.44
2	I	194	MPD	O2-C2	2.74	1.51	1.44
2	J	194	MPD	O2-C2	2.74	1.51	1.44
2	N	194	MPD	O2-C2	2.72	1.51	1.44
2	C	194	MPD	O2-C2	2.72	1.51	1.44
2	L	194	MPD	O2-C2	2.72	1.51	1.44
2	F	194	MPD	O2-C2	2.71	1.51	1.44
2	K	194	MPD	O2-C2	2.71	1.51	1.44
2	D	194	MPD	O2-C2	2.70	1.51	1.44
2	E	194	MPD	O2-C2	2.70	1.51	1.44
2	M	194	MPD	O2-C2	2.68	1.51	1.44
2	G	194	MPD	O2-C2	2.65	1.51	1.44
2	G	194	MPD	C3-C2	2.53	1.61	1.54
2	E	194	MPD	C3-C2	2.51	1.61	1.54
2	D	194	MPD	C3-C2	2.51	1.61	1.54
2	C	194	MPD	C3-C2	2.50	1.61	1.54
2	N	194	MPD	C3-C2	2.50	1.61	1.54
2	I	194	MPD	C3-C2	2.50	1.61	1.54
2	A	194	MPD	C3-C2	2.49	1.61	1.54
2	K	194	MPD	C3-C2	2.49	1.61	1.54
2	F	194	MPD	C3-C2	2.49	1.61	1.54
2	H	194	MPD	C3-C2	2.48	1.61	1.54
2	M	194	MPD	C3-C2	2.46	1.61	1.54

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	194	MPD	O2-C2-C3	-6.03	86.70	109.27
2	A	194	MPD	O2-C2-C3	-6.00	86.82	109.27
2	I	194	MPD	O2-C2-C3	-6.00	86.83	109.27
2	D	194	MPD	O2-C2-C3	-5.99	86.85	109.27
2	G	194	MPD	O2-C2-C3	-5.99	86.86	109.27
2	M	194	MPD	O2-C2-C3	-5.99	86.86	109.27
2	N	194	MPD	O2-C2-C3	-5.99	86.88	109.27
2	H	194	MPD	O2-C2-C3	-5.98	86.89	109.27
2	K	194	MPD	O2-C2-C3	-5.98	86.90	109.27
2	E	194	MPD	O2-C2-C3	-5.98	86.91	109.27
2	F	194	MPD	O2-C2-C3	-5.97	86.92	109.27
2	B	194	MPD	O2-C2-C3	-5.61	88.28	109.27
2	F	194	MPD	CM-C2-C3	-5.52	86.40	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	194	MPD	CM-C2-C3	-5.50	86.45	110.20
2	M	194	MPD	CM-C2-C3	-5.50	86.49	110.20
2	A	194	MPD	CM-C2-C3	-5.49	86.50	110.20
2	E	194	MPD	CM-C2-C3	-5.49	86.50	110.20
2	I	194	MPD	CM-C2-C3	-5.49	86.51	110.20
2	D	194	MPD	CM-C2-C3	-5.49	86.51	110.20
2	H	194	MPD	CM-C2-C3	-5.49	86.51	110.20
2	C	194	MPD	CM-C2-C3	-5.48	86.57	110.20
2	N	194	MPD	CM-C2-C3	-5.47	86.60	110.20
2	G	194	MPD	CM-C2-C3	-5.46	86.65	110.20
2	B	194	MPD	CM-C2-C3	-5.28	87.42	110.20
2	F	194	MPD	O2-C2-CM	4.79	122.92	107.99
2	A	194	MPD	O2-C2-CM	4.78	122.88	107.99
2	M	194	MPD	O2-C2-CM	4.76	122.81	107.99
2	D	194	MPD	O2-C2-CM	4.75	122.80	107.99
2	H	194	MPD	O2-C2-CM	4.75	122.79	107.99
2	K	194	MPD	O2-C2-CM	4.74	122.78	107.99
2	I	194	MPD	O2-C2-CM	4.74	122.76	107.99
2	C	194	MPD	O2-C2-CM	4.73	122.72	107.99
2	G	194	MPD	O2-C2-CM	4.69	122.61	107.99
2	E	194	MPD	O2-C2-CM	4.68	122.59	107.99
2	N	194	MPD	O2-C2-CM	4.68	122.57	107.99
2	B	194	MPD	C1-C2-C3	-4.37	91.36	110.20
2	B	194	MPD	O2-C2-C1	4.36	121.58	107.99
2	C	194	MPD	O2-C2-C1	4.31	121.42	107.99
2	G	194	MPD	O2-C2-C1	4.30	121.40	107.99
2	N	194	MPD	O2-C2-C1	4.30	121.39	107.99
2	E	194	MPD	O2-C2-C1	4.27	121.30	107.99
2	I	194	MPD	O2-C2-C1	4.27	121.28	107.99
2	M	194	MPD	O2-C2-C1	4.25	121.23	107.99
2	D	194	MPD	O2-C2-C1	4.25	121.22	107.99
2	K	194	MPD	O2-C2-C1	4.24	121.21	107.99
2	A	194	MPD	O2-C2-C1	4.24	121.20	107.99
2	H	194	MPD	O2-C2-C1	4.24	121.19	107.99
2	F	194	MPD	O2-C2-C1	4.22	121.13	107.99
2	B	194	MPD	O2-C2-CM	4.02	120.52	107.99
2	G	194	MPD	C1-C2-C3	-3.55	94.87	110.20
2	N	194	MPD	C1-C2-C3	-3.53	94.96	110.20
2	E	194	MPD	C1-C2-C3	-3.53	94.97	110.20
2	M	194	MPD	C1-C2-C3	-3.52	95.01	110.20
2	C	194	MPD	C1-C2-C3	-3.52	95.01	110.20
2	A	194	MPD	C1-C2-C3	-3.52	95.02	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	194	MPD	C1-C2-C3	-3.52	95.02	110.20
2	I	194	MPD	C1-C2-C3	-3.52	95.03	110.20
2	H	194	MPD	C1-C2-C3	-3.52	95.03	110.20
2	K	194	MPD	C1-C2-C3	-3.51	95.04	110.20
2	F	194	MPD	C1-C2-C3	-3.50	95.09	110.20
2	B	194	MPD	CM-C2-C1	3.21	117.82	110.63
2	E	194	MPD	CM-C2-C1	2.43	116.08	110.63
2	N	194	MPD	CM-C2-C1	2.40	116.00	110.63
2	H	194	MPD	CM-C2-C1	2.39	115.99	110.63
2	K	194	MPD	CM-C2-C1	2.39	115.98	110.63
2	J	194	MPD	O4-C4-C3	-2.38	101.87	111.35
2	G	194	MPD	CM-C2-C1	2.38	115.96	110.63
2	D	194	MPD	CM-C2-C1	2.37	115.94	110.63
2	L	194	MPD	O4-C4-C3	-2.37	101.94	111.35
2	I	194	MPD	CM-C2-C1	2.37	115.92	110.63
2	M	194	MPD	CM-C2-C1	2.36	115.92	110.63
2	F	194	MPD	CM-C2-C1	2.36	115.91	110.63
2	A	194	MPD	CM-C2-C1	2.35	115.88	110.63
2	C	194	MPD	CM-C2-C1	2.32	115.83	110.63

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	C	194	MPD	1	0
2	G	194	MPD	1	0
2	H	194	MPD	1	0
2	L	194	MPD	1	0
2	F	194	MPD	3	0
2	D	194	MPD	1	0
2	B	194	MPD	1	0
2	K	194	MPD	2	0
2	N	194	MPD	1	0
2	M	194	MPD	1	0
2	I	194	MPD	1	0
2	E	194	MPD	2	0
2	A	194	MPD	2	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.