



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:31 PM UTC

PDB ID : 1GTP / pdb_00001gtp
Title : GTP CYCLOHYDROLASE I
Authors : Nar, H.; Huber, R.; Meining, W.; Bacher, A.
Deposited on : 1995-09-16
Resolution : 3.00 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

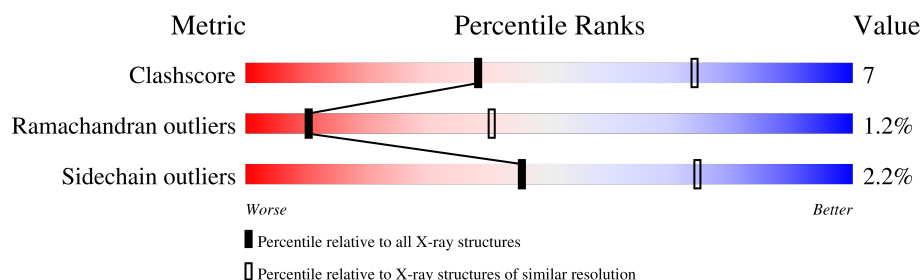
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	221	76% 23% .
1	B	221	78% 21% .
1	C	221	78% 21%
1	D	221	80% 18% .
1	E	221	78% 21% .
1	F	221	76% 24%
1	G	221	80% 19% .
1	H	221	75% 24% .

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Mol	Chain	Length	Quality of chain	
1	I	221		
1	J	221		•
1	K	221		•
1	L	221		•
1	M	221		•
1	N	221		•
1	O	221		•
1	P	221		•
1	Q	221		
1	R	221		
1	S	221		•
1	T	221		

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 43780 atoms, of which 8720 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 GTP CYCLOHYDROLASE I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	B	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	C	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	D	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	E	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	F	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	G	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	H	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	I	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	J	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	K	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	L	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	M	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	N	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	O	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	P	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	R	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	S	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	T	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	S	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	16	Total	H	O	0	0
			48	32	16		
3	B	14	Total	H	O	0	0
			42	28	14		
3	C	18	Total	H	O	0	0
			54	36	18		
3	D	16	Total	H	O	0	0
			48	32	16		
3	E	16	Total	H	O	0	0
			48	32	16		
3	F	16	Total	H	O	0	0
			48	32	16		

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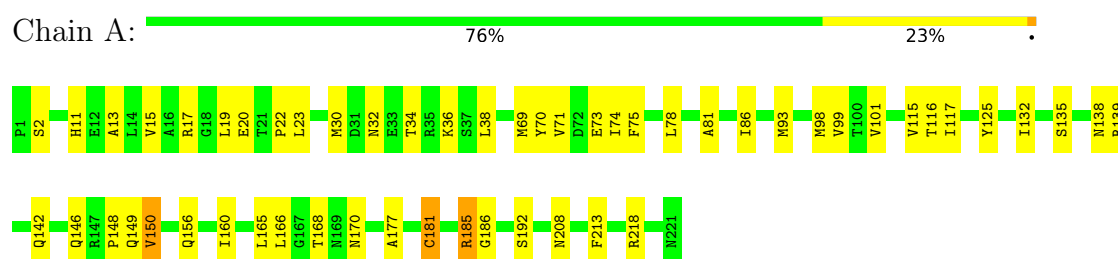
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	16	Total 48	H 32	O 16	0	0
3	H	16	Total 48	H 32	O 16	0	0
3	I	16	Total 48	H 32	O 16	0	0
3	J	16	Total 48	H 32	O 16	0	0
3	K	15	Total 45	H 30	O 15	0	0
3	L	17	Total 51	H 34	O 17	0	0
3	M	15	Total 45	H 30	O 15	0	0
3	N	17	Total 51	H 34	O 17	0	0
3	O	16	Total 48	H 32	O 16	0	0
3	P	17	Total 51	H 34	O 17	0	0
3	Q	15	Total 45	H 30	O 15	0	0
3	R	17	Total 51	H 34	O 17	0	0
3	S	16	Total 48	H 32	O 16	0	0
3	T	15	Total 45	H 30	O 15	0	0

3 Residue-property plots

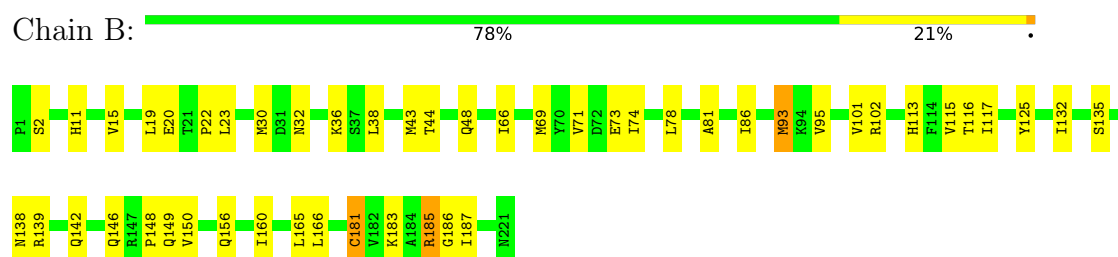
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

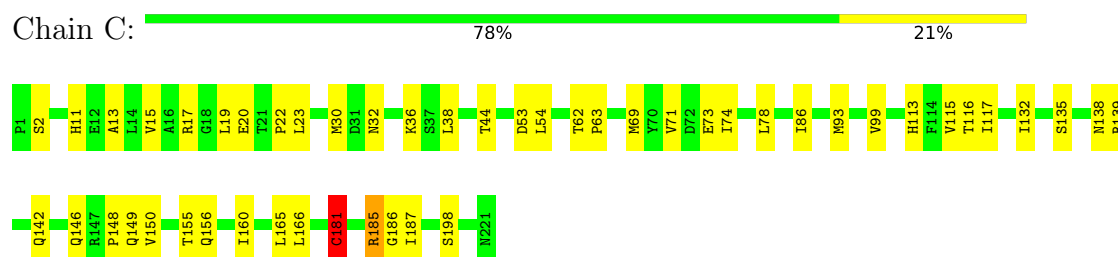
• Molecule 1: GTP CYCLOHYDROLASE I



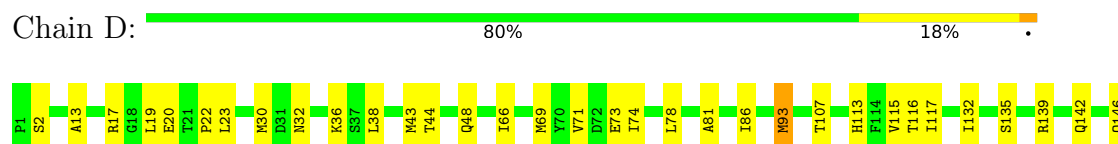
• Molecule 1: GTP CYCLOHYDROLASE I

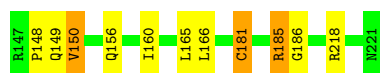


• Molecule 1: GTP CYCLOHYDROLASE I



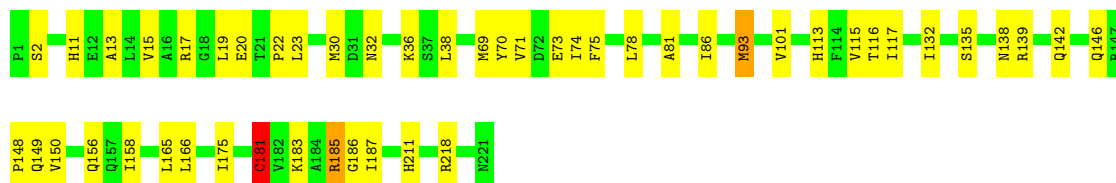
• Molecule 1: GTP CYCLOHYDROLASE I





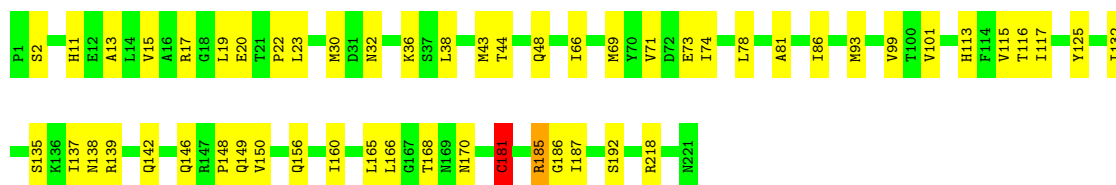
• Molecule 1: GTP CYCLOHYDROLASE I

Chain E: 78% 21%



• Molecule 1: GTP CYCLOHYDROLASE I

Chain F: 76% 24%



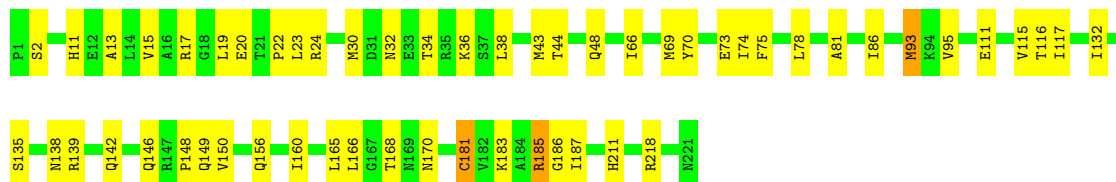
• Molecule 1: GTP CYCLOHYDROLASE I

Chain G: 80% 19%



• Molecule 1: GTP CYCLOHYDROLASE I

Chain H: 75% 24%



• Molecule 1: GTP CYCLOHYDROLASE I

Chain I: 79% 20%





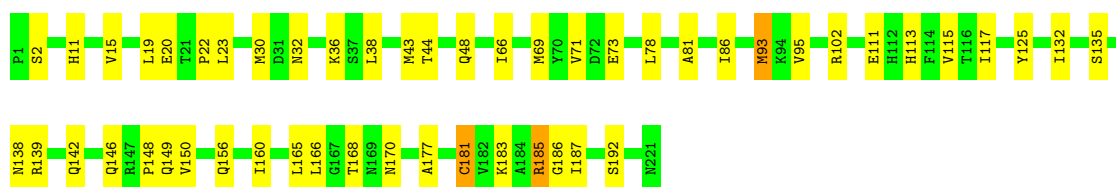
• Molecule 1: GTP CYCLOHYDROLASE I

Chain J: 80% 19%



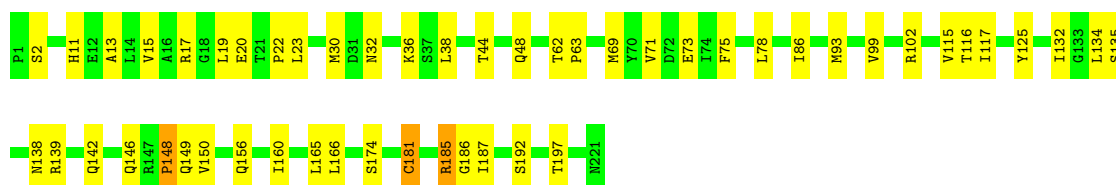
• Molecule 1: GTP CYCLOHYDROLASE I

Chain K: 77% 22%



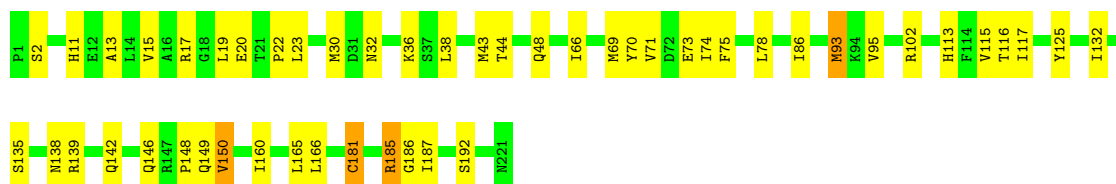
• Molecule 1: GTP CYCLOHYDROLASE I

Chain L: 77% 22%



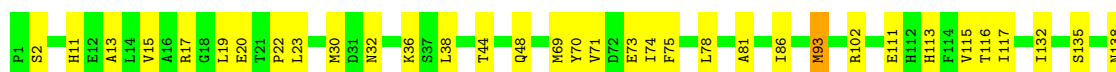
• Molecule 1: GTP CYCLOHYDROLASE I

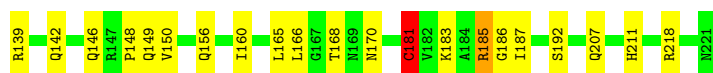
Chain M: 77% 21%



• Molecule 1: GTP CYCLOHYDROLASE I

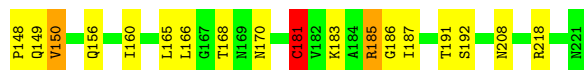
Chain N: 75% 24%





• Molecule 1: GTP CYCLOHYDROLASE I

Chain O: 77% 21%



• Molecule 1: GTP CYCLOHYDROLASE I

Chain P: 75% 24%



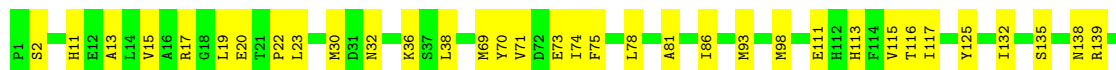
• Molecule 1: GTP CYCLOHYDROLASE I

Chain Q: 76% 24%



• Molecule 1: GTP CYCLOHYDROLASE I

Chain R: 78% 22%



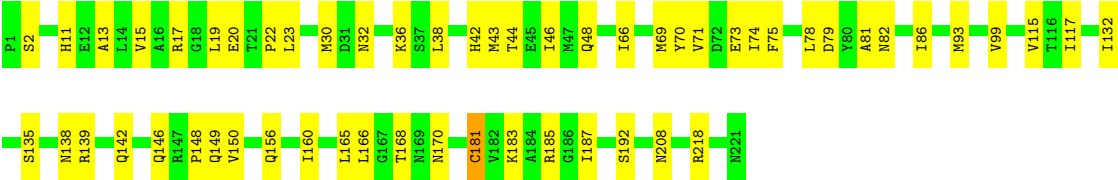
• Molecule 1: GTP CYCLOHYDROLASE I

Chain S: 81% 17%





● Molecule 1: GTP CYCLOHYDROLASE I



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	204.20Å 210.40Å 71.80Å 90.00° 95.80° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	92.5 (6.00-3.00)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	43780	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: SO4

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	0.52	0/1760	1.05	13/2384 (0.5%)
1	B	0.51	0/1760	1.03	12/2384 (0.5%)
1	C	0.51	0/1760	1.03	10/2384 (0.4%)
1	D	0.53	0/1760	1.04	10/2384 (0.4%)
1	E	0.52	0/1760	1.03	12/2384 (0.5%)
1	F	0.50	0/1760	1.03	11/2384 (0.5%)
1	G	0.52	0/1760	1.04	10/2384 (0.4%)
1	H	0.53	0/1760	1.04	11/2384 (0.5%)
1	I	0.51	0/1760	1.02	10/2384 (0.4%)
1	J	0.51	0/1760	1.03	12/2384 (0.5%)
1	K	0.50	0/1760	1.03	11/2384 (0.5%)
1	L	0.49	0/1760	1.03	9/2384 (0.4%)
1	M	0.52	0/1760	1.04	9/2384 (0.4%)
1	N	0.52	0/1760	1.03	12/2384 (0.5%)
1	O	0.51	0/1760	1.04	11/2384 (0.5%)
1	P	0.50	0/1760	1.04	14/2384 (0.6%)
1	Q	0.48	0/1760	1.03	9/2384 (0.4%)
1	R	0.52	0/1760	1.03	11/2384 (0.5%)
1	S	0.52	0/1760	1.03	8/2384 (0.3%)
1	T	0.50	0/1760	1.03	11/2384 (0.5%)
All	All	0.51	0/35200	1.03	216/47680 (0.5%)

There are no bond length outliers.

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	150	VAL	N-CA-C	-10.35	92.36	107.78
1	A	150	VAL	N-CA-C	-9.98	92.91	107.78
1	D	150	VAL	N-CA-C	-9.93	92.98	107.78
1	M	150	VAL	N-CA-C	-9.87	93.08	107.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	150	VAL	N-CA-C	-9.81	93.16	107.78
1	R	150	VAL	N-CA-C	-9.76	93.24	107.78
1	C	150	VAL	N-CA-C	-9.61	93.46	107.78
1	I	150	VAL	N-CA-C	-9.60	93.47	107.78
1	T	150	VAL	N-CA-C	-9.54	93.57	107.78
1	L	150	VAL	N-CA-C	-9.53	93.58	107.78
1	G	150	VAL	N-CA-C	-9.52	93.59	107.78
1	N	150	VAL	N-CA-C	-9.39	93.78	107.78
1	J	150	VAL	N-CA-C	-9.07	94.26	107.78
1	E	150	VAL	N-CA-C	-9.01	94.35	107.78
1	P	150	VAL	N-CA-C	-8.98	94.39	107.78
1	H	150	VAL	N-CA-C	-8.94	94.45	107.78
1	S	150	VAL	N-CA-C	-8.73	94.78	107.78
1	P	181	CYS	N-CA-C	-7.82	102.72	111.71
1	M	148	PRO	N-CA-C	-7.58	98.59	110.50
1	B	148	PRO	N-CA-C	-7.55	98.64	110.50
1	K	150	VAL	N-CA-C	-7.51	93.72	109.34
1	B	150	VAL	N-CA-C	-7.49	93.77	109.34
1	F	150	VAL	N-CA-C	-7.48	93.78	109.34
1	C	148	PRO	N-CA-C	-7.47	98.76	110.50
1	A	148	PRO	N-CA-C	-7.41	98.86	110.50
1	S	148	PRO	N-CA-C	-7.38	98.91	110.50
1	O	148	PRO	N-CA-C	-7.36	98.94	110.50
1	G	148	PRO	N-CA-C	-7.34	98.97	110.50
1	L	181	CYS	N-CA-C	-7.27	103.36	111.28
1	T	148	PRO	N-CA-C	-7.24	99.13	110.50
1	Q	73	GLU	N-CA-C	7.22	120.40	108.48
1	K	148	PRO	N-CA-C	-7.21	99.18	110.50
1	J	148	PRO	N-CA-C	-7.20	99.19	110.50
1	T	73	GLU	N-CA-C	7.16	120.30	108.48
1	P	148	PRO	N-CA-C	-7.15	99.27	110.50
1	I	148	PRO	N-CA-C	-7.15	99.27	110.50
1	R	148	PRO	N-CA-C	-7.13	99.30	110.50
1	F	73	GLU	N-CA-C	7.11	120.21	108.48
1	R	73	GLU	N-CA-C	7.09	120.17	108.48
1	S	73	GLU	N-CA-C	7.08	120.16	108.48
1	D	148	PRO	N-CA-C	-7.07	99.40	110.50
1	L	148	PRO	N-CA-C	-7.06	99.42	110.50
1	N	148	PRO	N-CA-C	-6.97	99.56	110.50
1	H	148	PRO	N-CA-C	-6.96	99.58	110.50
1	M	73	GLU	N-CA-C	6.90	119.86	108.48
1	H	73	GLU	N-CA-C	6.89	119.85	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	73	GLU	N-CA-C	6.87	119.81	108.48
1	B	73	GLU	N-CA-C	6.84	119.77	108.48
1	E	148	PRO	N-CA-C	-6.80	99.82	110.50
1	K	73	GLU	N-CA-C	6.80	119.69	108.48
1	A	181	CYS	N-CA-C	-6.78	103.92	111.71
1	Q	117	ILE	N-CA-C	-6.75	97.90	107.75
1	S	117	ILE	N-CA-C	-6.73	97.81	107.77
1	O	181	CYS	N-CA-C	-6.71	104.00	111.71
1	Q	148	PRO	N-CA-C	-6.69	99.99	110.50
1	S	181	CYS	N-CA-C	-6.69	104.02	111.71
1	Q	181	CYS	N-CA-C	-6.68	104.02	111.71
1	E	73	GLU	N-CA-C	6.68	119.50	108.48
1	C	73	GLU	N-CA-C	6.68	119.50	108.48
1	F	117	ILE	N-CA-C	-6.60	98.00	107.77
1	J	181	CYS	N-CA-C	-6.58	104.11	111.28
1	I	73	GLU	N-CA-C	6.56	119.31	108.48
1	K	181	CYS	N-CA-C	-6.55	104.14	111.28
1	T	71	VAL	N-CA-C	6.51	116.67	110.42
1	N	73	GLU	N-CA-C	6.51	119.22	108.48
1	L	73	GLU	N-CA-C	6.48	119.17	108.48
1	D	73	GLU	N-CA-C	6.46	119.13	108.48
1	E	181	CYS	N-CA-C	-6.44	104.30	111.71
1	H	181	CYS	N-CA-C	-6.44	104.31	111.71
1	P	117	ILE	N-CA-C	-6.41	98.28	107.77
1	N	181	CYS	N-CA-C	-6.36	104.39	111.71
1	I	117	ILE	N-CA-C	-6.30	98.44	107.77
1	K	117	ILE	N-CA-C	-6.29	98.45	107.77
1	O	73	GLU	N-CA-C	6.29	118.87	108.48
1	G	181	CYS	N-CA-C	-6.27	104.49	111.71
1	C	181	CYS	N-CA-C	-6.25	104.52	111.71
1	T	181	CYS	N-CA-C	-6.23	104.55	111.71
1	I	71	VAL	N-CA-C	6.21	116.38	110.42
1	B	149	GLN	N-CA-C	6.20	118.62	109.69
1	B	181	CYS	N-CA-C	-6.19	104.59	111.71
1	S	81	ALA	N-CA-C	-6.18	105.70	113.18
1	O	117	ILE	N-CA-C	-6.17	98.75	107.75
1	G	73	GLU	N-CA-C	6.13	118.59	108.48
1	D	71	VAL	N-CA-C	6.11	116.28	110.42
1	C	149	GLN	N-CA-C	6.10	118.47	109.69
1	J	117	ILE	N-CA-C	-6.09	98.86	107.75
1	N	71	VAL	N-CA-C	6.09	116.25	110.53
1	M	181	CYS	N-CA-C	-6.08	104.71	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	181	CYS	N-CA-C	-6.06	104.74	111.71
1	D	149	GLN	N-CA-C	6.06	118.41	109.69
1	R	81	ALA	N-CA-C	-6.04	105.40	112.89
1	R	71	VAL	N-CA-C	6.04	116.21	110.53
1	H	117	ILE	N-CA-C	-6.02	98.86	107.77
1	K	71	VAL	N-CA-C	5.98	116.16	110.42
1	J	116	THR	N-CA-C	5.98	118.67	110.24
1	M	117	ILE	N-CA-C	-5.98	99.02	107.75
1	A	73	GLU	N-CA-C	5.97	118.33	108.48
1	E	71	VAL	N-CA-C	5.96	116.13	110.53
1	K	81	ALA	N-CA-C	-5.96	105.97	113.18
1	F	148	PRO	N-CA-C	-5.95	100.21	112.47
1	H	116	THR	N-CA-C	5.95	118.63	110.24
1	S	116	THR	N-CA-C	5.94	118.62	110.24
1	I	181	CYS	N-CA-C	-5.94	104.88	111.71
1	P	73	GLU	N-CA-C	5.94	118.28	108.48
1	D	117	ILE	N-CA-C	-5.93	98.99	107.77
1	J	71	VAL	N-CA-C	5.91	116.10	110.42
1	B	117	ILE	N-CA-C	-5.91	99.13	107.75
1	E	117	ILE	N-CA-C	-5.89	99.06	107.77
1	C	117	ILE	N-CA-C	-5.88	99.17	107.75
1	P	149	GLN	N-CA-C	5.88	118.15	109.69
1	G	149	GLN	N-CA-C	5.87	118.14	109.69
1	L	117	ILE	N-CA-C	-5.86	99.19	107.75
1	Q	149	GLN	N-CA-C	5.86	118.12	109.69
1	D	181	CYS	N-CA-C	-5.86	104.98	111.71
1	G	117	ILE	N-CA-C	-5.82	99.16	107.77
1	E	149	GLN	N-CA-C	5.82	118.07	109.69
1	F	149	GLN	N-CA-C	5.81	118.05	109.69
1	C	116	THR	N-CA-C	5.80	118.42	110.24
1	R	117	ILE	N-CA-C	-5.80	99.28	107.75
1	O	71	VAL	N-CA-C	5.80	115.99	110.42
1	R	181	CYS	N-CA-C	-5.80	105.04	111.71
1	L	116	THR	N-CA-C	5.78	118.61	110.23
1	Q	71	VAL	N-CA-C	5.77	115.96	110.42
1	D	116	THR	N-CA-C	5.76	118.37	110.24
1	K	149	GLN	N-CA-C	5.75	117.97	109.69
1	H	149	GLN	N-CA-C	5.74	117.95	109.69
1	N	149	GLN	N-CA-C	5.74	117.95	109.69
1	A	116	THR	N-CA-C	5.73	118.54	110.23
1	O	183	LYS	N-CA-C	5.71	118.37	111.40
1	G	81	ALA	N-CA-C	-5.71	106.27	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	VAL	N-CA-C	5.71	115.90	110.42
1	N	81	ALA	N-CA-C	-5.71	106.27	113.18
1	A	117	ILE	N-CA-C	-5.71	99.42	107.75
1	F	71	VAL	N-CA-C	5.67	115.87	110.42
1	B	116	THR	N-CA-C	5.66	118.22	110.24
1	D	81	ALA	N-CA-C	-5.66	106.22	113.01
1	P	81	ALA	N-CA-C	-5.65	106.34	113.18
1	J	149	GLN	N-CA-C	5.64	117.81	109.69
1	J	183	LYS	N-CA-C	5.63	118.27	111.40
1	N	117	ILE	N-CA-C	-5.63	99.44	107.77
1	B	81	ALA	N-CA-C	-5.62	106.38	113.18
1	S	149	GLN	N-CA-C	5.61	117.77	109.69
1	Q	183	LYS	N-CA-C	5.61	118.24	111.40
1	K	183	LYS	N-CA-C	5.60	118.24	111.40
1	J	101	VAL	N-CA-C	-5.59	99.10	107.37
1	M	116	THR	N-CA-C	5.57	118.31	110.23
1	M	149	GLN	N-CA-C	5.56	117.69	109.69
1	P	111	GLU	N-CA-C	5.51	119.10	112.38
1	D	74	ILE	N-CA-C	5.50	120.78	109.34
1	H	183	LYS	N-CA-C	5.48	118.08	111.40
1	P	183	LYS	N-CA-C	5.47	118.07	111.40
1	I	74	ILE	N-CA-C	5.43	120.64	109.34
1	M	71	VAL	N-CA-C	5.43	115.63	110.42
1	P	116	THR	N-CA-C	5.42	118.09	110.23
1	T	149	GLN	N-CA-C	5.41	117.48	109.69
1	H	81	ALA	N-CA-C	-5.40	106.19	112.89
1	T	81	ALA	N-CA-C	-5.39	106.54	113.01
1	L	71	VAL	N-CA-C	5.38	115.59	110.42
1	P	71	VAL	N-CA-C	5.38	115.58	110.42
1	C	99	VAL	N-CA-C	-5.36	100.67	108.17
1	B	183	LYS	N-CA-C	5.36	117.93	111.40
1	G	183	LYS	N-CA-C	5.35	117.93	111.40
1	P	74	ILE	N-CA-C	5.33	120.43	109.34
1	R	149	GLN	N-CA-C	5.33	117.36	109.69
1	A	99	VAL	N-CA-C	-5.33	100.72	108.17
1	E	116	THR	N-CA-C	5.32	117.75	110.24
1	T	99	VAL	N-CA-C	-5.32	100.73	108.17
1	L	149	GLN	N-CA-C	5.31	117.34	109.69
1	F	74	ILE	N-CA-C	5.31	119.54	111.89
1	T	117	ILE	N-CA-C	-5.31	100.00	107.75
1	B	101	VAL	N-CA-C	-5.30	99.52	107.37
1	A	101	VAL	N-CA-C	-5.30	99.53	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	99	VAL	N-CA-C	-5.30	100.75	108.17
1	E	81	ALA	N-CA-C	-5.29	106.77	113.18
1	I	116	THR	N-CA-C	5.29	117.70	110.24
1	E	74	ILE	N-CA-C	5.28	120.32	109.34
1	R	74	ILE	N-CA-C	5.27	120.29	109.34
1	G	116	THR	N-CA-C	5.26	117.66	110.24
1	A	149	GLN	N-CA-C	5.26	117.26	109.69
1	E	183	LYS	N-CA-C	5.26	117.81	111.40
1	N	111	GLU	N-CA-C	5.26	118.80	112.38
1	C	71	VAL	N-CA-C	5.26	115.47	110.42
1	A	74	ILE	N-CA-C	5.24	120.25	109.34
1	F	99	VAL	N-CA-C	-5.24	100.83	108.17
1	A	71	VAL	N-CA-C	5.24	115.45	110.42
1	G	74	ILE	N-CA-C	5.24	120.24	109.34
1	J	74	ILE	N-CA-C	5.23	120.22	109.34
1	P	99	VAL	N-CA-C	-5.23	100.84	108.17
1	N	74	ILE	N-CA-C	5.23	120.21	109.34
1	K	111	GLU	N-CA-C	5.20	118.73	112.38
1	N	116	THR	N-CA-C	5.20	117.57	110.24
1	F	81	ALA	N-CA-C	-5.17	106.23	112.54
1	Q	116	THR	N-CA-C	5.17	117.73	110.23
1	B	74	ILE	N-CA-C	5.16	120.08	109.34
1	N	183	LYS	N-CA-C	5.16	117.69	111.40
1	I	183	LYS	N-CA-C	5.16	117.69	111.40
1	J	99	VAL	N-CA-C	-5.14	100.97	108.17
1	T	74	ILE	N-CA-C	5.14	120.03	109.34
1	E	101	VAL	N-CA-C	-5.13	99.78	107.37
1	H	111	GLU	N-CA-C	5.12	118.63	112.38
1	O	149	GLN	N-CA-C	5.12	117.06	109.69
1	O	191	THR	N-CA-C	5.11	120.37	114.04
1	K	177	ALA	N-CA-C	5.10	116.82	109.07
1	O	74	ILE	N-CA-C	5.10	119.94	109.34
1	O	116	THR	N-CA-C	5.10	117.62	110.23
1	R	116	THR	N-CA-C	5.10	117.62	110.23
1	C	74	ILE	N-CA-C	5.09	119.92	109.34
1	M	74	ILE	N-CA-C	5.08	119.90	109.34
1	P	101	VAL	N-CA-C	-5.05	99.90	107.37
1	T	183	LYS	N-CA-C	5.04	117.75	111.24
1	A	177	ALA	N-CA-C	5.03	116.72	109.07
1	R	111	GLU	N-CA-C	5.03	118.52	112.38
1	H	74	ILE	N-CA-C	5.02	119.78	109.34
1	I	101	VAL	N-CA-C	-5.01	99.95	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ALA	N-CA-C	-5.01	106.43	112.54
1	F	116	THR	N-CA-C	5.00	117.48	110.23

There are no chirality outliers.

There are no planarity outliers.

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	1732	404	1766	28	0
1	B	1732	404	1766	28	0
1	C	1732	404	1766	28	0
1	D	1732	404	1766	23	0
1	E	1732	404	1766	22	0
1	F	1732	404	1766	27	0
1	G	1732	404	1766	24	0
1	H	1732	404	1766	33	0
1	I	1732	404	1766	26	0
1	J	1732	404	1766	19	0
1	K	1732	404	1766	30	0
1	L	1732	404	1766	30	0
1	M	1732	404	1766	31	0
1	N	1732	404	1766	30	0
1	O	1732	404	1766	30	0
1	P	1732	404	1766	32	0
1	Q	1732	404	1766	28	0
1	R	1732	404	1766	26	0
1	S	1732	404	1766	25	0
1	T	1732	404	1766	31	0
2	A	10	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	10	0	0	0	0
2	N	5	0	0	0	0
2	O	5	0	0	0	0
2	P	5	0	0	0	0
2	Q	5	0	0	0	0
2	R	5	0	0	0	0
2	S	5	0	0	0	0
2	T	5	0	0	0	0
3	A	16	32	0	0	0
3	B	14	28	0	0	0
3	C	18	36	0	0	0
3	D	16	32	0	0	0
3	E	16	32	0	0	0
3	F	16	32	0	0	0
3	G	16	32	0	0	0
3	H	16	32	0	0	0
3	I	16	32	0	0	0
3	J	16	32	0	0	0
3	K	15	30	0	0	0
3	L	17	34	0	1	0
3	M	15	30	0	0	0
3	N	17	34	0	0	0
3	O	16	32	0	0	0
3	P	17	34	0	0	0
3	Q	15	30	0	1	0
3	R	17	34	0	0	0
3	S	16	32	0	0	0
3	T	15	30	0	0	0
All	All	35060	8720	35320	463	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 7.

All (463) 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:O:86:ILE:HG12	1:O:165:LEU:HD13	1.68	0.76
1:R:19:LEU:HD21	1:S:93:MET:HA	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:86:ILE:HG12	1:N:165:LEU:HD13	1.67	0.75
1:G:19:LEU:HD21	1:H:93:MET:HA	1.71	0.72
1:A:86:ILE:HG12	1:A:165:LEU:HD13	1.73	0.71
1:P:86:ILE:HG12	1:P:165:LEU:HD13	1.74	0.70
1:E:86:ILE:HG12	1:E:165:LEU:HD13	1.75	0.68
1:C:86:ILE:HG12	1:C:165:LEU:HD13	1.74	0.68
1:S:86:ILE:HG12	1:S:165:LEU:HD13	1.75	0.67
1:K:86:ILE:HG12	1:K:165:LEU:HD13	1.75	0.67
1:L:23:LEU:HD21	1:L:78:LEU:HD22	1.76	0.67
1:N:187:ILE:HD12	1:O:139:ARG:HG2	1.77	0.67
1:I:86:ILE:HG12	1:I:165:LEU:HD13	1.75	0.67
1:L:19:LEU:HD21	1:M:93:MET:HA	1.76	0.67
1:H:187:ILE:HD12	1:I:139:ARG:HG2	1.77	0.67
1:K:23:LEU:HD21	1:K:78:LEU:HD22	1.76	0.66
1:R:19:LEU:CD2	1:S:93:MET:HA	2.25	0.65
1:J:86:ILE:HG12	1:J:165:LEU:HD13	1.78	0.65
1:I:135:SER:O	1:I:139:ARG:HG3	1.98	0.64
1:Q:142:GLN:O	1:Q:146:GLN:HG2	1.97	0.64
1:S:187:ILE:HD12	1:T:139:ARG:HG2	1.78	0.64
1:B:86:ILE:HG12	1:B:165:LEU:HD13	1.79	0.64
1:L:86:ILE:HG12	1:L:165:LEU:HD13	1.81	0.63
1:F:86:ILE:HG12	1:F:165:LEU:HD13	1.81	0.62
1:C:19:LEU:HD21	1:D:93:MET:HA	1.81	0.62
1:M:142:GLN:O	1:M:146:GLN:HG2	2.00	0.62
1:Q:86:ILE:HG12	1:Q:165:LEU:HD13	1.81	0.62
1:D:86:ILE:HG12	1:D:165:LEU:HD13	1.80	0.61
1:G:19:LEU:CD2	1:H:93:MET:HA	2.30	0.61
1:L:19:LEU:CD2	1:M:93:MET:HA	2.31	0.61
1:I:23:LEU:HD21	1:I:78:LEU:HD22	1.83	0.60
1:D:23:LEU:HD21	1:D:78:LEU:HD22	1.82	0.60
1:R:86:ILE:HG12	1:R:165:LEU:HD13	1.82	0.60
1:P:93:MET:HA	1:T:19:LEU:HD21	1.83	0.60
1:E:142:GLN:O	1:E:146:GLN:HG2	2.01	0.60
1:O:23:LEU:HD21	1:O:78:LEU:HD22	1.83	0.60
1:P:23:LEU:HD21	1:P:78:LEU:HD22	1.83	0.60
1:H:30:MET:HE1	1:H:38:LEU:CD1	2.31	0.60
1:L:142:GLN:O	1:L:146:GLN:HG2	2.02	0.60
1:T:86:ILE:HG12	1:T:165:LEU:HD13	1.84	0.60
1:D:142:GLN:O	1:D:146:GLN:HG2	2.02	0.59
1:S:30:MET:HE1	1:S:38:LEU:CD1	2.32	0.59
1:C:23:LEU:HD21	1:C:78:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:142:GLN:O	1:H:146:GLN:HG2	2.02	0.59
1:I:142:GLN:O	1:I:146:GLN:HG2	2.02	0.59
1:S:135:SER:O	1:S:139:ARG:HG3	2.02	0.59
1:T:23:LEU:HD21	1:T:78:LEU:HD22	1.85	0.59
1:B:142:GLN:O	1:B:146:GLN:HG2	2.02	0.58
1:T:135:SER:O	1:T:139:ARG:HG3	2.03	0.58
1:M:23:LEU:HD21	1:M:78:LEU:HD22	1.83	0.58
1:G:86:ILE:HG12	1:G:165:LEU:HD13	1.84	0.58
1:Q:135:SER:O	1:Q:139:ARG:HG3	2.04	0.58
1:R:23:LEU:HD21	1:R:78:LEU:HD22	1.84	0.58
1:C:19:LEU:CD2	1:D:93:MET:HA	2.33	0.58
1:S:142:GLN:O	1:S:146:GLN:HG2	2.03	0.58
1:E:115:VAL:HG21	1:F:69:MET:HE1	1.86	0.58
1:F:135:SER:O	1:F:139:ARG:HG3	2.04	0.58
1:C:142:GLN:O	1:C:146:GLN:HG2	2.04	0.58
1:N:69:MET:HE1	1:Q:115:VAL:HG21	1.86	0.58
1:N:142:GLN:O	1:N:146:GLN:HG2	2.04	0.58
1:B:11:HIS:O	1:B:15:VAL:HG23	2.05	0.57
1:O:135:SER:O	1:O:139:ARG:HG3	2.03	0.57
1:B:135:SER:O	1:B:139:ARG:HG3	2.04	0.57
1:M:86:ILE:HG12	1:M:165:LEU:HD13	1.86	0.57
1:H:135:SER:O	1:H:139:ARG:HG3	2.04	0.57
1:C:32:ASN:O	1:C:36:LYS:HG3	2.05	0.57
1:N:23:LEU:HD21	1:N:78:LEU:HD22	1.86	0.57
1:B:23:LEU:HD21	1:B:78:LEU:HD22	1.86	0.56
1:J:23:LEU:HD21	1:J:78:LEU:HD22	1.87	0.56
1:G:23:LEU:HD21	1:G:78:LEU:HD22	1.86	0.56
1:C:115:VAL:HG21	1:H:69:MET:HE1	1.88	0.56
1:H:23:LEU:HD21	1:H:78:LEU:HD22	1.86	0.56
1:Q:19:LEU:HD12	1:Q:160:ILE:HD11	1.88	0.56
1:A:142:GLN:O	1:A:146:GLN:HG2	2.05	0.56
1:C:135:SER:O	1:C:139:ARG:HG3	2.06	0.56
1:E:23:LEU:HD21	1:E:78:LEU:HD22	1.87	0.56
1:F:23:LEU:HD21	1:F:78:LEU:HD22	1.87	0.56
1:K:11:HIS:O	1:K:15:VAL:HG23	2.06	0.56
1:L:135:SER:O	1:L:139:ARG:HG3	2.06	0.56
1:M:135:SER:O	1:M:139:ARG:HG3	2.06	0.56
1:E:69:MET:HE1	1:F:115:VAL:HG21	1.88	0.56
1:C:11:HIS:O	1:C:15:VAL:HG23	2.06	0.55
1:A:115:VAL:HG21	1:J:69:MET:HE1	1.89	0.55
1:K:142:GLN:O	1:K:146:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:HIS:O	1:G:15:VAL:HG23	2.06	0.55
1:P:93:MET:HA	1:T:19:LEU:CD2	2.36	0.55
1:K:93:MET:HA	1:O:19:LEU:CD2	2.37	0.55
1:M:115:VAL:HG21	1:R:69:MET:HE1	1.88	0.55
1:A:135:SER:O	1:A:139:ARG:HG3	2.06	0.55
1:K:187:ILE:HD12	1:L:139:ARG:HG2	1.88	0.55
1:N:115:VAL:HG21	1:Q:69:MET:HE1	1.88	0.55
1:I:19:LEU:HD21	1:J:93:MET:HA	1.88	0.55
1:E:30:MET:HE1	1:E:38:LEU:HD11	1.89	0.55
1:H:30:MET:HE1	1:H:38:LEU:HD11	1.89	0.55
1:A:23:LEU:HD21	1:A:78:LEU:HD22	1.87	0.55
1:H:86:ILE:HG12	1:H:165:LEU:HD13	1.88	0.55
1:R:135:SER:O	1:R:139:ARG:HG3	2.08	0.54
1:L:115:VAL:HG21	1:S:69:MET:HE1	1.90	0.54
1:S:23:LEU:HD21	1:S:78:LEU:HD22	1.89	0.54
1:A:30:MET:HE1	1:A:38:LEU:HD11	1.90	0.54
1:J:142:GLN:O	1:J:146:GLN:HG2	2.08	0.54
1:R:142:GLN:O	1:R:146:GLN:HG2	2.07	0.54
1:T:142:GLN:O	1:T:146:GLN:HG2	2.07	0.54
1:A:19:LEU:CD2	1:B:93:MET:HA	2.39	0.53
1:G:30:MET:HE1	1:G:38:LEU:CD1	2.38	0.53
1:G:30:MET:HE1	1:G:38:LEU:HD11	1.91	0.53
1:P:11:HIS:O	1:P:15:VAL:HG23	2.09	0.53
1:J:135:SER:O	1:J:139:ARG:HG3	2.08	0.53
1:K:93:MET:HA	1:O:19:LEU:HD21	1.90	0.53
1:H:34:THR:HG22	1:P:38:LEU:HD23	1.89	0.53
1:J:11:HIS:O	1:J:15:VAL:HG23	2.10	0.52
1:K:135:SER:O	1:K:139:ARG:HG3	2.10	0.52
1:A:69:MET:HE1	1:J:115:VAL:HG21	1.92	0.52
1:Q:11:HIS:O	1:Q:15:VAL:HG23	2.09	0.52
1:O:69:MET:HE1	1:P:115:VAL:HG21	1.92	0.52
1:H:32:ASN:O	1:H:36:LYS:HG3	2.09	0.51
1:L:32:ASN:O	1:L:36:LYS:HG3	2.10	0.51
1:D:135:SER:O	1:D:139:ARG:HG3	2.10	0.51
1:K:43:MET:HE2	1:K:66:ILE:CD1	2.41	0.51
1:F:32:ASN:O	1:F:36:LYS:HG3	2.10	0.51
1:Q:132:ILE:HB	1:Q:166:LEU:HD21	1.91	0.51
1:F:142:GLN:O	1:F:146:GLN:HG2	2.09	0.51
1:B:30:MET:HE1	1:B:38:LEU:CD1	2.41	0.51
1:K:115:VAL:HG21	1:T:69:MET:HE1	1.93	0.51
1:G:70:TYR:O	1:G:75:PHE:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:32:ASN:O	1:Q:36:LYS:HG3	2.11	0.51
1:A:32:ASN:O	1:A:36:LYS:HG3	2.10	0.51
1:Q:30:MET:HE1	1:Q:38:LEU:CD1	2.41	0.51
1:P:32:ASN:O	1:P:36:LYS:HG3	2.10	0.51
1:F:19:LEU:HD12	1:F:160:ILE:HD11	1.93	0.50
1:K:69:MET:HE1	1:T:115:VAL:HG21	1.93	0.50
1:S:30:MET:HE1	1:S:38:LEU:HD11	1.92	0.50
1:J:32:ASN:O	1:J:36:LYS:HG3	2.11	0.50
1:S:11:HIS:O	1:S:15:VAL:HG23	2.10	0.50
1:B:187:ILE:HD12	1:C:139:ARG:HG2	1.93	0.50
1:I:138:ASN:H	1:I:138:ASN:HD22	1.60	0.50
1:P:13:ALA:O	1:P:17:ARG:HD3	2.12	0.50
1:I:19:LEU:CD2	1:J:93:MET:HA	2.42	0.50
1:I:30:MET:HE1	1:I:38:LEU:HD11	1.94	0.50
1:A:139:ARG:HG2	1:E:187:ILE:HD12	1.94	0.50
1:I:30:MET:HE1	1:I:38:LEU:CD1	2.42	0.50
1:N:19:LEU:HD13	1:N:156:GLN:HB3	1.93	0.50
1:O:142:GLN:O	1:O:146:GLN:HG2	2.11	0.50
1:O:32:ASN:O	1:O:36:LYS:HG3	2.11	0.50
1:T:30:MET:HE1	1:T:38:LEU:CD1	2.42	0.50
1:A:19:LEU:HD12	1:A:160:ILE:HD11	1.94	0.49
1:E:135:SER:O	1:E:139:ARG:HG3	2.12	0.49
1:M:30:MET:HE1	1:M:38:LEU:CD1	2.42	0.49
1:S:19:LEU:HD12	1:S:160:ILE:CD1	2.41	0.49
1:S:19:LEU:HD12	1:S:160:ILE:HD11	1.94	0.49
1:A:19:LEU:HD12	1:A:160:ILE:CD1	2.42	0.49
1:F:43:MET:HE2	1:F:66:ILE:CD1	2.42	0.49
1:G:135:SER:O	1:G:139:ARG:HG3	2.12	0.49
1:L:11:HIS:O	1:L:15:VAL:HG23	2.12	0.49
1:Q:23:LEU:HD21	1:Q:78:LEU:HD22	1.93	0.49
1:B:138:ASN:HD22	1:B:138:ASN:H	1.60	0.49
1:N:135:SER:O	1:N:139:ARG:HG3	2.13	0.49
1:B:69:MET:HE1	1:I:115:VAL:HG21	1.95	0.49
1:E:30:MET:HE1	1:E:38:LEU:CD1	2.43	0.49
1:J:19:LEU:HD12	1:J:160:ILE:HD11	1.93	0.49
1:K:30:MET:HE1	1:K:38:LEU:CD1	2.43	0.49
1:N:19:LEU:HD12	1:N:160:ILE:HD11	1.94	0.49
1:A:19:LEU:HD21	1:B:93:MET:HA	1.93	0.49
1:R:32:ASN:O	1:R:36:LYS:HG3	2.12	0.49
1:K:125:TYR:CD2	1:K:166:LEU:HD13	2.48	0.49
1:O:11:HIS:O	1:O:15:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:30:MET:HE1	1:R:38:LEU:HD11	1.95	0.49
1:F:19:LEU:HD12	1:F:160:ILE:CD1	2.43	0.48
1:K:43:MET:HE2	1:K:66:ILE:HD12	1.95	0.48
1:P:44:THR:O	1:P:48:GLN:HG3	2.13	0.48
1:Q:113:HIS:HB2	1:Q:181:CYS:SG	2.52	0.48
1:Q:187:ILE:HD12	1:R:139:ARG:HG2	1.95	0.48
1:B:43:MET:HE2	1:B:66:ILE:CD1	2.43	0.48
1:F:30:MET:HE1	1:F:38:LEU:CD1	2.43	0.48
1:J:19:LEU:HD12	1:J:160:ILE:CD1	2.43	0.48
1:S:30:MET:HE2	1:S:34:THR:OG1	2.13	0.48
1:H:19:LEU:HD12	1:H:160:ILE:CD1	2.42	0.48
1:P:19:LEU:HD12	1:P:160:ILE:HD11	1.95	0.48
1:T:11:HIS:O	1:T:15:VAL:HG23	2.13	0.48
1:B:115:VAL:HG21	1:I:69:MET:HE1	1.95	0.48
1:C:30:MET:HE1	1:C:38:LEU:HD11	1.96	0.48
1:S:211:HIS:CE1	1:T:208:ASN:OD1	2.66	0.48
1:T:19:LEU:HD12	1:T:160:ILE:CD1	2.44	0.48
1:E:70:TYR:O	1:E:75:PHE:HB2	2.14	0.48
1:F:13:ALA:O	1:F:17:ARG:HD3	2.13	0.48
1:N:11:HIS:O	1:N:15:VAL:HG23	2.14	0.48
1:L:132:ILE:HB	1:L:166:LEU:HD21	1.94	0.48
1:H:30:MET:HE2	1:H:34:THR:OG1	2.14	0.47
1:O:185:ARG:HD2	1:P:69:MET:HE2	1.95	0.47
1:M:11:HIS:O	1:M:15:VAL:HG23	2.14	0.47
1:S:30:MET:HE1	1:S:38:LEU:HD12	1.96	0.47
1:G:142:GLN:O	1:G:146:GLN:HG2	2.14	0.47
1:H:138:ASN:H	1:H:138:ASN:HD22	1.61	0.47
1:L:69:MET:HE1	1:S:115:VAL:HG21	1.96	0.47
1:F:30:MET:HE1	1:F:38:LEU:HD11	1.97	0.47
1:O:19:LEU:HD12	1:O:160:ILE:CD1	2.44	0.47
1:B:19:LEU:HD12	1:B:160:ILE:HD11	1.95	0.47
1:E:138:ASN:HD22	1:E:138:ASN:H	1.62	0.47
1:Q:19:LEU:HD13	1:Q:156:GLN:HB3	1.96	0.47
1:N:70:TYR:O	1:N:75:PHE:HB2	2.15	0.47
1:D:44:THR:O	1:D:48:GLN:HG3	2.14	0.47
1:I:32:ASN:O	1:I:36:LYS:HG3	2.15	0.47
1:M:32:ASN:O	1:M:36:LYS:HG3	2.15	0.47
1:N:19:LEU:HD12	1:N:160:ILE:CD1	2.44	0.47
1:N:32:ASN:O	1:N:36:LYS:HG3	2.15	0.47
1:N:132:ILE:HB	1:N:166:LEU:HD21	1.97	0.47
1:S:13:ALA:O	1:S:17:ARG:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:13:ALA:O	1:T:17:ARG:HD3	2.15	0.47
1:P:187:ILE:HD12	1:Q:139:ARG:HG2	1.96	0.47
1:C:19:LEU:HD12	1:C:160:ILE:CD1	2.45	0.47
1:A:30:MET:HE1	1:A:38:LEU:CD1	2.44	0.47
1:I:43:MET:HE2	1:I:66:ILE:CD1	2.45	0.47
1:J:44:THR:O	1:J:48:GLN:HG3	2.15	0.47
1:Q:125:TYR:CD2	1:Q:166:LEU:HD13	2.50	0.47
1:H:43:MET:HE2	1:H:66:ILE:CD1	2.45	0.46
1:N:168:THR:HG22	1:N:170:ASN:H	1.80	0.46
1:D:30:MET:HE1	1:D:38:LEU:CD1	2.45	0.46
1:F:101:VAL:HG21	1:F:137:ILE:HD12	1.97	0.46
1:G:32:ASN:O	1:G:36:LYS:HG3	2.15	0.46
1:C:69:MET:HE1	1:H:115:VAL:HG21	1.97	0.46
1:J:30:MET:HE1	1:J:38:LEU:CD1	2.45	0.46
1:T:30:MET:HE1	1:T:38:LEU:HD11	1.98	0.46
1:H:11:HIS:O	1:H:15:VAL:HG23	2.15	0.46
1:P:135:SER:O	1:P:139:ARG:HG3	2.15	0.46
1:T:44:THR:O	1:T:48:GLN:HG3	2.15	0.46
1:A:11:HIS:O	1:A:15:VAL:HG23	2.16	0.46
1:F:132:ILE:HB	1:F:166:LEU:HD21	1.97	0.46
1:Q:30:MET:HE1	1:Q:38:LEU:HD11	1.98	0.46
1:Q:43:MET:HE2	1:Q:66:ILE:CD1	2.46	0.46
1:B:30:MET:HE1	1:B:38:LEU:HD11	1.98	0.46
1:P:30:MET:HE1	1:P:38:LEU:CD1	2.45	0.46
1:C:138:ASN:H	1:C:138:ASN:HD22	1.64	0.46
1:F:138:ASN:H	1:F:138:ASN:HD22	1.63	0.46
1:H:13:ALA:O	1:H:17:ARG:HD3	2.16	0.46
1:L:19:LEU:HD12	1:L:160:ILE:HD11	1.98	0.46
1:E:132:ILE:HB	1:E:166:LEU:HD21	1.97	0.46
1:H:30:MET:HE1	1:H:38:LEU:HD12	1.98	0.46
1:N:30:MET:HE1	1:N:38:LEU:CD1	2.46	0.46
1:R:168:THR:HG22	1:R:170:ASN:H	1.80	0.46
1:H:132:ILE:HB	1:H:166:LEU:HD21	1.97	0.46
1:S:19:LEU:HD13	1:S:156:GLN:HB3	1.98	0.46
1:B:19:LEU:HD12	1:B:160:ILE:CD1	2.47	0.45
1:C:30:MET:HE1	1:C:38:LEU:CD1	2.46	0.45
1:F:19:LEU:HD13	1:F:156:GLN:HB3	1.98	0.45
1:R:30:MET:HE1	1:R:38:LEU:CD1	2.45	0.45
1:B:185:ARG:HG2	1:B:186:GLY:H	1.81	0.45
1:K:30:MET:HE1	1:K:38:LEU:HD11	1.99	0.45
1:C:187:ILE:HD12	1:D:139:ARG:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:19:LEU:HD12	1:H:160:ILE:HD11	1.99	0.45
1:O:115:VAL:HG21	1:P:69:MET:HE1	1.98	0.45
1:A:138:ASN:H	1:A:138:ASN:HD22	1.64	0.45
1:K:19:LEU:HD13	1:K:156:GLN:HB3	1.99	0.45
1:M:19:LEU:HD12	1:M:160:ILE:HD11	1.98	0.45
1:K:168:THR:HG22	1:K:170:ASN:H	1.81	0.45
1:N:30:MET:HE1	1:N:38:LEU:HD11	1.98	0.45
1:O:168:THR:HG22	1:O:170:ASN:H	1.81	0.45
1:M:13:ALA:O	1:M:17:ARG:HD3	2.17	0.45
1:C:53:ASP:HA	1:H:24:ARG:HG3	1.98	0.45
1:D:115:VAL:HG21	1:G:69:MET:HE1	1.98	0.45
1:M:69:MET:HE1	1:R:113:HIS:HB3	1.98	0.45
1:D:32:ASN:O	1:D:36:LYS:HG3	2.16	0.45
1:F:11:HIS:O	1:F:15:VAL:HG23	2.17	0.45
1:K:19:LEU:HD12	1:K:160:ILE:CD1	2.47	0.45
1:C:113:HIS:HB2	1:C:181:CYS:SG	2.57	0.45
1:L:75:PHE:CE1	1:L:148:PRO:HG3	2.52	0.45
1:T:19:LEU:HD12	1:T:160:ILE:HD11	1.98	0.45
1:E:11:HIS:O	1:E:15:VAL:HG23	2.17	0.45
1:I:11:HIS:O	1:I:15:VAL:HG23	2.17	0.45
1:A:185:ARG:HG2	1:A:186:GLY:N	2.32	0.44
1:F:113:HIS:HB2	1:F:181:CYS:SG	2.56	0.44
1:O:185:ARG:HG2	1:O:186:GLY:N	2.32	0.44
1:P:19:LEU:HD12	1:P:160:ILE:CD1	2.48	0.44
1:R:70:TYR:O	1:R:75:PHE:HB2	2.17	0.44
1:B:132:ILE:HB	1:B:166:LEU:HD21	1.99	0.44
1:J:13:ALA:O	1:J:17:ARG:HD3	2.17	0.44
1:Q:101:VAL:HG21	1:Q:137:ILE:HD12	1.98	0.44
1:T:42:HIS:O	1:T:46:ILE:HG13	2.17	0.44
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.86	0.44
1:M:69:MET:HE1	1:R:115:VAL:HG21	1.98	0.44
1:M:185:ARG:HD2	1:R:69:MET:HE2	1.99	0.44
1:I:19:LEU:HD12	1:I:160:ILE:CD1	2.48	0.44
1:Q:44:THR:O	1:Q:48:GLN:HG3	2.17	0.44
1:A:70:TYR:O	1:A:75:PHE:HB2	2.17	0.44
1:I:43:MET:HE2	1:I:66:ILE:HD12	1.99	0.44
1:K:93:MET:HB2	1:K:95:VAL:HG23	1.99	0.44
1:L:138:ASN:HD22	1:L:138:ASN:H	1.66	0.44
1:M:70:TYR:O	1:M:75:PHE:HB2	2.17	0.44
1:N:192:SER:HA	1:O:102:ARG:O	2.17	0.44
1:G:13:ALA:O	1:G:17:ARG:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:TYR:CD2	1:G:166:LEU:HD13	2.53	0.44
1:O:19:LEU:HD12	1:O:160:ILE:HD11	2.00	0.44
1:T:19:LEU:HD23	1:T:19:LEU:HA	1.81	0.44
1:B:19:LEU:HD13	1:B:156:GLN:HB3	1.99	0.44
1:F:192:SER:HA	1:G:102:ARG:O	2.17	0.44
1:H:19:LEU:HD13	1:H:156:GLN:HB3	2.00	0.44
1:P:19:LEU:HD13	1:P:156:GLN:HB3	2.00	0.44
1:C:13:ALA:O	1:C:17:ARG:HD3	2.17	0.44
1:I:19:LEU:HD13	1:I:156:GLN:HB3	1.99	0.44
1:L:13:ALA:O	1:L:17:ARG:HD3	2.17	0.44
1:P:93:MET:HB2	1:P:95:VAL:HG23	1.99	0.44
1:B:185:ARG:HG2	1:B:186:GLY:N	2.33	0.44
1:C:185:ARG:HD2	1:H:69:MET:HE2	1.99	0.44
1:K:138:ASN:H	1:K:138:ASN:HD22	1.66	0.44
1:N:13:ALA:O	1:N:17:ARG:HD3	2.18	0.44
1:A:30:MET:HE2	1:A:34:THR:OG1	2.18	0.43
1:N:207:GLN:HG3	1:O:208:ASN:OD1	2.17	0.43
1:T:19:LEU:HD13	1:T:156:GLN:HB3	1.99	0.43
1:T:132:ILE:HB	1:T:166:LEU:HD21	2.00	0.43
1:C:132:ILE:HB	1:C:166:LEU:HD21	1.99	0.43
1:H:211:HIS:CE1	1:I:208:ASN:OD1	2.70	0.43
1:P:138:ASN:H	1:P:138:ASN:HD22	1.66	0.43
1:Q:105:THR:HG23	3:Q:228:HOH:O	2.18	0.43
1:K:102:ARG:O	1:O:192:SER:HA	2.18	0.43
1:L:30:MET:HE1	1:L:38:LEU:CD1	2.48	0.43
1:L:187:ILE:HD13	1:M:138:ASN:HB3	2.01	0.43
1:M:44:THR:O	1:M:48:GLN:HG3	2.18	0.43
1:T:79:ASP:HB3	1:T:82:ASN:ND2	2.34	0.43
1:M:19:LEU:HD21	1:N:93:MET:HA	1.99	0.43
1:P:187:ILE:HD13	1:Q:138:ASN:HB3	2.00	0.43
1:R:11:HIS:O	1:R:15:VAL:HG23	2.19	0.43
1:E:185:ARG:HG2	1:E:186:GLY:H	1.84	0.43
1:M:30:MET:HE1	1:M:38:LEU:HD11	2.00	0.43
1:N:211:HIS:CE1	1:O:208:ASN:OD1	2.72	0.43
1:O:13:ALA:O	1:O:17:ARG:HD3	2.18	0.43
1:O:113:HIS:HB3	1:P:69:MET:HE1	2.00	0.43
1:R:13:ALA:O	1:R:17:ARG:HD3	2.18	0.43
1:D:132:ILE:HB	1:D:166:LEU:HD21	2.00	0.43
1:D:69:MET:HE1	1:G:115:VAL:HG21	2.01	0.43
1:J:138:ASN:HD22	1:J:138:ASN:H	1.67	0.43
1:L:125:TYR:CD2	1:L:166:LEU:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:113:HIS:HB2	1:O:181:CYS:SG	2.58	0.43
1:F:187:ILE:HD12	1:G:139:ARG:HG2	2.01	0.43
1:G:138:ASN:HD22	1:G:138:ASN:H	1.66	0.43
1:H:44:THR:O	1:H:48:GLN:HG3	2.18	0.43
1:Q:19:LEU:HD12	1:Q:160:ILE:CD1	2.48	0.43
1:D:185:ARG:HG2	1:D:186:GLY:N	2.33	0.43
1:E:13:ALA:O	1:E:17:ARG:HD3	2.19	0.43
1:F:19:LEU:HA	1:F:19:LEU:HD23	1.84	0.43
1:I:125:TYR:CD2	1:I:166:LEU:HD13	2.52	0.43
1:K:192:SER:HA	1:L:102:ARG:O	2.18	0.43
1:P:142:GLN:O	1:P:146:GLN:HG2	2.19	0.43
1:K:138:ASN:HB3	1:O:187:ILE:HD13	2.01	0.43
1:S:32:ASN:O	1:S:36:LYS:HG3	2.18	0.43
1:T:32:ASN:O	1:T:36:LYS:HG3	2.19	0.43
1:D:19:LEU:HD12	1:D:160:ILE:CD1	2.48	0.42
1:M:19:LEU:CD2	1:N:93:MET:HA	2.49	0.42
1:M:43:MET:HE2	1:M:66:ILE:CD1	2.49	0.42
1:P:132:ILE:HB	1:P:166:LEU:HD21	1.99	0.42
1:B:43:MET:HE2	1:B:66:ILE:HD12	2.00	0.42
1:G:187:ILE:HD12	1:H:139:ARG:HA	2.01	0.42
1:L:19:LEU:HD12	1:L:160:ILE:CD1	2.50	0.42
1:L:19:LEU:HD13	1:L:156:GLN:HB3	2.01	0.42
1:L:44:THR:O	1:L:48:GLN:HG3	2.19	0.42
1:L:185:ARG:HG2	1:L:186:GLY:N	2.34	0.42
1:N:44:THR:O	1:N:48:GLN:HG3	2.18	0.42
1:T:168:THR:HG22	1:T:170:ASN:H	1.83	0.42
1:G:75:PHE:CE1	1:G:148:PRO:HG3	2.55	0.42
1:I:13:ALA:O	1:I:17:ARG:HD3	2.19	0.42
1:L:192:SER:HA	1:M:102:ARG:O	2.18	0.42
1:O:30:MET:HE1	1:O:38:LEU:HD11	2.00	0.42
1:P:102:ARG:O	1:T:192:SER:HA	2.19	0.42
1:P:125:TYR:CD2	1:P:166:LEU:HD13	2.55	0.42
1:R:132:ILE:HB	1:R:166:LEU:HD21	2.00	0.42
1:A:168:THR:HG22	1:A:170:ASN:H	1.83	0.42
1:K:132:ILE:HB	1:K:166:LEU:HD21	2.01	0.42
1:E:32:ASN:O	1:E:36:LYS:HG3	2.19	0.42
1:A:132:ILE:HB	1:A:166:LEU:HD21	2.00	0.42
1:B:32:ASN:O	1:B:36:LYS:HG3	2.19	0.42
1:K:113:HIS:HB3	1:T:69:MET:HE1	2.02	0.42
1:K:185:ARG:HD2	1:T:69:MET:HE2	2.00	0.42
1:L:174:SER:CB	1:L:197:THR:HG22	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:185:ARG:HG2	1:M:186:GLY:N	2.34	0.42
1:K:185:ARG:HG2	1:K:186:GLY:H	1.84	0.42
1:M:113:HIS:HB3	1:R:69:MET:HE1	2.02	0.42
1:O:185:ARG:HG2	1:O:186:GLY:H	1.84	0.42
1:R:125:TYR:CD2	1:R:166:LEU:HD13	2.55	0.42
1:B:93:MET:HB2	1:B:95:VAL:HG23	2.02	0.42
1:B:125:TYR:CD2	1:B:166:LEU:HD13	2.55	0.42
1:D:43:MET:HE2	1:D:66:ILE:CD1	2.50	0.42
1:G:44:THR:O	1:G:48:GLN:HG3	2.19	0.42
1:M:125:TYR:CD2	1:M:166:LEU:HD13	2.55	0.42
1:N:138:ASN:HD22	1:N:138:ASN:H	1.67	0.42
1:R:138:ASN:H	1:R:138:ASN:HD22	1.68	0.42
1:C:155:THR:HG22	1:C:198:SER:OG	2.19	0.42
1:J:30:MET:HE2	1:J:34:THR:OG1	2.20	0.42
1:L:185:ARG:HG2	1:L:186:GLY:H	1.85	0.42
1:C:19:LEU:HA	1:C:19:LEU:HD23	1.86	0.41
1:F:125:TYR:CD2	1:F:166:LEU:HD13	2.55	0.41
1:K:44:THR:O	1:K:48:GLN:HG3	2.20	0.41
1:P:185:ARG:HG2	1:P:186:GLY:N	2.35	0.41
1:A:125:TYR:CD2	1:A:166:LEU:HD13	2.55	0.41
1:D:19:LEU:CD2	1:E:93:MET:HA	2.50	0.41
1:M:93:MET:HB2	1:M:95:VAL:HG23	2.02	0.41
1:O:132:ILE:HB	1:O:166:LEU:HD21	2.01	0.41
1:C:185:ARG:HG2	1:C:186:GLY:N	2.35	0.41
1:D:13:ALA:O	1:D:17:ARG:HD3	2.20	0.41
1:G:132:ILE:HB	1:G:166:LEU:HD21	2.01	0.41
1:N:113:HIS:HB2	1:N:181:CYS:SG	2.61	0.41
1:O:53:ASP:HA	1:P:24:ARG:HG3	2.00	0.41
1:D:113:HIS:HB3	1:G:69:MET:HE1	2.03	0.41
1:F:43:MET:HE2	1:F:66:ILE:HD13	2.01	0.41
1:F:168:THR:HG22	1:F:170:ASN:H	1.85	0.41
1:I:19:LEU:HD23	1:I:19:LEU:HA	1.83	0.41
1:J:19:LEU:HD13	1:J:156:GLN:HB3	2.03	0.41
1:P:43:MET:HE2	1:P:66:ILE:CD1	2.50	0.41
1:R:98:MET:HE1	1:R:213:PHE:HA	2.02	0.41
1:S:185:ARG:HG2	1:S:186:GLY:H	1.85	0.41
1:A:98:MET:HE1	1:A:213:PHE:HA	2.02	0.41
1:B:69:MET:HE1	1:I:113:HIS:HB3	2.01	0.41
1:N:185:ARG:HG2	1:N:186:GLY:H	1.86	0.41
1:R:19:LEU:HD21	1:S:93:MET:CA	2.42	0.41
1:H:168:THR:HG22	1:H:170:ASN:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:132:ILE:HB	1:I:166:LEU:HD21	2.02	0.41
1:K:187:ILE:HD13	1:L:138:ASN:HB3	2.02	0.41
1:T:43:MET:HE2	1:T:66:ILE:CD1	2.50	0.41
1:A:208:ASN:OD1	1:E:211:HIS:CE1	2.73	0.41
1:D:19:LEU:HD21	1:E:93:MET:HA	2.03	0.41
1:D:185:ARG:HD2	1:G:69:MET:HE2	2.02	0.41
1:O:19:LEU:HD13	1:O:156:GLN:HB3	2.03	0.41
1:Q:79:ASP:HB3	1:Q:82:ASN:ND2	2.36	0.41
1:E:19:LEU:HD13	1:E:156:GLN:HB3	2.03	0.41
1:E:113:HIS:HB2	1:E:181:CYS:SG	2.61	0.41
1:A:13:ALA:O	1:A:17:ARG:HD3	2.20	0.41
1:D:185:ARG:HG2	1:D:186:GLY:H	1.85	0.41
1:L:134:LEU:HB3	3:L:232:HOH:O	2.21	0.41
1:M:19:LEU:HD12	1:M:160:ILE:CD1	2.51	0.41
1:Q:13:ALA:O	1:Q:17:ARG:HD3	2.21	0.41
1:Q:185:ARG:HG2	1:Q:186:GLY:H	1.86	0.41
1:S:93:MET:HB2	1:S:95:VAL:HG23	2.03	0.41
1:T:70:TYR:O	1:T:75:PHE:HB2	2.21	0.41
1:A:192:SER:HA	1:B:102:ARG:O	2.21	0.40
1:J:125:TYR:CD2	1:J:166:LEU:HD13	2.56	0.40
1:M:132:ILE:HB	1:M:166:LEU:HD21	2.02	0.40
1:M:187:ILE:HD12	1:N:139:ARG:HG2	2.04	0.40
1:M:192:SER:HA	1:N:102:ARG:O	2.21	0.40
1:P:185:ARG:HG2	1:P:186:GLY:H	1.85	0.40
1:Q:168:THR:HG22	1:Q:170:ASN:H	1.85	0.40
1:R:113:HIS:HB2	1:R:181:CYS:SG	2.62	0.40
1:S:185:ARG:HG2	1:S:186:GLY:N	2.36	0.40
1:C:44:THR:HG23	1:C:54:LEU:HD13	2.03	0.40
1:C:185:ARG:HD2	1:H:69:MET:CE	2.51	0.40
1:H:185:ARG:HG2	1:H:186:GLY:N	2.36	0.40
1:I:79:ASP:HB3	1:I:82:ASN:ND2	2.36	0.40
1:N:113:HIS:HB3	1:Q:69:MET:HE1	2.02	0.40
1:T:138:ASN:H	1:T:138:ASN:HD22	1.69	0.40
1:D:19:LEU:HD13	1:D:156:GLN:HB3	2.03	0.40
1:F:44:THR:O	1:F:48:GLN:HG3	2.21	0.40
1:P:138:ASN:HB3	1:T:187:ILE:HD13	2.03	0.40
1:P:208:ASN:O	1:P:212:GLU:HG3	2.21	0.40
1:B:44:THR:O	1:B:48:GLN:HG3	2.21	0.40
1:B:113:HIS:HB3	1:I:69:MET:HE1	2.04	0.40
1:C:62:THR:HB	1:C:63:PRO:HD3	2.04	0.40
1:E:158:ILE:HD12	1:E:175:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:70:TYR:O	1:H:75:PHE:HB2	2.22	0.40
1:O:30:MET:HE1	1:O:38:LEU:CD1	2.51	0.40
1:A:19:LEU:HD13	1:A:156:GLN:HB3	2.03	0.40
1:C:19:LEU:HD13	1:C:156:GLN:HB3	2.02	0.40
1:F:185:ARG:HG2	1:F:186:GLY:N	2.37	0.40
1:H:93:MET:HB2	1:H:95:VAL:HG23	2.04	0.40
1:K:32:ASN:O	1:K:36:LYS:HG3	2.21	0.40
1:L:62:THR:HB	1:L:63:PRO:HD3	2.03	0.40
1:R:159:LEU:O	1:R:163:GLN:HG3	2.22	0.40
1:S:70:TYR:O	1:S:75:PHE:HB2	2.21	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	219/221 (99%)	203 (93%)	13 (6%)	3 (1%)	9	36
1	B	219/221 (99%)	202 (92%)	15 (7%)	2 (1%)	14	48
1	C	219/221 (99%)	204 (93%)	13 (6%)	2 (1%)	14	48
1	D	219/221 (99%)	203 (93%)	13 (6%)	3 (1%)	9	36
1	E	219/221 (99%)	205 (94%)	11 (5%)	3 (1%)	9	36
1	F	219/221 (99%)	206 (94%)	10 (5%)	3 (1%)	9	36
1	G	219/221 (99%)	204 (93%)	12 (6%)	3 (1%)	9	36
1	H	219/221 (99%)	202 (92%)	14 (6%)	3 (1%)	9	36
1	I	219/221 (99%)	203 (93%)	14 (6%)	2 (1%)	14	48
1	J	219/221 (99%)	204 (93%)	12 (6%)	3 (1%)	9	36
1	K	219/221 (99%)	204 (93%)	13 (6%)	2 (1%)	14	48
1	L	219/221 (99%)	203 (93%)	14 (6%)	2 (1%)	14	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	14	48
1	N	219/221 (99%)	204 (93%)	12 (6%)	3 (1%)	9	36
1	O	219/221 (99%)	203 (93%)	13 (6%)	3 (1%)	9	36
1	P	219/221 (99%)	203 (93%)	14 (6%)	2 (1%)	14	48
1	Q	219/221 (99%)	204 (93%)	12 (6%)	3 (1%)	9	36
1	R	219/221 (99%)	205 (94%)	11 (5%)	3 (1%)	9	36
1	S	219/221 (99%)	203 (93%)	13 (6%)	3 (1%)	9	36
1	T	219/221 (99%)	206 (94%)	10 (5%)	3 (1%)	9	36
All	All	4380/4420 (99%)	4078 (93%)	249 (6%)	53 (1%)	10	40

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	SER
1	A	2	SER
1	B	2	SER
1	C	2	SER
1	D	2	SER
1	F	2	SER
1	G	2	SER
1	H	2	SER
1	I	2	SER
1	J	2	SER
1	K	2	SER
1	L	2	SER
1	M	2	SER
1	N	2	SER
1	O	2	SER
1	P	2	SER
1	Q	2	SER
1	R	2	SER
1	S	2	SER
1	T	2	SER
1	S	218	ARG
1	T	218	ARG
1	C	22	PRO
1	D	218	ARG
1	E	218	ARG
1	G	218	ARG

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Mol	Chain	Res	Type
1	H	22	PRO
1	J	218	ARG
1	N	22	PRO
1	P	22	PRO
1	Q	218	ARG
1	R	218	ARG
1	S	22	PRO
1	T	22	PRO
1	A	22	PRO
1	A	218	ARG
1	B	22	PRO
1	D	22	PRO
1	E	22	PRO
1	F	218	ARG
1	H	218	ARG
1	I	22	PRO
1	J	22	PRO
1	K	22	PRO
1	N	218	ARG
1	O	218	ARG
1	Q	22	PRO
1	R	22	PRO
1	F	22	PRO
1	G	22	PRO
1	L	22	PRO
1	M	22	PRO
1	O	22	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/194 (100%)	189 (97%)	5 (3%)	40	72
1	B	194/194 (100%)	190 (98%)	4 (2%)	47	75
1	C	194/194 (100%)	190 (98%)	4 (2%)	47	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	194/194 (100%)	188 (97%)	6 (3%)	35	68
1	E	194/194 (100%)	190 (98%)	4 (2%)	47	75
1	F	194/194 (100%)	190 (98%)	4 (2%)	47	75
1	G	194/194 (100%)	190 (98%)	4 (2%)	47	75
1	H	194/194 (100%)	190 (98%)	4 (2%)	47	75
1	I	194/194 (100%)	190 (98%)	4 (2%)	47	75
1	J	194/194 (100%)	190 (98%)	4 (2%)	47	75
1	K	194/194 (100%)	190 (98%)	4 (2%)	47	75
1	L	194/194 (100%)	190 (98%)	4 (2%)	47	75
1	M	194/194 (100%)	189 (97%)	5 (3%)	40	72
1	N	194/194 (100%)	190 (98%)	4 (2%)	47	75
1	O	194/194 (100%)	188 (97%)	6 (3%)	35	68
1	P	194/194 (100%)	190 (98%)	4 (2%)	47	75
1	Q	194/194 (100%)	190 (98%)	4 (2%)	47	75
1	R	194/194 (100%)	190 (98%)	4 (2%)	47	75
1	S	194/194 (100%)	189 (97%)	5 (3%)	40	72
1	T	194/194 (100%)	190 (98%)	4 (2%)	47	75
All	All	3880/3880 (100%)	3793 (98%)	87 (2%)	45	74

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	93	MET
1	A	150	VAL
1	A	181	CYS
1	A	185	ARG
1	B	20	GLU
1	B	93	MET
1	B	181	CYS
1	B	185	ARG
1	C	20	GLU
1	C	93	MET
1	C	181	CYS
1	C	185	ARG
1	D	20	GLU

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Mol	Chain	Res	Type
1	D	93	MET
1	D	107	THR
1	D	150	VAL
1	D	181	CYS
1	D	185	ARG
1	E	20	GLU
1	E	93	MET
1	E	181	CYS
1	E	185	ARG
1	F	20	GLU
1	F	93	MET
1	F	181	CYS
1	F	185	ARG
1	G	20	GLU
1	G	93	MET
1	G	181	CYS
1	G	185	ARG
1	H	20	GLU
1	H	93	MET
1	H	181	CYS
1	H	185	ARG
1	I	20	GLU
1	I	93	MET
1	I	181	CYS
1	I	185	ARG
1	J	20	GLU
1	J	93	MET
1	J	181	CYS
1	J	185	ARG
1	K	20	GLU
1	K	93	MET
1	K	181	CYS
1	K	185	ARG
1	L	20	GLU
1	L	93	MET
1	L	181	CYS
1	L	185	ARG
1	M	20	GLU
1	M	93	MET
1	M	150	VAL
1	M	181	CYS
1	M	185	ARG

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Mol	Chain	Res	Type
1	N	20	GLU
1	N	93	MET
1	N	181	CYS
1	N	185	ARG
1	O	20	GLU
1	O	63	PRO
1	O	93	MET
1	O	150	VAL
1	O	181	CYS
1	O	185	ARG
1	P	20	GLU
1	P	93	MET
1	P	181	CYS
1	P	185	ARG
1	Q	20	GLU
1	Q	93	MET
1	Q	181	CYS
1	Q	185	ARG
1	R	20	GLU
1	R	93	MET
1	R	181	CYS
1	R	185	ARG
1	S	20	GLU
1	S	93	MET
1	S	150	VAL
1	S	181	CYS
1	S	185	ARG
1	T	20	GLU
1	T	93	MET
1	T	181	CYS
1	T	185	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	82	ASN
1	A	138	ASN
1	A	163	GLN
1	B	48	GLN
1	B	51	ASN
1	B	82	ASN

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Mol	Chain	Res	Type
1	B	138	ASN
1	B	163	GLN
1	C	82	ASN
1	C	138	ASN
1	C	163	GLN
1	C	211	HIS
1	D	48	GLN
1	D	51	ASN
1	D	138	ASN
1	D	163	GLN
1	E	48	GLN
1	E	51	ASN
1	E	138	ASN
1	E	163	GLN
1	F	11	HIS
1	F	51	ASN
1	F	138	ASN
1	F	156	GLN
1	F	211	HIS
1	G	51	ASN
1	G	82	ASN
1	G	138	ASN
1	G	163	GLN
1	G	211	HIS
1	H	51	ASN
1	H	82	ASN
1	H	138	ASN
1	H	163	GLN
1	H	207	GLN
1	I	42	HIS
1	I	48	GLN
1	I	51	ASN
1	I	82	ASN
1	I	138	ASN
1	I	163	GLN
1	I	211	HIS
1	J	48	GLN
1	J	51	ASN
1	J	82	ASN
1	J	138	ASN
1	J	163	GLN
1	K	42	HIS

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Mol	Chain	Res	Type
1	K	48	GLN
1	K	82	ASN
1	K	138	ASN
1	K	163	GLN
1	L	48	GLN
1	L	82	ASN
1	L	138	ASN
1	L	163	GLN
1	L	211	HIS
1	M	48	GLN
1	M	51	ASN
1	M	138	ASN
1	M	163	GLN
1	M	211	HIS
1	N	48	GLN
1	N	51	ASN
1	N	82	ASN
1	N	138	ASN
1	N	163	GLN
1	N	207	GLN
1	N	211	HIS
1	O	82	ASN
1	O	138	ASN
1	O	163	GLN
1	P	48	GLN
1	P	82	ASN
1	P	138	ASN
1	P	163	GLN
1	Q	48	GLN
1	Q	82	ASN
1	Q	138	ASN
1	Q	163	GLN
1	R	138	ASN
1	R	211	HIS
1	S	51	ASN
1	S	138	ASN
1	S	163	GLN
1	T	51	ASN
1	T	82	ASN
1	T	138	ASN
1	T	163	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 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	SO4	C	222	-	4,4,4	0.50	0	6,6,6	0.20	0
2	SO4	E	222	-	4,4,4	0.49	0	6,6,6	0.26	0
2	SO4	A	222	-	4,4,4	0.60	0	6,6,6	0.23	0
2	SO4	J	222	-	4,4,4	0.54	0	6,6,6	0.36	0
2	SO4	K	222	-	4,4,4	0.55	0	6,6,6	0.37	0
2	SO4	P	222	-	4,4,4	0.48	0	6,6,6	0.40	0
2	SO4	R	222	-	4,4,4	0.54	0	6,6,6	0.38	0
2	SO4	L	223	-	4,4,4	0.59	0	6,6,6	0.44	0
2	SO4	F	222	-	4,4,4	0.49	0	6,6,6	0.23	0
2	SO4	N	222	-	4,4,4	0.52	0	6,6,6	0.33	0
2	SO4	A	223	-	4,4,4	0.54	0	6,6,6	0.37	0
2	SO4	O	222	-	4,4,4	0.50	0	6,6,6	0.24	0
2	SO4	D	222	-	4,4,4	0.58	0	6,6,6	0.39	0
2	SO4	I	222	-	4,4,4	0.46	0	6,6,6	0.14	0
2	SO4	H	222	-	4,4,4	0.65	0	6,6,6	0.51	0
2	SO4	T	222	-	4,4,4	0.47	0	6,6,6	0.19	0
2	SO4	L	222	-	4,4,4	0.49	0	6,6,6	0.15	0
2	SO4	S	222	-	4,4,4	0.61	0	6,6,6	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	Q	222	-	4,4,4	0.48	0	6,6,6	0.22	0
2	SO4	G	222	-	4,4,4	0.52	0	6,6,6	0.29	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.