



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:13 AM UTC

PDB ID : 1BBD / pdb_00001bbd
Title : THREE DIMENSIONAL STRUCTURE OF THE FAB FRAGMENT OF A
NEUTRALIZING ANTIBODY TO HUMAN RHINOVIRUS SEROTYPE 2
Authors : Tormo, J.; Blaas, D.; Fita, I.
Deposited on : 1992-05-05
Resolution : 2.80 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

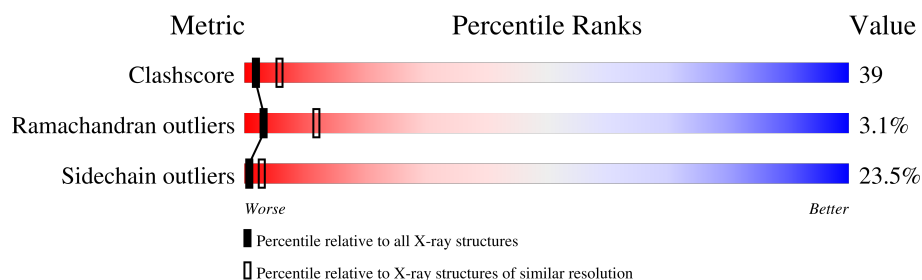
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	L	220	
2	H	218	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3342 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 IGG2A-KAPPA 8F5 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	219	Total	C	N	O	S	0	0	0
			1707	1063	286	351	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	12	THR	SER	conflict	GB 208622
L	14	THR	SER	conflict	GB 208622
L	15	THR	ALA	conflict	GB 208622
L	18	LYS	ARG	conflict	GB 208622
L	22	THR	SER	conflict	GB 208622
L	33	ARG	GLY	conflict	GB 208622
L	34	THR	ASN	conflict	GB 208622
L	38	TYR	PHE	conflict	GB 208622
L	40	THR	ALA	conflict	GB 208622
L	49	SER	PRO	conflict	GB 208622
L	56	TRP	GLY	conflict	GB 208622
L	80	SER	THR	conflict	GB 208622
L	83	GLY	SER	conflict	GB 208622
L	97	ASN	ASP	conflict	GB 208622
L	98	TYR	HIS	conflict	GB 208622
L	99	ASN	SER	conflict	GB 208622

- Molecule 2 is a protein called IGG2A-KAPPA 8F5 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	213	Total	C	N	O	S	0	0	0
			1625	1032	259	328	6			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	13	ARG	LYS	conflict	GB 2072133
H	16	ALA	THR	conflict	GB 2072133
H	24	THR	ALA	conflict	GB 2072133
H	32	ILE	THR	conflict	GB 2072133
H	35	HIS	TYR	conflict	GB 2072133
H	51	LEU	ILE	conflict	GB 2072133
H	57	TYR	ASN	conflict	GB 2072133
H	59	LYS	GLU	conflict	GB 2072133
H	60	TYR	PHE	conflict	GB 2072133
H	63	LYS	ARG	conflict	GB 2072133
H	65	GLN	LEU	conflict	GB 2072133
H	72	VAL	ALA	conflict	GB 2072133
H	82	HIS	GLN	conflict	GB 2072133
H	83	LEU	VAL	conflict	GB 2072133
H	97	ASP	-	insertion	GB 2072133
H	98	GLY	-	insertion	GB 2072133
H	99	TYR	-	insertion	GB 2072133
H	100	TYR	-	insertion	GB 2072133
H	101	SER	-	insertion	GB 2072133
H	102	TYR	HIS	conflict	GB 2072133
H	103	TYR	LEU	conflict	GB 2072133
H	104	ASP	HIS	conflict	GB 2072133
H	105	MET	GLY	conflict	GB 2072133
H	106	ASP	PRO	conflict	GB 2072133
H	110	PRO	GLN	conflict	GB 2072133
H	113	SER	LEU	conflict	GB 2072133
H	118	SER	ALA	conflict	GB 2072133

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	5	Total	O	0	0
			5	5		

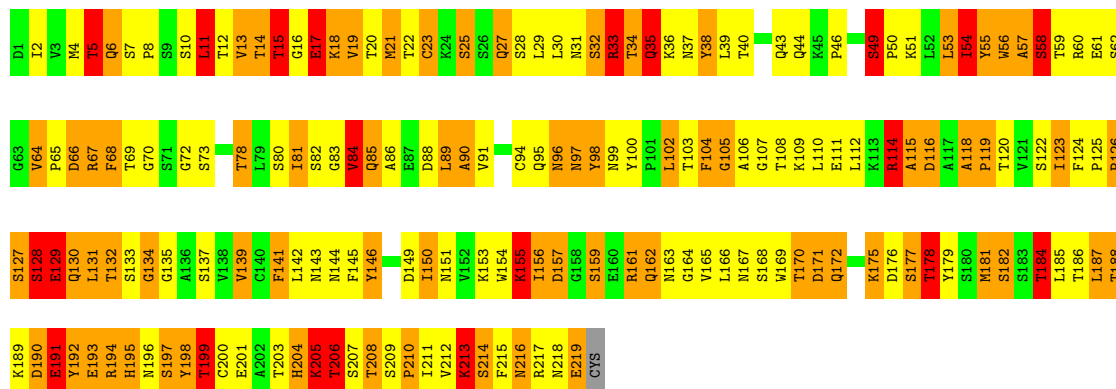
3 Residue-property plots

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.

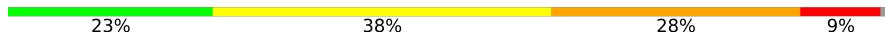
Note EDS was not executed.

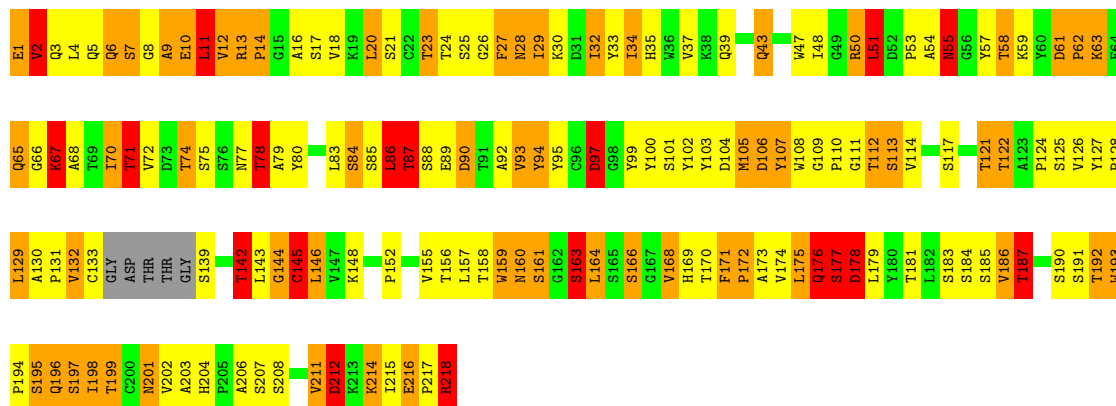
• Molecule 1: IGG2A-KAPPA 8F5 FAB (LIGHT CHAIN)

Chain L: 



• Molecule 2: IGG2A-KAPPA 8F5 FAB (HEAVY CHAIN)

Chain H: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.70Å 86.80Å 128.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3342	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	L	1.59	13/1744 (0.7%)	2.93	199/2370 (8.4%)
2	H	1.73	16/1669 (1.0%)	2.95	212/2285 (9.3%)
All	All	1.66	29/3413 (0.8%)	2.94	411/4655 (8.8%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	8	GLY	N-CA	9.05	1.58	1.45
2	H	125	SER	N-CA	8.65	1.56	1.46
2	H	7	SER	C-O	7.47	1.32	1.24
2	H	204	HIS	ND1-CE1	6.61	1.39	1.32
2	H	144	GLY	N-CA	6.58	1.53	1.45
2	H	169	HIS	CA-CB	-6.25	1.43	1.53
1	L	54	ILE	CA-CB	6.06	1.62	1.54
1	L	114	ARG	CD-NE	-5.96	1.38	1.46
1	L	171	ASP	N-CA	5.86	1.52	1.45
2	H	93	VAL	CA-C	5.85	1.60	1.52
1	L	198	TYR	N-CA	5.60	1.52	1.46
1	L	178	THR	CA-CB	5.41	1.61	1.53
1	L	57	ALA	C-O	5.41	1.30	1.24
2	H	201	ASN	C-O	5.37	1.30	1.24
2	H	129	LEU	N-CA	-5.34	1.38	1.46
2	H	112	THR	N-CA	-5.32	1.40	1.46
1	L	129	GLU	CA-CB	-5.23	1.45	1.53
1	L	108	THR	N-CA	-5.22	1.40	1.46
1	L	91	VAL	N-CA	5.15	1.52	1.46
1	L	135	GLY	CA-C	5.15	1.56	1.52
2	H	155	VAL	CA-C	5.15	1.58	1.52
1	L	59	THR	N-CA	5.14	1.52	1.45
1	L	135	GLY	N-CA	5.12	1.50	1.45
2	H	48	ILE	CA-CB	5.11	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	104	PHE	N-CA	5.09	1.52	1.46
2	H	121	THR	CA-CB	5.06	1.60	1.53
2	H	27	PHE	CA-CB	-5.06	1.45	1.53
2	H	7	SER	N-CA	-5.04	1.40	1.46
2	H	58	THR	C-N	-5.01	1.26	1.33

All (411) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	114	ARG	CD-NE-CZ	25.43	160.01	124.40
1	L	33	ARG	CD-NE-CZ	21.25	154.16	124.40
1	L	99	ASN	OD1-CG-ND2	14.23	136.83	122.60
2	H	86	LEU	CA-C-N	13.79	147.57	123.01
2	H	86	LEU	C-N-CA	13.79	147.57	123.01
2	H	7	SER	N-CA-C	13.62	125.82	110.97
1	L	129	GLU	CA-CB-CG	12.71	139.51	114.10
1	L	219	GLU	CA-CB-CG	12.59	139.28	114.10
2	H	27	PHE	CA-C-O	-11.85	108.34	121.25
2	H	125	SER	CA-C-O	-11.29	108.74	120.71
1	L	195	HIS	CA-CB-CG	-11.27	102.53	113.80
2	H	168	VAL	CA-C-O	-11.20	107.56	120.67
1	L	104	PHE	CA-CB-CG	10.77	124.57	113.80
2	H	47	TRP	CA-C-O	-10.69	108.73	120.92
2	H	173	ALA	CA-C-O	-10.68	109.92	121.56
2	H	10	GLU	O-C-N	10.59	135.32	123.25
1	L	67	ARG	N-CA-C	-10.54	100.16	113.23
2	H	107	TYR	CA-C-O	-10.54	108.63	120.54
2	H	169	HIS	CA-CB-CG	10.37	124.17	113.80
2	H	61	ASP	CA-CB-CG	10.29	122.89	112.60
2	H	7	SER	CA-C-O	-10.28	110.20	121.00
1	L	60	ARG	CA-C-O	-10.14	109.33	120.38
2	H	90	ASP	CA-CB-CG	9.96	122.56	112.60
1	L	6	GLN	OE1-CD-NE2	9.79	132.39	122.60
1	L	99	ASN	CA-CB-CG	-9.68	102.92	112.60
2	H	48	ILE	CA-C-O	9.55	130.83	120.32
2	H	171	PHE	CB-CA-C	9.52	120.70	109.47
2	H	125	SER	N-CA-C	-9.52	94.26	109.59
2	H	181	THR	O-C-N	9.48	134.80	123.33
1	L	107	GLY	CA-C-N	9.47	136.67	122.47
1	L	107	GLY	C-N-CA	9.47	136.67	122.47
1	L	51	LYS	CA-CB-CG	9.41	132.91	114.10
2	H	55	ASN	CA-CB-CG	-9.40	103.20	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	203	ALA	CA-C-O	-9.36	108.77	120.28
1	L	122	SER	CB-CA-C	9.29	129.74	109.94
1	L	97	ASN	CA-CB-CG	-9.23	103.37	112.60
2	H	179	LEU	CA-C-O	-9.16	110.73	120.99
2	H	6	GLN	CA-C-N	9.11	132.68	120.65
2	H	6	GLN	C-N-CA	9.11	132.68	120.65
2	H	172	PRO	CA-C-N	9.11	135.25	120.94
2	H	172	PRO	C-N-CA	9.11	135.25	120.94
2	H	161	SER	CA-C-O	-9.10	109.70	121.08
2	H	171	PHE	CA-C-O	9.10	130.95	119.67
2	H	203	ALA	O-C-N	9.08	134.44	123.36
2	H	16	ALA	CA-C-O	-9.07	110.16	121.50
1	L	60	ARG	NE-CZ-NH2	-9.06	111.04	119.20
2	H	105	MET	N-CA-CB	-9.05	95.28	110.57
2	H	148	LYS	N-CA-C	8.99	124.25	109.24
1	L	32	SER	O-C-N	8.97	131.31	122.07
1	L	172	GLN	N-CA-CB	8.95	123.34	109.83
1	L	145	PHE	CA-CB-CG	8.94	122.74	113.80
1	L	106	ALA	N-CA-C	8.93	124.23	113.16
1	L	60	ARG	NE-CZ-NH1	8.85	130.35	121.50
1	L	196	ASN	CA-C-N	-8.85	110.55	123.11
1	L	196	ASN	C-N-CA	-8.85	110.55	123.11
2	H	13	ARG	O-C-N	8.77	132.78	121.64
1	L	213	LYS	CA-C-O	-8.75	110.60	120.66
1	L	59	THR	CA-C-O	-8.62	112.16	121.56
2	H	169	HIS	N-CA-CB	8.60	125.26	110.81
1	L	2	ILE	CA-C-O	-8.59	112.74	121.59
2	H	2	VAL	CB-CA-C	8.56	125.63	111.51
2	H	178	ASP	CA-CB-CG	8.53	121.13	112.60
2	H	70	ILE	O-C-N	-8.53	113.89	122.93
2	H	199	THR	O-C-N	8.52	133.67	123.27
2	H	5	GLN	CA-C-O	-8.50	111.50	121.11
1	L	11	LEU	CB-CA-C	8.48	124.22	109.80
1	L	59	THR	N-CA-C	-8.47	98.56	110.50
1	L	54	ILE	N-CA-CB	-8.46	97.27	111.23
1	L	217	ARG	CA-C-O	-8.46	111.45	120.92
1	L	39	LEU	CA-C-O	-8.40	111.00	120.32
1	L	114	ARG	CA-C-O	8.40	130.30	121.31
2	H	158	THR	O-C-N	8.35	132.70	123.10
1	L	94	CYS	CA-C-O	-8.35	111.34	121.11
2	H	181	THR	CA-C-O	-8.31	110.63	120.60
1	L	215	PHE	O-C-N	-8.26	114.59	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	111	GLY	CA-C-N	8.22	134.54	122.86
2	H	111	GLY	C-N-CA	8.22	134.54	122.86
1	L	118	ALA	CA-C-O	8.21	127.99	120.60
2	H	107	TYR	O-C-N	8.17	132.53	123.22
2	H	184	SER	CA-C-O	-8.08	111.68	121.06
1	L	116	ASP	CA-CB-CG	8.06	120.66	112.60
2	H	43	GLN	OE1-CD-NE2	-8.04	114.56	122.60
2	H	7	SER	O-C-N	-8.02	113.69	122.03
2	H	148	LYS	N-CA-CB	-8.01	96.50	111.00
1	L	73	SER	CA-C-O	-7.94	112.76	121.33
2	H	207	SER	CA-C-O	7.91	127.97	119.03
2	H	122	THR	CB-CA-C	7.78	123.78	109.70
2	H	32	ILE	CA-C-O	7.75	129.58	121.67
1	L	170	THR	CA-C-O	-7.74	112.45	121.82
1	L	130	GLN	CG-CD-NE2	7.72	127.99	116.40
1	L	105	GLY	CA-C-O	-7.70	112.98	122.75
1	L	6	GLN	CA-C-O	-7.67	112.27	121.56
2	H	17	SER	CA-CB-OG	-7.65	95.80	111.10
1	L	72	GLY	CA-C-O	-7.64	117.25	122.22
1	L	33	ARG	NE-CZ-NH1	7.62	129.12	121.50
2	H	5	GLN	OE1-CD-NE2	7.56	130.16	122.60
2	H	195	SER	N-CA-C	-7.52	101.53	111.24
1	L	206	THR	CA-CB-OG1	-7.51	98.33	109.60
2	H	21	SER	CA-C-O	-7.47	112.39	121.06
1	L	130	GLN	OE1-CD-NE2	-7.45	115.15	122.60
2	H	86	LEU	CA-C-O	7.43	129.43	121.55
1	L	12	THR	CB-CA-C	7.38	122.14	110.19
2	H	33	TYR	CA-C-N	7.36	131.57	122.37
2	H	33	TYR	C-N-CA	7.36	131.57	122.37
2	H	58	THR	CA-CB-CG2	7.36	123.00	110.50
1	L	171	ASP	CA-C-O	-7.35	112.55	121.89
1	L	191	GLU	CB-CG-CD	7.34	125.08	112.60
1	L	94	CYS	N-CA-C	-7.34	97.90	109.50
1	L	170	THR	CA-CB-OG1	-7.29	98.66	109.60
2	H	212	ASP	CA-C-O	-7.29	112.30	120.32
2	H	117	SER	N-CA-CB	-7.28	100.49	111.56
1	L	49	SER	O-C-N	7.28	129.68	121.53
1	L	100	TYR	CA-C-O	-7.23	112.86	120.23
2	H	144	GLY	CA-C-O	-7.21	113.85	121.56
2	H	112	THR	N-CA-CB	7.20	121.79	110.84
1	L	210	PRO	CA-C-O	-7.18	113.39	121.43
2	H	166	SER	O-C-N	7.17	131.39	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	55	ASN	OD1-CG-ND2	7.15	129.75	122.60
1	L	14	THR	CA-CB-OG1	-7.14	98.89	109.60
2	H	61	ASP	N-CA-C	-7.12	100.68	109.65
1	L	120	THR	N-CA-C	-7.11	97.31	108.90
2	H	29	ILE	CB-CA-C	7.09	120.95	111.88
2	H	206	ALA	CA-C-O	-7.08	110.17	119.10
1	L	151	ASN	CA-CB-CG	7.08	119.68	112.60
1	L	211	ILE	N-CA-C	-7.08	98.12	108.87
2	H	158	THR	CA-C-O	-7.08	113.88	121.45
1	L	14	THR	CA-C-N	-7.07	110.94	120.90
1	L	14	THR	C-N-CA	-7.07	110.94	120.90
2	H	2	VAL	CA-CB-CG1	7.05	122.39	110.40
1	L	5	THR	O-C-N	6.97	132.21	123.28
1	L	6	GLN	O-C-N	6.96	132.08	123.10
1	L	210	PRO	O-C-N	6.94	131.81	122.99
1	L	211	ILE	O-C-N	6.93	130.87	122.83
1	L	91	VAL	CB-CA-C	6.91	121.12	110.83
2	H	101	SER	CA-C-N	6.91	129.84	120.38
2	H	101	SER	C-N-CA	6.91	129.84	120.38
1	L	132	THR	CA-C-O	6.88	128.27	120.90
2	H	202	VAL	CA-C-O	-6.88	112.96	120.67
1	L	54	ILE	CA-CB-CG2	6.88	122.19	110.50
2	H	27	PHE	CA-CB-CG	6.87	120.67	113.80
1	L	187	LEU	CA-C-O	-6.85	113.63	121.58
2	H	160	ASN	CB-CA-C	6.84	121.78	111.80
2	H	34	ILE	CB-CA-C	-6.83	102.70	110.96
2	H	78	THR	CA-C-O	-6.81	112.76	120.32
1	L	204	HIS	CA-CB-CG	6.80	120.61	113.80
2	H	6	GLN	CB-CG-CD	-6.79	101.05	112.60
2	H	87	THR	CA-CB-CG2	6.79	122.05	110.50
1	L	114	ARG	N-CA-C	6.78	117.54	108.38
2	H	195	SER	O-C-N	6.77	129.96	122.11
2	H	186	VAL	CA-C-N	-6.75	113.69	123.00
2	H	186	VAL	C-N-CA	-6.75	113.69	123.00
2	H	87	THR	CA-CB-OG1	-6.75	99.48	109.60
1	L	163	ASN	CB-CA-C	6.74	121.18	109.65
2	H	70	ILE	CB-CA-C	6.73	120.48	110.98
1	L	81	ILE	O-C-N	6.73	130.30	123.10
2	H	59	LYS	N-CA-CB	-6.69	99.16	111.13
1	L	107	GLY	CA-C-O	-6.68	117.88	122.22
2	H	164	LEU	CB-CA-C	6.68	120.82	110.67
2	H	32	ILE	CA-CB-CG2	6.67	121.83	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	187	LEU	O-C-N	6.65	132.06	122.94
2	H	160	ASN	N-CA-C	-6.65	102.50	111.54
2	H	146	LEU	CB-CA-C	6.64	121.86	109.71
2	H	218	ARG	NE-CZ-NH1	-6.62	114.88	121.50
1	L	197	SER	CB-CA-C	6.62	121.57	110.79
2	H	11	LEU	O-C-N	6.60	131.16	123.30
1	L	211	ILE	CA-C-O	-6.58	112.67	121.02
2	H	13	ARG	CA-C-O	-6.55	113.90	120.64
1	L	81	ILE	N-CA-C	-6.53	98.73	108.46
2	H	208	SER	CA-C-O	-6.53	113.97	122.45
2	H	17	SER	O-C-N	-6.50	115.99	123.33
1	L	196	ASN	CA-CB-CG	6.50	119.10	112.60
2	H	187	THR	CB-CA-C	6.49	120.95	109.72
2	H	10	GLU	CB-CA-C	-6.47	96.53	110.45
2	H	74	THR	CA-CB-OG1	-6.47	99.90	109.60
1	L	188	THR	N-CA-C	-6.46	102.20	110.53
2	H	176	GLN	N-CA-CB	-6.45	99.59	110.49
2	H	2	VAL	N-CA-CB	-6.44	99.77	110.14
2	H	53	PRO	CB-CA-C	6.44	121.51	112.11
1	L	217	ARG	CD-NE-CZ	-6.42	115.41	124.40
2	H	160	ASN	CA-C-O	6.42	128.99	121.54
2	H	168	VAL	N-CA-C	-6.42	99.24	108.48
1	L	208	THR	CA-C-O	6.41	125.83	118.97
1	L	66	ASP	CA-CB-CG	-6.41	106.19	112.60
2	H	124	PRO	CA-C-N	-6.41	113.64	122.93
2	H	124	PRO	C-N-CA	-6.41	113.64	122.93
2	H	16	ALA	O-C-N	6.40	130.02	121.83
2	H	122	THR	CA-C-O	-6.40	113.22	120.32
1	L	214	SER	O-C-N	6.39	131.02	122.96
1	L	108	THR	CA-CB-OG1	-6.39	100.02	109.60
2	H	103	TYR	CB-CA-C	6.39	120.76	109.65
2	H	37	VAL	N-CA-C	6.38	117.30	108.12
1	L	5	THR	CA-C-O	-6.37	112.42	120.20
1	L	102	LEU	CA-C-N	6.37	130.52	121.42
1	L	102	LEU	C-N-CA	6.37	130.52	121.42
1	L	208	THR	CB-CA-C	6.37	119.76	109.07
2	H	170	THR	CB-CA-C	6.37	121.53	109.37
2	H	83	LEU	CA-C-N	-6.35	112.15	122.82
2	H	83	LEU	C-N-CA	-6.35	112.15	122.82
2	H	156	THR	CA-C-O	-6.35	113.34	120.32
2	H	5	GLN	CG-CD-NE2	-6.32	106.93	116.40
1	L	132	THR	CB-CA-C	-6.30	100.73	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	175	LEU	CB-CA-C	6.19	120.02	109.80
1	L	175	LYS	CA-CB-CG	6.18	126.47	114.10
2	H	86	LEU	O-C-N	-6.18	115.21	122.81
1	L	192	TYR	N-CA-CB	6.18	120.94	110.49
2	H	18	VAL	CB-CA-C	6.16	120.55	110.69
1	L	95	GLN	CA-C-N	6.16	130.61	122.30
1	L	95	GLN	C-N-CA	6.16	130.61	122.30
1	L	58	SER	CA-C-N	-6.13	111.31	120.94
1	L	58	SER	C-N-CA	-6.13	111.31	120.94
2	H	124	PRO	N-CA-C	6.12	119.79	111.22
2	H	185	SER	CA-C-O	-6.12	114.30	121.46
2	H	27	PHE	O-C-N	6.12	129.40	123.04
1	L	154	TRP	CA-C-O	-6.11	114.23	120.71
2	H	121	THR	CA-C-O	-6.10	113.64	120.54
2	H	127	TYR	O-C-N	6.08	127.21	121.38
1	L	105	GLY	N-CA-C	-6.07	102.10	112.30
1	L	67	ARG	N-CA-CB	6.07	119.90	110.44
1	L	196	ASN	CA-C-O	-6.05	110.92	118.54
2	H	18	VAL	N-CA-CB	-6.04	100.75	111.93
2	H	84	SER	CA-CB-OG	-6.04	99.03	111.10
1	L	40	THR	CA-C-O	-5.99	114.34	121.11
1	L	168	SER	CA-C-O	-5.98	111.95	120.51
1	L	103	THR	O-C-N	-5.98	115.95	123.01
1	L	184	THR	CB-CA-C	5.95	120.48	109.70
1	L	84	VAL	N-CA-CB	-5.95	101.42	111.23
1	L	106	ALA	CA-C-O	-5.94	112.10	119.28
2	H	170	THR	CA-CB-OG1	-5.93	100.70	109.60
1	L	51	LYS	CA-C-N	5.93	129.29	120.87
1	L	51	LYS	C-N-CA	5.93	129.29	120.87
1	L	216	ASN	CA-C-O	-5.93	113.96	120.30
1	L	119	PRO	O-C-N	5.92	129.82	122.71
1	L	131	LEU	CA-C-N	5.92	128.53	120.54
1	L	131	LEU	C-N-CA	5.92	128.53	120.54
2	H	48	ILE	CB-CA-C	-5.91	104.75	111.55
1	L	159	SER	CB-CA-C	-5.90	99.53	109.50
1	L	35	GLN	CA-C-O	5.90	128.30	120.98
1	L	178	THR	N-CA-C	5.90	118.14	110.53
1	L	120	THR	CA-C-O	-5.90	113.99	120.36
1	L	123	ILE	CA-C-N	-5.87	112.08	122.48
1	L	123	ILE	C-N-CA	-5.87	112.08	122.48
1	L	128	SER	CA-C-N	-5.86	112.36	120.38
1	L	128	SER	C-N-CA	-5.86	112.36	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	63	LYS	N-CA-C	5.85	117.66	111.28
2	H	71	THR	CA-C-N	-5.85	113.92	122.58
2	H	71	THR	C-N-CA	-5.85	113.92	122.58
2	H	71	THR	CA-CB-OG1	-5.85	100.83	109.60
1	L	15	THR	CA-CB-OG1	-5.85	100.83	109.60
2	H	204	HIS	CA-C-N	5.84	125.32	119.24
2	H	204	HIS	C-N-CA	5.84	125.32	119.24
2	H	5	GLN	O-C-N	5.82	130.76	123.19
2	H	164	LEU	N-CA-CB	-5.82	100.05	109.60
2	H	218	ARG	CD-NE-CZ	-5.82	116.25	124.40
1	L	22	THR	CA-C-N	5.81	130.53	121.76
1	L	22	THR	C-N-CA	5.81	130.53	121.76
2	H	51	LEU	CA-C-O	5.80	127.33	120.66
2	H	65	GLN	CA-CB-CG	-5.80	102.51	114.10
1	L	171	ASP	CB-CA-C	5.79	120.47	110.45
1	L	213	LYS	O-C-N	5.78	130.32	123.27
2	H	7	SER	CB-CA-C	-5.78	102.06	110.96
2	H	86	LEU	CB-CA-C	5.77	119.96	109.62
1	L	122	SER	CA-CB-OG	5.77	122.64	111.10
2	H	155	VAL	CA-C-N	-5.75	114.99	123.05
2	H	155	VAL	C-N-CA	-5.75	114.99	123.05
2	H	71	THR	CA-CB-CG2	5.75	120.28	110.50
1	L	78	THR	CA-CB-CG2	5.75	120.27	110.50
2	H	179	LEU	N-CA-C	-5.74	99.97	108.99
2	H	77	ASN	CB-CG-ND2	5.72	124.99	116.40
1	L	149	ASP	CA-CB-CG	-5.72	106.88	112.60
1	L	141	PHE	CA-C-O	-5.72	114.15	120.38
1	L	27	GLN	N-CA-CB	5.72	120.26	111.46
1	L	56	TRP	CA-CB-CG	5.72	124.46	113.60
1	L	27	GLN	CA-C-O	-5.70	115.34	121.38
1	L	62	SER	CA-C-O	-5.69	115.53	120.88
2	H	208	SER	CA-CB-OG	-5.68	99.73	111.10
1	L	124	PHE	CB-CA-C	5.68	118.54	110.02
1	L	61	GLU	CA-C-O	5.67	128.46	121.94
1	L	95	GLN	N-CA-CB	-5.66	101.84	111.69
1	L	114	ARG	O-C-N	-5.65	116.94	122.99
1	L	33	ARG	CA-C-N	5.65	128.90	120.31
1	L	33	ARG	C-N-CA	5.65	128.90	120.31
2	H	173	ALA	CA-C-N	5.64	130.78	122.94
2	H	173	ALA	C-N-CA	5.64	130.78	122.94
2	H	4	LEU	CA-C-O	-5.63	114.24	120.38
1	L	217	ARG	NE-CZ-NH2	5.63	124.26	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	13	ARG	N-CA-C	-5.62	102.03	110.24
1	L	33	ARG	NH1-CZ-NH2	-5.62	111.99	119.30
1	L	102	LEU	N-CA-CB	-5.62	102.48	110.46
2	H	159	TRP	O-C-N	-5.62	116.61	123.30
2	H	113	SER	CA-C-O	-5.61	113.98	120.49
2	H	70	ILE	CA-C-N	5.60	131.28	122.21
2	H	70	ILE	C-N-CA	5.60	131.28	122.21
1	L	217	ARG	CA-CB-CG	5.59	125.29	114.10
1	L	67	ARG	CA-C-O	5.59	125.81	119.27
2	H	171	PHE	CA-CB-CG	5.58	119.38	113.80
1	L	103	THR	N-CA-C	5.58	119.01	110.20
1	L	131	LEU	CB-CA-C	5.57	120.04	110.79
2	H	191	SER	N-CA-C	-5.57	104.84	111.69
1	L	25	SER	CA-C-O	-5.57	114.68	121.36
2	H	34	ILE	N-CA-C	5.56	116.74	108.23
2	H	142	THR	N-CA-C	5.56	118.02	109.07
2	H	33	TYR	N-CA-CB	5.54	119.52	110.37
1	L	171	ASP	CA-CB-CG	5.53	118.13	112.60
2	H	173	ALA	O-C-N	5.53	129.38	122.86
2	H	145	CYS	CA-C-N	-5.52	115.21	122.99
2	H	145	CYS	C-N-CA	-5.52	115.21	122.99
1	L	157	ASP	CB-CG-OD1	-5.50	105.75	118.40
2	H	125	SER	O-C-N	5.48	130.17	123.21
1	L	11	LEU	N-CA-CB	-5.48	101.61	110.71
2	H	12	VAL	CA-CB-CG2	5.48	119.72	110.40
2	H	54	ALA	CA-C-N	5.48	131.30	121.66
2	H	54	ALA	C-N-CA	5.48	131.30	121.66
2	H	79	ALA	O-C-N	-5.48	116.84	123.03
1	L	128	SER	CB-CA-C	5.47	119.62	110.92
2	H	65	GLN	OE1-CD-NE2	5.47	128.07	122.60
2	H	161	SER	CB-CA-C	-5.47	103.07	111.66
1	L	108	THR	CA-CB-CG2	5.46	119.79	110.50
2	H	195	SER	N-CA-CB	5.46	118.10	110.07
2	H	144	GLY	N-CA-C	-5.45	101.51	110.56
1	L	78	THR	CA-CB-OG1	-5.45	101.42	109.60
2	H	109	GLY	N-CA-C	-5.45	105.40	112.10
2	H	7	SER	CA-C-N	-5.44	110.75	121.41
2	H	7	SER	C-N-CA	-5.44	110.75	121.41
1	L	57	ALA	CA-C-O	-5.44	112.73	120.51
1	L	2	ILE	N-CA-C	-5.42	102.59	109.80
1	L	49	SER	CA-C-O	-5.41	114.82	120.88
1	L	124	PHE	CA-CB-CG	5.41	119.21	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	211	ILE	N-CA-CB	5.41	118.02	110.56
2	H	106	ASP	CA-C-O	-5.40	114.49	120.60
1	L	143	ASN	O-C-N	5.40	130.07	123.21
1	L	44	GLN	N-CA-CB	5.40	119.18	110.65
2	H	164	LEU	N-CA-C	-5.40	101.37	109.15
1	L	64	VAL	O-C-N	5.40	127.25	121.10
1	L	177	SER	CA-C-N	5.40	133.00	121.45
1	L	177	SER	C-N-CA	5.40	133.00	121.45
2	H	75	SER	CA-C-N	-5.39	114.05	122.73
2	H	75	SER	C-N-CA	-5.39	114.05	122.73
2	H	178	ASP	N-CA-C	-5.39	103.85	111.56
1	L	139	VAL	O-C-N	5.38	128.62	123.14
1	L	84	VAL	CA-C-O	-5.37	114.07	120.78
2	H	67	LYS	N-CA-CB	-5.37	102.87	110.81
2	H	62	PRO	CA-C-N	5.36	127.46	120.28
2	H	62	PRO	C-N-CA	5.36	127.46	120.28
1	L	127	SER	CA-CB-OG	5.36	121.82	111.10
2	H	21	SER	CA-CB-OG	-5.36	100.39	111.10
2	H	128	PRO	CA-C-N	5.35	131.63	123.23
2	H	128	PRO	C-N-CA	5.35	131.63	123.23
1	L	197	SER	CA-C-O	-5.35	114.74	120.46
2	H	192	THR	O-C-N	5.34	128.25	122.11
2	H	155	VAL	N-CA-CB	5.33	121.80	111.93
1	L	119	PRO	CA-C-O	-5.33	114.64	122.31
1	L	90	ALA	CA-C-N	-5.31	116.61	123.19
1	L	90	ALA	C-N-CA	-5.31	116.61	123.19
1	L	129	GLU	CB-CA-C	5.31	119.70	110.68
1	L	22	THR	CA-CB-CG2	5.29	119.50	110.50
2	H	201	ASN	CA-C-N	-5.29	115.59	122.94
2	H	201	ASN	C-N-CA	-5.29	115.59	122.94
1	L	68	PHE	CA-CB-CG	-5.28	108.52	113.80
2	H	103	TYR	N-CA-C	-5.27	106.90	113.38
2	H	172	PRO	O-C-N	-5.27	115.53	122.64
2	H	55	ASN	CB-CA-C	-5.26	98.87	109.55
2	H	144	GLY	O-C-N	5.26	129.66	123.66
2	H	14	PRO	CA-C-O	-5.25	115.47	121.56
2	H	37	VAL	O-C-N	-5.25	117.53	123.20
1	L	55	TYR	O-C-N	-5.24	116.77	122.84
1	L	188	THR	CA-C-O	-5.23	115.93	121.94
1	L	123	ILE	CB-CG1-CD1	-5.22	102.84	113.80
1	L	191	GLU	CA-CB-CG	5.20	124.51	114.10
2	H	97	ASP	N-CA-CB	-5.20	102.98	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	206	THR	N-CA-CB	-5.18	101.95	110.14
1	L	27	GLN	N-CA-C	-5.18	101.04	108.60
1	L	162	GLN	CA-C-O	5.18	125.53	119.06
2	H	107	TYR	CA-CB-CG	-5.18	104.58	113.90
2	H	193	TRP	N-CA-C	5.17	117.68	109.40
1	L	214	SER	CB-CA-C	-5.17	99.14	110.67
2	H	94	TYR	CB-CA-C	-5.16	101.83	110.19
1	L	155	LYS	CA-C-O	-5.16	114.72	120.66
1	L	103	THR	CA-CB-OG1	-5.15	101.88	109.60
1	L	81	ILE	CA-C-O	-5.15	114.90	120.67
1	L	206	THR	OG1-CB-CG2	5.14	119.57	109.30
2	H	50	ARG	CG-CD-NE	-5.13	100.72	112.00
1	L	103	THR	CA-C-O	5.13	126.89	121.05
2	H	199	THR	CA-C-O	-5.12	114.77	120.66
1	L	8	PRO	CA-C-N	5.12	128.09	120.31
1	L	8	PRO	C-N-CA	5.12	128.09	120.31
2	H	50	ARG	CD-NE-CZ	5.11	131.55	124.40
1	L	115	ALA	CA-C-O	-5.11	115.57	121.19
1	L	34	THR	N-CA-CB	-5.10	102.37	110.28
1	L	203	THR	CA-CB-OG1	-5.10	101.95	109.60
2	H	23	THR	N-CA-C	5.09	118.10	109.76
1	L	157	ASP	O-C-N	-5.08	115.75	122.40
2	H	142	THR	OG1-CB-CG2	5.08	119.45	109.30
2	H	202	VAL	O-C-N	5.07	128.53	123.10
1	L	193	GLU	N-CA-C	5.07	118.56	112.38
2	H	29	ILE	CA-CB-CG2	5.07	119.12	110.50
1	L	38	TYR	CA-CB-CG	-5.07	104.78	113.90
2	H	4	LEU	O-C-N	-5.07	117.31	123.29
2	H	68	ALA	N-CA-C	5.07	118.33	110.17
1	L	199	THR	O-C-N	5.05	129.44	123.27
1	L	19	VAL	N-CA-CB	-5.05	102.44	112.24
2	H	112	THR	CB-CA-C	-5.05	102.99	110.62
1	L	23	CYS	CA-C-O	5.04	127.05	120.15
2	H	72	VAL	CA-C-N	-5.03	116.28	123.03
2	H	72	VAL	C-N-CA	-5.03	116.28	123.03
1	L	51	LYS	CA-C-O	-5.02	114.94	120.36
2	H	20	LEU	N-CA-C	-5.02	103.09	110.52
2	H	102	TYR	CA-C-N	-5.02	113.58	122.26
2	H	102	TYR	C-N-CA	-5.02	113.58	122.26
1	L	134	GLY	CA-C-N	5.01	126.51	121.35
1	L	134	GLY	C-N-CA	5.01	126.51	121.35
2	H	178	ASP	N-CA-CB	5.01	120.27	112.25

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	L	1707	0	1644	161	0
2	H	1625	0	1566	104	0
3	H	5	0	0	0	0
4	H	5	0	0	1	0
All	All	3342	0	3210	256	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 39.

All (256) 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:L:204:HIS:CD2	1:L:206:THR:HB	1.72	1.25
1:L:118:ALA:HB2	1:L:206:THR:CG2	1.76	1.16
2:H:176:GLN:O	2:H:177:SER:HB3	1.52	1.09
1:L:118:ALA:CB	1:L:206:THR:HG21	1.83	1.08
2:H:192:THR:HG23	2:H:196:GLN:NE2	1.68	1.07
1:L:118:ALA:HB2	1:L:206:THR:HG21	1.37	1.06
1:L:142:LEU:HD23	1:L:150:ILE:CD1	1.86	1.05
1:L:142:LEU:HD23	1:L:150:ILE:HD13	1.38	1.04
1:L:142:LEU:CD2	1:L:150:ILE:HD13	1.93	0.97
1:L:204:HIS:HD2	1:L:206:THR:HB	1.30	0.96
2:H:192:THR:HG23	2:H:196:GLN:HE21	1.23	0.92
1:L:118:ALA:HB2	1:L:206:THR:HG23	1.54	0.89
2:H:175:LEU:HD11	2:H:178:ASP:HA	1.53	0.89
1:L:190:ASP:O	1:L:192:TYR:N	2.08	0.86
1:L:167:ASN:HB3	1:L:181:MET:CE	2.07	0.83
1:L:190:ASP:O	1:L:191:GLU:C	2.21	0.83
1:L:176:ASP:OD1	1:L:178:THR:HB	1.79	0.83
1:L:188:THR:HG23	1:L:191:GLU:OE1	1.79	0.83
2:H:87:THR:HG22	2:H:89:GLU:H	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2:VAL:HG13	2:H:27:PHE:CD2	2.14	0.81
1:L:144:ASN:HD22	1:L:178:THR:HG21	1.44	0.81
1:L:204:HIS:CD2	1:L:206:THR:CB	2.61	0.80
1:L:144:ASN:ND2	1:L:178:THR:HG21	1.99	0.78
1:L:27:GLN:HG2	1:L:28:SER:N	1.98	0.78
1:L:144:ASN:HA	1:L:178:THR:CG2	2.15	0.77
1:L:141:PHE:HD1	1:L:182:SER:HB2	1.50	0.76
2:H:87:THR:CG2	2:H:89:GLU:H	2.00	0.75
2:H:175:LEU:O	2:H:176:GLN:HB2	1.85	0.74
2:H:65:GLN:HG3	2:H:66:GLY:N	2.02	0.74
2:H:201:ASN:ND2	2:H:212:ASP:OD1	2.22	0.73
1:L:144:ASN:HA	1:L:178:THR:HG23	1.70	0.73
1:L:218:ASN:O	1:L:219:GLU:CB	2.33	0.72
1:L:27:GLN:CG	1:L:28:SER:N	2.51	0.72
1:L:67:ARG:HH11	1:L:67:ARG:HG2	1.54	0.72
1:L:212:VAL:O	1:L:213:LYS:HD2	1.89	0.72
2:H:139:SER:C	2:H:190:SER:HB3	2.15	0.72
1:L:139:VAL:HG22	1:L:184:THR:HB	1.72	0.71
1:L:11:LEU:HD21	1:L:19:VAL:HG11	1.71	0.70
2:H:143:LEU:N	2:H:143:LEU:HD12	2.06	0.70
1:L:11:LEU:HD21	1:L:19:VAL:CG1	2.22	0.70
2:H:159:TRP:HZ3	2:H:215:ILE:CD1	2.05	0.70
1:L:131:LEU:O	1:L:134:GLY:HA2	1.92	0.69
2:H:87:THR:HG22	2:H:89:GLU:N	2.07	0.69
1:L:21:MET:O	1:L:78:THR:HA	1.92	0.69
1:L:17:GLU:O	1:L:83:GLY:N	2.24	0.69
1:L:118:ALA:CB	1:L:206:THR:CG2	2.53	0.69
1:L:11:LEU:HD11	1:L:19:VAL:HG13	1.74	0.68
2:H:23:THR:HG22	2:H:24:THR:O	1.93	0.68
1:L:141:PHE:CD1	1:L:182:SER:HB2	2.27	0.68
1:L:18:LYS:HB2	1:L:82:SER:HA	1.75	0.68
1:L:50:PRO:HG2	2:H:108:TRP:CZ3	2.30	0.67
1:L:17:GLU:HG3	1:L:18:LYS:H	1.59	0.67
2:H:86:LEU:HA	2:H:90:ASP:OD2	1.95	0.66
1:L:166:LEU:HD21	2:H:176:GLN:CD	2.22	0.65
1:L:53:LEU:C	1:L:54:ILE:CG1	2.69	0.65
1:L:118:ALA:HB1	1:L:206:THR:HG21	1.78	0.65
1:L:13:VAL:HG21	1:L:19:VAL:HG22	1.76	0.65
2:H:78:THR:HG21	2:H:80:TYR:CZ	2.32	0.65
1:L:13:VAL:HG13	1:L:17:GLU:HB3	1.78	0.64
1:L:161:ARG:NH2	1:L:191:GLU:OE2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:53:LEU:O	1:L:54:ILE:HG12	1.97	0.64
1:L:16:GLY:O	1:L:83:GLY:HA2	1.98	0.64
2:H:176:GLN:O	2:H:177:SER:CB	2.36	0.64
1:L:155:LYS:HA	1:L:159:SER:O	1.98	0.63
1:L:189:LYS:O	1:L:193:GLU:HG3	1.99	0.62
1:L:5:THR:HG22	1:L:5:THR:O	1.98	0.62
1:L:218:ASN:O	1:L:219:GLU:HG3	2.00	0.62
2:H:39:GLN:O	2:H:92:ALA:HB1	2.00	0.61
2:H:30:LYS:HE2	2:H:74:THR:HG21	1.82	0.61
1:L:4:MET:CE	1:L:23:CYS:SG	2.89	0.61
1:L:13:VAL:HG13	1:L:17:GLU:CB	2.30	0.61
1:L:218:ASN:O	1:L:219:GLU:HB2	2.01	0.61
2:H:214:LYS:HE2	2:H:216:GLU:OE1	2.01	0.61
1:L:167:ASN:HB3	1:L:181:MET:HE3	1.81	0.60
2:H:143:LEU:HD12	2:H:143:LEU:H	1.64	0.60
2:H:186:VAL:HG13	2:H:186:VAL:O	2.02	0.59
1:L:67:ARG:HG2	1:L:67:ARG:NH1	2.18	0.59
2:H:105:MET:HG2	2:H:107:TYR:CZ	2.38	0.59
1:L:119:PRO:HD3	1:L:204:HIS:CD2	2.38	0.58
2:H:175:LEU:CD1	2:H:178:ASP:HA	2.29	0.58
1:L:68:PHE:CE1	1:L:81:ILE:HG12	2.39	0.58
1:L:49:SER:HB3	2:H:95:TYR:CE2	2.39	0.58
1:L:50:PRO:HG2	2:H:108:TRP:CH2	2.39	0.58
2:H:87:THR:CG2	2:H:88:SER:N	2.67	0.57
1:L:144:ASN:HA	1:L:178:THR:HG21	1.86	0.57
1:L:10:SER:HA	1:L:109:LYS:O	2.05	0.57
1:L:31:ASN:O	1:L:35:GLN:N	2.37	0.57
2:H:67:LYS:HE3	2:H:84:SER:O	2.04	0.56
1:L:126:PRO:CD	1:L:192:TYR:CZ	2.89	0.56
1:L:25:SER:OG	1:L:27:GLN:O	2.18	0.56
1:L:53:LEU:C	1:L:54:ILE:HG12	2.29	0.56
1:L:156:ILE:HD13	1:L:198:TYR:CE2	2.40	0.56
2:H:97:ASP:OD2	2:H:106:ASP:OD1	2.22	0.56
1:L:27:GLN:HG3	1:L:28:SER:H	1.71	0.56
1:L:128:SER:O	1:L:129:GLU:C	2.48	0.56
2:H:34:ILE:O	2:H:34:ILE:HG22	2.04	0.56
1:L:14:THR:O	1:L:15:THR:C	2.47	0.56
2:H:171:PHE:O	2:H:172:PRO:C	2.46	0.56
2:H:99:TYR:OH	2:H:104:ASP:OD1	2.12	0.56
1:L:30:LEU:HD12	1:L:31:ASN:N	2.19	0.56
1:L:27:GLN:CG	1:L:28:SER:H	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:114:ARG:NH1	1:L:115:ALA:O	2.36	0.55
1:L:125:PRO:C	1:L:126:PRO:O	2.44	0.55
1:L:125:PRO:O	1:L:126:PRO:O	2.25	0.55
2:H:78:THR:CG2	2:H:80:TYR:CZ	2.89	0.55
2:H:3:GLN:HG2	2:H:25:SER:HB3	1.89	0.54
1:L:64:VAL:HG12	1:L:65:PRO:O	2.07	0.54
2:H:130:ALA:HB1	2:H:131:PRO:HD2	1.88	0.54
1:L:181:MET:HG3	1:L:182:SER:N	2.22	0.53
1:L:181:MET:CG	1:L:182:SER:N	2.70	0.53
1:L:216:ASN:HB3	1:L:219:GLU:HG3	1.90	0.52
1:L:31:ASN:HB2	1:L:38:TYR:HE2	1.73	0.52
2:H:2:VAL:HG22	2:H:26:GLY:O	2.08	0.52
1:L:66:ASP:C	1:L:66:ASP:OD1	2.53	0.52
2:H:1:GLU:N	2:H:1:GLU:CD	2.68	0.52
1:L:164:GLY:O	1:L:185:LEU:HA	2.10	0.52
1:L:204:HIS:HD2	1:L:206:THR:CB	2.12	0.52
1:L:218:ASN:O	1:L:219:GLU:CG	2.57	0.52
1:L:166:LEU:HD21	2:H:176:GLN:NE2	2.24	0.51
1:L:126:PRO:HD2	1:L:192:TYR:CZ	2.45	0.51
1:L:195:HIS:N	1:L:195:HIS:CD2	2.79	0.51
2:H:2:VAL:HG12	2:H:107:TYR:CZ	2.46	0.51
2:H:142:THR:HB	2:H:187:THR:HG22	1.92	0.51
1:L:88:ASP:O	1:L:110:LEU:HD23	2.11	0.51
2:H:9:ALA:HA	2:H:113:SER:O	2.10	0.51
1:L:53:LEU:O	1:L:64:VAL:HG21	2.11	0.50
1:L:29:LEU:HD22	1:L:98:TYR:HB2	1.94	0.50
1:L:131:LEU:O	1:L:134:GLY:CA	2.59	0.50
1:L:132:THR:C	1:L:134:GLY:N	2.68	0.50
1:L:55:TYR:OH	2:H:104:ASP:OD1	2.26	0.50
1:L:191:GLU:O	1:L:192:TYR:C	2.51	0.50
2:H:159:TRP:HZ3	2:H:215:ILE:HD11	1.76	0.50
1:L:156:ILE:O	1:L:157:ASP:C	2.53	0.50
1:L:165:VAL:HG22	1:L:185:LEU:HD13	1.93	0.50
2:H:30:LYS:CE	2:H:74:THR:HG21	2.41	0.50
1:L:172:GLN:NE2	1:L:177:SER:O	2.41	0.49
1:L:16:GLY:O	1:L:17:GLU:O	2.31	0.49
1:L:169:TRP:O	2:H:172:PRO:HG2	2.12	0.49
2:H:11:LEU:HB2	2:H:152:PRO:HG3	1.95	0.49
2:H:159:TRP:CZ3	2:H:215:ILE:HD11	2.47	0.49
1:L:132:THR:C	1:L:134:GLY:H	2.20	0.49
2:H:6:GLN:HG3	2:H:110:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:30:LEU:HD12	1:L:31:ASN:H	1.77	0.49
1:L:30:LEU:HD12	1:L:36:LYS:O	2.13	0.49
1:L:199:THR:HG22	1:L:201:GLU:HG2	1.95	0.49
2:H:61:ASP:OD1	2:H:63:LYS:CB	2.61	0.49
1:L:178:THR:HG23	1:L:179:TYR:N	2.28	0.48
2:H:211:VAL:CG2	2:H:212:ASP:N	2.76	0.48
1:L:126:PRO:HD2	1:L:192:TYR:OH	2.13	0.48
1:L:190:ASP:O	1:L:193:GLU:N	2.46	0.48
1:L:126:PRO:HG2	1:L:192:TYR:CE2	2.49	0.48
2:H:12:VAL:CG2	2:H:86:LEU:HD12	2.43	0.48
1:L:84:VAL:C	1:L:85:GLN:HG2	2.38	0.48
1:L:89:LEU:HD12	1:L:110:LEU:O	2.13	0.48
2:H:2:VAL:HA	2:H:25:SER:O	2.13	0.48
1:L:13:VAL:HG22	1:L:17:GLU:HG2	1.95	0.48
2:H:20:LEU:HD22	2:H:112:THR:HG21	1.96	0.48
1:L:58:SER:HB3	1:L:70:GLY:O	2.14	0.47
1:L:130:GLN:HE22	1:L:137:SER:HB2	1.79	0.47
2:H:100:TYR:HA	4:H:725:HOH:O	2.13	0.47
1:L:189:LYS:O	1:L:189:LYS:HG2	2.14	0.47
2:H:171:PHE:HA	2:H:172:PRO:HD3	1.82	0.47
2:H:62:PRO:O	2:H:65:GLN:HG2	2.15	0.47
2:H:159:TRP:CZ3	2:H:215:ILE:CD1	2.92	0.47
1:L:116:ASP:OD2	1:L:205:LYS:HD3	2.15	0.47
1:L:190:ASP:C	1:L:192:TYR:N	2.73	0.47
2:H:2:VAL:HG13	2:H:27:PHE:HD2	1.74	0.47
2:H:61:ASP:OD1	2:H:63:LYS:HB3	2.15	0.47
2:H:61:ASP:O	2:H:62:PRO:C	2.55	0.47
2:H:129:LEU:HB2	2:H:144:GLY:O	2.13	0.47
1:L:114:ARG:HD2	1:L:177:SER:HB2	1.96	0.46
1:L:114:ARG:HG2	1:L:146:TYR:CD2	2.50	0.46
1:L:4:MET:HB3	1:L:4:MET:HE3	1.53	0.46
1:L:85:GLN:O	1:L:86:ALA:C	2.58	0.46
1:L:156:ILE:HD13	1:L:198:TYR:HE2	1.80	0.46
1:L:67:ARG:HD2	1:L:81:ILE:HG22	1.98	0.46
1:L:199:THR:OG1	1:L:214:SER:OG	2.23	0.46
1:L:30:LEU:HD13	1:L:37:ASN:CG	2.41	0.46
1:L:199:THR:CG2	1:L:201:GLU:HG2	2.46	0.46
2:H:20:LEU:HD21	2:H:114:VAL:CG2	2.46	0.45
1:L:4:MET:HE3	1:L:23:CYS:SG	2.55	0.45
2:H:132:VAL:O	2:H:133:CYS:C	2.58	0.45
1:L:204:HIS:O	1:L:206:THR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:194:PRO:HG3	2:H:217:PRO:HG3	1.99	0.45
1:L:56:TRP:O	1:L:58:SER:N	2.49	0.45
2:H:1:GLU:O	2:H:1:GLU:OE2	2.35	0.45
2:H:87:THR:HG23	2:H:88:SER:N	2.30	0.45
1:L:104:PHE:C	1:L:105:GLY:O	2.59	0.45
1:L:123:ILE:HG21	1:L:123:ILE:HD13	1.71	0.45
2:H:2:VAL:HG13	2:H:27:PHE:CE2	2.52	0.44
2:H:30:LYS:HE3	2:H:74:THR:HB	1.98	0.44
1:L:21:MET:O	1:L:78:THR:CA	2.64	0.44
2:H:218:ARG:HH11	2:H:218:ARG:HD3	1.53	0.44
2:H:86:LEU:HD22	2:H:90:ASP:OD2	2.18	0.44
2:H:70:ILE:HA	2:H:80:TYR:O	2.18	0.44
2:H:157:LEU:C	2:H:157:LEU:HD23	2.42	0.44
2:H:193:TRP:HH2	2:H:217:PRO:HA	1.83	0.44
1:L:131:LEU:O	1:L:134:GLY:N	2.51	0.44
2:H:63:LYS:HB2	2:H:63:LYS:HE3	1.79	0.44
2:H:78:THR:HG22	2:H:80:TYR:CE2	2.52	0.44
1:L:31:ASN:O	1:L:35:GLN:HA	2.18	0.43
1:L:130:GLN:HE22	1:L:137:SER:CB	2.31	0.43
1:L:204:HIS:C	1:L:206:THR:N	2.74	0.43
2:H:1:GLU:CD	2:H:1:GLU:H3	2.26	0.43
2:H:65:GLN:HG3	2:H:66:GLY:H	1.79	0.43
1:L:29:LEU:HD22	1:L:98:TYR:CB	2.48	0.43
1:L:188:THR:CG2	1:L:191:GLU:OE1	2.59	0.43
1:L:209:SER:HA	1:L:210:PRO:HD3	1.88	0.43
2:H:145:CYS:O	2:H:183:SER:HA	2.18	0.43
2:H:61:ASP:C	2:H:63:LYS:N	2.76	0.43
1:L:96:ASN:OD1	1:L:96:ASN:C	2.61	0.43
2:H:87:THR:HG23	2:H:88:SER:H	1.84	0.43
1:L:126:PRO:HG2	1:L:192:TYR:CZ	2.54	0.43
1:L:123:ILE:HD12	1:L:200:CYS:CB	2.49	0.42
1:L:127:SER:O	1:L:128:SER:C	2.62	0.42
1:L:165:VAL:HG22	1:L:185:LEU:CD1	2.49	0.42
2:H:2:VAL:CG2	2:H:26:GLY:O	2.65	0.42
2:H:186:VAL:O	2:H:186:VAL:CG1	2.67	0.42
1:L:56:TRP:C	1:L:58:SER:H	2.28	0.42
2:H:28:ASN:N	2:H:28:ASN:ND2	2.67	0.42
2:H:94:TYR:CD1	2:H:94:TYR:N	2.88	0.42
2:H:159:TRP:O	2:H:160:ASN:C	2.61	0.42
2:H:197:SER:C	2:H:198:ILE:HD13	2.45	0.42
2:H:51:LEU:HD12	2:H:58:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:55:ASN:HB2	2:H:57:TYR:HD1	1.84	0.42
1:L:6:GLN:OE1	1:L:105:GLY:C	2.62	0.42
1:L:170:THR:HG23	2:H:171:PHE:CE2	2.55	0.41
1:L:156:ILE:N	1:L:159:SER:O	2.48	0.41
2:H:13:ARG:HA	2:H:14:PRO:HD3	1.89	0.41
1:L:97:ASN:HA	1:L:102:LEU:HD22	2.01	0.41
1:L:150:ILE:HG13	1:L:204:HIS:HB2	2.01	0.41
1:L:166:LEU:HD21	2:H:176:GLN:CG	2.50	0.41
1:L:194:ARG:HB3	1:L:195:HIS:CD2	2.55	0.41
2:H:71:THR:HG22	2:H:80:TYR:HD2	1.86	0.41
1:L:132:THR:HG22	1:L:133:SER:N	2.31	0.41
1:L:188:THR:N	1:L:191:GLU:OE1	2.50	0.41
2:H:35:HIS:HB2	2:H:97:ASP:OD1	2.21	0.41
2:H:55:ASN:OD1	2:H:55:ASN:N	2.50	0.41
1:L:53:LEU:HD12	1:L:53:LEU:HA	1.83	0.41
1:L:89:LEU:O	1:L:90:ALA:HB2	2.21	0.41
2:H:126:VAL:HA	2:H:146:LEU:O	2.21	0.41
1:L:6:GLN:OE1	1:L:105:GLY:HA3	2.20	0.41
1:L:162:GLN:HE21	1:L:162:GLN:HB2	1.60	0.41
2:H:23:THR:HG22	2:H:24:THR:N	2.35	0.41
2:H:157:LEU:HA	2:H:201:ASN:O	2.19	0.41
2:H:163:SER:HB2	2:H:164:LEU:H	1.64	0.41
1:L:31:ASN:HB2	1:L:38:TYR:CE2	2.54	0.41
2:H:32:ILE:HG21	2:H:32:ILE:HD13	1.79	0.41
2:H:26:GLY:O	2:H:27:PHE:HB3	2.21	0.40
1:L:187:LEU:HD23	1:L:187:LEU:HA	1.79	0.40
1:L:155:LYS:CA	1:L:159:SER:O	2.68	0.40
1:L:167:ASN:CB	1:L:181:MET:CE	2.91	0.40
2:H:20:LEU:HD21	2:H:114:VAL:HG21	2.03	0.40
1:L:32:SER:O	1:L:33:ARG:C	2.64	0.40
1:L:123:ILE:HD12	1:L:200:CYS:HB3	2.04	0.40
1:L:204:HIS:HD2	1:L:206:THR:CG2	2.33	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	L	217/220 (99%)	194 (89%)	14 (6%)	9 (4%)	2	8
2	H	209/218 (96%)	187 (90%)	18 (9%)	4 (2%)	6	22
All	All	426/438 (97%)	381 (89%)	32 (8%)	13 (3%)	3	12

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	17	GLU
1	L	33	ARG
1	L	191	GLU
1	L	190	ASP
1	L	205	LYS
2	H	176	GLN
2	H	177	SER
1	L	98	TYR
1	L	126	PRO
1	L	57	ALA
2	H	9	ALA
1	L	146	TYR
2	H	163	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	197/198 (100%)	149 (76%)	48 (24%)	1	2
2	H	186/190 (98%)	144 (77%)	42 (23%)	1	3
All	All	383/388 (99%)	293 (76%)	90 (24%)	1	3

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	7	SER
1	L	11	LEU
1	L	13	VAL
1	L	15	THR
1	L	17	GLU
1	L	18	LYS
1	L	20	THR
1	L	21	MET
1	L	34	THR
1	L	35	GLN
1	L	43	GLN
1	L	46	PRO
1	L	49	SER
1	L	53	LEU
1	L	54	ILE
1	L	58	SER
1	L	69	THR
1	L	80	SER
1	L	84	VAL
1	L	85	GLN
1	L	89	LEU
1	L	96	ASN
1	L	111	GLU
1	L	112	LEU
1	L	114	ARG
1	L	128	SER
1	L	129	GLU
1	L	150	ILE
1	L	153	LYS
1	L	155	LYS
1	L	156	ILE
1	L	161	ARG
1	L	171	ASP
1	L	175	LYS
1	L	178	THR
1	L	181	MET
1	L	182	SER
1	L	184	THR
1	L	186	THR
1	L	194	ARG
1	L	197	SER
1	L	199	THR

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Mol	Chain	Res	Type
1	L	205	LYS
1	L	206	THR
1	L	207	SER
1	L	208	THR
1	L	213	LYS
2	H	1	GLU
2	H	2	VAL
2	H	7	SER
2	H	10	GLU
2	H	11	LEU
2	H	28	ASN
2	H	29	ILE
2	H	43	GLN
2	H	50	ARG
2	H	51	LEU
2	H	55	ASN
2	H	67	LYS
2	H	71	THR
2	H	78	THR
2	H	85	SER
2	H	86	LEU
2	H	87	THR
2	H	93	VAL
2	H	97	ASP
2	H	121	THR
2	H	122	THR
2	H	132	VAL
2	H	142	THR
2	H	145	CYS
2	H	161	SER
2	H	163	SER
2	H	166	SER
2	H	168	VAL
2	H	174	VAL
2	H	177	SER
2	H	178	ASP
2	H	187	THR
2	H	195	SER
2	H	196	GLN
2	H	197	SER
2	H	198	ILE
2	H	199	THR

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Mol	Chain	Res	Type
2	H	211	VAL
2	H	212	ASP
2	H	214	LYS
2	H	216	GLU
2	H	218	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	31	ASN
1	L	44	GLN
1	L	48	GLN
1	L	144	ASN
1	L	162	GLN
1	L	163	ASN
1	L	196	ASN
2	H	28	ASN
2	H	39	GLN
2	H	169	HIS
2	H	196	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
3	SO4	H	720	-	4,4,4	0.65	0	6,6,6	0.49	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.