



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:34 AM UTC

PDB ID : 1IGC / pdb_00001igc
Title : IGG1 FAB FRAGMENT (MOPC21) COMPLEX WITH DOMAIN III OF PROTEIN G FROM STREPTOCOCCUS
Authors : Derrick, J.P.; Wigley, D.B.
Deposited on : 1994-08-05
Resolution : 2.60 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

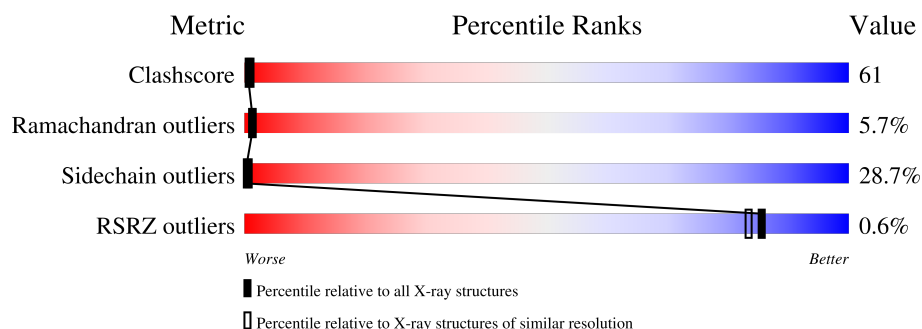
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	213	13% 33% 39% 14%
2	H	222	16% 42% 30% 13%
3	A	61	15% 51% 28% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4117 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 IGG1-KAPPA MOPC21 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1651	1025	277	340	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	92	ASN	TYR	conflict	UNP P01634
L	?	-	GLY	deletion	UNP P01634

- Molecule 2 is a protein called IGG1-KAPPA MOPC21 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1675	1057	281	327	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	5	VAL	LEU	conflict	UNP P01783
H	13	GLN	LYS	conflict	UNP P01783
H	18	ARG	LEU	conflict	UNP P01783
H	31	SER	ASP	conflict	UNP P01783
H	32	PHE	TYR	conflict	UNP P01783
H	58	LEU	ILE	conflict	UNP P01783
H	59	HIS	TYR	conflict	UNP P01783
H	75	PRO	ALA	conflict	UNP P01783
H	92	GLY	ALA	conflict	UNP P01783
H	?	-	ASP	deletion	UNP P01783
H	?	-	THR	deletion	UNP P01783
H	?	-	THR	deletion	UNP P01783
H	100	GLY	VAL	conflict	UNP P01783
H	101	ASN	SER	conflict	UNP P01783

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Chain	Residue	Modelled	Actual	Comment	Reference
H	102	TYR	GLY	conflict	UNP P01783
H	103	PRO	HIS	conflict	UNP P01783
H	106	ALA	VAL	conflict	UNP P01783
H	194	PRO	THR	conflict	UNP P01783
H	195	ARG	TRP	conflict	UNP P01783
H	198	GLU	GLN	conflict	UNP P01783

- Molecule 3 is a protein called STREPTOCOCCAL PROTEIN G (DOMAIN III).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	58	Total	C	N	O	0	0	0
			446	280	70	96			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	163	Total	O	0	0
			163	163		
4	H	145	Total	O	0	0
			145	145		
4	A	37	Total	O	0	0
			37	37		

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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.50Å 70.50Å 120.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.60) 98.4 (20.00-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.71 (at 2.59Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.168 , (Not available) 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 210.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4117	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.25	4/1687 (0.2%)	3.52	233/2291 (10.2%)
2	H	1.21	3/1722 (0.2%)	3.08	229/2352 (9.7%)
3	A	1.09	1/452 (0.2%)	2.87	55/613 (9.0%)
All	All	1.21	8/3861 (0.2%)	3.26	517/5256 (9.8%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	84	THR	CA-CB	10.65	1.61	1.53
1	L	30	VAL	N-CA	8.69	1.57	1.46
1	L	141	PRO	N-CD	7.06	1.57	1.47
1	L	51	ALA	N-CA	5.81	1.53	1.45
2	H	124	THR	CA-CB	5.64	1.60	1.53
3	A	7	THR	CA-CB	5.54	1.60	1.53
1	L	141	PRO	N-CA	-5.18	1.40	1.47
2	H	140	ASN	CA-C	5.12	1.59	1.52

All (517) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	140	TYR	CA-C-N	45.61	176.86	119.84
1	L	140	TYR	C-N-CA	45.61	176.86	119.84
1	L	140	TYR	O-C-N	29.51	155.26	121.32
2	H	38	ARG	CD-NE-CZ	28.71	164.60	124.40
2	H	67	ARG	CD-NE-CZ	24.04	158.05	124.40
1	L	141	PRO	N-CA-CB	22.21	126.57	103.25
2	H	43	LYS	CA-C-N	18.35	138.80	122.47
2	H	43	LYS	C-N-CA	18.35	138.80	122.47
2	H	195	ARG	CG-CD-NE	17.39	150.27	112.00
1	L	141	PRO	CA-N-CD	-17.31	87.77	112.00
1	L	137	ASN	CA-CB-CG	17.15	129.75	112.60
1	L	1	ASN	CA-CB-CG	16.63	129.23	112.60
1	L	153	GLU	CA-C-N	15.69	145.58	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	153	GLU	C-N-CA	15.69	145.58	120.94
2	H	42	GLU	CA-C-O	14.77	138.00	119.98
2	H	42	GLU	N-CA-CB	14.74	134.64	110.32
2	H	64	VAL	N-CA-CB	-14.65	93.36	112.26
1	L	154	ARG	N-CA-C	14.19	130.51	110.50
1	L	135	PHE	CA-CB-CG	13.94	127.74	113.80
1	L	207	SER	CA-C-N	13.66	147.62	121.54
1	L	207	SER	C-N-CA	13.66	147.62	121.54
1	L	209	ASN	CA-CB-CG	13.26	125.86	112.60
1	L	208	PHE	CA-CB-CG	13.14	126.94	113.80
2	H	140	ASN	N-CA-CB	12.84	127.66	110.59
2	H	140	ASN	N-CA-C	-12.58	98.41	113.88
1	L	189	ASN	CA-CB-CG	12.41	125.01	112.60
2	H	195	ARG	NE-CZ-NH1	12.39	133.89	121.50
1	L	210	ARG	CD-NE-CZ	11.90	141.06	124.40
1	L	141	PRO	N-CD-CG	11.89	121.03	103.20
3	A	13	ASN	OD1-CG-ND2	11.48	134.08	122.60
1	L	92	ASN	CA-CB-CG	11.40	124.00	112.60
2	H	32	PHE	CA-CB-CG	-11.31	102.49	113.80
1	L	206	LYS	CA-C-N	11.30	143.13	121.54
1	L	206	LYS	C-N-CA	11.30	143.13	121.54
1	L	58	VAL	CA-C-O	11.11	126.94	119.38
1	L	140	TYR	CA-C-O	-11.07	105.00	120.16
1	L	50	GLY	CA-C-O	-10.95	108.97	122.01
2	H	86	LEU	CB-CA-C	10.93	123.25	109.80
1	L	49	TYR	CA-C-O	-10.75	109.11	121.58
1	L	201	THR	CA-C-N	10.73	135.91	121.74
1	L	201	THR	C-N-CA	10.73	135.91	121.74
2	H	48	VAL	N-CA-C	10.65	120.53	111.90
1	L	81	GLU	CB-CG-CD	10.56	130.56	112.60
2	H	6	GLU	CB-CG-CD	10.48	130.42	112.60
1	L	74	THR	CA-C-O	-10.31	109.58	120.40
2	H	33	GLY	N-CA-C	-10.16	98.15	112.37
1	L	133	VAL	CA-CB-CG1	10.00	127.40	110.40
2	H	149	VAL	O-C-N	9.86	132.16	122.30
2	H	44	GLY	O-C-N	9.72	131.75	123.29
2	H	4	LEU	CA-C-O	-9.58	109.69	120.32
1	L	164	ASP	N-CA-C	-9.56	96.72	110.59
3	A	27	ASP	CA-CB-CG	9.55	122.15	112.60
1	L	3	VAL	CA-C-N	9.54	135.46	122.77
1	L	3	VAL	C-N-CA	9.54	135.46	122.77
1	L	19	VAL	CA-C-O	-9.53	111.17	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	12	ILE	O-C-N	9.53	132.85	123.03
1	L	41	GLU	CA-C-O	9.51	134.10	120.51
2	H	98	ARG	CD-NE-CZ	-9.51	111.09	124.40
1	L	196	THR	N-CA-CB	9.48	126.09	110.63
2	H	133	PRO	CA-C-N	9.45	139.94	121.41
2	H	133	PRO	C-N-CA	9.45	139.94	121.41
3	A	44	VAL	N-CA-CB	9.35	122.21	110.99
1	L	41	GLU	CA-C-N	9.33	137.89	121.75
1	L	41	GLU	C-N-CA	9.33	137.89	121.75
1	L	185	TYR	CA-C-O	9.31	130.42	120.55
1	L	95	PRO	CA-C-N	9.22	133.85	120.95
1	L	95	PRO	C-N-CA	9.22	133.85	120.95
1	L	92	ASN	OD1-CG-ND2	-9.20	113.40	122.60
1	L	154	ARG	N-CA-CB	-9.14	97.01	110.17
1	L	138	ASN	CA-C-O	-9.09	110.67	122.03
1	L	166	ASP	N-CA-C	-9.05	97.11	110.23
2	H	195	ARG	O-C-N	9.02	128.90	120.51
2	H	194	PRO	N-CA-C	8.99	131.00	112.47
2	H	162	ASN	OD1-CG-ND2	8.87	131.47	122.60
2	H	67	ARG	NE-CZ-NH1	-8.86	112.64	121.50
3	A	61	GLU	CB-CG-CD	8.84	127.62	112.60
2	H	127	SER	O-C-N	8.80	133.66	123.27
1	L	155	GLN	N-CA-C	8.78	129.51	110.80
1	L	140	TYR	C-N-CD	-8.73	89.21	125.00
1	L	48	ILE	CA-C-O	-8.69	111.14	120.36
1	L	212	GLU	N-CA-C	8.60	123.01	108.23
1	L	50	GLY	CA-C-N	-8.49	108.75	122.26
1	L	50	GLY	C-N-CA	-8.49	108.75	122.26
1	L	129	GLY	O-C-N	8.48	130.88	123.25
1	L	137	ASN	CA-C-O	8.47	131.02	121.11
1	L	61	ARG	N-CA-CB	8.43	123.28	110.30
2	H	171	HIS	N-CA-CB	8.37	124.40	110.59
1	L	137	ASN	CA-C-N	8.37	134.68	122.63
1	L	137	ASN	C-N-CA	8.37	134.68	122.63
3	A	10	LEU	O-C-N	8.36	132.97	123.27
1	L	182	LYS	N-CA-C	-8.35	101.86	110.97
2	H	43	LYS	N-CA-CB	8.29	124.50	110.49
2	H	190	VAL	N-CA-CB	-8.29	106.11	111.83
2	H	127	SER	CA-C-O	-8.27	111.22	120.32
1	L	61	ARG	CD-NE-CZ	-8.25	112.85	124.40
3	A	47	VAL	CB-CA-C	8.25	120.14	111.23
1	L	165	GLN	CA-C-O	-8.23	112.13	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	204	ILE	N-CA-C	-8.22	96.13	109.12
2	H	42	GLU	CB-CG-CD	8.19	126.53	112.60
1	L	199	THR	CA-C-O	8.18	128.14	119.14
2	H	221	ASP	CA-C-N	8.18	136.42	121.70
2	H	221	ASP	C-N-CA	8.18	136.42	121.70
1	L	38	GLN	OE1-CD-NE2	-8.13	114.47	122.60
2	H	195	ARG	CD-NE-CZ	8.12	135.77	124.40
1	L	51	ALA	N-CA-C	-8.12	103.16	113.72
2	H	32	PHE	N-CA-C	8.12	122.63	109.40
1	L	52	SER	N-CA-C	8.11	123.33	112.30
3	A	47	VAL	N-CA-CB	-8.10	102.00	111.39
1	L	30	VAL	CB-CA-C	8.08	124.54	111.29
3	A	6	THR	N-CA-CB	8.06	124.11	110.49
2	H	62	ASP	CA-C-N	8.04	131.06	120.28
2	H	62	ASP	C-N-CA	8.04	131.06	120.28
2	H	152	TYR	CA-C-O	8.04	131.21	121.72
1	L	151	ASP	N-CA-C	-8.04	99.27	111.56
2	H	74	ASN	O-C-N	7.97	127.57	120.48
3	A	31	ALA	CA-C-O	-7.96	112.00	120.92
2	H	214	ASP	CA-CB-CG	7.95	120.55	112.60
1	L	86	TYR	CA-C-O	7.94	128.91	120.33
1	L	139	PHE	CA-CB-CG	7.92	121.72	113.80
2	H	131	LEU	CB-CA-C	7.86	123.28	111.17
2	H	206	HIS	O-C-N	7.86	126.73	121.23
1	L	181	THR	N-CA-CB	7.84	122.49	110.49
2	H	221	ASP	CA-C-O	7.83	131.71	120.51
3	A	20	GLU	CA-CB-CG	7.82	129.74	114.10
1	L	207	SER	N-CA-C	7.79	127.40	110.80
1	L	123	GLU	O-C-N	7.79	130.37	122.12
2	H	49	ALA	CA-C-N	7.64	135.51	122.37
2	H	49	ALA	C-N-CA	7.64	135.51	122.37
2	H	153	PHE	CA-CB-CG	-7.64	106.16	113.80
1	L	77	SER	O-C-N	7.54	132.80	123.14
1	L	163	THR	N-CA-CB	-7.53	98.97	110.42
1	L	153	GLU	O-C-N	-7.52	114.18	123.36
2	H	144	THR	CB-CA-C	7.51	122.16	110.14
2	H	139	THR	N-CA-C	7.49	120.25	108.79
1	L	152	SER	N-CA-CB	7.48	123.13	110.49
1	L	154	ARG	CD-NE-CZ	-7.46	113.96	124.40
2	H	64	VAL	N-CA-C	7.45	120.06	112.90
2	H	213	VAL	N-CA-CB	-7.44	99.25	111.45
2	H	116	VAL	CA-C-O	-7.43	112.48	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	59	HIS	O-C-N	7.42	131.88	123.27
2	H	167	SER	N-CA-C	-7.42	103.36	113.30
1	L	160	ASN	CA-CB-CG	7.36	119.96	112.60
2	H	191	PRO	CA-C-N	7.36	130.44	120.44
2	H	191	PRO	C-N-CA	7.36	130.44	120.44
2	H	182	TYR	CA-C-O	-7.31	113.34	121.89
1	L	195	ALA	N-CA-C	7.30	120.44	107.80
3	A	22	THR	O-C-N	7.29	131.48	123.10
1	L	12	SER	O-C-N	7.24	131.92	123.30
2	H	172	THR	N-CA-C	-7.22	97.97	109.59
2	H	211	THR	CA-C-N	7.22	133.29	122.47
2	H	211	THR	C-N-CA	7.22	133.29	122.47
1	L	101	GLY	CA-C-O	-7.21	116.26	121.88
2	H	43	LYS	CA-C-O	7.20	130.80	120.51
1	L	199	THR	N-CA-C	-7.19	104.66	113.50
1	L	99	GLY	N-CA-C	-7.18	101.63	112.41
3	A	11	VAL	CA-C-N	-7.15	111.76	122.70
3	A	11	VAL	C-N-CA	-7.15	111.76	122.70
1	L	118	PHE	CA-CB-CG	7.13	120.94	113.80
1	L	50	GLY	N-CA-C	-7.13	98.75	112.02
2	H	181	LEU	CB-CA-C	7.12	121.91	109.80
2	H	127	SER	N-CA-C	-7.12	96.91	108.52
3	A	11	VAL	N-CA-C	-7.12	98.11	108.71
1	L	190	SER	CA-C-O	-7.11	112.83	121.36
1	L	56	THR	CB-CA-C	7.11	120.39	110.16
1	L	12	SER	CA-C-O	-7.09	112.70	120.36
1	L	60	ASP	CA-CB-CG	7.08	119.68	112.60
2	H	209	SER	CA-C-O	7.05	127.50	119.18
3	A	33	LYS	N-CA-CB	7.05	120.60	110.16
1	L	124	GLN	CA-C-N	7.02	129.57	120.44
1	L	124	GLN	C-N-CA	7.02	129.57	120.44
3	A	18	LYS	CA-C-O	-7.00	112.80	120.36
1	L	113	PRO	N-CA-C	7.00	122.21	111.57
2	H	187	SER	CA-C-N	6.98	132.63	121.95
2	H	187	SER	C-N-CA	6.98	132.63	121.95
2	H	32	PHE	O-C-N	6.98	132.30	123.23
2	H	123	THR	CB-CA-C	6.95	121.17	109.84
2	H	45	LEU	CB-CA-C	6.94	121.92	109.64
2	H	221	ASP	CA-CB-CG	-6.94	105.66	112.60
2	H	5	VAL	O-C-N	6.94	130.17	123.03
2	H	89	GLU	CB-CA-C	-6.93	96.82	110.27
2	H	65	LYS	CA-C-O	6.93	127.98	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	188	VAL	N-CA-CB	6.91	120.52	111.19
2	H	183	THR	CB-CA-C	6.90	121.53	109.80
2	H	164	GLY	N-CA-C	6.88	124.86	115.30
1	L	110	ASP	N-CA-CB	6.87	120.19	110.36
1	L	165	GLN	CA-C-N	-6.86	110.96	120.71
1	L	165	GLN	C-N-CA	-6.86	110.96	120.71
2	H	1	ASP	CA-CB-CG	-6.86	105.74	112.60
2	H	220	ARG	CA-C-N	6.84	134.61	121.54
2	H	220	ARG	C-N-CA	6.84	134.61	121.54
1	L	11	MET	CA-C-O	-6.84	112.58	120.31
1	L	40	PRO	CB-CA-C	6.83	122.83	111.56
2	H	133	PRO	CA-C-O	6.83	129.64	119.74
2	H	123	THR	CA-C-N	6.81	132.78	122.42
2	H	123	THR	C-N-CA	6.81	132.78	122.42
3	A	56	THR	CA-CB-CG2	6.79	122.04	110.50
2	H	112	GLN	CA-C-O	6.78	127.21	119.27
3	A	41	ASP	CA-CB-CG	6.78	119.38	112.60
1	L	83	LEU	CB-CA-C	6.77	120.96	110.67
3	A	56	THR	N-CA-CB	-6.76	99.10	110.80
3	A	13	ASN	CA-C-O	6.74	129.89	120.52
3	A	6	THR	CA-CB-OG1	-6.73	99.50	109.60
1	L	12	SER	CB-CA-C	-6.73	97.39	109.71
1	L	167	SER	CA-C-O	-6.72	113.30	120.42
1	L	178	LEU	O-C-N	6.70	131.20	123.29
1	L	182	LYS	O-C-N	6.70	129.00	122.03
1	L	124	GLN	CB-CG-CD	6.70	123.98	112.60
2	H	114	THR	CA-C-O	-6.69	112.04	120.20
1	L	108	ARG	CG-CD-NE	-6.68	97.30	112.00
1	L	39	LYS	O-C-N	6.64	128.84	121.53
2	H	59	HIS	CA-C-N	6.63	133.23	122.81
2	H	59	HIS	C-N-CA	6.63	133.23	122.81
2	H	107	MET	CA-C-N	6.63	134.20	121.54
2	H	107	MET	C-N-CA	6.63	134.20	121.54
3	A	42	ASN	O-C-N	6.61	130.61	122.34
1	L	190	SER	N-CA-CB	6.61	121.19	110.41
2	H	188	VAL	N-CA-C	-6.61	99.60	108.06
2	H	45	LEU	N-CA-CB	-6.60	99.36	109.92
2	H	63	THR	CA-CB-OG1	-6.59	99.72	109.60
1	L	164	ASP	CA-CB-CG	6.58	119.18	112.60
2	H	140	ASN	CA-CB-CG	-6.57	106.03	112.60
1	L	62	PHE	CA-CB-CG	6.56	120.36	113.80
1	L	146	VAL	O-C-N	6.56	129.83	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	172	THR	CB-CA-C	6.56	121.18	109.38
1	L	154	ARG	CA-C-O	-6.55	114.42	121.56
2	H	221	ASP	N-CA-C	6.55	124.75	110.80
1	L	140	TYR	CA-CB-CG	-6.53	102.15	113.90
2	H	66	GLY	CA-C-N	6.53	134.41	122.79
2	H	66	GLY	C-N-CA	6.53	134.41	122.79
1	L	37	GLN	CA-CB-CG	6.51	127.12	114.10
1	L	165	GLN	O-C-N	6.51	130.88	122.87
2	H	79	LEU	CB-CA-C	6.51	120.53	109.80
2	H	111	GLY	N-CA-C	-6.50	102.66	112.41
3	A	5	VAL	N-CA-C	6.49	117.48	111.45
2	H	212	LYS	N-CA-CB	6.48	122.17	110.95
1	L	138	ASN	O-C-N	6.48	130.62	122.91
2	H	61	ALA	N-CA-C	-6.48	100.89	110.48
2	H	194	PRO	CB-CA-C	-6.48	100.88	111.56
1	L	145	ASN	O-C-N	6.47	130.85	123.27
1	L	61	ARG	N-CA-C	-6.47	104.08	112.23
1	L	58	VAL	CB-CA-C	6.47	117.29	110.37
2	H	126	PRO	CA-C-N	6.43	132.05	123.05
2	H	126	PRO	C-N-CA	6.43	132.05	123.05
2	H	200	VAL	CA-C-O	-6.41	113.73	120.39
1	L	141	PRO	N-CA-C	-6.40	99.28	112.47
1	L	92	ASN	CB-CG-OD1	6.39	133.57	120.80
2	H	139	THR	CA-C-O	6.38	128.06	121.23
2	H	84	THR	N-CA-C	6.37	121.29	109.24
2	H	182	TYR	O-C-N	6.37	130.13	122.68
2	H	3	GLN	O-C-N	6.36	131.03	123.27
3	A	33	LYS	CA-C-O	-6.36	113.68	120.42
1	L	129	GLY	CA-C-O	-6.35	115.40	121.11
1	L	64	GLY	CA-C-O	-6.34	114.72	120.94
1	L	1	ASN	N-CA-CB	6.34	121.28	110.50
1	L	12	SER	N-CA-CB	6.33	121.32	110.68
1	L	208	PHE	N-CA-C	6.33	124.29	110.80
2	H	139	THR	N-CA-CB	-6.33	101.75	111.56
1	L	23	CYS	CB-CA-C	6.33	121.15	109.70
2	H	45	LEU	CA-C-O	6.33	128.27	121.44
2	H	189	THR	CA-C-O	6.32	126.94	120.24
2	H	60	TYR	CA-CB-CG	-6.29	102.58	113.90
1	L	212	GLU	CA-C-N	6.29	133.02	121.70
1	L	212	GLU	C-N-CA	6.29	133.02	121.70
1	L	185	TYR	N-CA-C	-6.28	104.44	111.28
1	L	102	THR	N-CA-CB	6.28	121.66	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	174	PRO	N-CD-CG	-6.28	93.78	103.20
1	L	151	ASP	CB-CA-C	6.27	122.75	111.03
3	A	14	GLY	N-CA-C	-6.26	104.00	112.57
3	A	37	GLN	N-CA-CB	6.25	119.12	110.07
1	L	155	GLN	CA-C-O	6.24	129.43	120.51
3	A	61	GLU	CG-CD-OE1	6.23	132.74	118.40
1	L	93	SER	N-CA-CB	-6.22	99.94	111.52
2	H	98	ARG	NE-CZ-NH1	-6.21	115.29	121.50
1	L	174	MET	N-CA-CB	-6.20	100.91	111.69
2	H	95	TYR	O-C-N	6.19	131.20	123.15
1	L	187	ARG	CA-C-O	-6.19	111.66	120.51
2	H	38	ARG	NE-CZ-NH2	6.17	124.75	119.20
1	L	209	ASN	OD1-CG-ND2	-6.16	116.44	122.60
3	A	60	THR	CB-CA-C	6.15	121.12	109.37
2	H	134	GLY	N-CA-C	6.14	127.74	113.18
2	H	141	SER	CA-C-N	6.14	131.19	122.72
2	H	141	SER	C-N-CA	6.14	131.19	122.72
1	L	164	ASP	CB-CA-C	6.13	122.10	110.51
1	L	22	THR	CA-CB-OG1	-6.12	100.41	109.60
3	A	39	ALA	CA-C-O	6.11	127.01	120.10
2	H	171	HIS	O-C-N	6.11	131.71	123.34
1	L	92	ASN	N-CA-CB	6.10	119.16	110.13
1	L	206	LYS	CA-C-O	6.10	127.03	120.32
1	L	34	SER	CA-C-O	-6.09	114.33	121.46
1	L	149	LYS	CA-C-N	6.09	132.93	121.97
1	L	149	LYS	C-N-CA	6.09	132.93	121.97
2	H	214	ASP	O-C-N	6.09	130.94	123.21
2	H	181	LEU	CA-C-O	-6.09	111.99	120.21
2	H	188	VAL	O-C-N	6.09	129.03	123.19
1	L	38	GLN	CG-CD-OE1	6.08	132.97	120.80
1	L	82	ASP	CA-C-O	-6.08	111.82	120.51
2	H	171	HIS	CB-CA-C	-6.07	101.38	110.24
2	H	90	ASP	N-CA-C	-6.06	105.64	113.16
2	H	3	GLN	N-CA-CB	6.05	121.95	111.00
2	H	180	ASP	CA-CB-CG	6.05	118.65	112.60
1	L	53	ASN	CA-C-O	-6.04	114.09	120.80
2	H	132	ALA	CB-CA-C	6.04	117.03	108.76
1	L	77	SER	CA-C-O	-6.04	112.32	120.47
2	H	40	ALA	CA-C-N	6.03	127.38	119.84
2	H	40	ALA	C-N-CA	6.03	127.38	119.84
1	L	122	SER	CA-C-N	6.03	128.36	120.28
1	L	122	SER	C-N-CA	6.03	128.36	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	30	THR	N-CA-C	-6.03	103.46	111.24
1	L	20	THR	CA-CB-OG1	-6.01	100.58	109.60
1	L	140	TYR	N-CA-CB	5.97	121.00	110.37
2	H	114	THR	CA-CB-OG1	-5.97	100.65	109.60
2	H	82	GLN	OE1-CD-NE2	5.95	128.55	122.60
2	H	214	ASP	N-CA-CB	5.95	120.26	110.69
1	L	153	GLU	CA-C-O	5.92	127.56	120.28
2	H	115	SER	O-C-N	5.91	129.64	122.96
1	L	171	THR	CA-C-N	5.91	133.32	122.92
1	L	171	THR	C-N-CA	5.91	133.32	122.92
1	L	40	PRO	CA-C-N	5.91	132.82	121.54
1	L	40	PRO	C-N-CA	5.91	132.82	121.54
2	H	194	PRO	CA-C-O	-5.90	109.86	120.60
3	A	13	ASN	N-CA-CB	5.90	120.48	110.87
2	H	67	ARG	NE-CZ-NH2	5.90	124.51	119.20
3	A	51	ASP	CA-CB-CG	5.89	118.49	112.60
1	L	117	ILE	CB-CA-C	5.89	119.89	110.82
1	L	212	GLU	CA-C-O	5.89	127.34	120.98
1	L	42	GLN	CA-C-O	-5.88	114.98	121.33
2	H	194	PRO	O-C-N	-5.88	114.70	122.64
3	A	40	ASN	CA-C-N	5.86	128.72	120.28
3	A	40	ASN	C-N-CA	5.86	128.72	120.28
1	L	43	SER	N-CA-C	-5.85	101.53	110.07
1	L	192	THR	CA-C-O	5.84	128.30	121.46
1	L	193	CYS	CA-C-O	-5.84	114.26	120.40
1	L	78	VAL	O-C-N	5.84	128.82	122.57
2	H	61	ALA	CA-C-N	5.83	128.37	120.38
2	H	61	ALA	C-N-CA	5.83	128.37	120.38
1	L	176	SER	N-CA-CB	5.83	120.13	110.63
3	A	39	ALA	CA-C-N	5.82	128.55	120.63
3	A	39	ALA	C-N-CA	5.82	128.55	120.63
3	A	46	GLY	CA-C-O	5.81	127.59	121.08
1	L	11	MET	O-C-N	5.80	129.91	123.52
1	L	68	ALA	CA-C-O	5.79	127.23	119.47
1	L	28	ASN	N-CA-C	5.79	118.87	110.42
1	L	41	GLU	CB-CG-CD	5.78	122.43	112.60
2	H	210	SER	O-C-N	5.78	129.97	122.86
1	L	54	ARG	CA-C-O	-5.76	114.45	121.36
1	L	70	ASP	CA-C-O	-5.76	114.14	120.30
2	H	42	GLU	N-CA-C	-5.75	98.43	107.93
1	L	62	PHE	N-CA-C	-5.74	101.13	110.20
2	H	145	LEU	CA-C-O	-5.74	114.61	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	44	VAL	O-C-N	5.74	129.40	123.03
2	H	216	LYS	N-CA-CB	5.72	118.39	109.97
3	A	36	LYS	CA-CB-CG	5.72	125.54	114.10
2	H	51	ILE	CA-CB-CG2	5.72	120.22	110.50
2	H	82	GLN	CA-C-O	-5.70	114.48	120.58
2	H	3	GLN	CA-C-O	-5.70	114.10	120.66
1	L	105	GLU	CA-CB-CG	5.70	125.49	114.10
2	H	170	VAL	CB-CA-C	5.69	119.13	111.28
2	H	183	THR	N-CA-C	-5.69	98.24	108.48
2	H	43	LYS	O-C-N	5.69	130.15	122.59
2	H	63	THR	N-CA-C	5.69	117.48	111.28
2	H	213	VAL	CB-CA-C	5.69	120.55	110.71
1	L	191	TYR	CA-C-O	-5.68	113.09	120.25
2	H	195	ARG	NE-CZ-NH2	-5.68	114.09	119.20
2	H	51	ILE	N-CA-CB	5.68	120.78	111.58
1	L	166	ASP	CB-CA-C	5.67	119.14	109.72
3	A	10	LEU	CA-C-O	-5.66	114.24	120.30
1	L	107	LYS	N-CA-CB	5.65	119.63	110.41
1	L	132	VAL	CA-C-N	5.65	130.80	122.94
1	L	132	VAL	C-N-CA	5.65	130.80	122.94
2	H	69	THR	CA-C-O	-5.65	114.25	120.24
2	H	77	ASN	N-CA-C	5.65	122.83	110.80
2	H	198	GLU	CA-CB-CG	5.64	125.39	114.10
2	H	101	ASN	CB-CA-C	5.63	119.68	109.37
1	L	137	ASN	OD1-CG-ND2	-5.62	116.98	122.60
2	H	193	SER	CA-C-N	5.62	126.87	119.84
2	H	193	SER	C-N-CA	5.62	126.87	119.84
2	H	200	VAL	O-C-N	5.61	129.14	123.20
2	H	132	ALA	CA-C-N	5.61	124.96	118.85
2	H	132	ALA	C-N-CA	5.61	124.96	118.85
2	H	140	ASN	CA-C-O	5.61	125.58	119.24
3	A	12	ILE	CA-C-O	-5.61	114.70	120.25
2	H	195	ARG	NH1-CZ-NH2	-5.60	112.02	119.30
2	H	127	SER	CA-C-N	5.58	130.12	123.19
2	H	127	SER	C-N-CA	5.58	130.12	123.19
2	H	66	GLY	N-CA-C	-5.58	107.84	114.48
1	L	166	ASP	N-CA-CB	5.57	118.25	109.83
1	L	190	SER	N-CA-C	-5.57	101.46	110.32
2	H	12	VAL	CA-C-O	5.57	127.18	121.28
1	L	210	ARG	NE-CZ-NH1	5.56	127.06	121.50
1	L	53	ASN	OD1-CG-ND2	-5.55	117.05	122.60
2	H	198	GLU	CB-CA-C	-5.55	100.16	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	89	GLU	CG-CD-OE2	-5.54	105.65	118.40
1	L	92	ASN	N-CA-C	-5.54	104.64	111.40
2	H	202	CYS	CA-C-O	-5.53	114.66	120.80
3	A	11	VAL	N-CA-CB	5.53	119.71	110.86
1	L	24	LYS	CB-CA-C	-5.53	101.29	110.14
3	A	6	THR	O-C-N	5.53	129.94	122.59
1	L	152	SER	CA-C-N	5.52	131.60	122.33
1	L	152	SER	C-N-CA	5.52	131.60	122.33
1	L	134	CYS	CA-C-O	-5.50	113.51	120.28
2	H	44	GLY	N-CA-C	-5.50	101.99	111.57
2	H	68	PHE	CA-CB-CG	5.50	119.30	113.80
2	H	27	PHE	CA-CB-CG	5.49	119.29	113.80
1	L	42	GLN	CA-C-N	-5.49	113.14	121.92
1	L	42	GLN	C-N-CA	-5.49	113.14	121.92
2	H	147	CYS	CA-C-N	5.48	130.73	123.05
2	H	147	CYS	C-N-CA	5.48	130.73	123.05
1	L	28	ASN	CA-C-O	5.48	126.43	120.95
3	A	13	ASN	CA-C-N	5.47	127.30	122.43
3	A	13	ASN	C-N-CA	5.47	127.30	122.43
2	H	105	TYR	CA-C-N	5.46	131.20	121.75
2	H	105	TYR	C-N-CA	5.46	131.20	121.75
2	H	184	LEU	CA-C-O	-5.46	115.23	121.40
2	H	143	VAL	CB-CA-C	-5.46	103.07	111.31
3	A	49	THR	CA-CB-OG1	-5.45	101.42	109.60
1	L	211	ASN	CA-C-O	-5.44	114.30	121.86
2	H	42	GLU	CA-C-N	5.44	131.92	121.54
2	H	42	GLU	C-N-CA	5.44	131.92	121.54
1	L	210	ARG	NE-CZ-NH2	-5.43	114.31	119.20
2	H	171	HIS	CA-C-N	-5.43	115.06	122.93
2	H	171	HIS	C-N-CA	-5.43	115.06	122.93
2	H	151	GLY	N-CA-C	5.42	123.11	115.30
1	L	189	ASN	OD1-CG-ND2	-5.41	117.19	122.60
1	L	97	THR	CA-CB-OG1	-5.41	101.49	109.60
1	L	108	ARG	N-CA-CB	-5.39	102.00	111.49
1	L	173	SER	N-CA-CB	5.39	120.67	111.66
2	H	95	TYR	N-CA-CB	5.38	120.91	111.55
3	A	56	THR	CA-CB-OG1	-5.38	101.53	109.60
2	H	68	PHE	N-CA-CB	5.37	119.34	110.69
2	H	92	GLY	CA-C-N	5.37	129.91	122.77
2	H	92	GLY	C-N-CA	5.37	129.91	122.77
1	L	109	ALA	CB-CA-C	5.36	118.62	109.72
3	A	16	THR	CA-CB-CG2	5.36	119.62	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	188	VAL	CA-CB-CG2	5.36	119.51	110.40
1	L	57	GLY	N-CA-C	5.35	123.32	115.08
1	L	188	HIS	CA-C-O	-5.35	115.73	121.45
2	H	189	THR	CB-CA-C	5.33	118.68	110.14
1	L	53	ASN	CB-CG-ND2	5.33	124.39	116.40
1	L	102	THR	N-CA-C	-5.32	99.77	108.76
1	L	46	LEU	N-CA-C	-5.32	102.41	110.28
2	H	59	HIS	N-CA-CB	5.32	121.42	111.53
1	L	165	GLN	OE1-CD-NE2	5.31	127.91	122.60
2	H	74	ASN	OD1-CG-ND2	5.30	127.91	122.60
1	L	67	SER	N-CA-C	5.30	122.09	110.80
2	H	96	CYS	N-CA-C	-5.30	100.26	108.90
1	L	164	ASP	CA-C-O	-5.30	115.69	121.89
2	H	35	HIS	CB-CA-C	-5.29	98.93	109.79
2	H	206	HIS	CA-C-N	5.29	124.74	119.24
2	H	206	HIS	C-N-CA	5.29	124.74	119.24
1	L	70	ASP	O-C-N	5.29	129.41	123.27
2	H	124	THR	CA-CB-OG1	-5.29	101.67	109.60
1	L	75	ILE	N-CA-CB	5.29	117.52	111.39
2	H	211	THR	N-CA-C	-5.29	101.09	109.76
1	L	49	TYR	CB-CA-C	5.29	120.77	110.30
1	L	204	ILE	CB-CA-C	5.29	119.56	111.68
2	H	85	SER	O-C-N	5.27	129.60	122.59
1	L	171	THR	CA-CB-OG1	-5.27	101.69	109.60
1	L	104	LEU	CB-CA-C	5.25	119.20	110.74
1	L	141	PRO	O-C-N	5.24	129.71	122.64
1	L	183	ASP	O-C-N	5.24	129.42	122.56
2	H	90	ASP	CB-CA-C	5.23	119.42	110.01
2	H	149	VAL	CA-C-N	5.23	132.12	122.92
2	H	149	VAL	C-N-CA	5.23	132.12	122.92
1	L	81	GLU	CG-CD-OE1	5.22	130.41	118.40
2	H	10	GLY	CA-C-O	-5.22	114.91	121.02
2	H	81	LEU	CB-CA-C	5.22	118.05	110.79
1	L	63	THR	OG1-CB-CG2	5.22	119.74	109.30
3	A	33	LYS	N-CA-C	-5.22	105.67	111.36
1	L	60	ASP	CA-C-O	-5.22	113.05	120.51
3	A	53	ALA	N-CA-C	-5.21	105.60	111.28
2	H	196	PRO	CA-N-CD	-5.21	104.71	112.00
2	H	39	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	L	28	ASN	OD1-CG-ND2	-5.20	117.40	122.60
2	H	8	GLY	CA-C-O	-5.19	113.26	119.07
2	H	36	TRP	CB-CA-C	5.17	119.25	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	112	ALA	O-C-N	5.17	128.20	121.64
2	H	155	GLU	CA-C-O	5.17	125.95	120.63
1	L	78	VAL	CA-C-O	-5.16	116.28	121.59
3	A	58	THR	CA-CB-OG1	-5.14	101.88	109.60
1	L	122	SER	N-CA-C	-5.14	105.68	111.28
2	H	149	VAL	CA-C-O	-5.14	115.64	121.09
2	H	37	VAL	CA-C-O	-5.13	114.37	120.78
2	H	169	GLY	CA-C-N	5.12	128.23	120.75
2	H	169	GLY	C-N-CA	5.12	128.23	120.75
1	L	40	PRO	CA-C-O	5.12	129.93	120.60
2	H	146	GLY	CA-C-N	5.12	130.96	121.94
2	H	146	GLY	C-N-CA	5.12	130.96	121.94
2	H	89	GLU	CA-C-O	-5.12	110.73	118.91
2	H	178	GLN	N-CA-C	-5.11	106.14	112.93
3	A	42	ASN	CA-C-O	-5.11	113.37	119.35
1	L	63	THR	CA-C-N	-5.10	117.66	122.66
1	L	63	THR	C-N-CA	-5.10	117.66	122.66
2	H	87	ARG	CA-C-O	-5.09	115.40	121.56
1	L	169	ASP	CA-C-N	5.09	131.27	121.54
1	L	169	ASP	C-N-CA	5.09	131.27	121.54
3	A	48	TRP	N-CA-C	5.09	117.41	108.56
2	H	105	TYR	CA-C-O	5.08	127.78	120.51
2	H	195	ARG	CA-C-N	5.08	126.19	119.84
2	H	195	ARG	C-N-CA	5.08	126.19	119.84
1	L	175	SER	CA-C-O	-5.08	113.20	120.15
2	H	51	ILE	N-CA-C	-5.08	100.76	108.17
1	L	72	THR	CA-C-N	5.07	130.14	122.99
1	L	72	THR	C-N-CA	5.07	130.14	122.99
2	H	62	ASP	N-CA-C	5.07	117.47	111.33
1	L	93	SER	N-CA-C	5.06	116.93	108.99
2	H	14	PRO	N-CA-C	-5.06	103.25	111.14
1	L	148	TRP	N-CA-CB	5.05	118.86	110.47
2	H	89	GLU	OE1-CD-OE2	5.05	135.01	122.90
1	L	14	SER	N-CA-C	-5.04	103.88	110.53
1	L	178	LEU	N-CA-C	-5.04	100.96	109.07
1	L	61	ARG	CB-CA-C	-5.04	100.11	110.38
2	H	74	ASN	CA-CB-CG	5.03	117.63	112.60
1	L	186	GLU	O-C-N	5.03	129.28	122.59
3	A	45	ASP	CA-C-O	-5.02	113.92	120.25
1	L	90	GLN	OE1-CD-NE2	5.01	127.61	122.60
2	H	41	PRO	CA-C-O	5.01	129.73	120.60
2	H	117	THR	CA-CB-CG2	5.01	119.01	110.50

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	1651	0	1578	209	0
2	H	1675	0	1621	208	0
3	A	446	0	433	41	0
4	A	37	0	0	5	0
4	H	145	0	0	18	0
4	L	163	0	0	11	0
All	All	4117	0	3632	448	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 61.

All (448) 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)
2:H:178:GLN:HE22	2:H:181:LEU:HB2	0.94	1.10
2:H:43:LYS:HG2	2:H:44:GLY:H	0.95	1.08
2:H:51:ILE:HD11	2:H:79:LEU:HD13	1.27	1.08
2:H:43:LYS:CG	2:H:44:GLY:H	1.55	1.08
2:H:193:SER:HB2	2:H:194:PRO:CD	1.83	1.07
2:H:193:SER:CB	2:H:194:PRO:HD3	1.85	1.07
2:H:196:PRO:HD2	2:H:197:SER:H	1.13	1.06
1:L:147:LYS:HG2	1:L:194:GLU:HB3	1.39	1.05
2:H:166:LEU:HB3	4:H:329:HOH:O	1.54	1.05
3:A:6:THR:HG22	3:A:25:ALA:O	1.56	1.05
1:L:8:PRO:O	1:L:9:LYS:HB2	1.57	1.02
1:L:163:THR:HG22	1:L:164:ASP:O	1.59	1.02
1:L:160:ASN:ND2	1:L:174:MET:HE1	1.74	1.01
2:H:51:ILE:HD11	2:H:79:LEU:CD1	1.90	1.00
2:H:178:GLN:NE2	2:H:181:LEU:HB2	1.74	1.00
2:H:51:ILE:HG12	2:H:70:ILE:HG12	1.43	1.00
1:L:191:TYR:O	1:L:207:SER:O	1.80	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:18:ARG:HG3	1:L:76:SER:HA	1.41	0.98
2:H:193:SER:HB2	2:H:194:PRO:HD3	0.99	0.98
2:H:51:ILE:CD1	2:H:79:LEU:HD13	1.93	0.97
1:L:17:GLU:HB2	4:L:269:HOH:O	1.64	0.97
2:H:43:LYS:HG2	2:H:44:GLY:N	1.74	0.96
1:L:8:PRO:HG3	1:L:11:MET:HE3	1.47	0.96
1:L:150:ILE:O	1:L:190:SER:O	1.84	0.95
1:L:17:GLU:HG3	1:L:18:ARG:N	1.77	0.95
2:H:87:ARG:HD2	2:H:88:SER:H	1.33	0.94
2:H:163:SER:H	2:H:203:ASN:ND2	1.65	0.94
1:L:13:MET:HG3	1:L:19:VAL:HG21	1.50	0.93
2:H:144:THR:HG21	4:H:275:HOH:O	1.67	0.93
1:L:150:ILE:CG2	1:L:151:ASP:H	1.83	0.91
2:H:163:SER:H	2:H:203:ASN:HD21	0.93	0.90
1:L:30:VAL:O	1:L:67:SER:O	1.89	0.90
1:L:69:THR:HG22	4:L:281:HOH:O	1.72	0.90
2:H:178:GLN:HE22	2:H:181:LEU:CB	1.83	0.90
3:A:27:ASP:HB2	3:A:30:THR:OG1	1.71	0.89
3:A:12:ILE:HD11	3:A:17:LEU:HD23	1.55	0.88
1:L:180:LEU:HD12	1:L:185:TYR:HB2	1.55	0.88
2:H:134:GLY:O	2:H:195:ARG:NH2	2.07	0.87
2:H:62:ASP:HA	2:H:65:LYS:HE3	1.59	0.85
2:H:163:SER:N	2:H:203:ASN:HD21	1.73	0.85
2:H:138:GLN:O	2:H:138:GLN:HG3	1.77	0.84
2:H:170:VAL:HG23	2:H:188:VAL:HG23	1.59	0.84
2:H:196:PRO:HD2	2:H:197:SER:N	1.93	0.84
1:L:30:VAL:CG2	1:L:31:THR:H	1.92	0.83
2:H:196:PRO:CD	2:H:197:SER:H	1.89	0.83
2:H:93:MET:HE3	2:H:113:GLY:C	2.03	0.83
2:H:51:ILE:CG1	2:H:70:ILE:HG12	2.07	0.83
1:L:61:ARG:NH2	1:L:82:ASP:OD2	2.12	0.82
2:H:144:THR:HB	2:H:189:THR:HB	1.61	0.82
1:L:150:ILE:HG23	1:L:151:ASP:N	1.95	0.81
1:L:184:GLU:O	1:L:188:HIS:CD2	2.33	0.81
1:L:136:LEU:N	1:L:136:LEU:HD12	1.95	0.80
1:L:147:LYS:HD3	1:L:194:GLU:HG2	1.62	0.80
2:H:193:SER:CB	2:H:194:PRO:CD	2.51	0.80
3:A:6:THR:CG2	3:A:25:ALA:O	2.31	0.79
3:A:12:ILE:HB	3:A:59:VAL:HG12	1.64	0.78
1:L:83:LEU:HD21	1:L:165:GLN:HB2	1.65	0.78
2:H:170:VAL:CG2	2:H:188:VAL:HG23	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:110:ASP:OD2	1:L:198:LYS:HE3	1.85	0.77
2:H:34:MET:HB3	2:H:79:LEU:HD22	1.66	0.76
1:L:150:ILE:CG2	1:L:151:ASP:N	2.43	0.75
1:L:61:ARG:HH22	1:L:82:ASP:CG	1.94	0.75
1:L:13:MET:HE2	1:L:19:VAL:HG23	1.69	0.75
1:L:115:VAL:CG1	1:L:134:CYS:SG	2.75	0.75
1:L:147:LYS:CG	1:L:194:GLU:HB3	2.15	0.75
2:H:166:LEU:C	4:H:329:HOH:O	2.28	0.75
1:L:41:GLU:HA	1:L:41:GLU:OE1	1.85	0.75
1:L:160:ASN:ND2	1:L:174:MET:CE	2.49	0.75
1:L:163:THR:CG2	1:L:164:ASP:O	2.35	0.75
1:L:8:PRO:CG	1:L:11:MET:HE3	2.16	0.75
2:H:38:ARG:HG3	2:H:48:VAL:HG21	1.69	0.74
2:H:121:ALA:HB2	4:H:362:HOH:O	1.86	0.74
2:H:38:ARG:HG3	2:H:48:VAL:CG2	2.19	0.73
2:H:76:LYS:O	2:H:78:THR:HG23	1.87	0.73
1:L:166:ASP:N	1:L:171:THR:O	2.19	0.73
1:L:186:GLU:O	1:L:210:ARG:NH2	2.22	0.73
1:L:13:MET:HG3	1:L:19:VAL:CG2	2.18	0.73
1:L:160:ASN:HD22	1:L:174:MET:HE1	1.53	0.73
2:H:145:LEU:HD12	2:H:188:VAL:HG12	1.71	0.73
2:H:180:ASP:O	2:H:181:LEU:HG	1.88	0.72
2:H:87:ARG:HD2	2:H:88:SER:N	2.05	0.72
1:L:142:LYS:O	1:L:162:TRP:CZ3	2.43	0.72
2:H:142:MET:HB3	4:H:282:HOH:O	1.90	0.71
1:L:212:GLU:HG2	4:L:305:HOH:O	1.90	0.71
1:L:87:HIS:ND1	4:L:216:HOH:O	2.23	0.71
2:H:79:LEU:HD12	2:H:80:PHE:H	1.55	0.71
2:H:99:TRP:O	2:H:108:ASP:HB2	1.91	0.70
1:L:30:VAL:HG22	1:L:31:THR:H	1.55	0.70
1:L:21:LEU:O	1:L:72:THR:HA	1.92	0.70
1:L:193:CYS:HB3	1:L:206:LYS:HB2	1.74	0.70
1:L:156:ASN:C	1:L:156:ASN:HD22	2.00	0.70
2:H:97:ALA:HB3	2:H:107:MET:HG2	1.73	0.70
2:H:153:PHE:CD1	2:H:153:PHE:C	2.69	0.70
1:L:83:LEU:HD23	1:L:167:SER:HA	1.74	0.69
3:A:52:ASP:O	3:A:55:LYS:HE2	1.92	0.69
2:H:175:ALA:HB1	2:H:182:TYR:HB3	1.74	0.69
1:L:95:PRO:HG3	4:H:268:HOH:O	1.92	0.69
1:L:21:LEU:HD22	1:L:102:THR:HG21	1.75	0.69
1:L:33:VAL:O	1:L:50:GLY:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:139:PHE:HZ	1:L:174:MET:HB2	1.58	0.69
1:L:108:ARG:NH1	1:L:109:ALA:O	2.25	0.69
1:L:185:TYR:CZ	1:L:210:ARG:HD3	2.27	0.69
1:L:142:LYS:O	1:L:162:TRP:CH2	2.45	0.69
1:L:185:TYR:CE2	1:L:210:ARG:HD3	2.28	0.69
1:L:8:PRO:O	1:L:9:LYS:CB	2.38	0.69
3:A:60:THR:CG2	4:A:98:HOH:O	2.38	0.68
2:H:157:VAL:CG2	2:H:184:LEU:HD21	2.23	0.68
2:H:94:TYR:O	2:H:113:GLY:HA2	1.94	0.68
1:L:79:GLN:HG2	1:L:80:ALA:N	2.09	0.68
2:H:51:ILE:HG12	2:H:70:ILE:CG1	2.22	0.68
1:L:150:ILE:HG22	1:L:151:ASP:H	1.58	0.67
1:L:133:VAL:HG11	2:H:131:LEU:HD13	1.77	0.67
1:L:43:SER:HB3	2:H:95:TYR:CE2	2.29	0.67
2:H:13:GLN:HB2	4:H:343:HOH:O	1.95	0.67
2:H:3:GLN:HG3	2:H:25:SER:OG	1.95	0.66
2:H:196:PRO:HB3	2:H:219:PRO:HG3	1.77	0.66
1:L:156:ASN:HD22	1:L:157:GLY:N	1.94	0.66
2:H:152:TYR:OH	2:H:184:LEU:HD23	1.95	0.66
2:H:145:LEU:HD13	2:H:200:VAL:HG11	1.78	0.66
1:L:160:ASN:HD22	1:L:174:MET:CE	2.09	0.66
1:L:182:LYS:NZ	1:L:182:LYS:HB3	2.11	0.66
2:H:161:TRP:HZ3	2:H:217:ILE:HD12	1.60	0.66
1:L:61:ARG:NH2	1:L:82:ASP:CG	2.53	0.65
1:L:139:PHE:O	1:L:140:TYR:CB	2.42	0.65
2:H:119:SER:O	4:H:237:HOH:O	2.14	0.65
2:H:145:LEU:CD1	2:H:200:VAL:HG11	2.27	0.65
2:H:2:VAL:HG22	2:H:27:PHE:HB3	1.79	0.65
2:H:99:TRP:O	2:H:106:ALA:O	2.15	0.65
2:H:150:LYS:HA	2:H:183:THR:HB	1.79	0.65
1:L:169:ASP:CG	1:L:169:ASP:O	2.39	0.64
1:L:90:GLN:HE22	1:L:92:ASN:H	1.43	0.64
2:H:34:MET:CB	2:H:79:LEU:HD22	2.27	0.64
1:L:139:PHE:O	1:L:140:TYR:HB2	1.98	0.64
2:H:178:GLN:HE21	2:H:179:SER:H	1.45	0.64
2:H:74:ASN:N	2:H:75:PRO:HD2	2.13	0.64
3:A:6:THR:HG23	3:A:8:TYR:CE2	2.33	0.63
2:H:209:SER:O	2:H:210:SER:OG	2.17	0.63
4:L:233:HOH:O	2:H:110:TRP:HD1	1.79	0.63
2:H:38:ARG:HG2	2:H:94:TYR:CE2	2.34	0.63
3:A:13:ASN:HB3	4:A:64:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:157:VAL:HG22	2:H:184:LEU:HD21	1.79	0.63
1:L:90:GLN:NE2	1:L:90:GLN:C	2.57	0.63
1:L:178:LEU:HD11	1:L:180:LEU:HD23	1.80	0.63
2:H:152:TYR:CE2	2:H:157:VAL:HG13	2.34	0.63
1:L:115:VAL:HG12	1:L:206:LYS:HG2	1.81	0.63
1:L:169:ASP:O	1:L:171:THR:N	2.31	0.62
2:H:151:GLY:O	2:H:181:LEU:HD22	1.98	0.62
1:L:8:PRO:HG3	1:L:11:MET:CE	2.25	0.62
1:L:2:ILE:HD13	1:L:29:VAL:HG12	1.83	0.61
1:L:128:GLY:HA2	1:L:182:LYS:HD3	1.83	0.61
2:H:13:GLN:HG3	4:H:345:HOH:O	2.00	0.61
2:H:209:SER:C	2:H:210:SER:OG	2.44	0.61
3:A:27:ASP:CB	3:A:30:THR:OG1	2.46	0.61
1:L:144:ILE:HG22	1:L:162:TRP:CH2	2.36	0.61
1:L:110:ASP:OD2	1:L:141:PRO:HD3	2.01	0.61
2:H:43:LYS:CG	2:H:44:GLY:N	2.40	0.60
2:H:134:GLY:C	2:H:195:ARG:NH2	2.59	0.60
3:A:26:VAL:HG22	3:A:27:ASP:H	1.66	0.60
1:L:30:VAL:CG2	1:L:31:THR:N	2.60	0.59
1:L:121:SER:O	1:L:125:LEU:HG	2.02	0.59
1:L:90:GLN:NE2	1:L:92:ASN:H	2.00	0.59
1:L:132:VAL:N	1:L:178:LEU:O	2.34	0.59
2:H:20:LEU:HD13	2:H:114:THR:CG2	2.33	0.59
1:L:150:ILE:HG23	1:L:151:ASP:H	1.55	0.59
1:L:192:THR:HA	1:L:206:LYS:O	2.02	0.59
3:A:28:ALA:O	3:A:57:PHE:HZ	1.85	0.59
2:H:35:HIS:HD2	2:H:47:TRP:NE1	2.01	0.59
3:A:5:VAL:HG22	3:A:25:ALA:O	2.03	0.59
1:L:124:GLN:OE1	1:L:131:SER:HB2	2.02	0.58
2:H:51:ILE:CG1	2:H:70:ILE:CG1	2.81	0.58
2:H:112:GLN:HA	2:H:112:GLN:HE21	1.67	0.58
2:H:141:SER:O	2:H:192:SER:OG	2.20	0.58
2:H:35:HIS:O	2:H:96:CYS:HA	2.03	0.58
2:H:163:SER:N	2:H:203:ASN:ND2	2.40	0.58
1:L:136:LEU:N	1:L:136:LEU:CD1	2.64	0.58
3:A:32:GLU:HA	3:A:35:PHE:HB2	1.84	0.58
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.49	0.58
2:H:93:MET:HE3	2:H:114:THR:N	2.19	0.58
2:H:195:ARG:N	2:H:196:PRO:HD3	2.18	0.58
2:H:38:ARG:NH1	2:H:90:ASP:HA	2.19	0.57
1:L:108:ARG:HG2	1:L:109:ALA:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:136:ALA:O	2:H:138:GLN:N	2.38	0.57
1:L:159:LEU:HD22	2:H:176:VAL:HG21	1.87	0.56
2:H:40:ALA:HB1	2:H:41:PRO:CD	2.34	0.56
1:L:17:GLU:HG3	1:L:18:ARG:H	1.69	0.56
1:L:148:TRP:O	1:L:154:ARG:HA	2.06	0.56
3:A:26:VAL:CG2	3:A:27:ASP:N	2.67	0.56
1:L:178:LEU:CD1	1:L:180:LEU:HD23	2.36	0.56
3:A:26:VAL:CG2	3:A:27:ASP:H	2.19	0.56
2:H:127:SER:HA	3:A:42:ASN:HD21	1.71	0.56
1:L:22:THR:HG22	1:L:24:LYS:HE2	1.86	0.56
1:L:182:LYS:HB3	1:L:182:LYS:HZ3	1.70	0.56
2:H:74:ASN:N	2:H:75:PRO:CD	2.68	0.56
2:H:180:ASP:C	2:H:181:LEU:HG	2.30	0.56
2:H:51:ILE:CD1	2:H:70:ILE:HG12	2.36	0.56
2:H:122:LYS:HZ1	2:H:123:THR:HG23	1.71	0.56
2:H:219:PRO:C	2:H:221:ASP:H	2.13	0.56
2:H:131:LEU:HD21	2:H:148:LEU:HD12	1.88	0.56
2:H:36:TRP:HD1	2:H:70:ILE:HD12	1.69	0.56
1:L:22:THR:CG2	1:L:24:LYS:HE2	2.36	0.55
1:L:147:LYS:HD3	1:L:194:GLU:CG	2.33	0.55
1:L:33:VAL:HA	1:L:89:GLY:O	2.06	0.55
1:L:166:ASP:OD1	1:L:168:LYS:HG3	2.07	0.55
2:H:6:GLU:HA	2:H:21:SER:O	2.05	0.55
2:H:11:LEU:HD11	2:H:119:SER:HB3	1.88	0.55
3:A:32:GLU:O	3:A:36:LYS:HG2	2.06	0.55
2:H:74:ASN:HB2	2:H:75:PRO:HD3	1.89	0.55
1:L:108:ARG:NH1	1:L:108:ARG:HG2	2.21	0.55
3:A:8:TYR:CE2	3:A:25:ALA:HB3	2.42	0.55
2:H:51:ILE:HG13	2:H:70:ILE:CD1	2.37	0.55
1:L:108:ARG:HG2	1:L:108:ARG:HH11	1.73	0.54
2:H:11:LEU:HD23	2:H:123:THR:HG22	1.89	0.54
2:H:189:THR:HG22	4:H:276:HOH:O	2.07	0.54
2:H:51:ILE:CG1	2:H:70:ILE:CD1	2.86	0.54
1:L:115:VAL:HG12	1:L:134:CYS:SG	2.48	0.54
2:H:97:ALA:CB	2:H:107:MET:HG2	2.37	0.54
1:L:196:THR:HG23	1:L:203:PRO:HA	1.89	0.54
1:L:182:LYS:O	1:L:186:GLU:CG	2.56	0.53
4:L:216:HOH:O	2:H:44:GLY:HA3	2.09	0.53
2:H:139:THR:OG1	2:H:141:SER:N	2.40	0.53
1:L:30:VAL:C	1:L:67:SER:O	2.51	0.53
3:A:37:GLN:HG3	3:A:37:GLN:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:38:ARG:HB3	2:H:94:TYR:CD2	2.44	0.53
1:L:183:ASP:HA	1:L:186:GLU:HB2	1.90	0.53
2:H:35:HIS:CG	2:H:107:MET:CE	2.92	0.53
2:H:168:SER:OG	2:H:169:GLY:N	2.38	0.53
1:L:115:VAL:CG1	1:L:206:LYS:HG2	2.39	0.52
1:L:79:GLN:CG	1:L:80:ALA:N	2.72	0.52
1:L:133:VAL:HG11	2:H:131:LEU:CD1	2.39	0.52
2:H:43:LYS:HG2	2:H:44:GLY:CA	2.37	0.52
2:H:97:ALA:HA	2:H:109:TYR:O	2.10	0.52
1:L:30:VAL:HG23	1:L:31:THR:H	1.70	0.52
1:L:32:TYR:O	1:L:90:GLN:HA	2.10	0.52
1:L:180:LEU:HD13	1:L:185:TYR:HA	1.91	0.52
2:H:42:GLU:HG3	2:H:43:LYS:N	2.24	0.52
1:L:197:HIS:C	1:L:199:THR:H	2.18	0.52
3:A:49:THR:HG23	4:A:98:HOH:O	2.10	0.52
1:L:147:LYS:CD	1:L:194:GLU:HB3	2.39	0.52
3:A:9:LYS:O	3:A:56:THR:HA	2.09	0.52
2:H:161:TRP:CZ3	2:H:217:ILE:HD12	2.45	0.51
2:H:1:ASP:O	2:H:26:GLY:HA3	2.09	0.51
1:L:45:LYS:HD3	4:L:231:HOH:O	2.11	0.51
2:H:195:ARG:N	2:H:196:PRO:CD	2.73	0.51
1:L:115:VAL:HG13	1:L:134:CYS:SG	2.50	0.51
1:L:136:LEU:HD23	1:L:144:ILE:CD1	2.40	0.51
2:H:68:PHE:HB3	2:H:81:LEU:HD11	1.92	0.51
1:L:79:GLN:HG2	1:L:81:GLU:H	1.76	0.51
1:L:116:SER:O	1:L:134:CYS:HA	2.10	0.51
2:H:2:VAL:HG13	2:H:27:PHE:CD1	2.46	0.51
2:H:5:VAL:HG23	2:H:5:VAL:O	2.10	0.51
3:A:60:THR:HG22	4:A:98:HOH:O	2.07	0.51
2:H:79:LEU:HD12	2:H:80:PHE:N	2.24	0.50
2:H:201:THR:CG2	2:H:214:ASP:HB3	2.41	0.50
1:L:59:PRO:C	1:L:61:ARG:H	2.20	0.50
2:H:6:GLU:OE1	2:H:6:GLU:N	2.42	0.50
2:H:35:HIS:HD2	2:H:47:TRP:CD1	2.30	0.50
2:H:35:HIS:CG	2:H:107:MET:HE3	2.47	0.50
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.28	0.50
1:L:115:VAL:O	1:L:206:LYS:HE2	2.11	0.50
1:L:149:LYS:HB3	1:L:154:ARG:HG2	1.92	0.49
1:L:196:THR:HG23	1:L:203:PRO:CA	2.42	0.49
2:H:178:GLN:NE2	2:H:179:SER:H	2.09	0.49
1:L:135:PHE:CE2	2:H:187:SER:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:150:ILE:HD13	1:L:155:GLN:NE2	2.27	0.49
2:H:68:PHE:CE1	2:H:83:MET:HB3	2.48	0.49
2:H:73:ASP:OD2	2:H:76:LYS:HD3	2.12	0.49
2:H:24:ALA:HB1	2:H:27:PHE:CE1	2.47	0.49
1:L:147:LYS:HG2	1:L:194:GLU:CB	2.26	0.49
2:H:43:LYS:HD3	2:H:44:GLY:O	2.13	0.49
2:H:72:ARG:CD	2:H:74:ASN:OD1	2.61	0.49
1:L:139:PHE:O	1:L:171:THR:HG22	2.13	0.49
1:L:150:ILE:N	1:L:153:GLU:O	2.43	0.49
1:L:175:SER:O	1:L:175:SER:OG	2.29	0.49
1:L:159:LEU:HD13	2:H:176:VAL:HG22	1.94	0.49
3:A:27:ASP:HB2	3:A:30:THR:HG1	1.75	0.49
1:L:160:ASN:OD1	1:L:176:SER:HB3	2.12	0.48
1:L:195:ALA:O	1:L:204:ILE:HD12	2.12	0.48
2:H:51:ILE:HG22	2:H:55:SER:HA	1.95	0.48
1:L:156:ASN:C	1:L:156:ASN:ND2	2.70	0.48
1:L:163:THR:HG23	4:L:288:HOH:O	2.12	0.48
1:L:4:MET:HE3	1:L:23:CYS:SG	2.53	0.48
1:L:108:ARG:HD3	1:L:109:ALA:O	2.14	0.48
2:H:34:MET:HB3	2:H:79:LEU:CD2	2.39	0.48
1:L:2:ILE:O	1:L:97:THR:HG21	2.13	0.48
2:H:35:HIS:CE1	2:H:107:MET:HE3	2.49	0.48
2:H:76:LYS:O	2:H:78:THR:CG2	2.57	0.48
2:H:214:ASP:O	3:A:17:LEU:HA	2.14	0.48
1:L:43:SER:HB2	1:L:44:PRO:CD	2.43	0.47
1:L:81:GLU:O	1:L:83:LEU:N	2.46	0.47
1:L:206:LYS:HD2	1:L:206:LYS:HA	1.41	0.47
2:H:19:LYS:HE3	2:H:80:PHE:CD2	2.49	0.47
2:H:38:ARG:HH12	2:H:90:ASP:HA	1.79	0.47
2:H:83:MET:HE1	2:H:94:TYR:CZ	2.49	0.47
2:H:138:GLN:O	2:H:138:GLN:CG	2.54	0.47
1:L:163:THR:HB	1:L:173:SER:H	1.78	0.47
2:H:141:SER:O	2:H:192:SER:N	2.47	0.47
3:A:6:THR:O	3:A:25:ALA:N	2.36	0.47
3:A:59:VAL:HG13	3:A:59:VAL:O	2.13	0.47
1:L:103:LYS:HG3	4:L:329:HOH:O	2.14	0.47
3:A:29:GLU:O	3:A:33:LYS:HD3	2.14	0.47
2:H:63:THR:HG23	2:H:64:VAL:HG23	1.96	0.47
2:H:161:TRP:HZ3	2:H:217:ILE:CD1	2.27	0.47
3:A:51:ASP:OD1	3:A:54:THR:HG23	2.15	0.47
1:L:133:VAL:HG21	2:H:148:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:185:TYR:HA	1:L:191:TYR:OH	2.14	0.47
2:H:3:GLN:CG	2:H:25:SER:OG	2.61	0.47
1:L:2:ILE:HD13	1:L:29:VAL:CG1	2.45	0.47
1:L:3:VAL:H	1:L:26:SER:HB3	1.79	0.47
2:H:129:TYR:HB2	2:H:148:LEU:HB3	1.97	0.47
2:H:164:GLY:C	2:H:166:LEU:H	2.22	0.47
2:H:55:SER:HB3	4:H:253:HOH:O	2.15	0.47
2:H:178:GLN:HE21	2:H:179:SER:N	2.12	0.47
1:L:90:GLN:C	1:L:90:GLN:CD	2.82	0.47
1:L:83:LEU:CD2	1:L:165:GLN:HB2	2.42	0.47
2:H:25:SER:HB3	4:H:286:HOH:O	2.15	0.47
3:A:12:ILE:CD1	3:A:44:VAL:HG21	2.44	0.47
1:L:28:ASN:CG	1:L:68:ALA:HB1	2.40	0.46
2:H:35:HIS:CD2	2:H:47:TRP:CD1	3.03	0.46
1:L:160:ASN:HB3	1:L:174:MET:CE	2.46	0.46
1:L:160:ASN:HB3	1:L:174:MET:HE3	1.97	0.46
2:H:40:ALA:HB1	2:H:41:PRO:HD2	1.97	0.46
2:H:52:SER:N	2:H:57:THR:O	2.45	0.46
1:L:110:ASP:CG	1:L:198:LYS:HE3	2.40	0.46
2:H:170:VAL:HG22	2:H:188:VAL:HG23	1.94	0.46
1:L:117:ILE:HD12	1:L:148:TRP:CZ3	2.50	0.46
1:L:79:GLN:HG2	1:L:80:ALA:H	1.79	0.46
2:H:36:TRP:HD1	2:H:70:ILE:CD1	2.29	0.46
1:L:58:VAL:HA	1:L:59:PRO:HD3	1.80	0.46
2:H:52:SER:OG	2:H:57:THR:N	2.42	0.46
2:H:58:LEU:HD23	4:H:351:HOH:O	2.16	0.46
2:H:138:GLN:HA	4:H:274:HOH:O	2.15	0.46
2:H:72:ARG:HD2	2:H:74:ASN:OD1	2.16	0.46
2:H:85:SER:O	2:H:86:LEU:C	2.59	0.46
2:H:93:MET:HE3	2:H:113:GLY:CA	2.45	0.46
2:H:122:LYS:HZ3	2:H:123:THR:H	1.64	0.46
3:A:10:LEU:HG	3:A:12:ILE:HG22	1.98	0.46
1:L:28:ASN:ND2	1:L:68:ALA:HB1	2.30	0.46
3:A:5:VAL:HG13	3:A:24:LYS:HB3	1.98	0.46
2:H:90:ASP:O	2:H:94:TYR:OH	2.31	0.45
2:H:176:VAL:HG13	4:H:279:HOH:O	2.16	0.45
1:L:139:PHE:HB2	1:L:140:TYR:H	1.36	0.45
1:L:182:LYS:C	1:L:186:GLU:HG3	2.42	0.45
2:H:124:THR:CG2	2:H:151:GLY:O	2.64	0.45
1:L:184:GLU:O	1:L:188:HIS:HD2	1.92	0.45
2:H:29:PHE:CE2	2:H:72:ARG:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:130:PRO:O	2:H:131:LEU:HD23	2.17	0.45
1:L:83:LEU:O	1:L:84:ALA:HB2	2.17	0.45
2:H:5:VAL:O	2:H:5:VAL:CG2	2.65	0.45
2:H:161:TRP:CZ3	2:H:217:ILE:CD1	3.00	0.45
3:A:12:ILE:CD1	3:A:17:LEU:HD23	2.38	0.45
2:H:201:THR:HG22	2:H:214:ASP:HB3	1.99	0.45
2:H:86:LEU:HD23	2:H:86:LEU:HA	1.67	0.45
1:L:41:GLU:HG3	4:L:348:HOH:O	2.16	0.44
1:L:80:ALA:O	1:L:81:GLU:C	2.57	0.44
1:L:186:GLU:C	1:L:188:HIS:H	2.25	0.44
3:A:28:ALA:O	3:A:57:PHE:CZ	2.68	0.44
1:L:94:TYR:HA	1:L:95:PRO:C	2.42	0.44
1:L:193:CYS:HB3	1:L:206:LYS:CB	2.46	0.44
1:L:180:LEU:HD12	1:L:185:TYR:CB	2.38	0.44
1:L:49:TYR:CD1	1:L:49:TYR:C	2.96	0.44
2:H:93:MET:CE	2:H:113:GLY:C	2.84	0.44
3:A:13:ASN:O	3:A:60:THR:HA	2.18	0.44
1:L:108:ARG:NH1	1:L:108:ARG:CG	2.81	0.44
1:L:125:LEU:O	1:L:126:THR:C	2.61	0.44
1:L:207:SER:HB2	1:L:208:PHE:H	1.37	0.44
2:H:51:ILE:HG13	2:H:70:ILE:HD13	2.00	0.44
2:H:166:LEU:CB	4:H:329:HOH:O	2.34	0.44
2:H:171:HIS:O	2:H:186:SER:HA	2.18	0.44
1:L:139:PHE:CZ	1:L:174:MET:HB2	2.47	0.44
2:H:35:HIS:CD2	2:H:47:TRP:NE1	2.83	0.44
2:H:122:LYS:HA	2:H:122:LYS:HE2	2.00	0.44
1:L:7:SER:HB2	4:L:354:HOH:O	2.16	0.44
1:L:12:SER:HA	1:L:105:GLU:O	2.17	0.44
1:L:61:ARG:NH2	1:L:82:ASP:OD1	2.35	0.44
1:L:108:ARG:HG2	1:L:109:ALA:H	1.83	0.44
1:L:30:VAL:HG22	1:L:31:THR:N	2.29	0.44
1:L:150:ILE:HB	1:L:153:GLU:O	2.18	0.43
2:H:62:ASP:HA	2:H:65:LYS:CE	2.39	0.43
2:H:171:HIS:CD2	4:H:231:HOH:O	2.71	0.43
1:L:155:GLN:HB3	1:L:156:ASN:H	1.35	0.43
1:L:159:LEU:HD23	1:L:159:LEU:HA	1.86	0.43
2:H:136:ALA:O	2:H:137:ALA:C	2.60	0.43
1:L:123:GLU:OE1	1:L:123:GLU:N	2.40	0.43
1:L:208:PHE:O	1:L:208:PHE:CD1	2.72	0.43
1:L:24:LYS:HB2	1:L:24:LYS:HE3	1.72	0.43
1:L:147:LYS:HD2	1:L:194:GLU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:68:PHE:CZ	2:H:83:MET:HE2	2.54	0.43
2:H:138:GLN:C	2:H:139:THR:HG22	2.43	0.43
3:A:7:THR:OG1	3:A:24:LYS:NZ	2.44	0.43
1:L:117:ILE:CD1	1:L:148:TRP:HZ3	2.32	0.43
3:A:32:GLU:HG3	4:A:86:HOH:O	2.18	0.43
1:L:17:GLU:O	1:L:78:VAL:HG23	2.19	0.42
1:L:90:GLN:CD	1:L:90:GLN:O	2.62	0.42
1:L:180:LEU:H	1:L:180:LEU:HG	1.66	0.42
2:H:126:PRO:HB2	2:H:149:VAL:HG13	2.00	0.42
1:L:88:CYS:O	1:L:98:PHE:HA	2.20	0.42
2:H:218:VAL:O	2:H:219:PRO:C	2.62	0.42
1:L:197:HIS:O	1:L:199:THR:N	2.51	0.42
2:H:157:VAL:HA	2:H:205:ALA:O	2.20	0.42
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.72	0.42
1:L:139:PHE:HE2	1:L:162:TRP:CZ3	2.38	0.42
2:H:45:LEU:H	2:H:45:LEU:HG	1.44	0.42
1:L:90:GLN:HE21	1:L:90:GLN:HB2	1.33	0.42
1:L:132:VAL:CG1	1:L:208:PHE:HE2	2.33	0.42
1:L:183:ASP:O	1:L:187:ARG:NH2	2.53	0.42
2:H:87:ARG:HD3	2:H:87:ARG:HA	1.84	0.42
2:H:124:THR:HG21	2:H:181:LEU:HD22	2.02	0.42
1:L:169:ASP:O	1:L:169:ASP:OD1	2.37	0.42
2:H:101:ASN:O	2:H:102:TYR:C	2.63	0.42
2:H:150:LYS:HG3	2:H:151:GLY:N	2.35	0.42
1:L:12:SER:C	1:L:13:MET:HG2	2.44	0.42
1:L:121:SER:HB3	1:L:123:GLU:OE1	2.20	0.42
2:H:124:THR:HG21	2:H:181:LEU:CD2	2.50	0.42
1:L:182:LYS:O	1:L:186:GLU:HG2	2.19	0.41
2:H:72:ARG:HD3	2:H:74:ASN:OD1	2.20	0.41
3:A:39:ALA:O	3:A:44:VAL:N	2.41	0.41
1:L:39:LYS:O	1:L:40:PRO:C	2.62	0.41
2:H:4:LEU:HD12	2:H:24:ALA:HA	2.01	0.41
2:H:6:GLU:H	2:H:6:GLU:CD	2.23	0.41
1:L:117:ILE:CD1	1:L:148:TRP:CZ3	3.03	0.41
1:L:196:THR:HG22	1:L:200:SER:O	2.20	0.41
2:H:210:SER:HA	4:H:364:HOH:O	2.19	0.41
1:L:71:PHE:CD1	1:L:71:PHE:N	2.89	0.41
1:L:178:LEU:HG	1:L:180:LEU:HD21	2.02	0.41
1:L:183:ASP:OD1	1:L:183:ASP:N	2.53	0.41
2:H:127:SER:HA	3:A:42:ASN:ND2	2.34	0.41
1:L:59:PRO:O	1:L:61:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:190:SER:HA	1:L:209:ASN:HA	2.02	0.41
2:H:159:VAL:HA	2:H:203:ASN:O	2.20	0.41
3:A:59:VAL:O	3:A:59:VAL:CG1	2.69	0.41
3:A:12:ILE:HB	3:A:59:VAL:CG1	2.42	0.41
2:H:38:ARG:CG	2:H:48:VAL:HG21	2.44	0.41
1:L:13:MET:CG	1:L:19:VAL:CG2	2.93	0.41
1:L:110:ASP:CG	1:L:198:LYS:NZ	2.79	0.41
1:L:112:ALA:HA	1:L:113:PRO:HD3	1.84	0.41
1:L:146:VAL:O	1:L:146:VAL:HG13	2.21	0.41
2:H:180:ASP:O	2:H:181:LEU:CG	2.66	0.41
1:L:136:LEU:O	1:L:139:PHE:HE1	2.04	0.41
1:L:55:TYR:CG	1:L:56:THR:N	2.84	0.40
1:L:79:GLN:CG	1:L:80:ALA:H	2.32	0.40
2:H:157:VAL:HG22	2:H:184:LEU:CD2	2.47	0.40
1:L:45:LYS:N	1:L:45:LYS:HD2	2.35	0.40
2:H:6:GLU:CD	2:H:113:GLY:H	2.29	0.40
2:H:28:THR:O	2:H:29:PHE:C	2.63	0.40
2:H:122:LYS:NZ	2:H:123:THR:HG23	2.35	0.40
2:H:133:PRO:HB3	2:H:138:GLN:HE21	1.86	0.40
2:H:184:LEU:HD12	2:H:184:LEU:C	2.46	0.40
1:L:33:VAL:HG21	1:L:71:PHE:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	21/213 (10%)	15 (71%)	4 (19%)	2 (10%)	0	0
2	H	184/222 (83%)	150 (82%)	22 (12%)	12 (6%)	1	1
3	A	56/61 (92%)	53 (95%)	2 (4%)	1 (2%)	6	14
All	All	261/496 (53%)	218 (84%)	28 (11%)	15 (6%)	1	1

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	43	LYS
2	H	85	SER
2	H	141	SER
2	H	168	SER
2	H	196	PRO
2	H	221	ASP
3	A	6	THR
1	L	9	LYS
2	H	137	ALA
2	H	193	SER
2	H	99	TRP
2	H	134	GLY
2	H	136	ALA
1	L	210	ARG
2	H	77	ASN

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	190/190 (100%)	130 (68%)	60 (32%)	0	0
2	H	169/189 (89%)	126 (75%)	43 (25%)	0	1
All	All	359/379 (95%)	256 (71%)	103 (29%)	0	1

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASN
1	L	10	SER
1	L	12	SER
1	L	14	SER
1	L	17	GLU
1	L	19	VAL
1	L	24	LYS
1	L	30	VAL

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Mol	Chain	Res	Type
1	L	41	GLU
1	L	45	LYS
1	L	65	SER
1	L	67	SER
1	L	72	THR
1	L	75	ILE
1	L	77	SER
1	L	81	GLU
1	L	82	ASP
1	L	83	LEU
1	L	90	GLN
1	L	93	SER
1	L	103	LYS
1	L	107	LYS
1	L	108	ARG
1	L	122	SER
1	L	132	VAL
1	L	136	LEU
1	L	139	PHE
1	L	142	LYS
1	L	144	ILE
1	L	145	ASN
1	L	147	LYS
1	L	150	ILE
1	L	153	GLU
1	L	156	ASN
1	L	159	LEU
1	L	161	SER
1	L	168	LYS
1	L	174	MET
1	L	175	SER
1	L	176	SER
1	L	178	LEU
1	L	179	THR
1	L	180	LEU
1	L	181	THR
1	L	182	LYS
1	L	183	ASP
1	L	184	GLU
1	L	187	ARG
1	L	192	THR
1	L	194	GLU

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Mol	Chain	Res	Type
1	L	196	THR
1	L	198	LYS
1	L	201	THR
1	L	206	LYS
1	L	207	SER
1	L	208	PHE
1	L	209	ASN
1	L	211	ASN
1	L	212	GLU
1	L	213	CYS
2	H	3	GLN
2	H	4	LEU
2	H	6	GLU
2	H	7	SER
2	H	13	GLN
2	H	20	LEU
2	H	38	ARG
2	H	42	GLU
2	H	51	ILE
2	H	53	SER
2	H	55	SER
2	H	58	LEU
2	H	64	VAL
2	H	78	THR
2	H	79	LEU
2	H	82	GLN
2	H	87	ARG
2	H	88	SER
2	H	107	MET
2	H	112	GLN
2	H	122	LYS
2	H	123	THR
2	H	126	PRO
2	H	138	GLN
2	H	139	THR
2	H	143	VAL
2	H	144	THR
2	H	145	LEU
2	H	148	LEU
2	H	165	SER
2	H	167	SER
2	H	176	VAL

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Mol	Chain	Res	Type
2	H	178	GLN
2	H	180	ASP
2	H	183	THR
2	H	185	SER
2	H	188	VAL
2	H	189	THR
2	H	190	VAL
2	H	192	SER
2	H	193	SER
2	H	197	SER
2	H	198	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	37	GLN
1	L	38	GLN
1	L	90	GLN
1	L	155	GLN
1	L	156	ASN
1	L	160	ASN
1	L	188	HIS
1	L	189	ASN
1	L	209	ASN
2	H	13	GLN
2	H	35	HIS
2	H	39	GLN
2	H	77	ASN
2	H	82	GLN
2	H	112	GLN
2	H	178	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	213/213 (100%)	-0.72	2 (0%) 81 78	9, 28, 59, 118	0
2	H	222/222 (100%)	-0.73	1 (0%) 87 85	9, 24, 62, 104	0
3	A	58/61 (95%)	-0.82	0 100 100	14, 30, 45, 71	0
All	All	493/496 (99%)	-0.74	3 (0%) 85 83	9, 26, 60, 118	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	212	GLU	3.6
2	H	134	GLY	3.0
1	L	213	CYS	2.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.