



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:00 AM UTC

PDB ID : 1OPG / pdb_00001opg
Title : OPG2 FAB FRAGMENT
Authors : Kodandapani, R.; Veerapandian, B.; Ely, K.R.
Deposited on : 1995-04-28
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
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

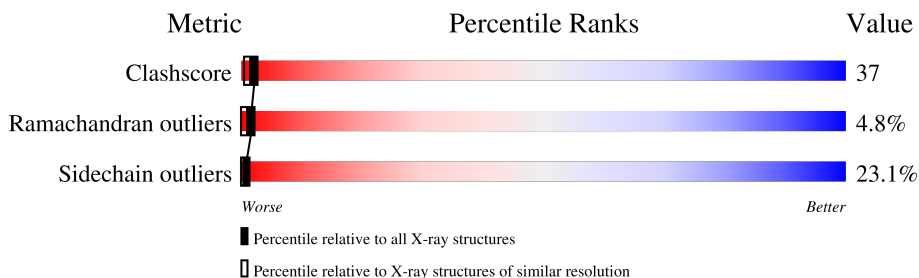
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	214	
2	H	227	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3966 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 OPG2 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1654	1023	280	344	7			

- Molecule 2 is a protein called OPG2 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	227	Total	C	N	O	S	0	11	0
			1824	1152	310	353	9			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	241	Total	O	0	0
			241	241		
3	H	247	Total	O	0	0
			247	247		

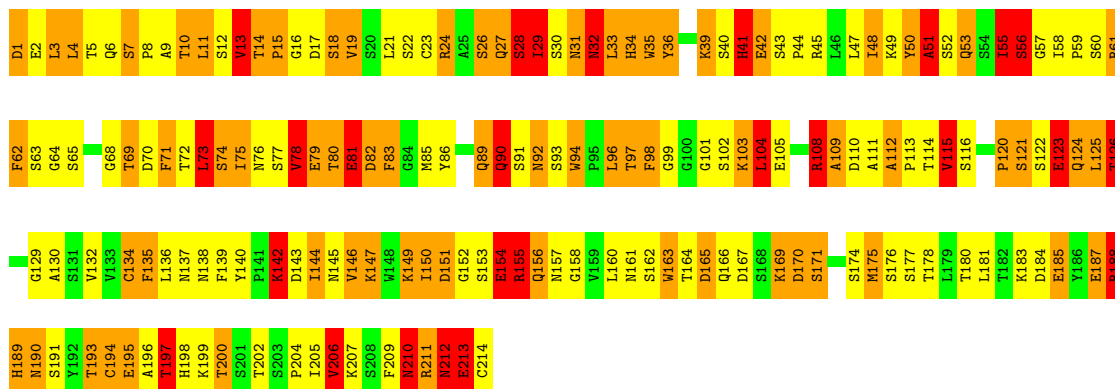
3 Residue-property plots

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.

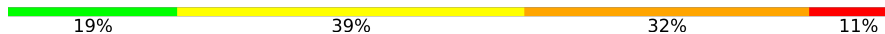
Note EDS was not executed.

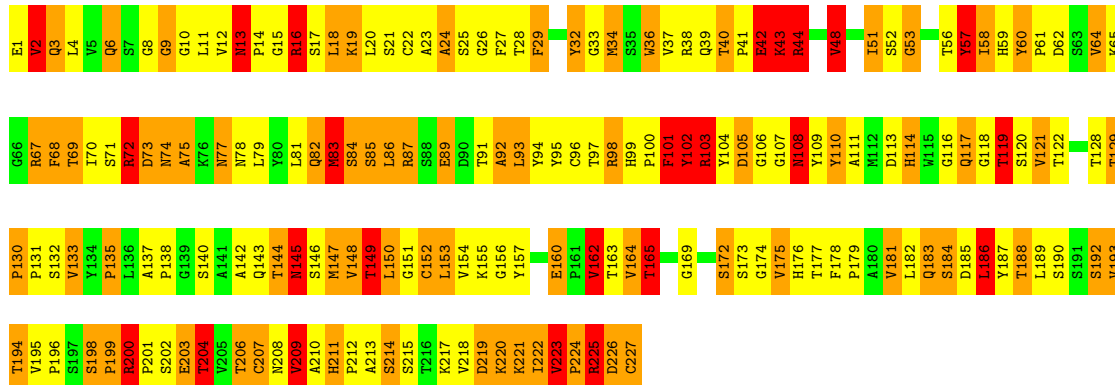
• Molecule 1: OPG2 FAB (LIGHT CHAIN)

Chain L: 



• Molecule 2: OPG2 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 2	Depositor
Cell constants a, b, c, α , β , γ	93.10Å 83.80Å 53.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.00)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3966	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	1.31	4/1691 (0.2%)	3.31	283/2293 (12.3%)
2	H	1.29	1/1877 (0.1%)	3.14	264/2560 (10.3%)
All	All	1.30	5/3568 (0.1%)	3.22	547/4853 (11.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	151	GLY	N-CA	6.88	1.52	1.45
1	L	180	THR	CA-CB	6.64	1.62	1.53
1	L	124	GLN	C-N	-6.29	1.24	1.33
1	L	194	CYS	N-CA	5.39	1.52	1.46
1	L	58	ILE	CA-CB	5.17	1.60	1.54

All (547) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	24	ARG	CD-NE-CZ	23.39	157.14	124.40
1	L	45	ARG	CD-NE-CZ	18.26	149.97	124.40
1	L	187	GLU	CA-CB-CG	15.72	145.53	114.10
2	H	39	GLN	CA-C-O	-15.61	103.42	120.43
1	L	103	LYS	CA-C-O	-15.45	103.08	120.69
2	H	4	LEU	CA-C-O	-14.24	105.06	120.30
2	H	14	PRO	CB-CA-C	14.15	128.58	111.46
2	H	9	GLY	CA-C-O	-13.85	109.11	121.58
1	L	24	ARG	NE-CZ-NH2	13.75	131.57	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	226	ASP	CA-C-O	13.61	138.03	122.37
2	H	145	ASN	N-CA-C	13.22	126.32	108.07
1	L	80	THR	CB-CA-C	12.94	131.51	110.81
1	L	92	ASN	OD1-CG-ND2	-12.70	109.90	122.60
1	L	81	GLU	CA-CB-CG	12.28	138.66	114.10
2	H	119	THR	N-CA-CB	12.04	132.79	111.00
2	H	226	ASP	CA-C-N	11.94	143.19	121.70
2	H	226	ASP	C-N-CA	11.94	143.19	121.70
1	L	3	LEU	O-C-N	11.81	137.35	123.30
1	L	92	ASN	CA-CB-CG	11.79	124.39	112.60
1	L	188	ARG	CD-NE-CZ	11.74	140.84	124.40
2	H	38	ARG	CD-NE-CZ	11.71	140.79	124.40
2	H	185	ASP	CA-CB-CG	11.69	124.29	112.60
2	H	39	GLN	CB-CG-CD	11.68	132.45	112.60
2	H	185	ASP	CA-C-O	-11.38	107.60	119.78
2	H	113	ASP	CA-CB-CG	11.33	123.93	112.60
2	H	32	TYR	O-C-N	11.26	137.01	123.27
2	H	155	LYS	O-C-N	11.24	137.81	123.19
1	L	90	GLN	CB-CG-CD	11.15	131.56	112.60
1	L	143	ASP	CA-CB-CG	11.13	123.73	112.60
1	L	137	ASN	OD1-CG-ND2	-11.03	111.57	122.60
1	L	209	PHE	CA-C-O	11.03	133.03	120.89
1	L	190	ASN	OD1-CG-ND2	-10.99	111.61	122.60
2	H	155	LYS	CA-C-O	-10.93	108.76	121.11
2	H	223	VAL	CB-CA-C	10.86	131.13	111.36
2	H	152	CYS	CA-C-O	-10.77	107.29	120.54
2	H	225	ARG	CA-C-O	10.73	134.81	121.82
2	H	103[A]	ARG	NE-CZ-NH2	-10.71	109.56	119.20
2	H	103[B]	ARG	NE-CZ-NH2	-10.71	109.56	119.20
1	L	210	ASN	CA-CB-CG	-10.68	101.92	112.60
1	L	3	LEU	CA-C-O	-10.52	109.00	120.36
2	H	188	THR	CA-CB-OG1	-10.47	93.90	109.60
2	H	222	ILE	CA-C-O	-10.31	110.95	120.34
1	L	155	ARG	CA-CB-CG	-10.29	93.52	114.10
2	H	200	ARG	CD-NE-CZ	10.24	138.74	124.40
1	L	81	GLU	CB-CG-CD	10.20	129.93	112.60
2	H	165	THR	N-CA-CB	-10.07	94.89	111.20
1	L	15	PRO	CA-C-O	-10.02	110.40	121.32
2	H	128	THR	CA-CB-OG1	-10.00	94.61	109.60
2	H	44	ARG	CD-NE-CZ	9.97	138.35	124.40
1	L	94	TRP	N-CA-C	-9.95	97.60	109.93
1	L	123	GLU	CA-CB-CG	9.92	133.93	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	84	SER	O-C-N	9.78	135.28	122.96
2	H	29	PHE	N-CA-C	9.76	121.92	111.28
2	H	103[A]	ARG	NE-CZ-NH1	9.68	131.18	121.50
2	H	103[B]	ARG	NE-CZ-NH1	9.68	131.18	121.50
2	H	84	SER	CA-C-O	-9.64	110.71	121.51
1	L	61	ARG	NE-CZ-NH2	9.60	127.83	119.20
2	H	43	LYS	N-CA-C	9.60	124.57	112.86
1	L	103	LYS	O-C-N	9.53	134.19	123.04
1	L	154	GLU	CA-CB-CG	9.51	133.12	114.10
2	H	43	LYS	CA-C-N	9.44	137.07	121.39
2	H	43	LYS	C-N-CA	9.44	137.07	121.39
1	L	3	LEU	N-CA-CB	9.43	126.52	110.68
2	H	13	ASN	CA-CB-CG	9.41	122.01	112.60
2	H	61	PRO	CB-CA-C	9.39	123.78	110.17
1	L	114	THR	N-CA-C	-9.39	93.22	108.52
2	H	204	THR	CA-C-O	9.32	131.31	120.69
2	H	225	ARG	CA-C-N	9.26	136.04	122.16
2	H	225	ARG	C-N-CA	9.26	136.04	122.16
1	L	80	THR	CA-C-O	-9.25	111.01	120.90
2	H	103[A]	ARG	CD-NE-CZ	9.21	137.30	124.40
2	H	103[B]	ARG	CD-NE-CZ	9.21	137.30	124.40
2	H	120	SER	CA-C-O	-9.21	110.58	120.80
1	L	134	CYS	CA-C-O	-9.08	110.55	120.36
2	H	195	VAL	N-CA-CB	-9.07	105.57	111.83
1	L	206	VAL	CA-CB-CG1	9.06	125.80	110.40
2	H	97	THR	CA-C-O	-9.04	110.57	121.06
2	H	206	THR	CA-CB-OG1	8.86	122.90	109.60
1	L	123	GLU	CA-C-N	8.73	132.50	120.63
1	L	123	GLU	C-N-CA	8.73	132.50	120.63
2	H	11	LEU	CA-C-N	8.70	135.24	122.71
2	H	11	LEU	C-N-CA	8.70	135.24	122.71
1	L	34	HIS	CA-C-N	8.60	134.87	123.00
1	L	34	HIS	C-N-CA	8.60	134.87	123.00
2	H	193	VAL	CA-C-O	-8.58	111.08	120.43
1	L	213	GLU	CA-C-N	8.58	137.14	121.70
1	L	213	GLU	C-N-CA	8.58	137.14	121.70
2	H	78	ASN	OD1-CG-ND2	-8.57	114.03	122.60
1	L	189	HIS	CA-C-O	-8.56	111.42	121.44
2	H	145	ASN	CA-C-O	8.50	132.78	121.47
1	L	132	VAL	N-CA-C	-8.47	96.25	108.11
2	H	69	THR	CA-C-O	8.47	130.54	120.20
2	H	25	SER	CA-C-O	-8.47	112.17	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	124	GLN	N-CA-C	-8.44	101.66	111.03
1	L	194	CYS	O-C-N	8.43	133.14	123.27
1	L	60	SER	N-CA-CB	-8.43	96.40	110.39
1	L	57	GLY	CA-C-O	8.40	128.34	119.01
2	H	42	GLU	CA-C-O	8.38	129.90	119.59
2	H	165	THR	CB-CA-C	8.38	125.91	109.66
2	H	73	ASP	CA-CB-CG	-8.37	104.23	112.60
1	L	176	SER	CA-C-O	-8.36	111.84	120.71
1	L	13	VAL	CA-C-O	8.30	130.08	121.28
2	H	222	ILE	CB-CA-C	-8.26	102.81	110.91
1	L	152	GLY	N-CA-C	8.23	124.87	115.08
1	L	212	ASN	CB-CG-ND2	8.22	128.73	116.40
2	H	210	ALA	O-C-N	8.19	133.24	123.33
1	L	124	GLN	N-CA-CB	8.18	121.84	109.98
2	H	183	GLN	CB-CG-CD	8.18	126.51	112.60
2	H	227	CYS	N-CA-CB	8.17	124.39	110.50
2	H	200	ARG	CB-CA-C	8.07	126.08	110.17
1	L	188	ARG	CA-CB-CG	8.04	130.17	114.10
1	L	4	LEU	CA-C-O	-8.02	111.64	120.38
1	L	89	GLN	CG-CD-NE2	-7.97	104.44	116.40
1	L	212	ASN	OD1-CG-ND2	-7.97	114.63	122.60
1	L	103	LYS	CA-C-N	-7.95	111.40	122.93
1	L	103	LYS	C-N-CA	-7.95	111.40	122.93
1	L	61	ARG	NE-CZ-NH1	-7.94	113.56	121.50
1	L	211	ARG	CD-NE-CZ	7.93	135.51	124.40
1	L	60	SER	CA-C-O	7.92	129.13	119.38
2	H	82	GLN	OE1-CD-NE2	7.91	130.51	122.60
2	H	200	ARG	NH1-CZ-NH2	-7.89	109.04	119.30
1	L	18	SER	CA-C-O	-7.88	112.41	121.47
2	H	67	ARG	O-C-N	7.87	131.70	122.25
1	L	4	LEU	O-C-N	7.85	132.55	123.29
1	L	58	ILE	CA-CB-CG2	7.81	123.78	110.50
1	L	145	ASN	OD1-CG-ND2	7.78	130.38	122.60
1	L	56	SER	CB-CA-C	-7.75	94.99	110.42
1	L	194	CYS	CB-CA-C	7.72	122.49	110.14
1	L	211	ARG	NE-CZ-NH2	-7.72	112.26	119.20
1	L	163	TRP	CA-C-O	-7.69	112.26	120.80
2	H	68	PHE	CA-CB-CG	7.68	121.48	113.80
2	H	114	HIS	CA-CB-CG	-7.68	106.12	113.80
1	L	205	ILE	N-CA-C	-7.68	98.77	109.21
1	L	76	ASN	N-CA-C	7.64	119.69	111.36
2	H	200	ARG	NE-CZ-NH2	7.64	126.08	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	101	GLY	CA-C-O	7.62	128.32	121.77
1	L	15	PRO	N-CA-C	-7.61	98.86	111.26
2	H	209	VAL	O-C-N	7.59	130.88	123.14
2	H	62	ASP	N-CA-C	7.57	120.41	111.71
2	H	110[A]	TYR	N-CA-C	7.56	120.77	107.61
2	H	110[B]	TYR	N-CA-C	7.56	120.77	107.61
2	H	199	PRO	N-CA-C	-7.55	96.91	112.47
1	L	125	LEU	CA-C-O	-7.55	109.71	120.51
2	H	223	VAL	N-CA-CB	-7.54	100.65	111.21
2	H	135	PRO	CB-CA-C	-7.54	102.29	111.11
1	L	137	ASN	CB-CG-ND2	7.53	127.69	116.40
1	L	41	HIS	CA-C-N	7.51	135.44	122.81
1	L	41	HIS	C-N-CA	7.51	135.44	122.81
2	H	97	THR	O-C-N	7.50	131.97	123.27
2	H	145	ASN	CA-C-N	7.50	134.26	121.14
2	H	145	ASN	C-N-CA	7.50	134.26	121.14
2	H	65	LYS	N-CA-CB	7.50	121.57	109.28
2	H	60	TYR	O-C-N	7.49	127.39	121.55
2	H	135	PRO	N-CA-CB	7.49	109.58	103.36
1	L	195	GLU	CA-CB-CG	7.47	129.05	114.10
1	L	10	THR	CA-C-O	-7.47	112.72	121.46
1	L	83	PHE	CA-CB-CG	7.46	121.27	113.80
1	L	76	ASN	CB-CA-C	7.44	123.50	110.85
1	L	62	PHE	CA-CB-CG	-7.41	106.39	113.80
1	L	178	THR	CA-C-O	-7.39	112.38	120.36
2	H	149	THR	CB-CA-C	7.35	122.60	109.38
1	L	198	HIS	CA-C-N	7.33	130.44	120.54
1	L	198	HIS	C-N-CA	7.33	130.44	120.54
2	H	29	PHE	CA-CB-CG	7.31	121.11	113.80
1	L	29	ILE	CA-C-O	7.30	129.91	120.78
1	L	210	ASN	O-C-N	7.30	131.90	123.29
2	H	48	VAL	N-CA-C	7.29	120.83	113.47
2	H	78	ASN	O-C-N	7.27	131.82	123.31
1	L	108	ARG	CA-C-O	-7.27	113.14	121.58
2	H	97	THR	CA-CB-OG1	-7.27	98.70	109.60
2	H	91	THR	N-CA-CB	7.23	120.75	109.69
1	L	3	LEU	N-CA-C	-7.21	97.15	108.90
1	L	153	SER	CA-C-N	7.19	130.96	120.82
1	L	153	SER	C-N-CA	7.19	130.96	120.82
1	L	4	LEU	CA-C-N	-7.14	112.93	123.00
1	L	4	LEU	C-N-CA	-7.14	112.93	123.00
1	L	24	ARG	CB-CA-C	7.14	121.72	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	76	ASN	OD1-CG-ND2	-7.13	115.47	122.60
1	L	150	ILE	O-C-N	7.13	130.62	122.99
1	L	98	PHE	CA-CB-CG	7.13	120.93	113.80
2	H	22	CYS	O-C-N	7.12	132.39	123.28
2	H	61	PRO	CA-C-O	-7.11	113.38	122.13
1	L	108	ARG	NE-CZ-NH2	7.09	125.58	119.20
1	L	51	ALA	N-CA-C	7.07	125.86	110.80
2	H	10	GLY	CA-C-O	-7.07	113.16	121.08
2	H	148	VAL	CB-CA-C	-7.07	100.08	110.62
1	L	94	TRP	CB-CA-C	7.07	119.65	109.26
1	L	5	THR	O-C-N	7.06	131.46	123.27
2	H	121	VAL	CA-C-O	-7.05	113.15	120.27
2	H	227	CYS	CA-CB-SG	-7.04	98.20	114.40
1	L	167	ASP	CA-CB-CG	-7.04	105.56	112.60
2	H	149	THR	CA-CB-CG2	7.01	122.42	110.50
2	H	82	GLN	CA-C-O	-7.01	112.96	120.46
1	L	198	HIS	CB-CA-C	6.98	123.19	109.66
2	H	163	THR	CA-CB-OG1	-6.97	99.14	109.60
2	H	150	LEU	CA-C-O	-6.97	113.29	121.44
1	L	96	LEU	N-CA-C	-6.94	100.45	110.24
2	H	40	THR	CB-CA-C	6.93	120.39	109.37
2	H	33	GLY	N-CA-C	-6.92	100.14	112.54
1	L	169	LYS	N-CA-CB	6.92	120.02	109.98
2	H	58	ILE	CB-CA-C	6.92	120.69	111.21
2	H	95	TYR	CA-C-O	-6.92	113.23	120.70
2	H	44	ARG	CA-CB-CG	6.91	127.92	114.10
1	L	15	PRO	O-C-N	6.90	131.27	122.85
1	L	155	ARG	NE-CZ-NH1	6.89	128.39	121.50
2	H	95	TYR	O-C-N	6.89	132.19	123.23
2	H	147	MET	CA-C-N	6.87	132.54	123.06
2	H	147	MET	C-N-CA	6.87	132.54	123.06
2	H	213	ALA	N-CA-C	6.87	119.64	111.33
2	H	132	SER	CA-C-N	-6.87	114.19	123.12
2	H	132	SER	C-N-CA	-6.87	114.19	123.12
1	L	44	PRO	CB-CA-C	6.87	120.02	111.23
1	L	137	ASN	N-CA-C	6.85	120.99	109.76
1	L	24	ARG	NH1-CZ-NH2	-6.82	110.43	119.30
1	L	53	GLN	OE1-CD-NE2	6.82	129.42	122.60
2	H	70	ILE	CA-C-N	6.82	133.30	122.59
2	H	70	ILE	C-N-CA	6.82	133.30	122.59
2	H	77	ASN	CA-CB-CG	6.77	119.37	112.60
2	H	20	LEU	CA-C-N	6.75	133.16	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	20	LEU	C-N-CA	6.75	133.16	122.62
1	L	29	ILE	CA-C-N	6.75	134.43	121.54
1	L	29	ILE	C-N-CA	6.75	134.43	121.54
2	H	44	ARG	CB-CA-C	-6.75	97.05	109.46
1	L	185	GLU	N-CA-C	-6.74	104.00	111.82
2	H	177	THR	CA-C-O	-6.74	113.15	120.36
1	L	60	SER	CA-C-N	6.73	129.97	120.28
1	L	60	SER	C-N-CA	6.73	129.97	120.28
1	L	18	SER	N-CA-C	-6.73	100.52	110.48
1	L	77	SER	N-CA-C	-6.71	96.82	108.69
1	L	177	SER	N-CA-CB	6.71	121.30	110.77
2	H	219	ASP	CA-C-O	-6.71	113.36	120.40
1	L	147	LYS	CA-C-O	-6.68	113.48	120.70
2	H	200	ARG	CA-CB-CG	6.68	127.46	114.10
2	H	162	VAL	CB-CA-C	6.68	120.70	110.55
2	H	2	VAL	N-CA-C	-6.67	95.46	109.34
2	H	3	GLN	CA-C-O	-6.67	112.92	120.32
1	L	123	GLU	CB-CG-CD	6.64	123.90	112.60
2	H	96	CYS	N-CA-CB	6.64	121.48	110.52
2	H	98	ARG	CA-C-O	-6.62	113.62	121.11
1	L	15	PRO	N-CA-CB	6.62	109.15	103.19
1	L	189	HIS	O-C-N	6.62	131.76	123.15
1	L	69	THR	CB-CA-C	6.62	121.34	109.29
1	L	5	THR	N-CA-CB	6.62	120.97	110.65
1	L	135	PHE	CA-C-O	-6.61	113.46	120.80
1	L	158	GLY	CA-C-O	-6.61	111.46	119.06
2	H	36	TRP	CA-C-O	-6.61	113.71	120.71
1	L	83	PHE	CA-C-O	6.60	128.00	120.54
1	L	200	THR	N-CA-CB	-6.60	98.30	110.18
1	L	115	VAL	CB-CA-C	6.59	120.97	110.82
2	H	187	TYR	CA-C-O	-6.58	113.95	121.72
2	H	209	VAL	CA-C-O	-6.57	113.23	120.72
2	H	23	ALA	CA-C-O	-6.57	113.12	120.54
1	L	149	LYS	CA-C-O	-6.55	112.22	120.28
1	L	155	ARG	NE-CZ-NH2	-6.53	113.32	119.20
2	H	175	VAL	N-CA-CB	6.52	123.27	111.21
1	L	195	GLU	CA-C-N	6.51	132.17	123.05
1	L	195	GLU	C-N-CA	6.51	132.17	123.05
2	H	213	ALA	N-CA-CB	-6.51	100.30	110.06
1	L	146	VAL	CA-C-N	-6.50	113.20	122.94
1	L	146	VAL	C-N-CA	-6.50	113.20	122.94
2	H	153	LEU	CB-CA-C	-6.48	98.51	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	115	VAL	CA-CB-CG2	6.46	121.39	110.40
1	L	165	ASP	N-CA-C	-6.46	102.20	110.53
1	L	175	MET	N-CA-CB	-6.45	99.58	110.99
1	L	29	ILE	CB-CG1-CD1	6.45	127.33	113.80
1	L	194	CYS	CA-C-O	-6.44	113.41	120.24
1	L	110	ASP	CA-CB-CG	6.44	119.04	112.60
1	L	17	ASP	OD1-CG-OD2	6.43	138.34	122.90
1	L	121	SER	CA-CB-OG	6.43	123.96	111.10
2	H	16	ARG	NH1-CZ-NH2	-6.42	110.95	119.30
1	L	205	ILE	CA-CB-CG2	6.42	121.42	110.50
2	H	212	PRO	CB-CA-C	6.42	124.05	113.20
1	L	121	SER	N-CA-CB	6.41	119.53	110.36
2	H	152	CYS	O-C-N	6.41	130.91	123.41
2	H	143	GLN	N-CA-C	-6.41	102.24	110.19
1	L	211	ARG	CB-CA-C	6.41	122.81	109.68
2	H	160	GLU	CG-CD-OE1	6.40	133.12	118.40
1	L	150	ILE	CA-C-O	-6.40	113.44	120.48
2	H	200	ARG	CA-C-O	-6.39	111.40	120.16
2	H	132	SER	CA-C-O	-6.38	113.42	120.38
1	L	126	THR	N-CA-CB	6.37	119.59	110.16
2	H	16	ARG	CB-CA-C	6.35	123.06	110.42
1	L	29	ILE	N-CA-C	6.34	122.53	109.34
2	H	192	SER	CA-CB-OG	6.30	123.70	111.10
1	L	140	TYR	CA-C-O	-6.29	111.54	120.16
2	H	11	LEU	CB-CA-C	6.28	120.10	109.80
2	H	37	VAL	CA-C-O	-6.28	113.71	120.36
1	L	122	SER	CA-C-O	6.26	127.12	119.11
2	H	62	ASP	CA-C-N	6.26	129.18	120.29
2	H	62	ASP	C-N-CA	6.26	129.18	120.29
2	H	220	LYS	N-CA-C	6.24	120.24	107.69
2	H	42	GLU	CA-CB-CG	6.24	126.58	114.10
1	L	4	LEU	N-CA-CB	6.23	120.35	110.57
1	L	151	ASP	CA-C-O	-6.20	113.90	121.28
2	H	184	SER	N-CA-CB	-6.17	100.06	110.49
2	H	19	LYS	CB-CG-CD	6.17	125.48	111.30
2	H	164	VAL	O-C-N	6.15	129.71	123.07
2	H	122	THR	CB-CA-C	-6.15	100.11	110.19
2	H	169	GLY	CA-C-N	6.14	133.26	121.54
2	H	169	GLY	C-N-CA	6.14	133.26	121.54
2	H	67	ARG	CG-CD-NE	-6.12	98.54	112.00
1	L	1	ASP	CA-C-O	-6.11	110.41	120.80
1	L	196	ALA	CB-CA-C	-6.11	100.17	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	199	LYS	CB-CA-C	-6.10	101.05	110.81
2	H	89	GLU	CA-C-O	-6.10	112.11	119.49
1	L	166	GLN	CB-CG-CD	6.08	122.94	112.60
2	H	150	LEU	N-CA-CB	-6.08	100.97	111.55
1	L	59	PRO	CA-C-O	6.08	129.86	122.08
2	H	119	THR	CB-CA-C	-6.07	97.32	109.35
1	L	188	ARG	CA-C-N	-6.07	113.07	122.59
1	L	188	ARG	C-N-CA	-6.07	113.07	122.59
1	L	207	LYS	CA-C-O	-6.06	112.83	120.28
1	L	61	ARG	CA-C-N	6.06	130.73	122.19
1	L	61	ARG	C-N-CA	6.06	130.73	122.19
2	H	188	THR	OG1-CB-CG2	6.05	121.41	109.30
1	L	150	ILE	CA-CB-CG2	6.05	120.78	110.50
2	H	156	GLY	N-CA-C	6.03	126.23	114.16
2	H	24	ALA	CA-C-O	-6.02	114.18	121.28
2	H	156	GLY	CA-C-O	6.01	126.67	119.82
2	H	24	ALA	O-C-N	6.01	130.01	123.10
2	H	160	GLU	CG-CD-OE2	-6.01	104.58	118.40
1	L	1	ASP	OD1-CG-OD2	6.00	137.31	122.90
1	L	103	LYS	CB-CA-C	-6.00	100.05	109.84
2	H	119	THR	N-CA-C	-5.99	99.23	109.24
1	L	77	SER	O-C-N	5.99	130.67	123.36
1	L	200	THR	CA-CB-OG1	-5.99	100.62	109.60
2	H	39	GLN	O-C-N	5.97	130.02	123.27
1	L	17	ASP	CB-CG-OD2	-5.97	104.68	118.40
1	L	155	ARG	CA-C-O	5.96	126.68	120.30
1	L	142	LYS	CB-CG-CD	5.96	125.00	111.30
1	L	197	THR	N-CA-CB	5.94	119.88	110.55
2	H	132	SER	O-C-N	5.94	130.30	123.29
1	L	109	ALA	N-CA-CB	5.93	118.83	110.36
2	H	65	LYS	O-C-N	5.92	131.18	123.07
2	H	13	ASN	O-C-N	5.92	128.16	121.53
1	L	72	THR	O-C-N	5.90	130.12	123.27
1	L	116	SER	N-CA-C	-5.90	99.03	109.06
1	L	114	THR	N-CA-CB	5.90	119.81	110.55
2	H	22	CYS	CA-C-O	-5.89	113.01	120.20
2	H	226	ASP	N-CA-C	-5.87	98.34	108.56
2	H	102[A]	TYR	N-CA-C	5.87	118.67	107.75
2	H	102[B]	TYR	N-CA-C	5.87	118.67	107.75
2	H	2	VAL	N-CA-CB	5.86	120.91	111.23
1	L	26	SER	CA-CB-OG	5.86	122.82	111.10
1	L	196	ALA	O-C-N	5.85	130.17	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	78	VAL	CB-CA-C	5.85	118.16	110.91
1	L	7	SER	CB-CA-C	-5.84	100.44	109.20
1	L	50	TYR	CA-C-N	5.84	132.70	121.54
1	L	50	TYR	C-N-CA	5.84	132.70	121.54
2	H	184	SER	CA-C-O	5.84	128.86	120.51
2	H	34	MET	N-CA-CB	5.83	121.70	111.55
2	H	44	ARG	NE-CZ-NH1	-5.83	115.67	121.50
2	H	32	TYR	CA-C-N	-5.82	115.28	121.45
2	H	32	TYR	C-N-CA	-5.82	115.28	121.45
2	H	59	HIS	CA-CB-CG	5.82	119.62	113.80
1	L	41	HIS	O-C-N	-5.82	114.86	122.59
1	L	89	GLN	OE1-CD-NE2	5.81	128.41	122.60
1	L	177	SER	O-C-N	5.80	130.06	123.27
1	L	202	THR	CB-CA-C	5.80	121.33	109.67
1	L	72	THR	CA-CB-OG1	-5.80	100.90	109.60
2	H	16	ARG	CA-C-N	5.80	131.85	122.29
2	H	16	ARG	C-N-CA	5.80	131.85	122.29
1	L	199	LYS	CA-C-O	5.79	127.10	120.90
2	H	102[A]	TYR	N-CA-CB	-5.79	100.83	110.39
2	H	102[B]	TYR	N-CA-CB	-5.79	100.83	110.39
1	L	34	HIS	O-C-N	-5.79	116.12	123.24
1	L	14	THR	N-CA-C	-5.78	102.37	109.65
2	H	82	GLN	CG-CD-NE2	-5.77	107.74	116.40
1	L	171	SER	CA-CB-OG	-5.77	99.57	111.10
2	H	131	PRO	N-CA-C	5.76	119.71	111.13
1	L	207	LYS	N-CA-CB	-5.75	101.14	110.81
1	L	82	ASP	N-CA-C	5.75	120.14	113.18
2	H	98	ARG	O-C-N	5.75	130.66	123.19
1	L	195	GLU	CB-CG-CD	5.74	122.36	112.60
2	H	34	MET	CB-CG-SD	-5.74	95.50	112.70
2	H	144	THR	CA-CB-CG2	5.74	120.25	110.50
2	H	79	LEU	CB-CA-C	5.73	119.10	109.48
2	H	72	ARG	CA-C-N	5.73	132.94	122.92
2	H	72	ARG	C-N-CA	5.73	132.94	122.92
2	H	44	ARG	CG-CD-NE	5.72	124.58	112.00
2	H	82	GLN	O-C-N	5.71	130.33	123.13
1	L	175	MET	CA-CB-CG	5.71	125.52	114.10
1	L	42	GLU	CB-CA-C	-5.70	98.61	109.66
1	L	39	LYS	N-CA-C	-5.70	102.49	110.35
1	L	170	ASP	CA-C-O	-5.67	113.09	119.95
1	L	79	GLU	CA-C-O	5.67	127.51	121.11
1	L	90	GLN	OE1-CD-NE2	-5.67	116.93	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	111	ALA	CB-CA-C	-5.67	100.17	109.80
2	H	188	THR	N-CA-C	-5.67	99.43	109.06
2	H	155	LYS	N-CA-C	5.66	118.77	109.72
2	H	87	ARG	CA-C-N	5.65	129.29	120.82
2	H	87	ARG	C-N-CA	5.65	129.29	120.82
2	H	200	ARG	O-C-N	5.65	127.81	121.32
1	L	126	THR	CA-C-O	5.64	126.40	120.42
1	L	126	THR	N-CA-C	5.64	117.51	111.36
1	L	10	THR	CA-CB-OG1	-5.63	101.15	109.60
1	L	97	THR	OG1-CB-CG2	-5.62	98.05	109.30
1	L	140	TYR	CA-CB-CG	-5.62	103.78	113.90
1	L	189	HIS	CA-CB-CG	5.62	119.42	113.80
1	L	194	CYS	N-CA-CB	-5.62	101.94	110.77
2	H	163	THR	CA-C-O	-5.61	114.30	120.36
1	L	61	ARG	CG-CD-NE	5.61	124.34	112.00
1	L	156	GLN	CA-C-O	5.61	126.57	119.78
2	H	226	ASP	O-C-N	-5.61	115.79	122.46
2	H	211	HIS	N-CA-CB	-5.60	103.30	111.20
2	H	72	ARG	N-CA-CB	5.60	121.01	111.66
1	L	144	ILE	CA-CB-CG2	5.60	120.02	110.50
2	H	93	LEU	CD1-CG-CD2	-5.60	98.48	110.80
2	H	93	LEU	CA-C-O	-5.60	114.33	120.43
1	L	181	LEU	CA-CB-CG	5.59	135.88	116.30
1	L	40	SER	O-C-N	5.59	129.46	122.86
1	L	214	CYS	N-CA-C	5.59	126.66	111.00
1	L	176	SER	O-C-N	5.59	130.31	123.21
2	H	181	VAL	CA-C-N	-5.59	114.31	122.19
2	H	181	VAL	C-N-CA	-5.59	114.31	122.19
2	H	193	VAL	O-C-N	5.59	129.10	123.07
2	H	16	ARG	CA-CB-CG	5.58	125.27	114.10
2	H	98	ARG	NE-CZ-NH1	5.57	127.07	121.50
2	H	102[A]	TYR	CA-C-O	5.57	126.85	120.84
2	H	102[B]	TYR	CA-C-O	5.57	126.85	120.84
1	L	18	SER	O-C-N	5.56	129.24	122.96
1	L	73	LEU	O-C-N	5.56	129.72	123.27
2	H	13	ASN	N-CA-C	-5.56	102.05	110.39
2	H	60	TYR	CA-C-O	-5.56	115.14	120.64
2	H	14	PRO	CA-C-O	5.55	127.36	121.03
2	H	75	ALA	CA-C-O	5.55	126.49	120.55
1	L	112	ALA	CA-C-O	5.55	125.89	120.23
1	L	27	GLN	N-CA-CB	-5.55	102.64	111.62
2	H	176	HIS	CA-C-O	-5.54	114.34	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	133	VAL	CB-CA-C	5.54	119.04	110.96
2	H	9	GLY	O-C-N	5.53	128.54	122.84
1	L	35	TRP	N-CA-C	5.53	117.97	109.07
2	H	119	THR	CA-C-O	-5.53	114.30	120.66
2	H	69	THR	O-C-N	-5.53	116.21	123.28
1	L	36	TYR	CB-CG-CD1	5.52	129.07	120.80
1	L	13	VAL	CB-CA-C	5.51	120.57	110.71
2	H	194	THR	CA-C-O	5.51	126.38	120.32
1	L	209	PHE	CB-CA-C	5.50	120.22	110.16
1	L	36	TYR	CB-CG-CD2	-5.49	112.57	120.80
2	H	17	SER	N-CA-C	5.49	117.74	109.23
2	H	144	THR	CA-C-O	-5.47	112.91	119.15
2	H	86	LEU	CB-CA-C	5.47	119.41	109.62
1	L	183	LYS	CA-C-O	5.46	126.26	120.10
1	L	40	SER	N-CA-C	-5.45	102.81	110.50
1	L	9	ALA	CA-C-N	5.45	131.96	122.81
1	L	9	ALA	C-N-CA	5.45	131.96	122.81
1	L	72	THR	CA-C-O	-5.43	114.76	121.06
1	L	108	ARG	CA-CB-CG	5.43	124.97	114.10
2	H	172	SER	N-CA-C	5.43	119.91	112.68
1	L	28	SER	CA-C-N	5.43	131.74	121.97
1	L	28	SER	C-N-CA	5.43	131.74	121.97
1	L	188	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	L	29	ILE	O-C-N	-5.42	115.80	122.57
1	L	212	ASN	O-C-N	-5.42	115.39	122.59
2	H	13	ASN	N-CA-CB	-5.41	102.31	109.78
1	L	28	SER	O-C-N	-5.39	115.42	122.59
2	H	207	CYS	N-CA-C	-5.39	100.11	108.90
1	L	105	GLU	CA-C-N	5.39	129.22	122.43
1	L	105	GLU	C-N-CA	5.39	129.22	122.43
2	H	120	SER	O-C-N	5.39	129.49	123.19
1	L	210	ASN	N-CA-CB	5.39	119.03	110.57
2	H	130	PRO	O-C-N	5.39	127.82	121.46
1	L	156	GLN	CA-C-N	5.38	128.99	121.24
1	L	156	GLN	C-N-CA	5.38	128.99	121.24
2	H	120	SER	CA-CB-OG	5.38	121.86	111.10
1	L	114	THR	O-C-N	5.38	129.61	123.27
1	L	189	HIS	CB-CA-C	5.37	120.80	109.79
2	H	70	ILE	CA-CB-CG1	-5.37	101.28	110.40
1	L	90	GLN	CG-CD-NE2	5.37	124.45	116.40
2	H	67	ARG	CD-NE-CZ	5.36	131.91	124.40
1	L	139	PHE	CA-CB-CG	5.36	119.16	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	61	PRO	N-CA-C	-5.35	102.83	111.77
2	H	137	ALA	N-CA-C	-5.35	102.75	110.40
2	H	217	LYS	CA-C-O	5.34	126.50	119.98
2	H	28	THR	OG1-CB-CG2	5.34	119.98	109.30
1	L	59	PRO	CA-C-N	5.34	129.64	120.72
1	L	59	PRO	C-N-CA	5.34	129.64	120.72
2	H	186	LEU	CD1-CG-CD2	-5.33	99.06	110.80
1	L	165	ASP	CA-C-O	-5.33	115.81	121.94
1	L	190	ASN	CB-CG-OD1	5.33	131.45	120.80
1	L	77	SER	N-CA-CB	5.32	119.75	110.81
2	H	194	THR	CA-C-N	5.32	130.06	122.24
2	H	194	THR	C-N-CA	5.32	130.06	122.24
1	L	36	TYR	CB-CA-C	-5.32	98.85	109.33
1	L	79	GLU	CG-CD-OE2	-5.32	106.17	118.40
1	L	198	HIS	CB-CG-ND1	-5.30	114.75	122.70
1	L	165	ASP	CA-CB-CG	-5.30	107.30	112.60
1	L	75	ILE	N-CA-C	-5.29	98.35	107.24
1	L	80	THR	N-CA-C	-5.28	104.77	111.11
2	H	65	LYS	CA-C-O	-5.28	115.09	120.80
2	H	62	ASP	CA-C-O	5.28	126.06	120.10
1	L	155	ARG	CB-CG-CD	5.27	123.43	111.30
1	L	55	ILE	CA-C-O	-5.27	114.20	120.78
2	H	16	ARG	O-C-N	-5.25	115.60	122.59
2	H	62	ASP	CA-CB-CG	-5.25	107.35	112.60
2	H	147	MET	N-CA-CB	-5.25	101.69	110.83
2	H	162	VAL	N-CA-CB	-5.25	103.62	112.44
1	L	166	GLN	O-C-N	5.25	129.29	122.89
1	L	16	GLY	CA-C-N	5.24	128.30	120.87
1	L	16	GLY	C-N-CA	5.24	128.30	120.87
2	H	130	PRO	CB-CA-C	5.23	117.30	110.92
1	L	71	PHE	CA-C-O	-5.22	114.66	120.66
1	L	167	ASP	O-C-N	5.21	129.01	122.86
2	H	177	THR	O-C-N	5.21	129.16	123.22
1	L	138	ASN	N-CA-C	5.21	117.53	111.02
2	H	162	VAL	CA-CB-CG2	5.21	119.26	110.40
2	H	72	ARG	CA-CB-CG	5.21	124.52	114.10
1	L	104	LEU	CB-CA-C	5.21	118.75	109.38
2	H	129	THR	O-C-N	5.21	127.41	121.94
2	H	108[A]	ASN	CA-CB-CG	5.20	117.80	112.60
2	H	108[B]	ASN	CA-CB-CG	5.20	117.80	112.60
2	H	38	ARG	NE-CZ-NH1	5.20	126.70	121.50
2	H	53	GLY	CA-C-O	-5.19	115.72	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	78	ASN	CA-C-O	-5.18	114.57	120.32
1	L	76	ASN	CA-C-O	-5.18	114.93	120.42
2	H	95	TYR	CA-CB-CG	5.17	123.20	113.90
1	L	42	GLU	CA-C-O	-5.15	115.43	121.46
1	L	9	ALA	O-C-N	-5.15	115.54	122.23
2	H	43	LYS	CB-CG-CD	5.14	123.12	111.30
2	H	162	VAL	CA-CB-CG1	5.14	119.14	110.40
1	L	102	SER	CB-CA-C	5.13	119.85	111.23
1	L	41	HIS	N-CA-CB	-5.13	101.83	110.49
1	L	193	THR	OG1-CB-CG2	5.13	119.55	109.30
2	H	222	ILE	O-C-N	5.11	127.18	121.97
1	L	164	THR	N-CA-C	-5.11	103.18	110.59
1	L	156	GLN	CG-CD-OE1	5.11	131.01	120.80
2	H	57	TYR	CB-CA-C	5.11	120.58	110.42
1	L	121	SER	CA-C-N	5.10	131.52	121.58
1	L	121	SER	C-N-CA	5.10	131.52	121.58
2	H	87	ARG	NE-CZ-NH2	5.09	123.78	119.20
2	H	83	MET	O-C-N	5.09	129.67	123.21
1	L	120	PRO	CB-CA-C	5.08	117.74	111.23
1	L	63	SER	CA-C-O	-5.08	114.82	120.66
1	L	116	SER	CB-CA-C	5.06	119.66	109.38
2	H	74	ASN	O-C-N	5.06	129.16	122.43
2	H	214	SER	CA-CB-OG	5.06	121.22	111.10
1	L	73	LEU	N-CA-C	-5.05	100.17	108.41
1	L	145	ASN	CB-CG-ND2	-5.05	108.82	116.40
1	L	113	PRO	CA-C-N	5.04	130.10	123.05
1	L	113	PRO	C-N-CA	5.04	130.10	123.05
2	H	92	ALA	CB-CA-C	-5.04	100.39	110.42
1	L	101	GLY	O-C-N	-5.03	118.41	122.64
1	L	180	THR	CA-C-O	-5.03	114.79	120.32
2	H	89	GLU	CA-CB-CG	5.02	124.14	114.10
1	L	55	ILE	CB-CA-C	5.02	119.52	111.29
1	L	74	SER	CA-C-O	-5.01	115.24	120.80
2	H	157	TYR	CA-C-O	-5.01	115.60	121.46

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	72	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1654	0	1570	109	4
2	H	1824	0	1754	148	7
3	H	247	0	0	26	1
3	L	241	0	0	28	7
All	All	3966	0	3324	252	10

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 37.

All (252) 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:107[B]:GLY:HA2	3:H:404:HOH:O	1.62	0.97
2:H:12:VAL:HG21	2:H:18:LEU:HG	1.50	0.93
2:H:107[B]:GLY:CA	3:H:404:HOH:O	2.14	0.92
2:H:9:GLY:H	2:H:119:THR:HG21	1.38	0.88
1:L:90:GLN:HE22	1:L:93:SER:H	1.16	0.88
1:L:195:GLU:HG2	1:L:206:VAL:HG12	1.54	0.87
2:H:165:THR:HG22	2:H:208:ASN:HB2	1.59	0.84
1:L:136:LEU:HG	3:L:296:HOH:O	1.80	0.81
2:H:102[A]:TYR:HB2	2:H:110[A]:TYR:OH	1.80	0.81
2:H:225:ARG:HB3	3:H:257:HOH:O	1.82	0.80
1:L:11:LEU:HD23	1:L:104:LEU:HD21	1.63	0.79
1:L:55:ILE:HG13	1:L:56:SER:H	1.47	0.78
2:H:102[B]:TYR:HB2	2:H:110[B]:TYR:OH	1.83	0.78
2:H:1:GLU:HA	2:H:3:GLN:HE21	1.51	0.76
1:L:210:ASN:ND2	3:L:376:HOH:O	2.17	0.76
2:H:200:ARG:HB3	2:H:201:PRO:CD	2.16	0.76
2:H:94:TYR:O	2:H:118:GLY:HA2	1.87	0.74
2:H:140:SER:OG	2:H:200:ARG:NH1	2.20	0.74
2:H:198:SER:OG	2:H:199:PRO:HD3	1.88	0.74
1:L:146:VAL:HG22	3:L:296:HOH:O	1.88	0.74
2:H:72:ARG:NE	2:H:74:ASN:HD21	1.86	0.73
2:H:201:PRO:HA	2:H:223:VAL:CG1	2.18	0.73
1:L:29:ILE:HG22	1:L:92:ASN:OD1	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:82:GLN:HG3	3:H:332:HOH:O	1.88	0.73
2:H:164:VAL:HG13	3:H:300:HOH:O	1.88	0.73
1:L:21:LEU:HD11	1:L:104:LEU:HD11	1.71	0.72
2:H:200:ARG:HB3	2:H:201:PRO:HD3	1.73	0.70
2:H:2:VAL:H	2:H:26:GLY:HA3	1.56	0.70
2:H:225:ARG:HG2	2:H:227:CYS:O	1.92	0.70
1:L:135:PHE:CE2	2:H:192:SER:HB3	2.26	0.69
2:H:6:GLN:NE2	2:H:6:GLN:H	1.91	0.69
2:H:6:GLN:H	2:H:6:GLN:HE21	1.39	0.69
1:L:144:ILE:HG22	1:L:163:TRP:CZ3	2.29	0.68
1:L:31:ASN:ND2	3:L:388:HOH:O	2.27	0.68
2:H:73:ASP:OD1	2:H:75:ALA:HB3	1.93	0.68
1:L:4:LEU:HD22	1:L:23:CYS:SG	2.34	0.68
2:H:103[B]:ARG:HA	3:H:462:HOH:O	1.94	0.67
1:L:169:LYS:HB2	3:L:414:HOH:O	1.94	0.67
2:H:107[B]:GLY:O	2:H:108[B]:ASN:HB2	1.95	0.67
1:L:108:ARG:NH1	1:L:109:ALA:O	2.28	0.67
2:H:225:ARG:H	2:H:225:ARG:HD2	1.60	0.67
2:H:184:SER:O	2:H:186:LEU:HD12	1.94	0.66
1:L:90:GLN:NE2	1:L:93:SER:H	1.91	0.66
2:H:18:LEU:O	2:H:83:MET:HG2	1.95	0.66
1:L:42:GLU:HG2	1:L:43:SER:N	2.09	0.66
2:H:223:VAL:O	2:H:225:ARG:N	2.30	0.65
1:L:184:ASP:HB3	3:L:270:HOH:O	1.97	0.64
2:H:200:ARG:HA	2:H:224:PRO:HG2	1.79	0.64
1:L:28:SER:OG	1:L:29:ILE:N	2.21	0.63
1:L:49:LYS:HB2	1:L:53:GLN:O	1.98	0.63
1:L:211:ARG:O	1:L:212:ASN:HB3	1.98	0.63
2:H:83:MET:CE	2:H:121:VAL:HG11	2.28	0.63
1:L:55:ILE:HG13	1:L:56:SER:N	2.11	0.63
2:H:200:ARG:CD	2:H:201:PRO:HD3	2.28	0.63
2:H:204:THR:HA	2:H:223:VAL:HG22	1.79	0.63
1:L:197:THR:HG23	1:L:204:PRO:HB3	1.81	0.62
2:H:201:PRO:HA	2:H:223:VAL:HG13	1.80	0.62
2:H:103[A]:ARG:HA	3:H:462:HOH:O	1.98	0.62
1:L:31:ASN:HA	3:L:432:HOH:O	1.99	0.62
1:L:52:SER:HA	1:L:64:GLY:O	1.99	0.61
1:L:39:LYS:HE2	3:L:254:HOH:O	1.98	0.61
2:H:1:GLU:HA	2:H:3:GLN:NE2	2.15	0.61
1:L:13:VAL:HG23	3:L:358:HOH:O	2.00	0.61
1:L:39:LYS:HZ3	1:L:81:GLU:C	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:15:PRO:HA	1:L:78:VAL:O	2.00	0.61
2:H:72:ARG:HE	2:H:74:ASN:HD21	1.48	0.60
1:L:142:LYS:NZ	3:L:313:HOH:O	2.34	0.60
2:H:182:LEU:HD21	3:H:328:HOH:O	2.01	0.60
1:L:80:THR:O	1:L:83:PHE:HD1	1.83	0.60
2:H:172:SER:OG	2:H:173:SER:N	2.32	0.60
2:H:101[B]:PHE:CB	2:H:103[B]:ARG:HH11	2.14	0.60
2:H:1:GLU:OE1	2:H:3:GLN:NE2	2.33	0.60
2:H:200:ARG:CB	2:H:201:PRO:HD3	2.31	0.60
2:H:201:PRO:HA	2:H:223:VAL:HG12	1.82	0.60
2:H:147:MET:O	3:H:396:HOH:O	2.16	0.60
2:H:107[A]:GLY:HA2	3:H:459:HOH:O	2.01	0.60
2:H:6:GLN:HE22	2:H:117:GLN:H	1.48	0.59
2:H:200:ARG:HD3	2:H:224:PRO:HB2	1.85	0.59
1:L:108:ARG:HD3	1:L:109:ALA:O	2.02	0.59
2:H:32:TYR:CG	2:H:98:ARG:HD2	2.38	0.59
2:H:200:ARG:HD2	2:H:201:PRO:HD3	1.84	0.59
2:H:174:GLY:HA2	3:H:275:HOH:O	2.01	0.59
1:L:126:THR:HA	3:L:395:HOH:O	2.03	0.58
2:H:83:MET:HE3	2:H:121:VAL:HG11	1.85	0.58
1:L:6:GLN:HE21	1:L:99:GLY:HA3	1.68	0.58
2:H:51:ILE:HG13	2:H:58:ILE:HG22	1.85	0.58
1:L:32:ASN:N	1:L:32:ASN:ND2	2.49	0.57
2:H:64:VAL:HG22	2:H:68:PHE:CD2	2.40	0.57
1:L:90:GLN:HB2	3:L:441:HOH:O	2.03	0.57
1:L:91:SER:HB2	2:H:110[A]:TYR:H	1.69	0.57
2:H:196:PRO:O	2:H:199:PRO:HD2	2.04	0.57
2:H:99:HIS:HB3	2:H:110[B]:TYR:CD1	2.40	0.57
2:H:149:THR:HG23	3:H:242:HOH:O	2.04	0.57
1:L:61:ARG:NH1	1:L:82:ASP:OD2	2.34	0.57
2:H:6:GLN:OE1	2:H:116:GLY:HA3	2.05	0.57
2:H:58:ILE:HD12	2:H:60:TYR:OH	2.05	0.56
2:H:222:ILE:O	2:H:225:ARG:CZ	2.53	0.56
2:H:140:SER:CB	2:H:200:ARG:HH12	2.18	0.56
1:L:32:ASN:N	1:L:32:ASN:HD22	2.03	0.56
2:H:108[B]:ASN:O	2:H:109[B]:TYR:CD1	2.58	0.56
2:H:58:ILE:HG13	2:H:60:TYR:CE2	2.41	0.56
2:H:104[B]:TYR:O	2:H:105[B]:ASP:HB2	2.05	0.56
1:L:89:GLN:HB2	1:L:98:PHE:CD2	2.41	0.56
1:L:41:HIS:HA	3:L:298:HOH:O	2.06	0.56
2:H:67:ARG:HD2	2:H:85:SER:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:101[B]:PHE:HB2	2:H:103[B]:ARG:HH11	1.71	0.56
2:H:135:PRO:HB3	2:H:222:ILE:HD13	1.88	0.56
2:H:67:ARG:HB3	2:H:84:SER:O	2.07	0.55
2:H:133:VAL:HB	2:H:218:VAL:HG11	1.88	0.55
2:H:16:ARG:HH11	2:H:16:ARG:HB2	1.71	0.55
2:H:208:ASN:ND2	3:H:306:HOH:O	2.33	0.55
2:H:208:ASN:ND2	2:H:219:ASP:OD1	2.35	0.55
1:L:144:ILE:HG22	1:L:163:TRP:HZ3	1.72	0.54
2:H:13:ASN:HB2	2:H:16:ARG:HD2	1.88	0.54
2:H:43:LYS:HE3	2:H:43:LYS:HA	1.90	0.54
2:H:12:VAL:CG2	2:H:18:LEU:HG	2.30	0.54
2:H:102[B]:TYR:HB2	2:H:110[B]:TYR:HH	1.73	0.54
1:L:191:SER:HB3	3:L:329:HOH:O	2.08	0.53
2:H:48:VAL:O	2:H:64:VAL:HG11	2.08	0.53
1:L:115:VAL:HB	1:L:136:LEU:HD13	1.89	0.53
1:L:62:PHE:CE1	1:L:75:ILE:HG12	2.43	0.53
2:H:15:GLY:N	2:H:86:LEU:O	2.30	0.53
2:H:108[B]:ASN:ND2	3:H:459:HOH:O	2.41	0.53
2:H:208:ASN:N	3:H:300:HOH:O	2.42	0.53
2:H:221:LYS:H	2:H:221:LYS:HE3	1.74	0.53
2:H:83:MET:HB2	2:H:86:LEU:HD21	1.92	0.52
2:H:93:LEU:HD21	3:H:354:HOH:O	2.09	0.52
1:L:3:LEU:HD12	3:L:404:HOH:O	2.09	0.52
2:H:41:PRO:O	2:H:43:LYS:HD2	2.09	0.52
1:L:11:LEU:HD23	1:L:104:LEU:CD2	2.35	0.52
2:H:48:VAL:HG12	2:H:64:VAL:HG21	1.92	0.52
2:H:149:THR:C	2:H:150:LEU:HD12	2.35	0.52
2:H:99:HIS:HB3	2:H:110[A]:TYR:CD1	2.45	0.51
1:L:34:HIS:O	1:L:89:GLN:N	2.37	0.51
1:L:28:SER:O	1:L:29:ILE:HG13	2.09	0.51
2:H:24:ALA:HB1	2:H:27:PHE:CE1	2.46	0.51
1:L:136:LEU:HD23	1:L:175:MET:SD	2.51	0.51
1:L:28:SER:O	1:L:68:GLY:O	2.28	0.51
1:L:204:PRO:HG2	3:L:300:HOH:O	2.10	0.51
1:L:212:ASN:OD1	1:L:213:GLU:N	2.39	0.50
2:H:103[B]:ARG:C	2:H:105[B]:ASP:H	2.19	0.50
2:H:221:LYS:H	2:H:221:LYS:CE	2.25	0.50
1:L:154:GLU:HG3	3:L:262:HOH:O	2.09	0.50
1:L:42:GLU:HG2	1:L:43:SER:H	1.75	0.50
2:H:52:SER:O	2:H:72:ARG:NH1	2.45	0.50
1:L:36:TYR:HE2	1:L:89:GLN:HB3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:61:ARG:HH22	1:L:82:ASP:CG	2.19	0.50
2:H:175:VAL:HG22	3:H:274:HOH:O	2.12	0.50
2:H:73:ASP:OD1	2:H:73:ASP:C	2.54	0.50
2:H:140:SER:HA	2:H:200:ARG:HH22	1.77	0.50
2:H:87:ARG:HG3	2:H:87:ARG:HH11	1.77	0.49
1:L:155:ARG:NH2	1:L:185:GLU:OE2	2.44	0.49
2:H:9:GLY:N	2:H:119:THR:HG21	2.18	0.49
3:L:393:HOH:O	2:H:149:THR:HG21	2.12	0.49
2:H:101[A]:PHE:HB2	2:H:103[A]:ARG:HH11	1.76	0.49
2:H:43:LYS:HD2	2:H:43:LYS:N	2.28	0.49
2:H:188:THR:O	3:H:248:HOH:O	2.20	0.49
1:L:151:ASP:OD2	1:L:189:HIS:HB3	2.11	0.49
1:L:189:HIS:HE1	3:L:336:HOH:O	1.96	0.49
2:H:8:GLY:HA2	3:H:385:HOH:O	2.13	0.49
1:L:6:GLN:HE21	1:L:99:GLY:CA	2.26	0.48
1:L:123:GLU:HA	3:L:319:HOH:O	2.13	0.48
1:L:124:GLN:HG2	1:L:129:GLY:O	2.12	0.48
1:L:82:ASP:O	1:L:86:TYR:OH	2.25	0.48
1:L:121:SER:O	1:L:125:LEU:HG	2.14	0.48
1:L:39:LYS:NZ	1:L:81:GLU:O	2.39	0.48
1:L:149:LYS:HB2	1:L:193:THR:HB	1.95	0.48
2:H:211:HIS:ND1	2:H:214:SER:OG	2.43	0.48
1:L:163:TRP:N	1:L:163:TRP:CD1	2.82	0.48
2:H:200:ARG:CB	2:H:201:PRO:CD	2.86	0.48
2:H:72:ARG:HE	2:H:74:ASN:ND2	2.11	0.47
2:H:133:VAL:O	2:H:220:LYS:HE3	2.14	0.47
1:L:31:ASN:O	1:L:50:TYR:HA	2.15	0.47
2:H:42:GLU:N	2:H:42:GLU:OE1	2.47	0.47
2:H:130:PRO:HB3	2:H:214:SER:OG	2.14	0.47
1:L:80:THR:O	1:L:83:PHE:CD1	2.67	0.47
2:H:29:PHE:CD2	2:H:77:ASN:HA	2.49	0.47
1:L:97:THR:HA	3:L:369:HOH:O	2.15	0.47
1:L:155:ARG:HD3	1:L:157:ASN:O	2.14	0.47
2:H:58:ILE:HG13	2:H:60:TYR:HE2	1.79	0.47
1:L:31:ASN:ND2	3:L:432:HOH:O	2.49	0.46
2:H:53:GLY:HA3	2:H:102[A]:TYR:HE2	1.80	0.46
2:H:202:SER:OG	2:H:203:GLU:N	2.49	0.46
1:L:49:LYS:O	1:L:53:GLN:HB2	2.16	0.46
1:L:155:ARG:NH1	3:L:429:HOH:O	2.48	0.46
1:L:149:LYS:C	1:L:150:ILE:HD12	2.41	0.45
2:H:130:PRO:HB3	2:H:214:SER:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:170:ASP:O	1:L:171:SER:HB2	2.16	0.45
2:H:29:PHE:O	2:H:72:ARG:NH2	2.50	0.45
2:H:222:ILE:O	2:H:225:ARG:NH1	2.49	0.45
2:H:40:THR:OG1	2:H:44:ARG:HD2	2.16	0.45
2:H:89:GLU:HG3	3:H:353:HOH:O	2.16	0.45
1:L:90:GLN:HE21	1:L:92:ASN:HB3	1.81	0.45
2:H:198:SER:H	2:H:199:PRO:CD	2.30	0.45
2:H:53:GLY:HA3	2:H:102[B]:TYR:HE2	1.81	0.44
1:L:79:GLU:O	1:L:80:THR:C	2.60	0.44
1:L:21:LEU:HD11	1:L:104:LEU:CD1	2.45	0.44
1:L:211:ARG:O	1:L:212:ASN:CB	2.64	0.44
2:H:178:PHE:O	2:H:189:LEU:HG	2.17	0.44
2:H:182:LEU:HG	2:H:183:GLN:N	2.33	0.44
2:H:6:GLN:HE22	2:H:117:GLN:N	2.13	0.44
1:L:32:ASN:HB2	1:L:92:ASN:HB2	2.00	0.43
1:L:35:TRP:CE3	1:L:73:LEU:HD12	2.53	0.43
1:L:169:LYS:HD2	1:L:169:LYS:HA	1.90	0.43
2:H:214:SER:O	2:H:215:SER:C	2.61	0.43
2:H:225:ARG:CG	2:H:227:CYS:O	2.64	0.43
1:L:32:ASN:ND2	2:H:109[A]:TYR:CD2	2.86	0.43
1:L:31:ASN:C	1:L:33:LEU:H	2.27	0.43
1:L:112:ALA:HB2	1:L:200:THR:HG21	2.01	0.43
2:H:114:HIS:CE1	3:H:468:HOH:O	2.71	0.43
1:L:39:LYS:NZ	1:L:81:GLU:C	2.76	0.43
2:H:181:VAL:HG22	3:H:248:HOH:O	2.18	0.43
1:L:11:LEU:HD11	3:L:438:HOH:O	2.18	0.43
1:L:14:THR:O	1:L:15:PRO:C	2.60	0.43
2:H:6:GLN:HA	2:H:21:SER:O	2.19	0.43
2:H:43:LYS:HD2	2:H:43:LYS:H	1.83	0.43
1:L:26:SER:OG	1:L:27:GLN:OE1	2.15	0.43
2:H:36:TRP:NE1	2:H:81:LEU:HB2	2.34	0.42
1:L:120:PRO:HG3	1:L:130:ALA:HB1	2.01	0.42
1:L:18:SER:HA	1:L:75:ILE:O	2.19	0.42
1:L:19:VAL:HG13	1:L:75:ILE:HB	2.01	0.42
2:H:162:VAL:HG23	2:H:211:HIS:CD2	2.54	0.42
2:H:100[A]:PRO:HD3	2:H:111:ALA:O	2.19	0.42
1:L:8:PRO:HB3	3:L:292:HOH:O	2.19	0.42
1:L:48:ILE:HG21	1:L:64:GLY:HA3	2.02	0.42
1:L:174:SER:HB3	2:H:178:PHE:HE2	1.84	0.42
2:H:1:GLU:CA	2:H:3:GLN:HE21	2.27	0.42
2:H:178:PHE:HA	2:H:179:PRO:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:197:THR:HG21	3:L:240:HOH:O	2.18	0.42
1:L:197:THR:HG23	1:L:204:PRO:HA	2.02	0.42
1:L:10:THR:HG23	3:L:302:HOH:O	2.20	0.41
2:H:174:GLY:O	2:H:193:VAL:HA	2.20	0.41
2:H:133:VAL:HG21	2:H:209:VAL:HG13	2.01	0.41
1:L:51:ALA:O	1:L:64:GLY:C	2.63	0.41
2:H:145:ASN:ND2	3:H:457:HOH:O	2.53	0.41
1:L:85:MET:HE3	1:L:85:MET:HB2	1.81	0.41
1:L:155:ARG:HH11	1:L:155:ARG:HB2	1.85	0.41
2:H:165:THR:O	3:H:300:HOH:O	2.21	0.41
1:L:71:PHE:CD1	1:L:71:PHE:N	2.89	0.41
1:L:96:LEU:H	1:L:96:LEU:HG	1.67	0.41
2:H:6:GLN:NE2	2:H:118:GLY:H	2.19	0.41
2:H:64:VAL:CG2	2:H:68:PHE:CD2	3.03	0.41
2:H:146:SER:HB3	3:H:273:HOH:O	2.20	0.41
1:L:61:ARG:HH11	1:L:61:ARG:HD2	1.66	0.41
2:H:100[B]:PRO:HD3	2:H:111:ALA:O	2.21	0.40
1:L:155:ARG:HG2	1:L:156:GLN:N	2.35	0.40
2:H:107[B]:GLY:O	2:H:108[B]:ASN:CB	2.67	0.40
2:H:160:GLU:HB2	3:H:293:HOH:O	2.20	0.40
1:L:91:SER:HB2	2:H:110[B]:TYR:H	1.85	0.40
2:H:102[A]:TYR:HB2	2:H:110[A]:TYR:HH	1.80	0.40
1:L:188:ARG:CD	3:L:341:HOH:O	2.69	0.40
2:H:64:VAL:HG22	2:H:68:PHE:CE2	2.56	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:333:HOH:O	3:L:333:HOH:O[2_975]	1.54	0.66
2:H:77:ASN:CB	3:H:273:HOH:O[2_985]	1.72	0.48
2:H:87:ARG:CB	3:L:436:HOH:O[4_476]	1.74	0.46
2:H:16:ARG:NH1	3:L:374:HOH:O[4_476]	1.75	0.45
1:L:161:ASN:OD1	2:H:106[A]:GLY:CA[3_845]	1.81	0.39
1:L:190:ASN:OD1	3:L:333:HOH:O[2_975]	1.82	0.38
2:H:57:TYR:N	3:L:303:HOH:O[3_855]	2.03	0.17
1:L:161:ASN:OD1	2:H:106[A]:GLY:C[3_845]	2.10	0.10
1:L:190:ASN:ND2	3:L:333:HOH:O[2_975]	2.10	0.10
2:H:87:ARG:CG	3:L:318:HOH:O[4_476]	2.12	0.08

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	212/214 (99%)	190 (90%)	12 (6%)	10 (5%)	2	0
2	H	236/227 (104%)	198 (84%)	24 (10%)	14 (6%)	1	0
All	All	448/441 (102%)	388 (87%)	36 (8%)	24 (5%)	2	0

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	28	SER
1	L	30	SER
1	L	51	ALA
1	L	56	SER
1	L	212	ASN
2	H	105[A]	ASP
2	H	105[B]	ASP
2	H	108[A]	ASN
2	H	108[B]	ASN
2	H	200	ARG
2	H	223	VAL
1	L	41	HIS
2	H	57	TYR
1	L	213	GLU
2	H	142	ALA
2	H	198	SER
2	H	224	PRO
2	H	92	ALA
2	H	101[A]	PHE
2	H	101[B]	PHE
1	L	11	LEU
2	H	2	VAL
1	L	32	ASN
1	L	29	ILE

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	193/193 (100%)	148 (77%)	45 (23%)	1	0
2	H	202/193 (105%)	155 (77%)	47 (23%)	1	0
All	All	395/386 (102%)	303 (77%)	92 (23%)	1	0

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	2	GLU
1	L	7	SER
1	L	12	SER
1	L	13	VAL
1	L	19	VAL
1	L	22	SER
1	L	24	ARG
1	L	29	ILE
1	L	31	ASN
1	L	32	ASN
1	L	33	LEU
1	L	41	HIS
1	L	47	LEU
1	L	48	ILE
1	L	55	ILE
1	L	65	SER
1	L	69	THR
1	L	70	ASP
1	L	73	LEU
1	L	74	SER
1	L	78	VAL
1	L	81	GLU
1	L	90	GLN
1	L	94	TRP
1	L	103	LYS
1	L	104	LEU

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Mol	Chain	Res	Type
1	L	108	ARG
1	L	115	VAL
1	L	123	GLU
1	L	126	THR
1	L	134	CYS
1	L	142	LYS
1	L	147	LYS
1	L	154	GLU
1	L	155	ARG
1	L	160	LEU
1	L	162	SER
1	L	165	ASP
1	L	187	GLU
1	L	188	ARG
1	L	194	CYS
1	L	197	THR
1	L	206	VAL
1	L	210	ASN
2	H	6	GLN
2	H	13	ASN
2	H	16	ARG
2	H	18	LEU
2	H	19	LYS
2	H	34	MET
2	H	42	GLU
2	H	43	LYS
2	H	44	ARG
2	H	48	VAL
2	H	51	ILE
2	H	56	THR
2	H	64	VAL
2	H	69	THR
2	H	71	SER
2	H	83	MET
2	H	85	SER
2	H	101[A]	PHE
2	H	101[B]	PHE
2	H	102[A]	TYR
2	H	102[B]	TYR
2	H	103[A]	ARG
2	H	103[B]	ARG
2	H	117	GLN

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Mol	Chain	Res	Type
2	H	119	THR
2	H	129	THR
2	H	138	PRO
2	H	144	THR
2	H	145	ASN
2	H	148	VAL
2	H	149	THR
2	H	152	CYS
2	H	153	LEU
2	H	154	VAL
2	H	162	VAL
2	H	165	THR
2	H	186	LEU
2	H	190	SER
2	H	194	THR
2	H	203	GLU
2	H	204	THR
2	H	206	THR
2	H	207	CYS
2	H	209	VAL
2	H	221	LYS
2	H	225	ARG
2	H	226	ASP

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	6	GLN
1	L	53	GLN
1	L	90	GLN
1	L	137	ASN
1	L	138	ASN
2	H	3	GLN
2	H	6	GLN
2	H	74	ASN
2	H	99	HIS
2	H	145	ASN
2	H	183	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](#)

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

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.