



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 12:13 PM UTC

PDB ID : 1QGC / pdb_00001qgc
Title : STRUCTURE OF THE COMPLEX OF A FAB FRAGMENT OF A NEUTRALIZING ANTIBODY WITH FOOT AND MOUTH DISEASE VIRUS
Authors : Fita, I.
Deposited on : 1999-04-23
Resolution : 30.00 Å(reported)
Based on initial model : 1FMD

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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

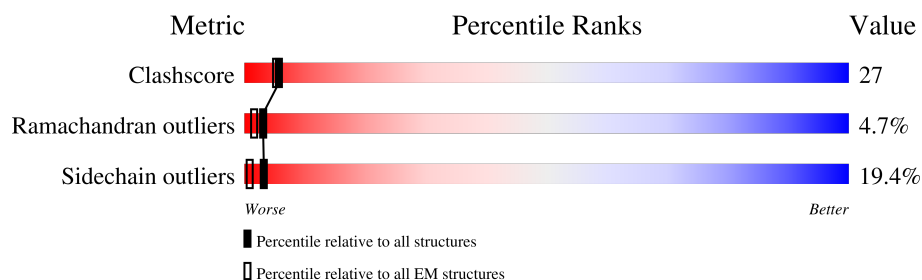
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 30.00 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	207	50% 27% 11% • 12%
2	2	218	52% 38% 10% •
3	3	219	51% 33% 16% •
4	4	218	33% 42% 20% 5%
5	A	220	37% 40% 21% •
6	5	24	12% 38% 33% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OCS	4	218	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8279 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 PROTEIN (VIRUS CAPSID PROTEIN VP1).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	183	Total	C	N	O	S	0	0
			1416	893	253	267	3		

- Molecule 2 is a protein called PROTEIN (VIRUS CAPSID PROTEIN VP2).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	218	Total	C	N	O	S	0	0
			1680	1061	296	316	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	50	ALA	GLY	conflict	UNP Q9QCE2

- Molecule 3 is a protein called PROTEIN (VIRUS CAPSID PROTEIN VP3).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	219	Total	C	N	O	S	0	0
			1690	1075	277	327	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	168	THR	ALA	conflict	UNP P15072

- Molecule 4 is a protein called PROTEIN (IMMUNOGLOBULIN LIGHT CHAIN).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	218	Total	C	N	O	S	0	0
			1683	1042	287	347	7		

- Molecule 5 is a protein called PROTEIN (IMMUNOGLOBULIN HEAVY CHAIN).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	220	Total 1644	C 1039	N 275	O 320	S 10	0	0

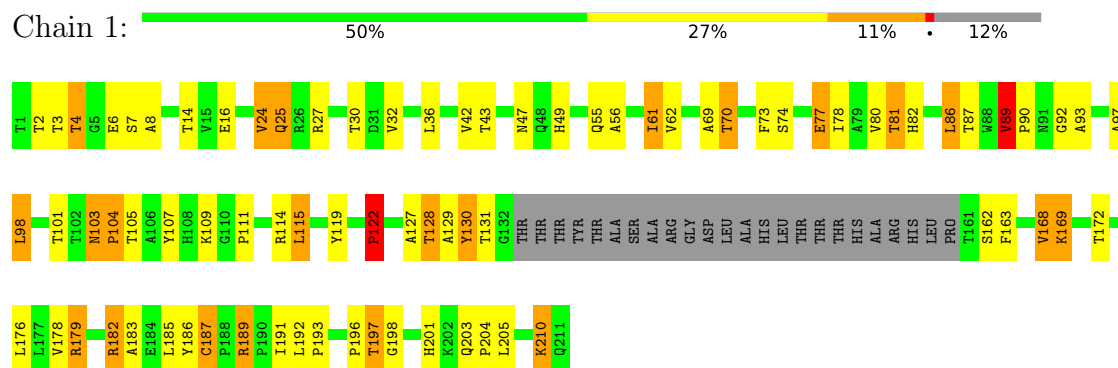
- Molecule 6 is a protein called PROTEIN (GH-LOOP FROM VIRUS CAPSID PROTEIN VP1).

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5	24	Total 166	C 102	N 29	O 35	0	0

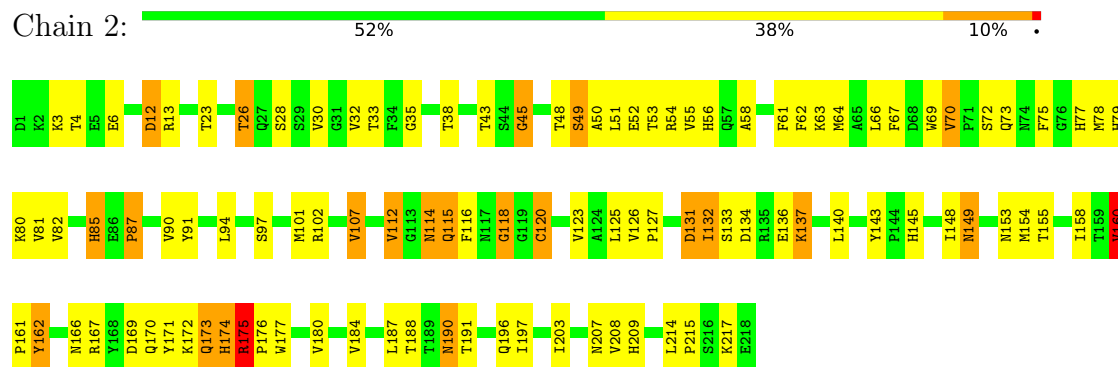
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PROTEIN (VIRUS CAPSID PROTEIN VP1)



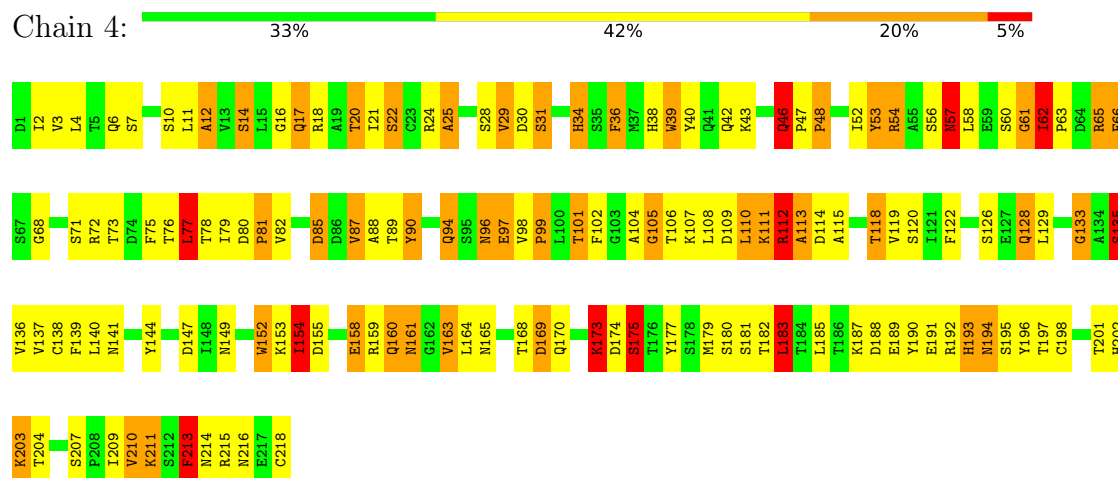
• Molecule 2: PROTEIN (VIRUS CAPSID PROTEIN VP2)



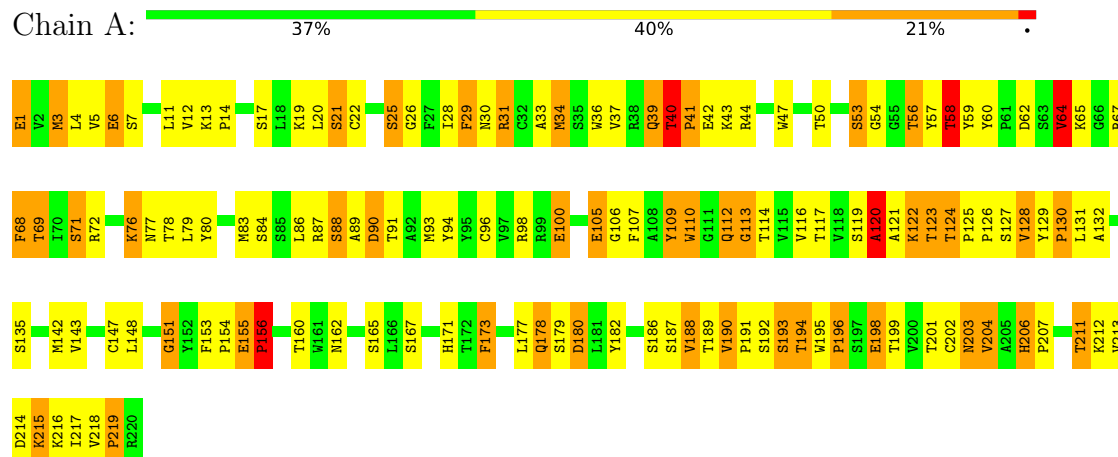
• Molecule 3: PROTEIN (VIRUS CAPSID PROTEIN VP3)



- Molecule 4: PROTEIN (IMMUNOGLOBULIN LIGHT CHAIN)



- Molecule 5: PROTEIN (IMMUNOGLOBULIN HEAVY CHAIN)



- Molecule 6: PROTEIN (GH-LOOP FROM VIRUS CAPSID PROTEIN VP1)



4 Data and refinement statistics

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 30.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-30.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8279	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OCS

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	1	0.70	0/1449	1.18	16/1982 (0.8%)
2	2	0.67	0/1723	1.24	17/2352 (0.7%)
3	3	0.68	0/1739	1.30	25/2377 (1.1%)
4	4	1.59	19/1713 (1.1%)	2.50	109/2329 (4.7%)
5	A	1.34	8/1685 (0.5%)	2.62	108/2300 (4.7%)
6	5	1.05	0/168	2.26	13/232 (5.6%)
All	All	1.08	27/8477 (0.3%)	1.90	288/11572 (2.5%)

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
3	3	0	1
4	4	0	6
5	A	0	3
All	All	0	10

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	112	ARG	C-N	-28.58	0.93	1.33
5	A	206	HIS	CD2-NE2	-7.48	1.29	1.37
4	4	210	VAL	CA-CB	6.95	1.64	1.54
4	4	89	THR	CA-CB	6.89	1.63	1.53
4	4	82	VAL	CA-CB	6.85	1.63	1.53
5	A	171	HIS	CA-CB	-6.79	1.44	1.53
5	A	171	HIS	CD2-NE2	-6.56	1.30	1.37
4	4	193	HIS	CD2-NE2	-6.40	1.30	1.37
4	4	38	HIS	CD2-NE2	-6.27	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	96	CYS	CA-CB	-6.06	1.45	1.53
4	4	34	HIS	CD2-NE2	-5.95	1.31	1.37
4	4	54	ARG	NE-CZ	5.82	1.39	1.33
5	A	180	ASP	CA-C	5.77	1.60	1.52
4	4	63	PRO	CA-CB	-5.69	1.46	1.53
4	4	54	ARG	CA-CB	5.61	1.58	1.53
4	4	28	SER	CA-CB	5.59	1.62	1.53
4	4	48	PRO	CA-CB	-5.52	1.45	1.53
5	A	171	HIS	CG-ND1	-5.51	1.32	1.38
5	A	109	TYR	CA-CB	5.50	1.62	1.53
4	4	202	HIS	CD2-NE2	-5.42	1.31	1.37
4	4	39	TRP	CG-CD2	-5.24	1.34	1.43
4	4	154	ILE	CA-CB	5.18	1.61	1.54
4	4	198	CYS	CA-CB	-5.13	1.46	1.53
5	A	130	PRO	CA-CB	-5.13	1.46	1.53
4	4	38	HIS	CG-ND1	-5.11	1.32	1.38
4	4	180	SER	CA-CB	-5.11	1.45	1.53
4	4	54	ARG	CA-C	-5.00	1.47	1.53

All (288) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	120	ALA	CA-C-N	-35.38	65.92	122.87
5	A	120	ALA	C-N-CA	-35.38	65.92	122.87
4	4	112	ARG	CA-C-N	-29.25	65.67	121.54
4	4	112	ARG	C-N-CA	-29.25	65.67	121.54
5	A	120	ALA	O-C-N	16.97	152.88	122.34
5	A	188	VAL	CB-CA-C	-12.53	91.95	110.62
5	A	107	PHE	CA-CB-CG	12.09	125.89	113.80
5	A	178	GLN	N-CA-C	-11.34	92.93	109.59
5	A	182	TYR	N-CA-C	11.14	125.51	110.35
4	4	102	PHE	CA-CB-CG	10.99	124.79	113.80
4	4	112	ARG	O-C-N	10.72	135.85	123.31
6	5	149	THR	N-CA-C	-10.62	100.04	113.43
5	A	180	ASP	CA-CB-CG	10.56	123.16	112.60
2	2	137	LYS	N-CA-C	-10.21	100.56	113.23
2	2	118	GLY	N-CA-C	-9.76	99.35	112.81
5	A	62	ASP	N-CA-C	9.58	122.61	111.11
5	A	219	PRO	N-CA-C	9.49	125.28	111.13
5	A	105	GLU	N-CA-CB	-9.47	100.43	111.79
5	A	124	THR	CA-CB-OG1	-9.04	96.03	109.60
2	2	4	THR	N-CA-C	8.98	117.37	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	136	VAL	N-CA-C	-8.89	94.91	107.80
5	A	57	TYR	N-CA-C	-8.84	91.98	110.80
4	4	161	ASN	OD1-CG-ND2	-8.73	113.87	122.60
4	4	194	ASN	N-CA-C	8.69	124.49	112.93
5	A	124	THR	CB-CA-C	8.66	120.63	108.76
4	4	79	ILE	N-CA-C	-8.65	95.12	107.75
4	4	203	LYS	N-CA-C	8.58	123.17	112.87
5	A	64	VAL	N-CA-CB	-8.50	102.21	112.33
4	4	147	ASP	CA-CB-CG	8.49	121.09	112.60
5	A	187	SER	CA-C-O	-8.40	111.81	120.71
5	A	39	GLN	CA-CB-CG	-8.38	97.33	114.10
4	4	161	ASN	CB-CG-ND2	8.25	128.77	116.40
6	5	148	THR	O-C-N	8.23	132.81	123.27
3	3	159	ILE	CA-C-N	8.20	128.21	119.76
3	3	159	ILE	C-N-CA	8.20	128.21	119.76
4	4	114	ASP	CA-CB-CG	8.12	120.72	112.60
4	4	20	THR	N-CA-CB	-8.07	97.93	110.85
4	4	111	LYS	N-CA-C	-8.05	97.75	109.59
6	5	136	TYR	O-C-N	8.03	133.27	122.59
5	A	127	SER	CA-CB-OG	7.92	126.94	111.10
4	4	216	ASN	CA-CB-CG	7.86	120.46	112.60
6	5	149	THR	O-C-N	7.81	132.57	122.10
6	5	152	ALA	N-CA-C	-7.79	101.65	112.25
3	3	170	THR	N-CA-C	-7.76	102.14	111.69
5	A	188	VAL	N-CA-CB	7.72	124.82	111.39
4	4	149	ASN	OD1-CG-ND2	-7.70	114.90	122.60
4	4	31	SER	N-CA-C	-7.70	97.34	109.50
5	A	34	MET	N-CA-C	7.67	121.90	109.40
4	4	133	GLY	O-C-N	-7.63	118.08	123.95
4	4	54	ARG	N-CA-C	-7.56	92.98	108.18
4	4	96	ASN	CA-C-O	-7.49	111.80	120.49
5	A	98	ARG	CB-CG-CD	-7.46	94.13	111.30
4	4	149	ASN	CA-CB-CG	7.43	120.03	112.60
5	A	100	GLU	N-CA-CB	-7.41	97.75	111.53
3	3	188	GLN	N-CA-C	-7.38	96.52	109.06
2	2	149	ASN	CA-C-N	7.37	129.05	119.84
2	2	149	ASN	C-N-CA	7.37	129.05	119.84
5	A	177	LEU	CB-CA-C	-7.36	99.28	111.41
5	A	112	GLN	OE1-CD-NE2	-7.35	115.25	122.60
4	4	105	GLY	CA-C-O	-7.33	116.35	122.29
5	A	217	ILE	CA-C-N	7.32	129.70	123.33
5	A	217	ILE	C-N-CA	7.32	129.70	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	118	THR	CA-CB-OG1	-7.32	98.62	109.60
4	4	29	VAL	N-CA-CB	-7.29	102.86	112.26
5	A	58	THR	N-CA-CB	-7.29	99.19	110.85
4	4	110	LEU	N-CA-C	7.27	120.58	108.73
5	A	112	GLN	N-CA-CB	-7.26	99.85	110.53
4	4	36	PHE	CA-C-N	7.24	133.19	122.99
4	4	36	PHE	C-N-CA	7.24	133.19	122.99
4	4	213	PHE	CA-CB-CG	7.17	120.97	113.80
4	4	65	ARG	O-C-N	7.11	131.96	122.43
1	1	109	LYS	N-CA-C	-7.04	95.80	110.80
5	A	113	GLY	N-CA-C	6.99	120.88	111.72
3	3	31	ASN	N-CA-C	6.98	118.51	109.64
4	4	54	ARG	CA-CB-CG	6.97	128.05	114.10
5	A	178	GLN	CA-CB-CG	6.85	127.79	114.10
4	4	198	CYS	N-CA-C	-6.84	97.59	108.73
4	4	53	TYR	N-CA-C	6.83	123.20	113.02
5	A	179	SER	CA-C-O	-6.82	113.50	122.03
6	5	141	ARG	O-C-N	6.77	131.59	122.59
1	1	81	THR	N-CA-C	-6.74	96.68	108.20
3	3	54	PHE	N-CA-C	6.72	121.01	110.32
5	A	58	THR	CB-CA-C	6.72	121.67	109.37
4	4	61	GLY	N-CA-C	-6.71	97.29	113.18
5	A	203	ASN	OD1-CG-ND2	-6.69	115.91	122.60
4	4	128	GLN	OE1-CD-NE2	-6.69	115.91	122.60
5	A	3	MET	N-CA-C	6.69	119.25	107.61
2	2	160	VAL	CA-C-N	6.67	126.84	120.31
2	2	160	VAL	C-N-CA	6.67	126.84	120.31
6	5	153	ARG	N-CA-C	-6.66	96.62	110.80
4	4	57	ASN	CB-CG-ND2	6.65	126.37	116.40
4	4	62	ILE	CA-C-N	6.62	126.58	119.76
4	4	62	ILE	C-N-CA	6.62	126.58	119.76
5	A	30	ASN	CA-CB-CG	6.62	119.22	112.60
4	4	97	GLU	N-CA-C	6.61	124.88	110.80
5	A	124	THR	CA-CB-CG2	6.59	121.71	110.50
3	3	197	ASP	N-CA-C	6.58	119.78	110.23
5	A	151	GLY	O-C-N	6.58	131.25	122.70
4	4	174	ASP	CA-CB-CG	6.55	119.15	112.60
5	A	37	VAL	N-CA-C	-6.55	98.18	108.86
4	4	163	VAL	CA-C-O	6.54	127.53	120.53
5	A	56	THR	CA-C-N	6.51	133.97	121.54
5	A	56	THR	C-N-CA	6.51	133.97	121.54
3	3	189	ILE	N-CA-C	-6.50	106.22	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	26	THR	CB-CA-C	-6.47	103.41	111.43
4	4	202	HIS	CB-CG-CD2	-6.46	122.80	131.20
4	4	96	ASN	CA-CB-CG	6.45	119.05	112.60
1	1	77	GLU	N-CA-C	-6.43	98.13	109.06
4	4	214	ASN	CA-CB-CG	6.42	119.02	112.60
4	4	30	ASP	CB-CA-C	-6.41	98.95	109.53
5	A	42	GLU	CA-CB-CG	6.37	126.85	114.10
4	4	38	HIS	CB-CG-CD2	-6.36	122.93	131.20
5	A	105	GLU	CA-CB-CG	6.36	126.82	114.10
4	4	28	SER	CA-CB-OG	6.35	123.80	111.10
5	A	179	SER	O-C-N	-6.34	115.36	122.91
4	4	96	ASN	N-CA-C	-6.33	99.57	109.25
5	A	68	PHE	CA-CB-CG	6.30	120.10	113.80
4	4	63	PRO	CA-C-O	-6.29	114.17	121.34
2	2	45	GLY	CA-C-N	6.29	125.85	119.19
2	2	45	GLY	C-N-CA	6.29	125.85	119.19
4	4	195	SER	CA-CB-OG	6.26	123.63	111.10
1	1	183	ALA	N-CA-C	6.23	119.02	110.24
4	4	57	ASN	CA-CB-CG	6.22	118.82	112.60
5	A	31	ARG	CA-CB-CG	6.22	126.53	114.10
4	4	201	THR	N-CA-CB	-6.21	99.75	111.00
5	A	64	VAL	N-CA-C	-6.20	107.21	113.47
4	4	54	ARG	NE-CZ-NH1	6.17	127.67	121.50
5	A	193	SER	N-CA-C	-6.15	97.70	110.80
4	4	12	ALA	N-CA-C	-6.14	99.70	109.59
1	1	47	ASN	N-CA-C	-6.10	105.01	112.88
3	3	217	ALA	N-CA-C	-6.08	98.49	108.41
5	A	186	SER	N-CA-CB	-6.06	100.62	110.81
5	A	156	PRO	CA-N-CD	-6.05	103.03	111.50
5	A	171	HIS	CB-CG-CD2	-6.04	123.35	131.20
4	4	194	ASN	CA-CB-CG	-6.04	106.56	112.60
4	4	62	ILE	N-CA-C	-6.03	95.85	108.88
4	4	75	PHE	CA-C-O	-6.03	114.39	121.44
1	1	103	ASN	N-CA-C	-6.02	102.29	110.36
3	3	32	PRO	CA-C-N	6.02	126.96	119.98
3	3	32	PRO	C-N-CA	6.02	126.96	119.98
3	3	61	VAL	CA-C-N	6.00	127.34	119.84
3	3	61	VAL	C-N-CA	6.00	127.34	119.84
4	4	104	ALA	N-CA-C	5.99	120.20	113.01
4	4	38	HIS	CB-CG-ND1	5.99	131.68	122.70
5	A	203	ASN	CB-CG-ND2	5.99	125.38	116.40
4	4	46	GLN	N-CA-C	-5.98	102.53	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	198	ALA	N-CA-C	5.94	119.33	109.46
5	A	162	ASN	OD1-CG-ND2	-5.94	116.66	122.60
3	3	201	VAL	N-CA-C	5.94	117.03	108.48
1	1	119	TYR	N-CA-C	-5.94	101.25	110.10
4	4	87	VAL	N-CA-C	-5.94	101.88	109.30
6	5	141	ARG	NE-CZ-NH2	5.93	124.53	119.20
3	3	77	PHE	N-CA-C	5.92	117.25	108.60
2	2	51	LEU	N-CA-C	-5.92	105.37	113.30
4	4	158	GLU	CA-CB-CG	-5.87	102.37	114.10
4	4	85	ASP	CA-CB-CG	5.85	118.45	112.60
4	4	56	SER	N-CA-C	5.84	121.28	114.04
4	4	202	HIS	CB-CG-ND1	5.82	131.44	122.70
5	A	125	PRO	CB-CA-C	5.82	118.02	110.92
5	A	34	MET	O-C-N	-5.81	115.68	123.23
5	A	64	VAL	CB-CA-C	5.80	116.88	110.62
1	1	4	THR	N-CA-C	-5.79	99.08	108.41
4	4	7	SER	CA-C-O	-5.79	113.92	120.46
4	4	194	ASN	OD1-CG-ND2	-5.79	116.81	122.60
4	4	57	ASN	OD1-CG-ND2	-5.78	116.83	122.60
4	4	149	ASN	CB-CG-ND2	5.78	125.06	116.40
5	A	173	PHE	CA-C-N	5.77	127.05	119.84
5	A	173	PHE	C-N-CA	5.77	127.05	119.84
1	1	162	SER	N-CA-C	5.77	119.84	112.34
4	4	108	LEU	N-CA-C	-5.74	100.35	109.76
5	A	68	PHE	N-CA-C	5.74	119.17	109.76
5	A	180	ASP	N-CA-C	5.74	123.02	110.80
6	5	152	ALA	O-C-N	5.72	130.32	121.63
5	A	155	GLU	N-CA-C	-5.71	102.46	109.65
5	A	190	VAL	CA-CB-CG2	-5.69	100.73	110.40
2	2	175	ARG	N-CA-C	-5.68	99.54	109.48
4	4	136	VAL	CA-C-O	-5.68	114.45	120.53
5	A	77	ASN	OD1-CG-ND2	-5.67	116.92	122.60
5	A	201	THR	CA-CB-OG1	-5.66	101.11	109.60
4	4	141	ASN	CA-CB-CG	5.64	118.24	112.60
5	A	177	LEU	N-CA-CB	5.63	118.45	110.46
3	3	31	ASN	CA-C-N	-5.59	115.63	119.66
3	3	31	ASN	C-N-CA	-5.59	115.63	119.66
2	2	148	ILE	N-CA-C	-5.59	100.28	108.11
5	A	77	ASN	CA-CB-CG	5.59	118.19	112.60
4	4	139	PHE	N-CA-C	-5.59	99.91	109.24
2	2	112	VAL	N-CA-C	5.59	116.42	107.98
4	4	29	VAL	CB-CA-C	5.58	118.12	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	39	GLY	N-CA-C	5.57	122.52	114.10
5	A	93	MET	N-CA-C	-5.55	99.47	108.52
5	A	40	THR	CA-C-N	5.55	126.78	119.84
5	A	40	THR	C-N-CA	5.55	126.78	119.84
4	4	22	SER	O-C-N	-5.54	116.85	123.06
5	A	30	ASN	CA-C-N	-5.54	114.92	123.17
5	A	30	ASN	C-N-CA	-5.54	114.92	123.17
5	A	194	THR	N-CA-C	-5.54	102.29	111.37
5	A	212	LYS	N-CA-C	-5.53	100.00	109.24
4	4	99	PRO	N-CD-CG	-5.53	94.91	103.20
4	4	201	THR	CB-CA-C	5.53	120.30	109.35
6	5	135	ALA	CA-C-N	-5.52	111.00	121.54
6	5	135	ALA	C-N-CA	-5.52	111.00	121.54
4	4	66	PHE	N-CA-C	5.51	117.72	108.96
5	A	206	HIS	CA-C-N	5.51	126.72	119.84
5	A	206	HIS	C-N-CA	5.51	126.72	119.84
1	1	128	THR	N-CA-C	-5.50	106.25	113.12
3	3	30	TYR	N-CA-C	5.48	117.69	107.99
5	A	178	GLN	OE1-CD-NE2	-5.47	117.12	122.60
3	3	32	PRO	N-CA-C	-5.47	104.73	110.58
5	A	50	THR	CA-CB-OG1	-5.45	101.42	109.60
5	A	112	GLN	CB-CA-C	5.45	119.20	109.29
1	1	210	LYS	N-CA-C	5.44	117.66	111.02
4	4	34	HIS	CB-CG-CD2	-5.44	124.13	131.20
4	4	165	ASN	OD1-CG-ND2	-5.43	117.17	122.60
5	A	39	GLN	CG-CD-NE2	5.43	124.54	116.40
4	4	17	GLN	CG-CD-NE2	5.41	124.51	116.40
4	4	6	GLN	CA-C-O	-5.40	114.89	121.05
5	A	56	THR	CA-CB-OG1	-5.36	101.56	109.60
5	A	98	ARG	N-CA-C	-5.35	100.46	108.96
4	4	68	GLY	O-C-N	-5.34	118.61	123.36
5	A	17	SER	CA-C-N	5.33	130.97	121.75
5	A	17	SER	C-N-CA	5.33	130.97	121.75
5	A	58	THR	CA-CB-CG2	5.32	119.55	110.50
1	1	24	VAL	CB-CA-C	-5.32	103.94	111.38
5	A	1	GLU	CA-C-O	-5.32	111.77	120.80
5	A	71	SER	CA-CB-OG	5.31	121.73	111.10
4	4	135	SER	N-CA-C	-5.30	100.75	109.40
4	4	118	THR	N-CA-CB	-5.30	101.73	109.95
4	4	3	VAL	N-CA-CB	-5.29	104.05	111.25
5	A	29	PHE	CA-CB-CG	5.28	119.08	113.80
6	5	140	ALA	N-CA-C	-5.28	102.04	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	216	ASN	CB-CA-C	-5.27	99.29	110.31
5	A	47	TRP	CE2-CD2-CG	-5.27	100.87	107.20
3	3	154	LYS	N-CA-C	5.27	118.70	110.32
5	A	186	SER	CA-CB-OG	5.27	121.64	111.10
4	4	128	GLN	CB-CG-CD	5.27	121.56	112.60
5	A	1	GLU	N-CA-C	-5.26	96.26	111.00
4	4	20	THR	CB-CA-C	5.26	118.99	109.37
4	4	152	TRP	CE2-CD2-CG	-5.25	100.90	107.20
5	A	42	GLU	CA-C-N	5.25	129.79	122.08
5	A	42	GLU	C-N-CA	5.25	129.79	122.08
4	4	119	VAL	CA-C-O	-5.25	114.93	120.39
1	1	89	VAL	CA-C-N	5.24	125.14	119.85
1	1	89	VAL	C-N-CA	5.24	125.14	119.85
3	3	50	ALA	N-CA-C	5.23	117.06	111.36
4	4	120	SER	CA-C-O	-5.23	115.05	120.70
5	A	198	GLU	CB-CG-CD	5.22	121.48	112.60
3	3	102	THR	CA-C-N	-5.20	115.34	122.57
3	3	102	THR	C-N-CA	-5.20	115.34	122.57
2	2	177	TRP	N-CA-C	5.20	118.02	109.76
5	A	219	PRO	CA-C-N	5.20	131.05	121.70
5	A	219	PRO	C-N-CA	5.20	131.05	121.70
4	4	216	ASN	CB-CG-ND2	5.18	124.18	116.40
4	4	89	THR	CB-CA-C	5.18	118.30	109.75
1	1	56	ALA	N-CA-C	-5.18	103.56	110.55
5	A	196	PRO	N-CA-CB	5.18	108.29	102.60
4	4	188	ASP	N-CA-C	5.16	116.98	111.36
5	A	171	HIS	CB-CA-C	-5.16	101.73	110.19
5	A	132	ALA	N-CA-C	-5.15	103.65	110.40
4	4	202	HIS	CA-CB-CG	5.15	118.95	113.80
4	4	30	ASP	N-CA-CB	5.14	118.56	110.23
4	4	173	LYS	N-CA-CB	5.13	119.17	110.49
5	A	58	THR	CA-CB-OG1	-5.13	101.91	109.60
4	4	71	SER	CA-CB-OG	5.11	121.32	111.10
5	A	76	LYS	O-C-N	5.10	128.32	121.99
5	A	56	THR	N-CA-C	5.10	116.81	108.55
4	4	209	ILE	CA-CB-CG2	-5.10	101.83	110.50
5	A	5	VAL	N-CA-C	5.09	115.10	107.51
4	4	25	ALA	N-CA-C	-5.09	101.42	109.76
5	A	90	ASP	N-CA-C	5.09	119.11	113.01
4	4	40	TYR	CA-C-O	5.08	127.39	121.44
5	A	110	TRP	CE2-CD2-CG	-5.07	101.12	107.20
1	1	115	LEU	N-CA-C	5.07	116.89	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	106	GLY	O-C-N	5.07	127.08	122.88
4	4	154	ILE	CA-C-O	5.06	127.10	120.78
5	A	206	HIS	CB-CG-CD2	-5.05	124.64	131.20
5	A	128	VAL	CA-C-O	5.05	125.93	120.53
4	4	183	LEU	N-CA-C	-5.05	101.01	109.24
4	4	118	THR	CB-CA-C	5.04	118.06	109.84
5	A	165	SER	N-CA-C	5.04	119.64	111.37
4	4	77	LEU	N-CA-C	-5.04	102.06	110.17
4	4	122	PHE	CA-CB-CG	-5.02	108.78	113.80
2	2	145	HIS	N-CA-C	5.02	115.94	108.86
5	A	36	TRP	CE2-CD2-CG	-5.02	101.18	107.20
4	4	29	VAL	N-CA-C	-5.01	108.08	112.90
4	4	193	HIS	CB-CG-CD2	-5.01	124.68	131.20
6	5	142	GLY	N-CA-C	-5.01	101.32	113.18
2	2	75	PHE	N-CA-C	5.00	117.36	110.35
4	4	175	SER	N-CA-C	5.00	121.46	110.80

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	30	TYR	Sidechain
4	4	112	ARG	Mainchain
4	4	190	TYR	Sidechain
4	4	46	GLN	Peptide
4	4	80	ASP	Peptide
4	4	90	TYR	Sidechain
4	4	98	VAL	Peptide
5	A	109	TYR	Sidechain
5	A	120	ALA	Mainchain
5	A	155	GLU	Peptide

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	1	1416	0	1415	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	1680	0	1608	69	0
3	3	1690	0	1603	87	0
4	4	1683	0	1605	76	0
5	A	1644	0	1620	97	0
6	5	166	0	161	86	0
All	All	8279	0	8012	443	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 27.

All (443) 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)
5:A:13:LYS:CE	5:A:122:LYS:HE3	1.29	1.60
5:A:13:LYS:HE3	5:A:122:LYS:CE	1.49	1.41
3:3:173:HIS:CE1	6:5:141:ARG:HH22	1.42	1.37
6:5:136:TYR:O	6:5:150:THR:CG2	1.75	1.33
6:5:148:THR:HB	6:5:152:ALA:N	1.48	1.27
6:5:134:THR:CG2	6:5:147:LEU:HD22	1.65	1.27
6:5:136:TYR:C	6:5:150:THR:HG21	1.59	1.25
6:5:135:ALA:O	6:5:136:TYR:CB	1.79	1.20
5:A:119:SER:HB3	5:A:153:PHE:CZ	1.75	1.20
6:5:134:THR:CG2	6:5:147:LEU:HB3	1.72	1.19
6:5:134:THR:HG21	6:5:147:LEU:HD22	1.15	1.15
5:A:13:LYS:NZ	5:A:121:ALA:C	2.07	1.13
5:A:11:LEU:HD12	5:A:154:PRO:HD3	1.26	1.11
1:1:127:ALA:H	6:5:155:LEU:HD21	1.11	1.11
6:5:148:THR:CB	6:5:152:ALA:HB2	1.78	1.11
6:5:149:THR:HG23	6:5:154:THR:HG23	1.21	1.10
6:5:134:THR:CG2	6:5:147:LEU:CD2	2.30	1.09
6:5:133:THR:OG1	6:5:147:LEU:CA	2.01	1.09
4:4:109:ASP:CG	4:4:177:TYR:OH	1.96	1.08
6:5:134:THR:HG22	6:5:147:LEU:CD2	1.84	1.07
6:5:134:THR:HG23	6:5:147:LEU:HB3	1.35	1.07
3:3:173:HIS:CE1	6:5:141:ARG:NH2	2.22	1.06
6:5:149:THR:CG2	6:5:154:THR:HG23	1.85	1.05
6:5:136:TYR:O	6:5:150:THR:CB	2.04	1.04
5:A:119:SER:CB	5:A:153:PHE:CZ	2.41	1.03
5:A:11:LEU:HD21	5:A:121:ALA:O	1.60	1.01
1:1:127:ALA:HB3	6:5:155:LEU:HD11	1.44	0.98
4:4:58:LEU:HD22	4:4:62:ILE:HD11	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:134:THR:CG2	6:5:147:LEU:CB	2.43	0.96
6:5:133:THR:O	6:5:134:THR:O	1.83	0.95
6:5:133:THR:OG1	6:5:147:LEU:C	2.10	0.95
6:5:154:THR:O	6:5:155:LEU:HB2	1.67	0.95
6:5:136:TYR:O	6:5:150:THR:HB	1.64	0.94
2:2:48:THR:HG21	2:2:52:GLU:HB3	1.49	0.94
5:A:119:SER:HB3	5:A:153:PHE:HZ	1.32	0.94
1:1:127:ALA:N	6:5:155:LEU:HD21	1.83	0.93
6:5:149:THR:O	6:5:154:THR:OG1	1.87	0.93
6:5:134:THR:HG22	6:5:147:LEU:CB	2.00	0.92
5:A:13:LYS:CE	5:A:122:LYS:CE	2.25	0.92
6:5:148:THR:HB	6:5:152:ALA:CA	1.98	0.92
6:5:148:THR:OG1	6:5:152:ALA:HB2	1.72	0.89
4:4:112:ARG:NH2	4:4:115:ALA:HB2	1.89	0.88
1:1:127:ALA:O	6:5:155:LEU:HD22	1.73	0.88
5:A:13:LYS:NZ	5:A:122:LYS:HE3	1.89	0.88
6:5:136:TYR:N	6:5:150:THR:OG1	2.06	0.87
6:5:133:THR:OG1	6:5:148:THR:N	2.06	0.87
6:5:148:THR:CB	6:5:152:ALA:CB	2.53	0.87
3:3:78:ASP:HB3	3:3:179:CYS:SG	2.13	0.87
6:5:136:TYR:C	6:5:150:THR:CG2	2.35	0.87
6:5:152:ALA:O	6:5:153:ARG:O	1.92	0.87
1:1:127:ALA:H	6:5:155:LEU:CD2	1.87	0.86
1:1:70:THR:HG23	1:1:187:CYS:HB2	1.56	0.86
4:4:111:LYS:HA	4:4:144:TYR:CZ	2.11	0.85
6:5:136:TYR:O	6:5:150:THR:HG22	1.75	0.85
1:1:92:GLY:HA3	3:3:169:TYR:CE1	2.13	0.84
4:4:107:LYS:HE2	4:4:169:ASP:OD1	1.79	0.83
2:2:70:VAL:HG22	2:2:73:GLN:HE21	1.41	0.83
5:A:13:LYS:NZ	5:A:121:ALA:O	2.09	0.83
2:2:70:VAL:H	2:2:73:GLN:NE2	1.77	0.82
4:4:109:ASP:CB	4:4:177:TYR:OH	2.27	0.82
6:5:134:THR:HG21	6:5:147:LEU:CD2	1.99	0.82
6:5:135:ALA:O	6:5:136:TYR:HB2	1.00	0.82
4:4:112:ARG:CZ	4:4:115:ALA:HB2	2.08	0.82
5:A:13:LYS:HZ1	5:A:122:LYS:N	1.77	0.82
6:5:133:THR:OG1	6:5:147:LEU:N	2.11	0.82
3:3:86:MET:HE3	3:3:89:THR:HG21	1.62	0.81
6:5:133:THR:HG1	6:5:148:THR:N	1.79	0.81
4:4:110:LEU:HD12	4:4:175:SER:OG	1.80	0.81
6:5:152:ALA:C	6:5:153:ARG:O	2.24	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:13:LYS:HZ2	5:A:121:ALA:C	1.89	0.81
3:3:190:THR:HG22	3:3:191:HIS:H	1.45	0.80
2:2:58:ALA:HB3	2:2:208:VAL:HG21	1.63	0.80
3:3:173:HIS:NE2	6:5:141:ARG:NH2	2.28	0.79
4:4:12:ALA:HB1	4:4:144:TYR:OH	1.81	0.79
5:A:160:THR:HB	5:A:203:ASN:HB2	1.65	0.78
1:1:127:ALA:HB3	6:5:155:LEU:CD1	2.11	0.78
6:5:133:THR:HG1	6:5:148:THR:H	1.29	0.78
6:5:149:THR:HG23	6:5:154:THR:CG2	2.10	0.77
5:A:1:GLU:O	5:A:26:GLY:HA3	1.85	0.76
5:A:64:VAL:HG13	5:A:68:PHE:HB2	1.67	0.76
5:A:13:LYS:NZ	5:A:122:LYS:N	2.31	0.76
4:4:129:LEU:HD22	4:4:187:LYS:HG3	1.68	0.75
4:4:110:LEU:H	4:4:170:GLN:CD	1.94	0.75
1:1:203:GLN:HB2	1:1:204:PRO:HD2	1.69	0.75
3:3:103:GLY:HA3	3:3:209:PHE:HA	1.67	0.75
1:1:6:GLU:HG2	2:2:153:ASN:ND2	2.01	0.75
6:5:148:THR:HB	6:5:151:ALA:C	2.11	0.75
5:A:11:LEU:HG	5:A:153:PHE:HE1	1.52	0.74
3:3:219:GLN:HA	3:3:219:GLN:NE2	2.00	0.74
5:A:119:SER:CB	5:A:153:PHE:HZ	1.89	0.73
3:3:52:PRO:HB3	3:3:204:SER:HB3	1.70	0.73
4:4:110:LEU:H	4:4:170:GLN:NE2	1.85	0.73
4:4:109:ASP:OD1	4:4:177:TYR:OH	2.07	0.73
2:2:70:VAL:HG22	2:2:73:GLN:NE2	2.05	0.72
2:2:126:VAL:HG13	2:2:143:TYR:CE1	2.25	0.72
6:5:134:THR:HG22	6:5:147:LEU:HD23	1.72	0.72
6:5:133:THR:OG1	6:5:147:LEU:HA	1.88	0.71
1:1:163:PHE:CE1	6:5:156:PRO:HD2	2.25	0.71
1:1:6:GLU:HB2	2:2:30:VAL:HG21	1.73	0.71
1:1:163:PHE:CZ	6:5:156:PRO:HD2	2.26	0.70
1:1:80:VAL:HG22	1:1:176:LEU:CD1	2.20	0.70
5:A:13:LYS:HZ1	5:A:122:LYS:CA	2.06	0.69
3:3:143:ILE:HD12	3:3:143:ILE:H	1.57	0.69
4:4:112:ARG:HG3	4:4:113:ALA:O	1.93	0.69
5:A:13:LYS:HZ1	5:A:122:LYS:CB	2.05	0.69
5:A:119:SER:OG	5:A:121:ALA:HB3	1.93	0.68
4:4:164:LEU:HD21	5:A:178:GLN:HB2	1.76	0.68
4:4:110:LEU:H	4:4:170:GLN:HE22	1.41	0.68
3:3:89:THR:HG23	3:3:92:ALA:H	1.58	0.67
6:5:148:THR:CB	6:5:152:ALA:CA	2.72	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:120:ALA:O	5:A:122:LYS:NZ	2.27	0.67
6:5:133:THR:HG1	6:5:147:LEU:N	1.92	0.67
3:3:190:THR:HG22	3:3:191:HIS:N	2.10	0.66
6:5:134:THR:CG2	6:5:147:LEU:CG	2.73	0.66
3:3:64:VAL:HG11	3:3:74:LEU:HB3	1.78	0.66
2:2:67:PHE:HB3	2:2:79:HIS:HD2	1.60	0.66
5:A:126:PRO:HD2	5:A:211:THR:HG21	1.78	0.66
4:4:128:GLN:HG3	5:A:129:TYR:CE2	2.31	0.66
1:1:97:ALA:HB2	3:3:217:ALA:HB2	1.78	0.66
4:4:129:LEU:HD23	4:4:133:GLY:O	1.96	0.66
4:4:111:LYS:HA	4:4:144:TYR:CE1	2.31	0.65
3:3:13:ASN:H	3:3:13:ASN:ND2	1.93	0.65
2:2:107:VAL:HG21	2:2:125:LEU:HD21	1.78	0.65
3:3:44:TYR:O	3:3:47:VAL:HG22	1.96	0.65
6:5:148:THR:HB	6:5:152:ALA:CB	2.22	0.65
1:1:114:ARG:O	1:1:115:LEU:HD23	1.97	0.65
5:A:191:PRO:HG2	5:A:194:THR:OG1	1.96	0.65
6:5:134:THR:HG22	6:5:147:LEU:CG	2.26	0.64
4:4:110:LEU:N	4:4:170:GLN:HE22	1.95	0.64
1:1:182:ARG:HH11	1:1:182:ARG:HG2	1.62	0.64
2:2:3:LYS:CB	2:2:12:ASP:HB2	2.28	0.64
2:2:70:VAL:O	2:2:73:GLN:HG2	1.98	0.64
4:4:58:LEU:HD21	4:4:66:PHE:O	1.98	0.64
4:4:196:TYR:HB2	4:4:213:PHE:CE1	2.34	0.63
1:1:122:PRO:HB3	3:3:100:GLN:HE21	1.63	0.63
5:A:13:LYS:HE3	5:A:122:LYS:HE3	0.64	0.63
3:3:78:ASP:CB	3:3:179:CYS:SG	2.84	0.63
6:5:154:THR:O	6:5:155:LEU:CB	2.42	0.63
1:1:107:TYR:HB2	3:3:14:MET:HB3	1.82	0.62
1:1:70:THR:HB	1:1:189:ARG:NH1	2.14	0.62
3:3:67:ARG:HE	3:3:72:ARG:NE	1.97	0.62
3:3:86:MET:O	3:3:88:ASN:N	2.32	0.62
6:5:136:TYR:CA	6:5:150:THR:HG21	2.30	0.62
1:1:89:VAL:HG13	1:1:93:ALA:HB3	1.81	0.62
1:1:182:ARG:HH11	1:1:182:ARG:CG	2.13	0.61
4:4:110:LEU:N	4:4:170:GLN:OE1	2.33	0.61
1:1:89:VAL:CG1	1:1:93:ALA:HB3	2.29	0.61
2:2:85:HIS:O	2:2:87:PRO:HD3	2.00	0.61
2:2:160:VAL:HG22	2:2:161:PRO:HD2	1.83	0.61
5:A:119:SER:OG	5:A:121:ALA:CB	2.48	0.61
1:1:86:LEU:HD12	1:1:87:THR:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:133:THR:C	6:5:134:THR:O	2.44	0.61
1:1:86:LEU:HD11	1:1:168:VAL:HG13	1.82	0.61
4:4:54:ARG:HB2	4:4:57:ASN:HD21	1.66	0.60
4:4:90:TYR:O	4:4:105:GLY:HA2	2.01	0.60
5:A:13:LYS:NZ	5:A:122:LYS:CA	2.65	0.60
1:1:196:PRO:HB3	1:1:201:HIS:HB2	1.84	0.60
4:4:109:ASP:HB3	4:4:177:TYR:OH	2.00	0.60
4:4:110:LEU:HB2	4:4:175:SER:HB3	1.84	0.60
3:3:191:HIS:CG	3:3:194:ALA:HB3	2.37	0.59
5:A:13:LYS:HD3	5:A:120:ALA:HA	1.83	0.59
2:2:70:VAL:H	2:2:73:GLN:HE21	1.46	0.59
1:1:122:PRO:HB3	3:3:100:GLN:NE2	2.17	0.59
6:5:149:THR:HG22	6:5:154:THR:HG23	1.83	0.59
3:3:185:CYS:HB2	3:3:187:TYR:CE1	2.38	0.59
4:4:111:LYS:HA	4:4:144:TYR:OH	2.02	0.59
1:1:70:THR:HG22	1:1:189:ARG:HG2	1.84	0.59
5:A:119:SER:HB3	5:A:153:PHE:CE1	2.34	0.59
3:3:187:TYR:N	3:3:187:TYR:CD1	2.70	0.59
6:5:134:THR:HG22	6:5:147:LEU:CA	2.33	0.59
3:3:78:ASP:HB3	3:3:179:CYS:HG	1.67	0.58
4:4:153:LYS:HB2	4:4:197:THR:HB	1.85	0.58
3:3:78:ASP:OD2	3:3:179:CYS:SG	2.62	0.58
3:3:195:ASP:O	3:3:196:ALA:HB3	2.02	0.58
5:A:128:VAL:HG21	5:A:204:VAL:HG11	1.85	0.58
3:3:63:TYR:HA	3:3:200:VAL:HA	1.84	0.58
5:A:13:LYS:CD	5:A:122:LYS:HE3	2.25	0.58
6:5:133:THR:O	6:5:133:THR:HG23	2.04	0.57
3:3:212:ARG:HD3	3:3:213:LEU:HD22	1.86	0.57
5:A:11:LEU:CG	5:A:153:PHE:HE1	2.17	0.57
1:1:92:GLY:HA3	3:3:169:TYR:HE1	1.66	0.57
4:4:4:LEU:HD23	4:4:25:ALA:HA	1.85	0.57
5:A:13:LYS:NZ	5:A:122:LYS:HB3	2.20	0.57
3:3:14:MET:HG3	3:3:15:VAL:N	2.18	0.57
5:A:11:LEU:HD11	5:A:122:LYS:HA	1.86	0.57
2:2:101:MET:HE2	2:2:171:TYR:CE2	2.38	0.57
6:5:133:THR:OG1	6:5:146:HIS:C	2.47	0.57
6:5:149:THR:HA	6:5:154:THR:HA	1.87	0.57
4:4:140:LEU:HD13	4:4:179:MET:HE3	1.85	0.56
4:4:189:GLU:HA	4:4:192:ARG:HD3	1.88	0.56
5:A:11:LEU:HG	5:A:153:PHE:CE1	2.37	0.56
3:3:94:LEU:HD12	3:3:211:LEU:HD23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:135:ASN:N	3:3:135:ASN:HD22	2.04	0.56
4:4:12:ALA:HA	4:4:109:ASP:O	2.05	0.56
3:3:102:THR:HA	3:3:161:TYR:CE2	2.40	0.56
1:1:78:ILE:HG22	1:1:178:VAL:HG12	1.88	0.56
2:2:126:VAL:HG13	2:2:143:TYR:CD1	2.41	0.55
6:5:151:ALA:C	6:5:153:ARG:H	2.14	0.55
1:1:61:ILE:HG23	1:1:62:VAL:N	2.21	0.55
2:2:114:ASN:ND2	2:2:116:PHE:H	2.04	0.55
1:1:73:PHE:CD1	1:1:73:PHE:C	2.85	0.55
3:3:102:THR:HA	3:3:161:TYR:CD2	2.41	0.55
3:3:120:ARG:HH11	3:3:146:GLU:HG2	1.72	0.55
1:1:129:ALA:O	1:1:130:TYR:HB2	2.07	0.54
4:4:10:SER:HA	4:4:107:LYS:O	2.08	0.54
4:4:185:LEU:HD23	4:4:189:GLU:HG3	1.89	0.54
5:A:215:LYS:HZ2	5:A:215:LYS:HB3	1.71	0.54
2:2:70:VAL:N	2:2:73:GLN:NE2	2.53	0.54
5:A:22:CYS:HB3	5:A:79:LEU:HB3	1.88	0.54
3:3:121:TYR:CE2	3:3:199:LEU:HD22	2.43	0.54
4:4:31:SER:HB2	4:4:96:ASN:OD1	2.07	0.54
3:3:93:GLY:O	3:3:96:GLN:HG2	2.08	0.54
1:1:89:VAL:HG13	1:1:93:ALA:CB	2.38	0.53
3:3:161:TYR:CE1	3:3:163:SER:HB3	2.42	0.53
5:A:142:MET:HB3	5:A:189:THR:CG2	2.38	0.53
1:1:105:THR:O	3:3:15:VAL:HA	2.09	0.53
2:2:115:GLN:HE21	2:2:115:GLN:N	2.07	0.53
4:4:168:THR:HG23	5:A:173:PHE:CD1	2.43	0.53
5:A:13:LYS:CE	5:A:122:LYS:HB3	2.38	0.53
3:3:135:ASN:HD22	3:3:135:ASN:H	1.54	0.53
3:3:161:TYR:CD1	3:3:161:TYR:C	2.86	0.53
1:1:92:GLY:CA	3:3:169:TYR:CE1	2.89	0.53
3:3:167:TYR:CE2	3:3:212:ARG:HG2	2.43	0.53
5:A:13:LYS:NZ	5:A:122:LYS:CE	2.64	0.53
5:A:60:TYR:OH	5:A:69:THR:HA	2.09	0.53
2:2:54:ARG:HE	2:2:56:HIS:CD2	2.27	0.52
2:2:58:ALA:CB	2:2:208:VAL:HG21	2.37	0.52
4:4:53:TYR:CE1	5:A:105:GLU:HG3	2.44	0.52
5:A:119:SER:O	5:A:121:ALA:O	2.26	0.52
1:1:86:LEU:CD1	1:1:168:VAL:HG13	2.39	0.52
3:3:191:HIS:HB2	3:3:194:ALA:HB3	1.91	0.52
5:A:40:THR:HG23	5:A:44:ARG:O	2.08	0.52
6:5:133:THR:HG21	6:5:148:THR:C	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:6:GLU:CD	5:A:113:GLY:H	2.18	0.52
3:3:97:TYR:O	3:3:214:PRO:HA	2.10	0.52
5:A:11:LEU:HD11	5:A:153:PHE:CD1	2.45	0.52
5:A:11:LEU:CD1	5:A:122:LYS:HA	2.40	0.52
3:3:107:LEU:HD23	3:3:159:ILE:HD11	1.91	0.51
6:5:148:THR:OG1	6:5:152:ALA:CB	2.51	0.51
2:2:26:THR:HG22	2:2:28:SER:H	1.76	0.51
6:5:135:ALA:O	6:5:136:TYR:CG	2.57	0.51
1:1:130:TYR:CD1	6:5:155:LEU:HD12	2.46	0.51
5:A:54:GLY:HA2	5:A:72:ARG:HD3	1.91	0.51
1:1:6:GLU:HG2	2:2:153:ASN:HD21	1.75	0.51
3:3:79:VAL:HG23	3:3:183:TRP:HA	1.91	0.51
5:A:13:LYS:HZ2	5:A:120:ALA:C	2.19	0.51
1:1:73:PHE:CD1	1:1:74:SER:N	2.79	0.51
2:2:162:TYR:CD1	2:2:162:TYR:C	2.89	0.51
5:A:13:LYS:HZ1	5:A:122:LYS:HB3	1.73	0.51
2:2:118:GLY:H	2:2:188:THR:HB	1.76	0.51
2:2:64:MET:O	2:2:64:MET:HG3	2.10	0.51
3:3:73:LEU:HD21	3:3:76:LYS:HB3	1.92	0.51
5:A:94:TYR:O	5:A:113:GLY:HA2	2.11	0.51
3:3:89:THR:CG2	3:3:92:ALA:H	2.24	0.50
3:3:89:THR:HG22	3:3:92:ALA:CB	2.41	0.50
3:3:89:THR:HG22	3:3:92:ALA:HB3	1.92	0.50
3:3:212:ARG:O	3:3:213:LEU:HB2	2.11	0.50
1:1:82:HIS:CE1	1:1:86:LEU:HB2	2.46	0.50
5:A:41:PRO:C	5:A:43:LYS:H	2.20	0.50
2:2:48:THR:C	2:2:50:ALA:N	2.69	0.50
2:2:115:GLN:H	2:2:115:GLN:NE2	2.08	0.50
3:3:168:THR:HG22	3:3:169:TYR:N	2.27	0.50
2:2:166:ASN:HD22	3:3:165:ALA:HA	1.77	0.50
4:4:16:GLY:HA2	4:4:81:PRO:HB2	1.93	0.50
6:5:133:THR:HG21	6:5:148:THR:O	2.11	0.50
5:A:33:ALA:HB3	5:A:100:GLU:HB3	1.92	0.50
6:5:133:THR:O	6:5:134:THR:C	2.55	0.49
2:2:114:ASN:HD21	2:2:116:PHE:HB2	1.77	0.49
5:A:156:PRO:O	5:A:206:HIS:HD2	1.95	0.49
2:2:12:ASP:O	2:2:13:ARG:HB2	2.12	0.49
2:2:48:THR:O	2:2:48:THR:HG22	2.13	0.49
2:2:214:LEU:HB3	2:2:215:PRO:HD2	1.94	0.49
4:4:94:GLN:NE2	4:4:96:ASN:O	2.44	0.49
6:5:148:THR:C	6:5:152:ALA:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:110:LEU:O	4:4:144:TYR:CE2	2.66	0.49
3:3:102:THR:HG22	3:3:103:GLY:N	2.28	0.49
4:4:4:LEU:HA	4:4:24:ARG:O	2.12	0.49
1:1:86:LEU:HD12	1:1:86:LEU:C	2.37	0.48
3:3:43:ASN:HD21	3:3:45:LEU:HB2	1.78	0.48
4:4:163:VAL:HA	4:4:182:THR:O	2.12	0.48
4:4:155:ASP:OD1	4:4:193:HIS:HB3	2.14	0.48
5:A:58:THR:HG22	5:A:60:TYR:HE1	1.78	0.48
5:A:194:THR:O	5:A:198:GLU:HB2	2.13	0.48
1:1:80:VAL:HG21	1:1:86:LEU:HD21	1.96	0.48
3:3:219:GLN:HA	3:3:219:GLN:HE21	1.76	0.48
4:4:34:HIS:HB2	4:4:36:PHE:CE1	2.48	0.48
4:4:109:ASP:OD1	4:4:177:TYR:CE1	2.67	0.48
4:4:58:LEU:HD22	4:4:62:ILE:CD1	2.31	0.48
3:3:67:ARG:HH21	3:3:72:ARG:HD3	1.78	0.48
5:A:13:LYS:NZ	5:A:122:LYS:CB	2.75	0.48
2:2:126:VAL:HG13	2:2:127:PRO:HD2	1.95	0.47
1:1:7:SER:O	1:1:8:ALA:HB3	2.13	0.47
1:1:127:ALA:CA	6:5:155:LEU:HD21	2.45	0.47
1:1:130:TYR:CE2	2:2:174:HIS:HD2	2.32	0.47
5:A:59:TYR:CE2	6:5:143:ASP:HA	2.49	0.47
2:2:70:VAL:HG23	2:2:72:SER:H	1.78	0.47
6:5:134:THR:HG22	6:5:147:LEU:HA	1.95	0.47
4:4:14:SER:HB2	4:4:17:GLN:HG3	1.97	0.47
1:1:130:TYR:CZ	2:2:174:HIS:CD2	3.03	0.47
2:2:78:MET:HE3	2:2:80:LYS:HE2	1.97	0.47
3:3:190:THR:CG2	3:3:191:HIS:H	2.22	0.47
3:3:195:ASP:O	3:3:196:ALA:CB	2.62	0.47
5:A:128:VAL:CG2	5:A:204:VAL:HG11	2.44	0.47
3:3:56:MET:HE3	3:3:88:ASN:HD21	1.80	0.47
1:1:182:ARG:HH11	1:1:182:ARG:HB3	1.80	0.47
5:A:11:LEU:CD1	5:A:123:THR:H	2.28	0.47
1:1:69:ALA:C	1:1:189:ARG:HG3	2.40	0.47
5:A:87:ARG:HG3	5:A:89:ALA:HB3	1.96	0.46
3:3:104:THR:HG23	3:3:158:SER:HB3	1.97	0.46
3:3:104:THR:CG2	3:3:158:SER:HB3	2.45	0.46
2:2:120:CYS:O	2:2:184:VAL:HG22	2.16	0.46
4:4:160:GLN:HG2	4:4:161:ASN:ND2	2.30	0.46
5:A:87:ARG:HD2	5:A:88:SER:N	2.31	0.46
5:A:117:THR:HG22	5:A:153:PHE:CZ	2.50	0.46
1:1:90:PRO:HG2	3:3:99:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:166:ASN:ND2	3:3:165:ALA:HA	2.30	0.46
3:3:190:THR:CG2	3:3:191:HIS:N	2.79	0.46
1:1:36:LEU:HD11	1:1:185:LEU:HD11	1.97	0.46
1:1:49:HIS:CE1	1:1:55:GLN:HE22	2.34	0.46
2:2:115:GLN:N	2:2:115:GLN:NE2	2.64	0.46
2:2:118:GLY:N	2:2:188:THR:HB	2.31	0.46
3:3:129:GLY:O	3:3:130:MET:HE3	2.15	0.46
5:A:199:THR:HG22	5:A:216:LYS:NZ	2.30	0.46
2:2:62:PHE:CD1	2:2:62:PHE:C	2.94	0.46
3:3:123:VAL:HG12	3:3:147:TRP:HZ3	1.81	0.46
3:3:168:THR:HG22	3:3:169:TYR:H	1.81	0.46
4:4:196:TYR:N	4:4:196:TYR:CD1	2.84	0.46
2:2:33:THR:HB	2:2:158:ILE:HG12	1.96	0.46
3:3:211:LEU:HD12	3:3:211:LEU:HA	1.81	0.46
4:4:25:ALA:O	4:4:73:THR:HG23	2.15	0.45
5:A:11:LEU:HD13	5:A:123:THR:H	1.81	0.45
2:2:132:ILE:HD13	2:2:137:LYS:HG2	1.98	0.45
4:4:109:ASP:HA	4:4:170:GLN:OE1	2.16	0.45
5:A:195:TRP:CG	5:A:196:PRO:HA	2.52	0.45
1:1:127:ALA:HB3	1:1:163:PHE:HE2	1.79	0.45
2:2:61:PHE:HA	2:2:203:ILE:O	2.16	0.45
4:4:138:CYS:HB3	4:4:181:SER:HB3	1.99	0.45
5:A:211:THR:HG23	5:A:213:VAL:HG23	1.98	0.45
4:4:152:TRP:O	4:4:153:LYS:HD2	2.17	0.45
6:5:151:ALA:C	6:5:153:ARG:N	2.73	0.45
6:5:155:LEU:O	6:5:156:PRO:O	2.35	0.45
5:A:83:MET:HE1	5:A:116:VAL:HG21	1.99	0.45
5:A:87:ARG:O	5:A:90:ASP:HB2	2.16	0.45
1:1:130:TYR:CE2	2:2:174:HIS:CD2	3.05	0.44
2:2:54:ARG:NH1	2:2:207:ASN:HA	2.32	0.44
5:A:54:GLY:H	5:A:72:ARG:NH1	2.16	0.44
3:3:77:PHE:O	3:3:183:TRP:HB3	2.17	0.44
5:A:143:VAL:HG21	5:A:192:SER:HB2	1.99	0.44
6:5:135:ALA:O	6:5:136:TYR:CD1	2.70	0.44
2:2:171:TYR:C	2:2:173:GLN:H	2.26	0.44
1:1:77:GLU:HB3	1:1:179:ARG:HB3	1.99	0.44
1:1:25:GLN:H	1:1:25:GLN:NE2	2.16	0.44
2:2:91:TYR:CE1	2:2:101:MET:HE1	2.52	0.44
6:5:140:ALA:HA	6:5:145:ALA:HB1	2.00	0.44
2:2:70:VAL:N	2:2:73:GLN:HE21	2.15	0.44
3:3:56:MET:HE2	3:3:59:ASN:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:73:GLN:OE1	2:2:77:HIS:CE1	2.71	0.44
4:4:48:PRO:HD2	5:A:110:TRP:CE3	2.53	0.44
1:1:61:ILE:CG2	1:1:62:VAL:N	2.81	0.43
3:3:15:VAL:HG12	3:3:17:THR:H	1.82	0.43
4:4:211:LYS:HA	4:4:211:LYS:HD2	1.65	0.43
4:4:128:GLN:OE1	4:4:135:SER:N	2.51	0.43
1:1:98:LEU:HG	1:1:169:LYS:HB2	1.99	0.43
4:4:46:GLN:HA	4:4:47:PRO:HD2	1.86	0.43
1:1:163:PHE:HB2	6:5:155:LEU:HB3	1.98	0.43
5:A:142:MET:HB3	5:A:189:THR:HG22	1.99	0.43
1:1:197:THR:HG23	1:1:198:GLY:H	1.83	0.43
2:2:188:THR:HG22	2:2:190:ASN:ND2	2.33	0.43
3:3:74:LEU:HD11	3:3:188:GLN:HB2	2.00	0.43
3:3:100:GLN:HA	3:3:168:THR:O	2.19	0.43
4:4:187:LYS:HG2	4:4:191:GLU:OE1	2.17	0.43
5:A:119:SER:HB2	5:A:153:PHE:CZ	2.45	0.43
1:1:6:GLU:CD	1:1:6:GLU:H	2.26	0.43
4:4:21:ILE:HG23	4:4:106:THR:HG21	2.00	0.43
1:1:80:VAL:HG22	1:1:176:LEU:HD11	1.98	0.43
4:4:36:PHE:HB2	4:4:96:ASN:HB2	2.00	0.43
1:1:129:ALA:HB3	1:1:189:ARG:NH1	2.34	0.43
2:2:214:LEU:HD23	3:3:127:PRO:HG2	1.99	0.43
1:1:61:ILE:HG23	1:1:62:VAL:HG23	2.01	0.43
5:A:21:SER:HB3	5:A:78:THR:CG2	2.49	0.43
3:3:191:HIS:C	3:3:191:HIS:CD2	2.97	0.42
1:1:103:ASN:O	1:1:105:THR:N	2.52	0.42
5:A:11:LEU:HD11	5:A:153:PHE:HD1	1.84	0.42
5:A:67:ARG:HB3	5:A:84:SER:O	2.19	0.42
2:2:118:GLY:CA	2:2:188:THR:HB	2.49	0.42
6:5:143:ASP:OD1	6:5:143:ASP:N	2.49	0.42
6:5:145:ALA:HA	6:5:148:THR:OG1	2.20	0.42
2:2:69:TRP:CE2	2:2:187:LEU:HB2	2.54	0.42
4:4:53:TYR:CD1	5:A:105:GLU:HG3	2.55	0.42
1:1:104:PRO:HG3	3:3:17:THR:HG21	2.02	0.42
2:2:217:LYS:HE2	2:2:217:LYS:HB3	1.81	0.42
5:A:130:PRO:HG3	5:A:215:LYS:HB3	2.02	0.42
6:5:149:THR:C	6:5:151:ALA:N	2.72	0.42
1:1:14:THR:HB	1:1:16:GLU:OE1	2.19	0.42
2:2:173:GLN:O	2:2:174:HIS:HB2	2.20	0.42
4:4:110:LEU:CA	4:4:170:GLN:HE22	2.32	0.42
5:A:60:TYR:HB2	5:A:65:LYS:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:202:CYS:O	5:A:214:ASP:HA	2.19	0.42
6:5:155:LEU:HD12	6:5:155:LEU:HA	1.81	0.42
3:3:161:TYR:C	3:3:161:TYR:HD1	2.28	0.41
4:4:76:THR:HG22	4:4:77:LEU:O	2.20	0.41
5:A:123:THR:HA	5:A:153:PHE:O	2.20	0.41
5:A:195:TRP:CH2	5:A:219:PRO:HB3	2.55	0.41
6:5:136:TYR:N	6:5:150:THR:CB	2.83	0.41
4:4:65:ARG:HD2	4:4:81:PRO:HD2	2.02	0.41
5:A:13:LYS:HE3	5:A:122:LYS:CD	2.37	0.41
2:2:137:LYS:O	2:2:140:LEU:HB2	2.20	0.41
4:4:129:LEU:O	4:4:187:LYS:HD3	2.21	0.41
5:A:58:THR:CG2	5:A:60:TYR:HE1	2.33	0.41
2:2:48:THR:O	2:2:50:ALA:N	2.52	0.41
2:2:101:MET:HE2	2:2:171:TYR:HE2	1.83	0.41
4:4:109:ASP:OD1	4:4:177:TYR:CZ	2.73	0.41
5:A:13:LYS:HZ1	5:A:122:LYS:CE	2.33	0.41
5:A:29:PHE:HE1	5:A:34:MET:HE2	1.86	0.41
1:1:192:LEU:HD21	2:2:136:GLU:HB3	2.03	0.41
3:3:111:PHE:CZ	3:3:113:GLY:HA3	2.55	0.41
3:3:112:THR:HB	3:3:198:ALA:O	2.20	0.41
4:4:39:TRP:HB2	4:4:52:ILE:HB	2.03	0.41
1:1:186:TYR:CD1	1:1:186:TYR:N	2.88	0.41
2:2:67:PHE:HB3	2:2:79:HIS:CD2	2.49	0.41
1:1:182:ARG:HH11	1:1:182:ARG:CB	2.34	0.41
2:2:54:ARG:HB2	2:2:209:HIS:NE2	2.36	0.41
2:2:82:VAL:HB	2:2:175:ARG:NH1	2.36	0.41
3:3:17:THR:O	3:3:17:THR:HG23	2.21	0.41
4:4:2:ILE:O	4:4:101:THR:HG21	2.20	0.41
4:4:87:VAL:O	4:4:88:ALA:HB2	2.20	0.41
4:4:193:HIS:O	4:4:215:ARG:HD3	2.21	0.41
5:A:129:TYR:HD2	5:A:148:LEU:HD23	1.85	0.41
4:4:42:GLN:HE22	5:A:39:GLN:NE2	2.19	0.41
4:4:189:GLU:HA	4:4:192:ARG:HB2	2.01	0.41
2:2:45:GLY:HA3	2:2:167:ARG:HE	1.85	0.40
2:2:48:THR:HB	2:2:52:GLU:OE1	2.21	0.40
4:4:46:GLN:HB3	4:4:47:PRO:O	2.21	0.40
6:5:140:ALA:HB2	6:5:152:ALA:C	2.47	0.40
3:3:143:ILE:HD12	3:3:143:ILE:N	2.31	0.40
4:4:18:ARG:HH21	4:4:78:THR:HG21	1.86	0.40
5:A:3:MET:HB3	5:A:25:SER:HB2	2.02	0.40
5:A:28:ILE:CG2	5:A:31:ARG:HG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:54:ARG:HB2	2:2:209:HIS:CD2	2.56	0.40
4:4:159:ARG:HG2	4:4:183:LEU:HD21	2.03	0.40
5:A:19:LYS:HD3	5:A:80:TYR:HD2	1.86	0.40
5:A:119:SER:HB2	5:A:153:PHE:HZ	1.77	0.40
3:3:190:THR:O	3:3:191:HIS:HB3	2.22	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 PDB entries followed by that with respect to all EM entries.

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	1	179/207 (86%)	154 (86%)	17 (10%)	8 (4%)	2	17
2	2	216/218 (99%)	177 (82%)	29 (13%)	10 (5%)	2	17
3	3	217/219 (99%)	182 (84%)	25 (12%)	10 (5%)	2	17
4	4	216/218 (99%)	185 (86%)	21 (10%)	10 (5%)	2	17
5	A	218/220 (99%)	187 (86%)	24 (11%)	7 (3%)	3	21
6	5	22/24 (92%)	12 (54%)	5 (23%)	5 (23%)	0	1
All	All	1068/1106 (97%)	897 (84%)	121 (11%)	50 (5%)	3	16

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	6	GLU
2	2	35	GLY
2	2	174	HIS
3	3	87	SER
3	3	219	GLN
4	4	60	SER
4	4	113	ALA

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Mol	Chain	Res	Type
4	4	173	LYS
5	A	53	SER
5	A	156	PRO
5	A	193	SER
6	5	134	THR
6	5	136	TYR
6	5	151	ALA
6	5	153	ARG
2	2	49	SER
2	2	173	GLN
3	3	14	MET
3	3	59	ASN
3	3	71	GLN
4	4	175	SER
5	A	123	THR
5	A	151	GLY
5	A	180	ASP
1	1	193	PRO
4	4	72	ARG
5	A	91	THR
1	1	104	PRO
1	1	130	TYR
1	1	187	CYS
2	2	85	HIS
2	2	190	ASN
3	3	196	ALA
6	5	155	LEU
1	1	111	PRO
2	2	131	ASP
2	2	176	PRO
3	3	15	VAL
3	3	83	ALA
4	4	97	GLU
1	1	61	ILE
3	3	24	PRO
3	3	180	VAL
4	4	81	PRO
1	1	32	VAL
4	4	99	PRO
1	1	122	PRO
2	2	87	PRO
4	4	61	GLY

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Mol	Chain	Res	Type
4	4	154	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 PDB entries followed by that with respect to all EM entries.

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	1	154/173 (89%)	126 (82%)	28 (18%)	2	9
2	2	177/187 (95%)	138 (78%)	39 (22%)	1	6
3	3	177/177 (100%)	138 (78%)	39 (22%)	1	6
4	4	192/192 (100%)	162 (84%)	30 (16%)	2	12
5	A	183/183 (100%)	149 (81%)	34 (19%)	1	8
6	5	16/17 (94%)	12 (75%)	4 (25%)	0	4
All	All	899/929 (97%)	725 (81%)	174 (19%)	3	7

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	2	THR
1	1	3	THR
1	1	4	THR
1	1	24	VAL
1	1	25	GLN
1	1	27	ARG
1	1	30	THR
1	1	42	VAL
1	1	43	THR
1	1	70	THR
1	1	81	THR
1	1	86	LEU
1	1	89	VAL
1	1	98	LEU
1	1	101	THR
1	1	122	PRO
1	1	128	THR

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Mol	Chain	Res	Type
1	1	131	THR
1	1	168	VAL
1	1	169	LYS
1	1	172	THR
1	1	179	ARG
1	1	182	ARG
1	1	189	ARG
1	1	191	ILE
1	1	197	THR
1	1	205	LEU
1	1	210	LYS
2	2	12	ASP
2	2	23	THR
2	2	32	VAL
2	2	38	THR
2	2	43	THR
2	2	49	SER
2	2	53	THR
2	2	55	VAL
2	2	63	LYS
2	2	66	LEU
2	2	70	VAL
2	2	81	VAL
2	2	90	VAL
2	2	94	LEU
2	2	97	SER
2	2	102	ARG
2	2	107	VAL
2	2	112	VAL
2	2	114	ASN
2	2	115	GLN
2	2	120	CYS
2	2	123	VAL
2	2	131	ASP
2	2	132	ILE
2	2	133	SER
2	2	134	ASP
2	2	149	ASN
2	2	154	MET
2	2	155	THR
2	2	160	VAL
2	2	162	TYR

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Mol	Chain	Res	Type
2	2	169	ASP
2	2	170	GLN
2	2	172	LYS
2	2	175	ARG
2	2	180	VAL
2	2	191	THR
2	2	196	GLN
2	2	197	ILE
3	3	13	ASN
3	3	17	THR
3	3	35	THR
3	3	42	THR
3	3	45	LEU
3	3	53	THR
3	3	56	MET
3	3	58	GLU
3	3	59	ASN
3	3	69	ASP
3	3	76	LYS
3	3	78	ASP
3	3	89	THR
3	3	100	GLN
3	3	107	LEU
3	3	112	THR
3	3	130	MET
3	3	135	ASN
3	3	137	GLU
3	3	151	LEU
3	3	153	SER
3	3	161	TYR
3	3	177	THR
3	3	179	CYS
3	3	180	VAL
3	3	183	TRP
3	3	184	VAL
3	3	185	CYS
3	3	186	VAL
3	3	187	TYR
3	3	191	HIS
3	3	200	VAL
3	3	201	VAL
3	3	207	LYS

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Mol	Chain	Res	Type
3	3	211	LEU
3	3	212	ARG
3	3	213	LEU
3	3	218	ARG
3	3	219	GLN
4	4	11	LEU
4	4	14	SER
4	4	20	THR
4	4	22	SER
4	4	29	VAL
4	4	43	LYS
4	4	46	GLN
4	4	57	ASN
4	4	62	ILE
4	4	77	LEU
4	4	85	ASP
4	4	94	GLN
4	4	101	THR
4	4	118	THR
4	4	126	SER
4	4	135	SER
4	4	137	VAL
4	4	154	ILE
4	4	158	GLU
4	4	160	GLN
4	4	169	ASP
4	4	173	LYS
4	4	183	LEU
4	4	194	ASN
4	4	203	LYS
4	4	204	THR
4	4	207	SER
4	4	210	VAL
4	4	211	LYS
4	4	213	PHE
5	A	4	LEU
5	A	6	GLU
5	A	7	SER
5	A	12	VAL
5	A	14	PRO
5	A	20	LEU
5	A	21	SER

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Mol	Chain	Res	Type
5	A	25	SER
5	A	40	THR
5	A	41	PRO
5	A	53	SER
5	A	56	THR
5	A	58	THR
5	A	64	VAL
5	A	69	THR
5	A	71	SER
5	A	76	LYS
5	A	86	LEU
5	A	88	SER
5	A	112	GLN
5	A	114	THR
5	A	122	LYS
5	A	124	THR
5	A	131	LEU
5	A	135	SER
5	A	147	CYS
5	A	167	SER
5	A	188	VAL
5	A	190	VAL
5	A	204	VAL
5	A	207	PRO
5	A	211	THR
5	A	215	LYS
5	A	218	VAL
6	5	139	SER
6	5	143	ASP
6	5	148	THR
6	5	155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	17	ASN
1	1	25	GLN
1	1	55	GLN
1	1	82	HIS
1	1	99	ASN
1	1	108	HIS
2	2	19	ASN

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Mol	Chain	Res	Type
2	2	56	HIS
2	2	73	GLN
2	2	114	ASN
2	2	115	GLN
2	2	117	ASN
2	2	149	ASN
2	2	153	ASN
2	2	166	ASN
2	2	190	ASN
3	3	13	ASN
3	3	43	ASN
3	3	88	ASN
3	3	100	GLN
3	3	135	ASN
3	3	152	ASN
3	3	191	HIS
3	3	219	GLN
4	4	17	GLN
4	4	38	HIS
4	4	57	ASN
4	4	161	ASN
4	4	194	ASN
4	4	216	ASN
5	A	39	GLN
5	A	77	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OCS	4	218	4	5,6,9	4.00	2 (40%)	3,7,13	3.65	2 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OCS	4	218	4	-	4/6/6/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	218	OCS	CB-CA	8.43	1.62	1.53
4	4	218	OCS	CB-SG	2.12	1.85	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	218	OCS	CB-CA-C	4.74	114.61	109.89
4	4	218	OCS	CA-CB-SG	4.06	123.08	114.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	4	218	OCS	OXT-C-CA-CB
4	4	218	OCS	O-C-CA-CB
4	4	218	OCS	N-CA-CB-SG
4	4	218	OCS	OXT-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	112:ARG	C	113:ALA	N	0.93