



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:16 PM UTC

PDB ID : 1MCP / pdb_00001mcp
Title : PHOSPHOCHOLINE BINDING IMMUNOGLOBULIN FAB MC/PC603.
AN X-RAY DIFFRACTION STUDY AT 2.7 ANGSTROMS
Authors : Satow, Y.; Cohen, G.H.; Padlan, E.A.; Davies, D.R.
Deposited on : 1984-07-09
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

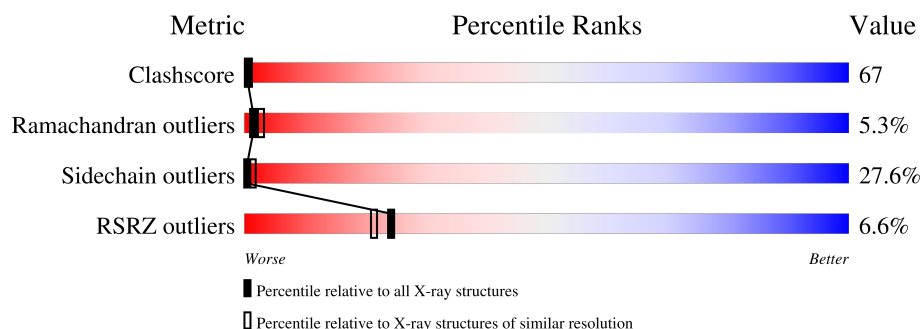
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	L	220	
2	H	222	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3544 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 IGA-KAPPA MCPC603 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	220	Total	C	N	O	S	0	0	0
			1692	1048	286	350	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	112	ILE	LEU	conflict	GB 208622

- Molecule 2 is a protein called IGA-KAPPA MCPC603 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1709	1079	286	334	10			

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



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

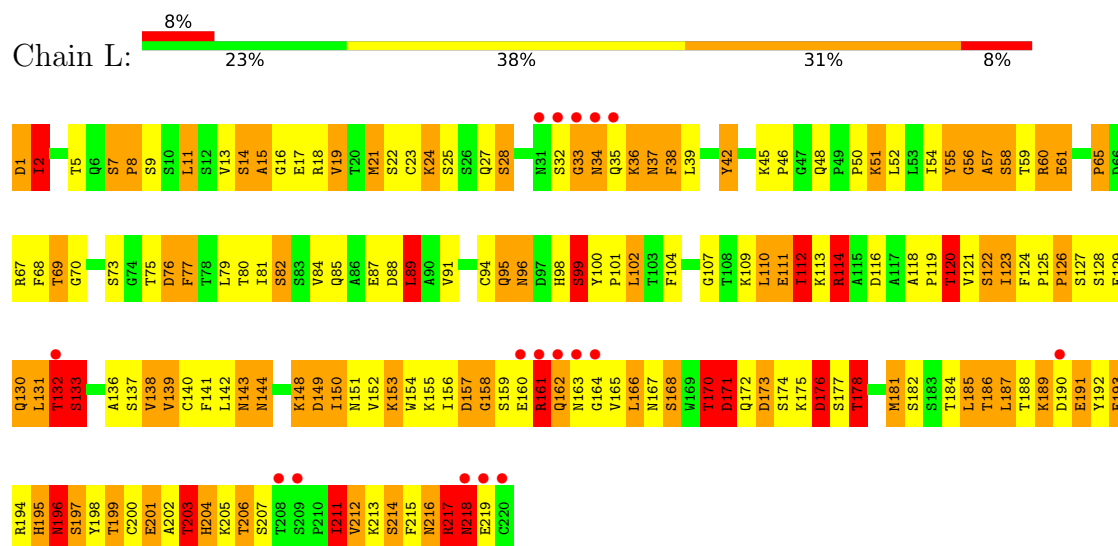
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	62	Total	O		0	0
			62	62			
4	H	76	Total	O		0	0
			76	76			

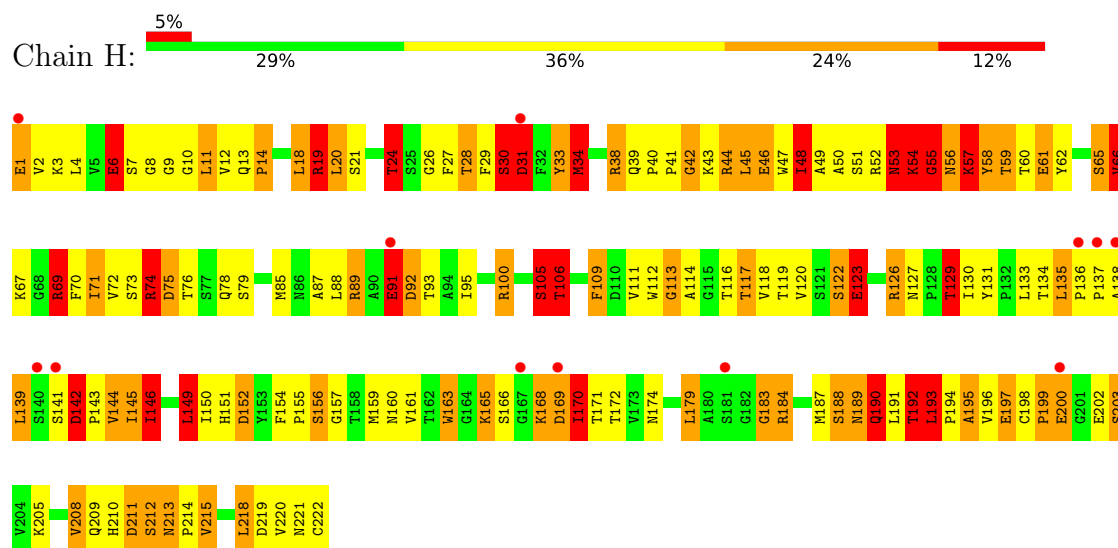
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: IGA-KAPPA MCPC603 FAB (LIGHT CHAIN)



• Molecule 2: IGA-KAPPA MCPC603 FAB (HEAVY CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	162.53Å 162.53Å 60.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.70 140.76 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70) 92.8 (140.76-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.225 , (Not available) 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 77.9	EDS
L-test for twinning ¹	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.053 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3544	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L	1.50	10/1728 (0.6%)	2.54	125/2344 (5.3%)
2	H	1.50	13/1753 (0.7%)	2.46	117/2389 (4.9%)
All	All	1.50	23/3481 (0.7%)	2.50	242/4733 (5.1%)

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
1	L	0	3
2	H	0	5
All	All	0	8

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	42	GLY	N-CA	7.68	1.56	1.45
2	H	24	THR	CA-CB	7.28	1.63	1.53
2	H	149	LEU	CA-CB	-6.81	1.44	1.53
1	L	57	ALA	N-CA	6.79	1.55	1.46
2	H	106	THR	CA-CB	6.78	1.63	1.53
1	L	114	ARG	CD-NE	-6.55	1.37	1.46
2	H	55	GLY	N-CA	6.03	1.54	1.45
1	L	107	GLY	N-CA	5.89	1.50	1.45
2	H	126	ARG	NE-CZ	5.85	1.39	1.33
2	H	100	ARG	N-CA	5.80	1.53	1.46
2	H	100	ARG	NE-CZ	-5.62	1.26	1.33
1	L	15	ALA	N-CA	5.62	1.53	1.46
1	L	178	THR	CA-CB	5.59	1.62	1.53
1	L	33	GLY	N-CA	5.59	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	146	ILE	N-CA	5.45	1.52	1.46
1	L	212	VAL	CA-CB	5.35	1.61	1.54
2	H	73	SER	N-CA	5.21	1.52	1.45
2	H	184	ARG	NE-CZ	5.17	1.38	1.33
1	L	159	SER	CA-C	5.13	1.58	1.52
1	L	184	THR	CA-CB	5.10	1.61	1.53
2	H	117	THR	CB-OG1	5.05	1.51	1.43
2	H	41	PRO	C-O	5.03	1.30	1.24
1	L	141	PHE	CA-CB	-5.03	1.46	1.53

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	114	ARG	CD-NE-CZ	19.05	151.07	124.40
2	H	100	ARG	CD-NE-CZ	17.34	148.68	124.40
1	L	157	ASP	CA-CB-CG	16.64	129.24	112.60
1	L	37	ASN	CA-CB-CG	15.42	128.02	112.60
2	H	56	ASN	OD1-CG-ND2	14.28	136.88	122.60
1	L	141	PHE	CA-CB-CG	14.23	128.03	113.80
2	H	127	ASN	CA-CB-CG	13.43	126.03	112.60
1	L	114	ARG	NE-CZ-NH1	13.34	134.84	121.50
2	H	126	ARG	CD-NE-CZ	-13.29	105.79	124.40
1	L	196	ASN	CA-CB-CG	-12.88	99.72	112.60
1	L	211	ILE	CB-CA-C	12.88	128.35	110.84
1	L	2	ILE	CB-CA-C	12.48	128.50	110.77
1	L	60	ARG	CD-NE-CZ	12.02	141.22	124.40
1	L	109	LYS	CA-CB-CG	11.69	137.47	114.10
2	H	92	ASP	CA-CB-CG	11.21	123.81	112.60
1	L	176	ASP	CA-CB-CG	-11.17	101.43	112.60
2	H	126	ARG	CG-CD-NE	11.04	136.29	112.00
1	L	60	ARG	NE-CZ-NH2	11.04	129.13	119.20
1	L	191	GLU	CB-CG-CD	11.01	131.31	112.60
2	H	152	ASP	CA-CB-CG	10.33	122.93	112.60
2	H	6	GLU	CB-CG-CD	10.18	129.91	112.60
2	H	169	ASP	CA-CB-CG	-10.12	102.47	112.60
1	L	56	GLY	CA-C-O	-10.03	108.33	122.58
1	L	213	LYS	N-CA-CB	9.56	124.82	110.29
2	H	129	THR	CB-CA-C	9.46	124.91	110.62
2	H	56	ASN	CA-CB-CG	-9.34	103.27	112.60
2	H	126	ARG	NE-CZ-NH2	-9.31	110.82	119.20
1	L	16	GLY	N-CA-C	-9.03	103.48	115.40
1	L	48	GLN	O-C-N	9.03	127.49	121.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	56	GLY	N-CA-C	-8.83	93.91	112.45
2	H	184	ARG	CD-NE-CZ	-8.83	112.04	124.40
2	H	89	ARG	CD-NE-CZ	8.78	136.69	124.40
2	H	100	ARG	CA-CB-CG	8.57	131.23	114.10
2	H	189	ASN	CA-CB-CG	-8.42	104.18	112.60
2	H	24	THR	CA-C-O	-8.42	111.45	120.46
2	H	54	LYS	CA-C-O	-8.34	108.58	120.51
1	L	21	MET	CA-C-O	-8.26	111.58	121.66
2	H	183	GLY	N-CA-C	-8.20	103.34	115.72
1	L	102	LEU	CA-C-O	-8.14	112.04	121.16
1	L	2	ILE	CA-CB-CG1	8.12	124.20	110.40
2	H	215	VAL	CA-C-O	-8.02	113.56	121.58
2	H	189	ASN	OD1-CG-ND2	7.92	130.53	122.60
1	L	69	THR	CA-C-O	-7.91	111.88	121.06
2	H	189	ASN	N-CA-CB	-7.91	97.55	110.59
1	L	32	SER	N-CA-C	-7.89	103.73	112.72
1	L	57	ALA	N-CA-C	-7.74	103.86	113.38
1	L	114	ARG	NH1-CZ-NH2	-7.66	109.34	119.30
2	H	109	PHE	CA-CB-CG	7.65	121.45	113.80
1	L	132	THR	CB-CA-C	7.62	125.59	110.42
1	L	54	ILE	CA-C-O	-7.46	112.31	120.67
1	L	212	VAL	N-CA-CB	-7.46	98.92	111.23
2	H	34	MET	CB-CA-C	7.43	122.97	109.37
2	H	149	LEU	CB-CA-C	7.41	122.60	110.22
1	L	149	ASP	CB-CA-C	7.39	120.34	110.06
1	L	58	SER	N-CA-C	7.38	125.56	113.89
1	L	143	ASN	N-CA-C	7.36	121.43	109.59
2	H	31	ASP	CA-CB-CG	-7.31	105.29	112.60
2	H	192	THR	CB-CA-C	7.27	123.25	109.37
2	H	61	GLU	CA-CB-CG	7.22	128.55	114.10
2	H	19	ARG	CD-NE-CZ	7.20	134.48	124.40
2	H	213	ASN	N-CA-C	7.15	118.89	110.31
2	H	151	HIS	N-CA-C	7.12	120.79	108.76
2	H	6	GLU	CG-CD-OE1	7.04	134.59	118.40
1	L	102	LEU	N-CA-C	-7.03	99.88	110.28
2	H	19	ARG	NH1-CZ-NH2	-7.03	110.17	119.30
2	H	127	ASN	CB-CG-ND2	6.96	126.84	116.40
2	H	48	ILE	O-C-N	-6.90	113.95	122.57
2	H	11	LEU	CA-C-N	6.87	132.46	121.95
2	H	11	LEU	C-N-CA	6.87	132.46	121.95
2	H	146	ILE	CA-C-O	-6.87	114.83	121.63
2	H	126	ARG	NE-CZ-NH1	6.85	128.35	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	45	LEU	N-CA-C	-6.79	99.47	110.20
1	L	203	THR	CB-CA-C	6.75	122.02	111.77
1	L	94	CYS	O-C-N	6.67	131.87	123.19
2	H	19	ARG	NE-CZ-NH1	6.67	128.17	121.50
2	H	193	LEU	CB-CA-C	6.67	118.99	109.92
1	L	60	ARG	NH1-CZ-NH2	-6.65	110.65	119.30
1	L	176	ASP	CA-C-O	-6.65	111.58	118.90
1	L	159	SER	N-CA-C	-6.64	96.93	108.69
2	H	146	ILE	N-CA-CB	-6.64	100.07	112.36
2	H	170	ILE	O-C-N	6.64	130.87	122.57
2	H	74	ARG	CA-CB-CG	6.62	127.33	114.10
2	H	4	LEU	CA-C-O	-6.61	113.23	120.24
1	L	185	LEU	CA-CB-CG	6.59	139.36	116.30
1	L	77	PHE	CA-C-O	-6.56	113.78	121.46
1	L	120	THR	N-CA-C	-6.55	99.02	109.76
2	H	33	TYR	O-C-N	6.53	130.85	122.89
2	H	24	THR	N-CA-CB	-6.50	99.68	110.47
1	L	112	ILE	CB-CA-C	6.49	120.50	110.83
2	H	69	ARG	CD-NE-CZ	-6.47	115.35	124.40
2	H	219	ASP	O-C-N	6.42	130.84	123.27
1	L	24	LYS	CA-CB-CG	6.37	126.84	114.10
2	H	106	THR	N-CA-CB	-6.30	101.35	110.87
1	L	185	LEU	CA-C-O	-6.28	113.41	120.32
2	H	146	ILE	CA-CB-CG1	6.28	121.07	110.40
1	L	158	GLY	CA-C-N	6.28	132.87	122.33
1	L	158	GLY	C-N-CA	6.28	132.87	122.33
2	H	151	HIS	CA-CB-CG	6.27	120.07	113.80
1	L	37	ASN	OD1-CG-ND2	-6.26	116.34	122.60
2	H	218	LEU	CA-C-N	6.26	131.82	123.05
2	H	218	LEU	C-N-CA	6.26	131.82	123.05
2	H	100	ARG	NE-CZ-NH1	6.26	127.76	121.50
2	H	160	ASN	CA-C-O	-6.26	113.61	120.43
1	L	144	ASN	CA-CB-CG	6.20	118.80	112.60
2	H	127	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	L	116	ASP	CA-CB-CG	-6.16	106.44	112.60
2	H	54	LYS	N-CA-C	-6.15	97.71	110.80
1	L	81	ILE	N-CA-C	-6.14	98.89	107.80
2	H	122	SER	CA-CB-OG	-6.10	98.89	111.10
1	L	59	THR	CA-C-N	6.10	130.22	121.50
1	L	59	THR	C-N-CA	6.10	130.22	121.50
2	H	135	LEU	O-C-N	6.10	127.69	121.72
2	H	33	TYR	CA-C-O	-6.07	114.36	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	193	LEU	N-CA-CB	-6.06	102.34	110.77
2	H	213	ASN	CA-CB-CG	6.06	118.66	112.60
1	L	65	PRO	CB-CA-C	6.03	118.88	110.98
2	H	213	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	L	57	ALA	CB-CA-C	6.02	120.13	109.65
1	L	184	THR	CA-CB-OG1	-6.01	100.58	109.60
2	H	149	LEU	N-CA-CB	6.00	120.25	110.17
1	L	94	CYS	N-CA-C	-5.97	100.17	109.72
1	L	111	GLU	CA-C-O	-5.96	114.49	121.46
2	H	212	SER	N-CA-C	5.95	120.38	113.18
1	L	55	TYR	CA-C-O	-5.94	114.69	121.58
2	H	91	GLU	CA-CB-CG	5.94	125.97	114.10
2	H	151	HIS	CA-C-O	5.93	126.91	120.32
2	H	100	ARG	NE-CZ-NH2	-5.90	113.89	119.20
2	H	211	ASP	CA-C-N	5.89	133.06	121.58
2	H	211	ASP	C-N-CA	5.89	133.06	121.58
2	H	105	SER	N-CA-C	-5.88	103.58	112.04
2	H	66	VAL	N-CA-CB	-5.86	101.56	111.23
2	H	163	TRP	CB-CA-C	5.83	120.05	109.37
1	L	196	ASN	CB-CG-ND2	-5.81	107.69	116.40
1	L	173	ASP	CA-CB-CG	-5.81	106.79	112.60
2	H	169	ASP	CB-CA-C	-5.80	101.09	110.77
1	L	204	HIS	CA-CB-CG	-5.79	108.01	113.80
2	H	56	ASN	CB-CG-OD1	-5.78	109.24	120.80
1	L	166	LEU	CA-CB-CG	5.76	136.47	116.30
1	L	131	LEU	N-CA-CB	-5.75	101.38	109.94
1	L	77	PHE	O-C-N	5.74	130.80	123.11
2	H	156	SER	N-CA-CB	5.74	119.09	110.19
1	L	120	THR	CA-C-O	-5.73	114.44	120.80
1	L	61	GLU	CB-CG-CD	5.72	122.33	112.60
1	L	58	SER	CA-C-O	-5.72	112.56	119.03
2	H	189	ASN	CA-C-O	-5.65	112.37	120.11
1	L	28	SER	CA-C-O	-5.64	114.98	121.19
2	H	156	SER	N-CA-C	-5.64	103.92	112.04
2	H	24	THR	CA-CB-OG1	-5.63	101.15	109.60
1	L	219	GLU	N-CA-C	-5.63	104.36	111.11
1	L	28	SER	O-C-N	5.62	129.79	122.87
2	H	71	ILE	CA-CB-CG2	5.59	120.01	110.50
1	L	2	ILE	N-CA-CB	-5.59	104.37	111.64
2	H	30	SER	CA-C-O	-5.57	112.54	120.51
2	H	65	SER	O-C-N	5.54	128.51	122.20
2	H	71	ILE	CB-CA-C	5.54	118.41	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	160	ASN	CA-CB-CG	-5.53	107.07	112.60
2	H	31	ASP	CA-C-N	5.52	131.67	122.73
2	H	31	ASP	C-N-CA	5.52	131.67	122.73
1	L	16	GLY	CA-C-O	-5.48	113.23	119.04
1	L	165	VAL	N-CA-C	5.48	115.88	107.77
2	H	172	THR	CA-CB-OG1	-5.44	101.44	109.60
1	L	21	MET	N-CA-C	-5.43	102.00	110.42
1	L	199	THR	O-C-N	5.41	130.18	123.15
1	L	196	ASN	OD1-CG-ND2	5.40	128.00	122.60
2	H	48	ILE	CA-C-O	-5.39	114.04	120.78
1	L	59	THR	CA-C-O	-5.39	114.39	120.43
2	H	53	ASN	CA-C-O	-5.38	115.69	121.56
2	H	145	ILE	N-CA-CB	5.38	120.30	111.58
1	L	197	SER	N-CA-C	-5.36	100.00	108.73
2	H	24	THR	OG1-CB-CG2	5.36	120.01	109.30
2	H	190	GLN	CB-CG-CD	5.35	121.70	112.60
1	L	61	GLU	CG-CD-OE1	5.35	130.71	118.40
1	L	126	PRO	CB-CA-C	5.34	118.06	111.23
1	L	16	GLY	O-C-N	5.33	129.16	122.28
1	L	168	SER	CB-CA-C	-5.33	102.46	110.24
1	L	182	SER	N-CA-C	-5.32	100.73	109.40
2	H	74	ARG	NH1-CZ-NH2	-5.32	112.39	119.30
2	H	55	GLY	N-CA-C	-5.32	100.58	113.18
2	H	87	ALA	CA-C-O	-5.31	115.39	122.03
2	H	46	GLU	CA-C-N	5.30	129.94	122.09
2	H	46	GLU	C-N-CA	5.30	129.94	122.09
1	L	186	THR	CA-CB-OG1	-5.30	101.65	109.60
2	H	127	ASN	CA-C-O	-5.29	114.94	120.70
1	L	56	GLY	CA-C-N	-5.29	113.12	122.26
1	L	56	GLY	C-N-CA	-5.29	113.12	122.26
2	H	195	ALA	CA-C-O	-5.28	113.38	119.61
1	L	199	THR	CA-CB-OG1	-5.28	101.68	109.60
1	L	162	GLN	N-CA-CB	-5.28	101.57	110.49
2	H	40	PRO	CB-CA-C	5.27	117.35	110.92
1	L	70	GLY	CA-C-O	-5.27	116.73	121.47
1	L	191	GLU	CG-CD-OE1	5.27	130.52	118.40
2	H	54	LYS	CB-CA-C	-5.26	99.94	110.42
1	L	176	ASP	CB-CG-OD1	-5.26	106.30	118.40
1	L	89	LEU	CA-C-O	-5.26	112.99	120.51
1	L	138	VAL	CA-C-O	-5.23	114.89	120.59
1	L	218	ASN	CB-CA-C	5.23	120.82	110.42
2	H	129	THR	N-CA-C	-5.22	98.72	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	149	ASP	CA-CB-CG	5.22	117.82	112.60
1	L	212	VAL	CA-C-O	-5.21	114.27	120.78
2	H	76	THR	CA-CB-OG1	-5.21	101.79	109.60
2	H	169	ASP	CA-C-O	-5.21	114.72	120.60
1	L	107	GLY	N-CA-C	-5.20	106.73	112.04
2	H	46	GLU	CG-CD-OE2	-5.20	106.45	118.40
1	L	159	SER	O-C-N	5.19	129.69	123.36
1	L	50	PRO	CB-CA-C	5.18	117.73	110.95
1	L	82	SER	CA-C-O	-5.18	114.01	119.97
2	H	53	ASN	O-C-N	5.18	128.97	122.86
2	H	39	GLN	O-C-N	5.18	127.47	121.47
2	H	113	GLY	N-CA-C	-5.17	104.69	112.60
1	L	91	VAL	N-CA-CB	5.17	120.78	111.21
1	L	57	ALA	CA-C-O	5.17	125.04	119.15
1	L	9	SER	O-C-N	5.17	128.49	122.24
1	L	113	LYS	N-CA-CB	5.16	118.81	110.41
1	L	185	LEU	O-C-N	5.15	129.35	123.27
2	H	170	ILE	CA-C-O	-5.15	114.34	120.78
2	H	146	ILE	CB-CG1-CD1	-5.14	103.01	113.80
1	L	187	LEU	CB-CA-C	5.12	121.61	113.37
1	L	68	PHE	CA-CB-CG	5.11	118.91	113.80
1	L	7	SER	N-CA-CB	-5.11	102.49	111.17
1	L	137	SER	CA-C-O	-5.10	114.84	120.30
1	L	39	LEU	CA-C-O	-5.10	114.66	120.32
2	H	215	VAL	N-CA-C	-5.10	101.73	109.78
1	L	94	CYS	CA-C-O	-5.09	115.36	121.11
2	H	18	LEU	O-C-N	5.08	129.07	123.33
2	H	46	GLU	CA-C-O	-5.06	114.70	120.32
1	L	1	ASP	CB-CA-C	5.06	119.71	110.10
1	L	14	SER	N-CA-CB	5.05	118.17	110.44
1	L	125	PRO	CB-CA-C	-5.05	104.76	110.92
1	L	69	THR	O-C-N	5.05	129.12	123.27
1	L	132	THR	CA-CB-OG1	5.04	117.16	109.60
1	L	42	TYR	CA-C-O	-5.04	115.21	121.11
1	L	170	THR	N-CA-C	-5.04	104.03	110.53
1	L	25	SER	CA-C-O	-5.03	115.57	121.46
1	L	21	MET	O-C-N	5.03	128.72	123.03
1	L	159	SER	CA-C-O	-5.03	114.09	120.28
1	L	99	SER	O-C-N	5.03	128.54	123.26
1	L	89	LEU	O-C-N	5.03	129.28	122.59
1	L	34	ASN	N-CA-C	-5.02	107.54	113.97
2	H	14	PRO	N-CA-C	-5.02	103.08	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	65	SER	CB-CA-C	-5.02	100.73	110.46
1	L	171	ASP	CA-C-O	-5.01	115.76	121.82
1	L	8	PRO	O-C-N	5.00	130.60	121.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	126	ARG	Sidechain
2	H	129	THR	Mainchain
2	H	19	ARG	Sidechain
2	H	44	ARG	Sidechain
2	H	54	LYS	Mainchain
1	L	161	ARG	Sidechain
1	L	2	ILE	Mainchain
1	L	217	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	1692	0	1622	237	14
2	H	1709	0	1648	217	13
3	H	5	0	0	1	0
4	H	76	0	0	8	1
4	L	62	0	0	16	0
All	All	3544	0	3270	444	15

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 67.

All (444) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:153:LYS:NZ	1:L:161:ARG:HD3	1.37	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:169:ASP:O	2:H:170:ILE:HG13	1.42	1.17
1:L:34:ASN:CB	1:L:36:LYS:HE3	1.72	1.17
1:L:160:GLU:O	1:L:161:ARG:HG3	1.44	1.15
1:L:201:GLU:CB	1:L:212:VAL:HG22	1.76	1.14
2:H:169:ASP:CG	2:H:194:PRO:HD3	1.71	1.14
1:L:152:VAL:HG21	1:L:181:MET:HE2	1.16	1.13
2:H:136:PRO:HG2	2:H:139:LEU:HG	1.28	1.12
1:L:14:SER:O	1:L:15:ALA:HB3	1.48	1.11
2:H:49:ALA:CB	2:H:72:VAL:HG21	1.80	1.11
1:L:34:ASN:HB3	1:L:36:LYS:CE	1.81	1.09
1:L:199:THR:HG22	1:L:214:SER:HB2	1.28	1.07
1:L:157:ASP:CG	1:L:195:HIS:HB3	1.78	1.07
2:H:131:TYR:HB2	2:H:149:LEU:CD1	1.85	1.06
1:L:153:LYS:NZ	1:L:161:ARG:CD	2.19	1.05
2:H:49:ALA:HB1	2:H:72:VAL:CG2	1.86	1.04
1:L:153:LYS:CD	1:L:161:ARG:HG2	1.87	1.04
2:H:8:GLY:O	2:H:20:LEU:CD2	2.07	1.03
1:L:201:GLU:HB2	1:L:212:VAL:HG22	1.39	1.02
1:L:195:HIS:O	1:L:218:ASN:ND2	1.93	1.01
1:L:14:SER:O	1:L:15:ALA:CB	2.09	1.00
1:L:34:ASN:HB2	1:L:36:LYS:HE3	1.41	1.00
2:H:49:ALA:HB1	2:H:72:VAL:HG21	1.01	0.99
1:L:216:ASN:O	1:L:217:ARG:CG	2.12	0.97
2:H:24:THR:HG22	2:H:24:THR:O	1.60	0.97
2:H:138:ALA:O	2:H:139:LEU:HD23	1.64	0.96
2:H:138:ALA:C	2:H:139:LEU:HD23	1.89	0.96
2:H:169:ASP:OD2	2:H:194:PRO:HD3	1.65	0.96
2:H:11:LEU:HD13	2:H:155:PRO:HG3	1.45	0.96
1:L:191:GLU:HA	1:L:194:ARG:HD2	1.47	0.94
1:L:34:ASN:CB	1:L:36:LYS:CE	2.42	0.94
1:L:152:VAL:HG21	1:L:181:MET:CE	1.98	0.94
1:L:153:LYS:HZ2	1:L:161:ARG:HD3	0.88	0.92
1:L:188:THR:OG1	1:L:191:GLU:HB2	1.67	0.92
2:H:52:ARG:HE	2:H:59:THR:HG22	1.32	0.92
2:H:49:ALA:CB	2:H:72:VAL:CG2	2.44	0.91
2:H:136:PRO:HG2	2:H:139:LEU:CG	1.99	0.90
1:L:201:GLU:HB3	1:L:212:VAL:HG22	1.52	0.90
2:H:136:PRO:HD2	2:H:139:LEU:HD12	1.54	0.90
1:L:190:ASP:HA	4:L:346:HOH:O	1.71	0.90
2:H:169:ASP:OD1	2:H:169:ASP:C	2.13	0.90
2:H:54:LYS:HB2	2:H:58:TYR:OH	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:153:LYS:HZ3	1:L:161:ARG:CG	1.86	0.89
1:L:96:ASN:ND2	1:L:98:HIS:H	1.71	0.88
1:L:34:ASN:HB3	1:L:36:LYS:HE2	1.53	0.88
1:L:1:ASP:HB3	4:L:226:HOH:O	1.73	0.87
1:L:216:ASN:O	1:L:217:ARG:HG2	1.73	0.87
1:L:198:TYR:HB2	1:L:215:PHE:CE2	2.09	0.87
2:H:169:ASP:OD2	2:H:194:PRO:CD	2.24	0.86
1:L:153:LYS:HZ3	1:L:161:ARG:HD3	1.37	0.86
2:H:131:TYR:HB2	2:H:149:LEU:HD11	1.54	0.86
1:L:37:ASN:HD22	1:L:57:ALA:HB2	1.41	0.86
1:L:67:ARG:NH1	1:L:88:ASP:OD2	2.09	0.86
2:H:105:SER:HB2	2:H:106:THR:HG22	1.58	0.86
2:H:1:GLU:HG3	4:H:305:HOH:O	1.74	0.85
1:L:160:GLU:O	1:L:161:ARG:CG	2.24	0.85
1:L:176:ASP:OD1	1:L:176:ASP:N	2.05	0.84
1:L:212:VAL:HG12	1:L:212:VAL:O	1.75	0.84
2:H:54:LYS:O	2:H:54:LYS:CG	2.18	0.84
2:H:202:GLU:O	2:H:203:SER:HB3	1.73	0.84
2:H:142:ASP:C	2:H:142:ASP:OD1	2.18	0.84
2:H:150:ILE:HG21	2:H:159:MET:HE3	1.58	0.84
1:L:153:LYS:HD2	1:L:161:ARG:HG2	1.61	0.82
1:L:1:ASP:CB	4:L:226:HOH:O	2.25	0.82
1:L:153:LYS:HZ2	1:L:161:ARG:CD	1.82	0.82
2:H:66:VAL:HG13	2:H:70:PHE:HB2	1.60	0.82
1:L:42:TYR:OH	1:L:95:GLN:NE2	2.13	0.81
1:L:151:ASN:OD1	1:L:203:THR:HG22	1.79	0.81
1:L:128:SER:O	1:L:132:THR:HG23	1.80	0.81
2:H:93:THR:HG23	2:H:119:THR:HA	1.61	0.81
1:L:173:ASP:OD2	1:L:173:ASP:C	2.21	0.81
2:H:38:ARG:NH2	2:H:46:GLU:OE2	2.15	0.80
1:L:150:ILE:HG23	1:L:150:ILE:O	1.80	0.80
1:L:153:LYS:HD2	1:L:161:ARG:NE	1.97	0.79
2:H:131:TYR:HB2	2:H:149:LEU:HD13	1.65	0.79
1:L:217:ARG:O	1:L:218:ASN:CB	2.30	0.79
2:H:62:TYR:HE1	2:H:72:VAL:HG23	1.47	0.79
1:L:202:ALA:N	1:L:211:ILE:O	2.16	0.79
1:L:24:LYS:HD3	1:L:76:ASP:OD1	1.83	0.79
2:H:196:VAL:O	2:H:196:VAL:HG22	1.83	0.78
1:L:153:LYS:HD2	1:L:161:ARG:CG	2.12	0.78
1:L:188:THR:OG1	1:L:191:GLU:CB	2.30	0.78
1:L:153:LYS:HD2	1:L:161:ARG:CD	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:196:ASN:HD22	1:L:196:ASN:N	1.80	0.77
1:L:152:VAL:CG2	1:L:181:MET:HE2	2.08	0.76
1:L:216:ASN:O	1:L:217:ARG:HG3	1.84	0.76
2:H:161:VAL:HG11	2:H:189:ASN:ND2	1.99	0.76
2:H:202:GLU:O	2:H:203:SER:CB	2.33	0.76
1:L:216:ASN:C	1:L:217:ARG:HG3	2.10	0.76
1:L:153:LYS:HZ3	1:L:161:ARG:CD	1.88	0.76
1:L:18:ARG:O	4:L:349:HOH:O	2.04	0.75
1:L:42:TYR:CE1	1:L:95:GLN:NE2	2.54	0.75
1:L:201:GLU:HA	1:L:211:ILE:O	1.86	0.75
1:L:157:ASP:CB	1:L:195:HIS:HB3	2.15	0.75
2:H:53:ASN:O	2:H:55:GLY:N	2.19	0.75
1:L:170:THR:HG23	1:L:171:ASP:O	1.88	0.74
2:H:54:LYS:O	2:H:54:LYS:CD	2.35	0.74
2:H:145:ILE:CG2	2:H:190:GLN:HE21	1.99	0.74
2:H:169:ASP:CG	2:H:194:PRO:CD	2.58	0.74
2:H:42:GLY:O	2:H:43:LYS:HG2	1.88	0.74
2:H:161:VAL:CG1	2:H:189:ASN:ND2	2.52	0.73
1:L:11:LEU:CD2	1:L:19:VAL:CG2	2.66	0.73
2:H:52:ARG:NE	2:H:59:THR:HG22	2.03	0.73
1:L:197:SER:HA	1:L:216:ASN:HB3	1.70	0.72
1:L:96:ASN:HD22	1:L:98:HIS:H	1.36	0.72
1:L:173:ASP:OD2	1:L:174:SER:N	2.22	0.72
2:H:117:THR:HG21	2:H:157:GLY:HA2	1.71	0.72
2:H:6:GLU:HA	2:H:21:SER:O	1.89	0.72
2:H:163:TRP:NE1	2:H:189:ASN:HD21	1.88	0.72
2:H:136:PRO:O	2:H:138:ALA:N	2.23	0.72
1:L:114:ARG:HD2	1:L:176:ASP:O	1.90	0.72
2:H:62:TYR:CE1	2:H:72:VAL:HG23	2.25	0.72
2:H:123:GLU:O	4:H:310:HOH:O	2.07	0.71
1:L:42:TYR:HE1	1:L:95:GLN:HE21	1.35	0.71
2:H:1:GLU:O	2:H:26:GLY:HA3	1.90	0.71
1:L:153:LYS:HD2	1:L:161:ARG:HE	1.55	0.71
2:H:89:ARG:HE	2:H:91:GLU:CD	1.98	0.71
1:L:153:LYS:CD	1:L:161:ARG:CG	2.67	0.71
2:H:105:SER:CB	2:H:106:THR:HG22	2.20	0.71
1:L:195:HIS:H	1:L:195:HIS:CD2	2.08	0.71
1:L:201:GLU:HB2	1:L:212:VAL:CG2	2.19	0.71
2:H:136:PRO:HD2	2:H:139:LEU:CD1	2.19	0.70
1:L:17:GLU:OE2	4:L:301:HOH:O	2.08	0.70
1:L:187:LEU:HD11	1:L:192:TYR:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:145:ILE:CD1	2:H:192:THR:HB	2.21	0.70
2:H:31:ASP:HA	2:H:53:ASN:HB2	1.73	0.70
2:H:24:THR:O	2:H:24:THR:CG2	2.30	0.69
1:L:157:ASP:OD1	1:L:195:HIS:HB3	1.91	0.69
1:L:198:TYR:CB	1:L:215:PHE:CE2	2.74	0.69
1:L:55:TYR:C	1:L:56:GLY:O	2.29	0.69
1:L:153:LYS:HD3	1:L:161:ARG:HG2	1.73	0.69
1:L:156:ILE:HG23	1:L:198:TYR:CE1	2.27	0.69
1:L:11:LEU:CD2	1:L:19:VAL:HG22	2.23	0.69
1:L:151:ASN:OD1	1:L:203:THR:CG2	2.40	0.69
2:H:75:ASP:OD2	2:H:78:GLN:HB2	1.93	0.69
1:L:187:LEU:CD1	1:L:192:TYR:HB2	2.23	0.69
2:H:54:LYS:HB2	2:H:58:TYR:CZ	2.27	0.69
1:L:173:ASP:OD2	1:L:175:LYS:N	2.26	0.69
2:H:30:SER:O	2:H:31:ASP:HB3	1.92	0.69
1:L:114:ARG:HD2	1:L:177:SER:HB2	1.74	0.68
1:L:37:ASN:HD21	1:L:73:SER:HA	1.58	0.68
2:H:10:GLY:HA3	4:H:275:HOH:O	1.92	0.68
2:H:163:TRP:HE1	2:H:189:ASN:ND2	1.92	0.68
1:L:162:GLN:HG3	1:L:163:ASN:H	1.59	0.68
2:H:56:ASN:C	2:H:57:LYS:HG2	2.18	0.68
2:H:145:ILE:HD12	2:H:192:THR:HB	1.76	0.67
2:H:169:ASP:OD1	2:H:170:ILE:N	2.26	0.67
1:L:131:LEU:O	1:L:133:SER:N	2.19	0.67
1:L:67:ARG:HH12	1:L:88:ASP:CG	2.02	0.67
2:H:170:ILE:HG12	2:H:193:LEU:HB2	1.76	0.67
2:H:88:LEU:HB3	2:H:120:VAL:HG21	1.76	0.67
2:H:145:ILE:HG23	2:H:190:GLN:HE21	1.59	0.67
1:L:34:ASN:HD22	1:L:36:LYS:NZ	1.93	0.67
2:H:24:THR:HG21	2:H:29:PHE:CD1	2.30	0.67
2:H:136:PRO:CG	2:H:139:LEU:CD1	2.73	0.67
1:L:172:GLN:HG2	1:L:177:SER:HA	1.77	0.66
1:L:11:LEU:HD21	1:L:19:VAL:HG22	1.76	0.66
2:H:6:GLU:OE2	2:H:113:GLY:HA3	1.95	0.66
2:H:8:GLY:O	2:H:20:LEU:HD22	1.95	0.66
1:L:131:LEU:C	1:L:133:SER:H	2.02	0.66
1:L:216:ASN:C	1:L:217:ARG:CG	2.65	0.66
2:H:145:ILE:CG2	2:H:190:GLN:NE2	2.58	0.66
2:H:159:MET:SD	2:H:208:VAL:HG12	2.36	0.66
1:L:176:ASP:OD2	1:L:178:THR:OG1	2.14	0.66
2:H:29:PHE:CE2	2:H:74:ARG:HD3	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:PHE:CD1	2:H:135:LEU:HG	2.31	0.65
1:L:11:LEU:HD22	1:L:19:VAL:HG21	1.78	0.65
2:H:8:GLY:O	2:H:20:LEU:HD23	1.96	0.65
2:H:44:ARG:HG3	2:H:45:LEU:O	1.96	0.65
1:L:37:ASN:ND2	1:L:77:PHE:HE2	1.94	0.65
2:H:31:ASP:HA	2:H:53:ASN:CB	2.25	0.65
1:L:120:THR:HG22	4:L:344:HOH:O	1.97	0.65
1:L:131:LEU:HD21	1:L:136:ALA:HB2	1.78	0.65
1:L:155:LYS:HG2	1:L:160:GLU:H	1.61	0.65
1:L:42:TYR:CZ	1:L:95:GLN:NE2	2.65	0.65
2:H:48:ILE:HG13	2:H:49:ALA:H	1.62	0.65
1:L:156:ILE:O	1:L:197:SER:O	2.15	0.65
2:H:136:PRO:CG	2:H:139:LEU:HD11	2.27	0.65
1:L:153:LYS:HZ3	1:L:161:ARG:CB	2.10	0.64
1:L:34:ASN:HB3	1:L:36:LYS:HE3	1.43	0.64
1:L:162:GLN:CG	1:L:163:ASN:N	2.59	0.64
2:H:150:ILE:CG2	2:H:159:MET:HE3	2.27	0.64
1:L:218:ASN:OD1	1:L:218:ASN:C	2.38	0.63
1:L:11:LEU:CD2	1:L:19:VAL:HG21	2.29	0.63
1:L:201:GLU:CB	1:L:212:VAL:CG2	2.67	0.63
2:H:159:MET:SD	2:H:208:VAL:CG1	2.87	0.63
2:H:54:LYS:O	2:H:54:LYS:HG2	1.94	0.63
2:H:136:PRO:CG	2:H:139:LEU:HG	2.18	0.63
1:L:162:GLN:CG	1:L:163:ASN:H	2.11	0.63
1:L:37:ASN:ND2	1:L:73:SER:HA	2.13	0.62
2:H:53:ASN:C	2:H:55:GLY:N	2.56	0.62
2:H:163:TRP:NE1	2:H:189:ASN:ND2	2.46	0.62
1:L:89:LEU:HD23	1:L:110:LEU:O	1.99	0.62
1:L:217:ARG:O	1:L:218:ASN:HB3	1.98	0.62
1:L:201:GLU:CA	1:L:211:ILE:O	2.47	0.62
2:H:50:ALA:O	2:H:60:THR:HA	1.98	0.62
2:H:8:GLY:O	2:H:20:LEU:HD21	2.00	0.61
2:H:9:GLY:O	2:H:212:SER:HB3	1.99	0.61
2:H:53:ASN:C	2:H:53:ASN:HD22	2.08	0.61
1:L:51:LYS:O	1:L:51:LYS:HG3	1.99	0.61
1:L:162:GLN:HG2	1:L:164:GLY:H	1.66	0.61
1:L:198:TYR:N	1:L:215:PHE:O	2.24	0.61
1:L:196:ASN:N	1:L:196:ASN:ND2	2.49	0.61
2:H:161:VAL:HG11	2:H:189:ASN:HD22	1.63	0.61
2:H:56:ASN:O	2:H:57:LYS:O	2.18	0.60
2:H:142:ASP:OD1	2:H:143:PRO:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:176:ASP:O	1:L:177:SER:HB2	2.01	0.60
2:H:66:VAL:HG13	2:H:70:PHE:CB	2.30	0.60
1:L:121:VAL:HG12	1:L:122:SER:N	2.16	0.59
2:H:19:ARG:NE	4:H:293:HOH:O	2.35	0.59
1:L:142:LEU:HD13	1:L:181:MET:HG2	1.84	0.59
1:L:186:THR:O	1:L:186:THR:HG23	2.03	0.59
2:H:52:ARG:NH1	3:H:223:SO4:O3	2.36	0.59
1:L:157:ASP:HB2	1:L:195:HIS:HB3	1.83	0.59
1:L:197:SER:HA	1:L:216:ASN:HA	1.83	0.59
2:H:7:SER:HB2	4:H:279:HOH:O	2.03	0.58
1:L:201:GLU:HB3	1:L:212:VAL:CG2	2.30	0.58
2:H:56:ASN:C	2:H:56:ASN:OD1	2.44	0.58
1:L:196:ASN:O	1:L:216:ASN:HA	2.04	0.58
2:H:136:PRO:CD	2:H:139:LEU:CD1	2.81	0.58
2:H:169:ASP:O	2:H:170:ILE:CG1	2.35	0.58
1:L:153:LYS:NZ	1:L:161:ARG:CG	2.54	0.57
1:L:204:HIS:ND1	1:L:206:THR:OG1	2.34	0.57
1:L:168:SER:O	1:L:181:MET:HA	2.04	0.57
1:L:153:LYS:CE	1:L:161:ARG:HG2	2.33	0.57
2:H:169:ASP:OD2	2:H:194:PRO:HG3	2.05	0.57
2:H:130:ILE:HD12	2:H:208:VAL:HG21	1.86	0.57
2:H:52:ARG:NH2	2:H:59:THR:CG2	2.67	0.56
1:L:150:ILE:O	1:L:150:ILE:CG2	2.50	0.56
1:L:157:ASP:HB2	1:L:195:HIS:CB	2.35	0.56
2:H:142:ASP:HA	2:H:143:PRO:C	2.30	0.56
1:L:187:LEU:HD11	1:L:192:TYR:CB	2.35	0.56
2:H:29:PHE:CZ	2:H:74:ARG:HD3	2.41	0.56
1:L:149:ASP:O	4:L:327:HOH:O	2.17	0.56
2:H:66:VAL:HG13	2:H:70:PHE:CG	2.40	0.56
2:H:66:VAL:CG1	2:H:70:PHE:HB2	2.32	0.56
2:H:69:ARG:NH2	2:H:92:ASP:OD1	2.38	0.56
2:H:169:ASP:OD2	2:H:194:PRO:CG	2.53	0.56
2:H:28:THR:HG22	2:H:28:THR:O	2.06	0.56
1:L:101:PRO:HB3	2:H:47:TRP:CZ3	2.41	0.56
2:H:52:ARG:NE	2:H:59:THR:CG2	2.69	0.56
2:H:56:ASN:C	2:H:57:LYS:CG	2.75	0.56
2:H:145:ILE:HG21	2:H:190:GLN:NE2	2.20	0.56
1:L:189:LYS:HD3	4:L:306:HOH:O	2.05	0.55
2:H:136:PRO:CG	2:H:139:LEU:CG	2.79	0.55
1:L:96:ASN:ND2	1:L:96:ASN:C	2.64	0.55
1:L:126:PRO:HG2	1:L:192:TYR:CZ	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:217:ARG:O	1:L:218:ASN:HB2	2.06	0.55
1:L:153:LYS:HZ3	1:L:161:ARG:HB3	1.70	0.55
2:H:12:VAL:HG21	2:H:18:LEU:HG	1.89	0.55
2:H:52:ARG:HH21	2:H:59:THR:CG2	2.20	0.55
2:H:75:ASP:OD1	2:H:75:ASP:C	2.50	0.55
1:L:196:ASN:HD22	1:L:196:ASN:H	1.55	0.55
2:H:42:GLY:HA3	4:H:253:HOH:O	2.06	0.55
2:H:69:ARG:HH22	2:H:92:ASP:CG	2.14	0.55
1:L:202:ALA:O	1:L:211:ILE:N	2.32	0.55
2:H:169:ASP:O	2:H:169:ASP:CG	2.49	0.55
2:H:179:LEU:HD21	2:H:183:GLY:C	2.32	0.55
1:L:200:CYS:O	1:L:212:VAL:HA	2.06	0.55
1:L:37:ASN:HD22	1:L:57:ALA:CB	2.17	0.55
2:H:19:ARG:CD	4:H:293:HOH:O	2.55	0.54
2:H:42:GLY:C	2:H:43:LYS:CG	2.79	0.54
1:L:131:LEU:CD2	1:L:136:ALA:HB2	2.37	0.54
2:H:24:THR:HG21	2:H:29:PHE:HB2	1.90	0.54
1:L:196:ASN:O	1:L:217:ARG:N	2.38	0.54
2:H:136:PRO:O	2:H:139:LEU:HG	2.06	0.54
2:H:130:ILE:HG22	2:H:218:LEU:HD22	1.90	0.54
2:H:145:ILE:HD13	2:H:192:THR:HB	1.90	0.54
2:H:165:LYS:NZ	2:H:197:GLU:O	2.40	0.54
1:L:11:LEU:HD22	1:L:19:VAL:CG2	2.34	0.54
1:L:121:VAL:CG1	1:L:122:SER:N	2.71	0.53
1:L:212:VAL:O	1:L:212:VAL:CG1	2.43	0.53
1:L:198:TYR:HB2	1:L:215:PHE:CD2	2.42	0.53
1:L:124:PHE:CE1	2:H:135:LEU:HG	2.43	0.53
2:H:31:ASP:OD1	2:H:31:ASP:C	2.49	0.53
2:H:163:TRP:HE1	2:H:189:ASN:HD21	1.50	0.53
2:H:161:VAL:HG12	2:H:189:ASN:ND2	2.24	0.53
2:H:163:TRP:HE1	2:H:189:ASN:CG	2.17	0.52
2:H:31:ASP:C	2:H:53:ASN:HB3	2.35	0.52
1:L:110:LEU:CD1	1:L:112:ILE:HD13	2.39	0.52
2:H:135:LEU:HB3	2:H:139:LEU:HB2	1.92	0.52
1:L:152:VAL:CG2	1:L:181:MET:CE	2.79	0.52
1:L:156:ILE:O	1:L:198:TYR:HA	2.10	0.52
1:L:193:GLU:HA	1:L:218:ASN:OD1	2.09	0.52
2:H:161:VAL:HG21	2:H:187:MET:CE	2.40	0.52
2:H:198:CYS:N	2:H:199:PRO:CD	2.73	0.52
1:L:15:ALA:C	1:L:17:GLU:H	2.17	0.52
1:L:161:ARG:O	1:L:162:GLN:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:24:THR:HG23	2:H:27:PHE:CZ	2.45	0.52
2:H:163:TRP:C	2:H:165:LYS:H	2.19	0.52
1:L:55:TYR:OH	4:L:320:HOH:O	2.10	0.51
1:L:36:LYS:NZ	2:H:105:SER:O	2.36	0.51
1:L:101:PRO:HB3	2:H:47:TRP:HZ3	1.76	0.51
1:L:101:PRO:CB	2:H:47:TRP:CZ3	2.94	0.51
2:H:2:VAL:HG12	2:H:111:VAL:HG21	1.93	0.51
1:L:127:SER:O	1:L:131:LEU:HG	2.10	0.51
2:H:29:PHE:C	2:H:31:ASP:H	2.18	0.51
1:L:24:LYS:HA	1:L:75:THR:O	2.10	0.51
2:H:42:GLY:O	2:H:43:LYS:CG	2.59	0.51
2:H:56:ASN:C	2:H:57:LYS:O	2.53	0.51
2:H:196:VAL:O	2:H:196:VAL:CG2	2.57	0.51
1:L:1:ASP:OD1	1:L:101:PRO:HG3	2.11	0.50
2:H:202:GLU:OE1	2:H:202:GLU:HA	2.12	0.50
2:H:152:ASP:OD2	2:H:184:ARG:NH1	2.44	0.50
1:L:139:VAL:CG1	2:H:133:LEU:HD21	2.42	0.50
2:H:145:ILE:HG23	2:H:190:GLN:NE2	2.23	0.50
1:L:77:PHE:HB3	4:L:313:HOH:O	2.12	0.50
2:H:144:VAL:CG2	2:H:195:ALA:HA	2.41	0.50
1:L:38:PHE:CD1	1:L:38:PHE:N	2.79	0.50
1:L:197:SER:HA	1:L:216:ASN:CB	2.41	0.50
2:H:31:ASP:CA	2:H:53:ASN:HB2	2.42	0.49
2:H:144:VAL:O	2:H:145:ILE:HD13	2.12	0.49
2:H:210:HIS:O	2:H:211:ASP:C	2.55	0.49
1:L:89:LEU:HD11	1:L:172:GLN:HB3	1.95	0.49
2:H:11:LEU:HD11	2:H:154:PHE:HE2	1.77	0.49
1:L:37:ASN:ND2	1:L:57:ALA:HB2	2.21	0.49
1:L:131:LEU:C	1:L:133:SER:N	2.65	0.49
1:L:167:ASN:ND2	1:L:181:MET:HE1	2.28	0.49
1:L:193:GLU:HA	1:L:218:ASN:CG	2.37	0.49
1:L:216:ASN:ND2	4:L:295:HOH:O	2.46	0.49
2:H:13:GLN:O	2:H:14:PRO:C	2.55	0.49
1:L:197:SER:CA	1:L:216:ASN:HB3	2.41	0.49
2:H:52:ARG:HE	2:H:59:THR:CG2	2.14	0.49
2:H:134:THR:HG21	2:H:221:ASN:O	2.12	0.48
2:H:213:ASN:HB3	2:H:214:PRO:HD2	1.94	0.48
1:L:162:GLN:HG2	1:L:164:GLY:N	2.28	0.48
2:H:141:SER:O	2:H:142:ASP:HB3	2.13	0.48
1:L:34:ASN:O	1:L:35:GLN:HB2	2.13	0.48
2:H:136:PRO:HG3	2:H:139:LEU:HD11	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:196:ASN:ND2	1:L:197:SER:N	2.61	0.48
2:H:52:ARG:NH2	2:H:59:THR:HG21	2.28	0.48
1:L:112:ILE:H	1:L:172:GLN:HE22	1.60	0.48
1:L:110:LEU:HD11	1:L:112:ILE:CD1	2.43	0.47
1:L:7:SER:HA	1:L:8:PRO:C	2.38	0.47
1:L:38:PHE:N	1:L:38:PHE:HD1	2.12	0.47
1:L:130:GLN:HB2	2:H:131:TYR:CE2	2.49	0.47
2:H:163:TRP:CE3	2:H:191:LEU:HD22	2.48	0.47
2:H:169:ASP:C	2:H:170:ILE:HG13	2.33	0.47
1:L:201:GLU:HB3	1:L:212:VAL:HA	1.96	0.47
1:L:110:LEU:HD11	1:L:112:ILE:HD13	1.95	0.47
1:L:96:ASN:ND2	1:L:98:HIS:N	2.52	0.47
1:L:104:PHE:O	4:L:303:HOH:O	2.20	0.47
2:H:109:PHE:HD1	2:H:112:TRP:CZ2	2.32	0.47
1:L:13:VAL:O	1:L:112:ILE:HA	2.15	0.47
1:L:128:SER:O	1:L:129:GLU:C	2.55	0.47
2:H:49:ALA:HA	2:H:61:GLU:O	2.14	0.47
1:L:114:ARG:CD	1:L:177:SER:HB2	2.42	0.47
1:L:110:LEU:CD1	1:L:112:ILE:CD1	2.93	0.47
1:L:42:TYR:HE1	1:L:95:GLN:NE2	1.96	0.47
1:L:143:ASN:O	1:L:144:ASN:HB2	2.15	0.47
1:L:5:THR:O	1:L:23:CYS:HA	2.16	0.46
1:L:188:THR:OG1	1:L:191:GLU:HB3	2.14	0.46
2:H:174:ASN:OD1	2:H:189:ASN:OD1	2.33	0.46
1:L:157:ASP:HA	1:L:197:SER:O	2.16	0.46
2:H:34:MET:HB3	2:H:34:MET:HE3	1.62	0.46
2:H:134:THR:HG22	2:H:135:LEU:H	1.80	0.46
2:H:200:GLU:C	2:H:202:GLU:N	2.72	0.46
1:L:100:TYR:HA	1:L:101:PRO:C	2.41	0.46
1:L:201:GLU:HA	1:L:212:VAL:HA	1.97	0.46
1:L:19:VAL:O	1:L:80:THR:HG23	2.15	0.46
1:L:191:GLU:CA	1:L:194:ARG:HD2	2.33	0.46
2:H:29:PHE:O	2:H:31:ASP:N	2.49	0.46
2:H:203:SER:HA	2:H:220:VAL:O	2.15	0.46
1:L:153:LYS:CD	1:L:161:ARG:CD	2.89	0.46
1:L:19:VAL:O	1:L:80:THR:HA	2.16	0.45
2:H:54:LYS:O	2:H:54:LYS:HD2	2.14	0.45
2:H:30:SER:O	2:H:54:LYS:HB3	2.16	0.45
2:H:135:LEU:HB3	2:H:139:LEU:HD12	1.98	0.45
2:H:198:CYS:O	2:H:222:CYS:HB3	2.16	0.45
2:H:52:ARG:CZ	2:H:59:THR:CG2	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:34:ASN:HD22	1:L:36:LYS:CE	2.29	0.45
1:L:187:LEU:CD1	1:L:192:TYR:CA	2.95	0.45
2:H:6:GLU:OE2	2:H:114:ALA:N	2.50	0.45
2:H:194:PRO:HB2	2:H:197:GLU:HB2	1.99	0.45
1:L:153:LYS:NZ	1:L:161:ARG:HG2	2.32	0.45
2:H:85:MET:HE2	2:H:88:LEU:HD21	1.99	0.45
1:L:214:SER:HB3	4:L:292:HOH:O	2.17	0.45
2:H:24:THR:HG21	2:H:29:PHE:HD1	1.77	0.45
1:L:140:CYS:HB2	1:L:154:TRP:CZ2	2.53	0.44
1:L:201:GLU:HB3	1:L:212:VAL:CA	2.47	0.44
2:H:89:ARG:HG3	2:H:91:GLU:HG3	1.99	0.44
2:H:131:TYR:CB	2:H:149:LEU:HD11	2.36	0.44
2:H:205:LYS:HB2	2:H:205:LYS:HE3	1.64	0.44
1:L:13:VAL:CG2	1:L:84:VAL:HG11	2.47	0.44
1:L:112:ILE:H	1:L:172:GLN:NE2	2.15	0.44
1:L:188:THR:HG1	1:L:191:GLU:HB2	1.79	0.44
2:H:179:LEU:HD23	2:H:179:LEU:HA	1.80	0.44
1:L:193:GLU:HA	1:L:218:ASN:ND2	2.33	0.44
1:L:87:GLU:HG3	4:L:284:HOH:O	2.16	0.44
2:H:89:ARG:NE	2:H:91:GLU:CD	2.72	0.44
1:L:148:LYS:O	1:L:150:ILE:HG22	2.17	0.44
1:L:187:LEU:CD1	1:L:192:TYR:CB	2.95	0.44
2:H:54:LYS:HB2	2:H:58:TYR:HH	1.79	0.44
1:L:123:ILE:O	2:H:135:LEU:HD21	2.18	0.44
2:H:188:SER:OG	4:H:289:HOH:O	2.21	0.44
2:H:38:ARG:NH2	2:H:46:GLU:CD	2.76	0.43
2:H:134:THR:CG2	2:H:221:ASN:O	2.66	0.43
1:L:139:VAL:HG11	2:H:133:LEU:HD21	2.00	0.43
1:L:110:LEU:CD1	1:L:110:LEU:C	2.92	0.43
1:L:131:LEU:HD23	1:L:131:LEU:HA	1.41	0.43
1:L:201:GLU:C	1:L:211:ILE:O	2.61	0.43
2:H:93:THR:HA	2:H:118:VAL:O	2.18	0.43
1:L:187:LEU:HD12	1:L:187:LEU:C	2.44	0.43
2:H:57:LYS:O	2:H:59:THR:N	2.48	0.43
1:L:144:ASN:HA	1:L:178:THR:HB	2.01	0.42
2:H:33:TYR:C	2:H:34:MET:HG2	2.41	0.42
1:L:87:GLU:HG3	4:L:339:HOH:O	2.19	0.42
1:L:96:ASN:ND2	1:L:98:HIS:HB3	2.34	0.42
2:H:78:GLN:O	2:H:79:SER:HB2	2.19	0.42
1:L:196:ASN:ND2	1:L:196:ASN:C	2.64	0.42
2:H:56:ASN:O	2:H:57:LYS:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:56:ASN:OD1	2:H:56:ASN:N	2.47	0.42
2:H:136:PRO:C	2:H:138:ALA:N	2.77	0.42
2:H:52:ARG:O	2:H:74:ARG:NH2	2.53	0.42
1:L:142:LEU:HD21	1:L:202:ALA:HB2	2.01	0.42
1:L:192:TYR:C	1:L:194:ARG:H	2.27	0.42
2:H:44:ARG:HE	2:H:44:ARG:HB3	1.72	0.42
2:H:169:ASP:HB3	2:H:194:PRO:CG	2.50	0.42
1:L:96:ASN:HD21	1:L:99:SER:H	1.67	0.42
2:H:6:GLU:OE2	2:H:113:GLY:CA	2.64	0.42
2:H:52:ARG:CZ	2:H:59:THR:HG22	2.50	0.42
1:L:118:ALA:HA	1:L:119:PRO:HD3	1.90	0.41
1:L:65:PRO:C	1:L:67:ARG:H	2.28	0.41
2:H:146:ILE:HG21	2:H:146:ILE:HD13	1.54	0.41
1:L:45:LYS:HB3	1:L:46:PRO:CD	2.50	0.41
1:L:197:SER:HA	1:L:216:ASN:CA	2.50	0.41
2:H:156:SER:O	2:H:157:GLY:C	2.62	0.41
2:H:159:MET:HG2	2:H:187:MET:CE	2.50	0.41
1:L:96:ASN:ND2	1:L:98:HIS:CB	2.84	0.41
2:H:56:ASN:O	2:H:57:LYS:HB2	2.21	0.41
2:H:136:PRO:HG2	2:H:136:PRO:O	2.20	0.41
2:H:170:ILE:HA	2:H:192:THR:O	2.20	0.41
2:H:135:LEU:HD22	2:H:139:LEU:CB	2.51	0.41
2:H:29:PHE:C	2:H:31:ASP:N	2.78	0.41
1:L:85:GLN:O	1:L:88:ASP:HB2	2.20	0.41
1:L:142:LEU:HD13	1:L:181:MET:CG	2.48	0.41
2:H:169:ASP:O	2:H:194:PRO:CD	2.69	0.41
1:L:170:THR:CG2	1:L:171:ASP:O	2.64	0.40
1:L:187:LEU:HD11	1:L:192:TYR:HA	2.03	0.40
1:L:197:SER:CB	1:L:216:ASN:HB3	2.51	0.40
1:L:211:ILE:C	1:L:212:VAL:HG23	2.47	0.40
2:H:70:PHE:N	2:H:70:PHE:CD1	2.87	0.40
2:H:193:LEU:HA	2:H:194:PRO:HD3	1.99	0.40
1:L:17:GLU:HG3	4:L:301:HOH:O	2.21	0.40

All (15) 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)
1:L:132:THR:OG1	2:H:19:ARG:NH2[4_665]	1.05	1.15
1:L:15:ALA:O	2:H:1:GLU:OE2[2_665]	1.22	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:132:THR:OG1	2:H:19:ARG:CZ[4_665]	1.34	0.86
1:L:132:THR:CB	2:H:19:ARG:NH2[4_665]	1.41	0.79
4:H:230:HOH:O	4:H:329:HOH:O[4_664]	1.58	0.62
1:L:132:THR:CA	2:H:19:ARG:NH2[4_665]	1.89	0.31
1:L:15:ALA:O	2:H:1:GLU:CD[2_665]	1.91	0.29
1:L:15:ALA:C	2:H:1:GLU:OE2[2_665]	1.94	0.26
1:L:132:THR:O	2:H:19:ARG:NH2[4_665]	1.98	0.22
1:L:132:THR:OG1	2:H:19:ARG:NE[4_665]	1.99	0.21
1:L:132:THR:O	2:H:19:ARG:NH1[4_665]	2.01	0.19
1:L:132:THR:O	2:H:19:ARG:CZ[4_665]	2.03	0.17
1:L:18:ARG:NH1	1:L:61:GLU:OE1[2_665]	2.09	0.11
1:L:132:THR:C	2:H:19:ARG:NH1[4_665]	2.16	0.04
1:L:132:THR:C	2:H:19:ARG:NH2[4_665]	2.19	0.01

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	218/220 (99%)	183 (84%)	26 (12%)	9 (4%)	2	5
2	H	220/222 (99%)	192 (87%)	14 (6%)	14 (6%)	1	1
All	All	438/442 (99%)	375 (86%)	40 (9%)	23 (5%)	1	3

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	132	THR
1	L	218	ASN
2	H	30	SER
2	H	31	ASP
2	H	54	LYS
2	H	168	LYS
2	H	170	ILE

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Mol	Chain	Res	Type
2	H	199	PRO
2	H	203	SER
1	L	161	ARG
2	H	123	GLU
1	L	133	SER
1	L	158	GLY
1	L	193	GLU
2	H	57	LYS
1	L	196	ASN
1	L	217	ARG
2	H	58	TYR
2	H	137	PRO
2	H	142	ASP
2	H	48	ILE
1	L	33	GLY
2	H	55	GLY

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	195/195 (100%)	138 (71%)	57 (29%)	0	1
2	H	189/189 (100%)	140 (74%)	49 (26%)	0	2
All	All	384/384 (100%)	278 (72%)	106 (28%)	0	1

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	ILE
1	L	11	LEU
1	L	19	VAL
1	L	21	MET
1	L	22	SER
1	L	27	GLN
1	L	28	SER

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Mol	Chain	Res	Type
1	L	36	LYS
1	L	38	PHE
1	L	51	LYS
1	L	52	LEU
1	L	58	SER
1	L	60	ARG
1	L	69	THR
1	L	76	ASP
1	L	79	LEU
1	L	82	SER
1	L	89	LEU
1	L	95	GLN
1	L	96	ASN
1	L	99	SER
1	L	102	LEU
1	L	110	LEU
1	L	111	GLU
1	L	112	ILE
1	L	114	ARG
1	L	120	THR
1	L	122	SER
1	L	123	ILE
1	L	130	GLN
1	L	132	THR
1	L	133	SER
1	L	138	VAL
1	L	139	VAL
1	L	148	LYS
1	L	150	ILE
1	L	153	LYS
1	L	166	LEU
1	L	170	THR
1	L	171	ASP
1	L	176	ASP
1	L	178	THR
1	L	181	MET
1	L	185	LEU
1	L	189	LYS
1	L	195	HIS
1	L	196	ASN
1	L	201	GLU
1	L	203	THR

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Mol	Chain	Res	Type
1	L	205	LYS
1	L	206	THR
1	L	207	SER
1	L	211	ILE
1	L	214	SER
1	L	216	ASN
1	L	217	ARG
1	L	218	ASN
2	H	1	GLU
2	H	3	LYS
2	H	6	GLU
2	H	20	LEU
2	H	24	THR
2	H	28	THR
2	H	30	SER
2	H	34	MET
2	H	38	ARG
2	H	51	SER
2	H	53	ASN
2	H	54	LYS
2	H	57	LYS
2	H	59	THR
2	H	65	SER
2	H	66	VAL
2	H	67	LYS
2	H	69	ARG
2	H	71	ILE
2	H	74	ARG
2	H	75	ASP
2	H	91	GLU
2	H	95	ILE
2	H	100	ARG
2	H	105	SER
2	H	106	THR
2	H	116	THR
2	H	122	SER
2	H	123	GLU
2	H	129	THR
2	H	139	LEU
2	H	142	ASP
2	H	144	VAL
2	H	146	ILE

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Mol	Chain	Res	Type
2	H	149	LEU
2	H	165	LYS
2	H	166	SER
2	H	168	LYS
2	H	171	THR
2	H	179	LEU
2	H	188	SER
2	H	190	GLN
2	H	192	THR
2	H	193	LEU
2	H	197	GLU
2	H	200	GLU
2	H	208	VAL
2	H	209	GLN
2	H	215	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	34	ASN
1	L	37	ASN
1	L	95	GLN
1	L	96	ASN
1	L	172	GLN
1	L	195	HIS
1	L	196	ASN
1	L	216	ASN
2	H	53	ASN
2	H	101	ASN
2	H	189	ASN
2	H	210	HIS
2	H	216	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	H	223	-	4,4,4	0.73	0	6,6,6	0.34	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	223	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	L	220/220 (100%)	0.04	17 (7%)	19 17	2, 13, 31, 41	0
2	H	222/222 (100%)	-0.17	12 (5%)	31 27	2, 10, 24, 35	0
All	All	442/442 (100%)	-0.07	29 (6%)	24 21	2, 11, 30, 41	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	33	GLY	6.3
1	L	220	CYS	5.1
1	L	32	SER	4.8
2	H	181	SER	4.6
1	L	219	GLU	4.6
2	H	141	SER	4.0
1	L	163	ASN	3.9
1	L	31	ASN	3.5
1	L	34	ASN	3.4
1	L	162	GLN	3.3
2	H	169	ASP	3.2
1	L	208	THR	3.1
1	L	161	ARG	3.1
2	H	1	GLU	3.1
2	H	136	PRO	3.0
1	L	164	GLY	2.9
2	H	137	PRO	2.9
2	H	138	ALA	2.9
1	L	160	GLU	2.8
1	L	218	ASN	2.8
1	L	35	GLN	2.6
2	H	200	GLU	2.5
1	L	190	ASP	2.5
2	H	167	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	209	SER	2.2
2	H	140	SER	2.2
1	L	132	THR	2.2
2	H	31	ASP	2.1
2	H	91	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	H	223	5/5	0.98	0.10	26,26,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.