



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:45 PM UTC

PDB ID : 7F52 / pdb_00007f52
Title : Crystal Structure of IBV Nsp2
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Deposited on : 2021-06-21
Resolution : 2.56 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

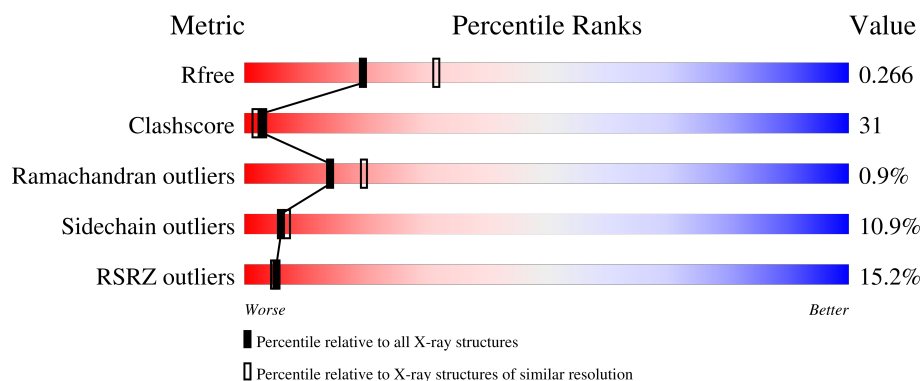
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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))
R_{free}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	A	673	12% 51% 26% 8% 13%
1	B	673	14% 48% 28% 8% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9717 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 Non-structural protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	584	Total	C	N	O	S	0	0	0
			4584	2980	775	804	25			
1	B	584	Total	C	N	O	S	0	0	0
			4584	2980	775	804	25			

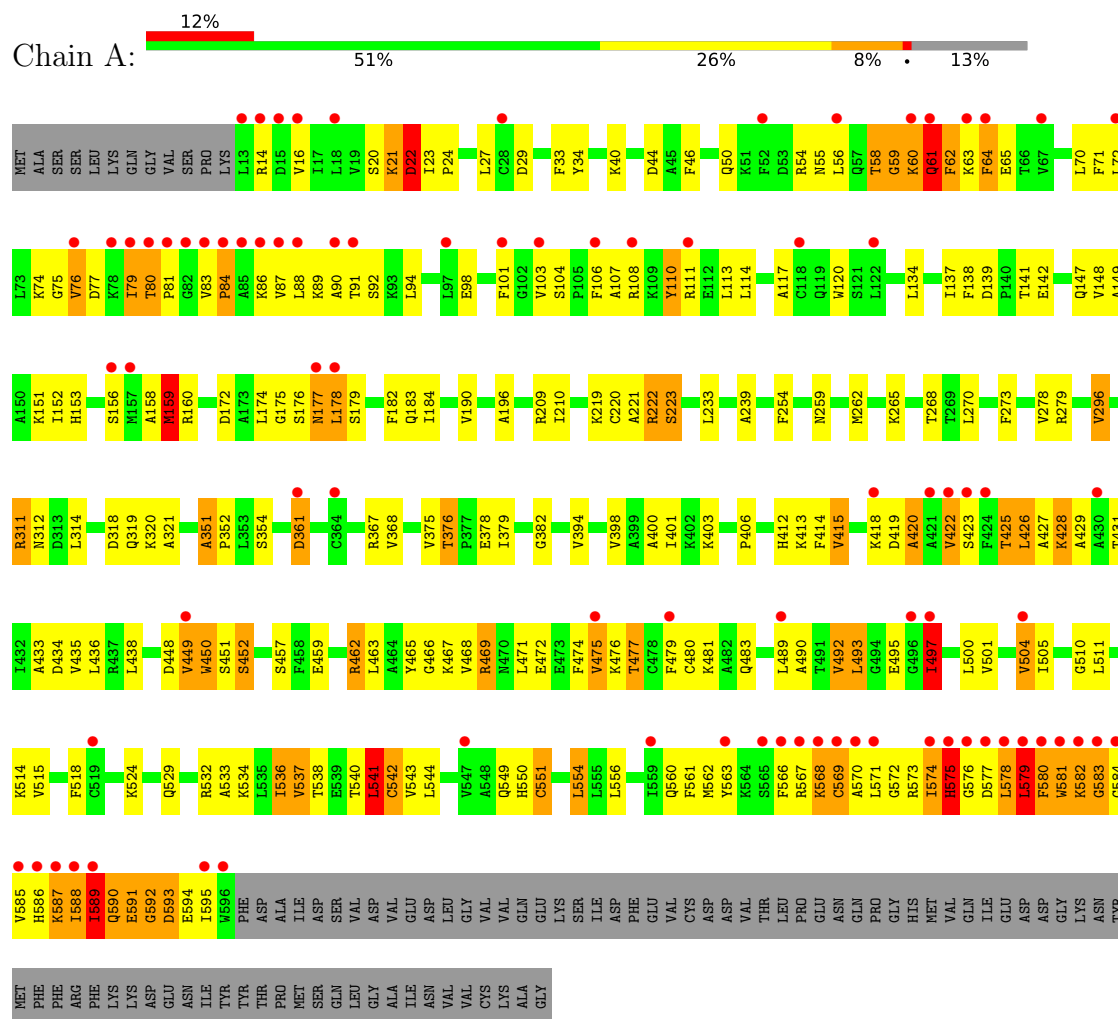
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	291	Total	O	0	0
			291	291		
2	B	258	Total	O	0	0
			258	258		

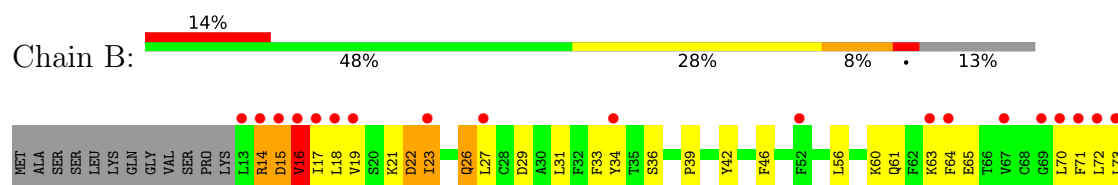
3 Residue-property plots [i](#)

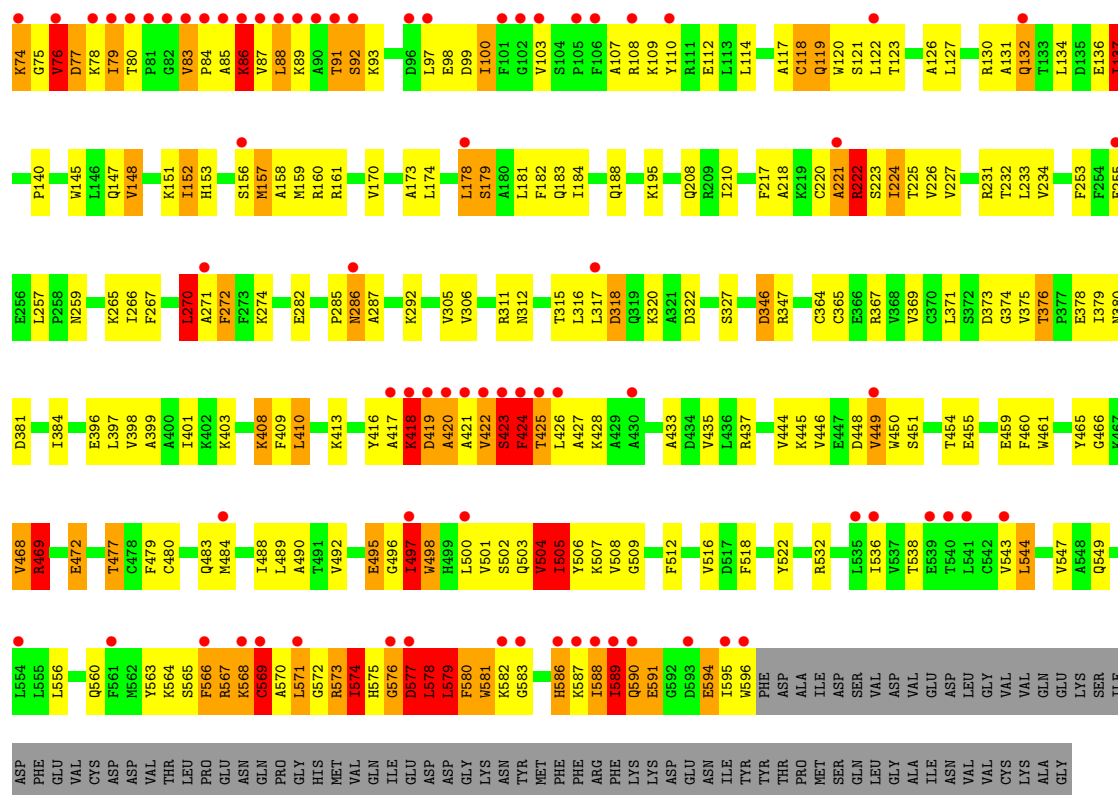
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Non-structural protein 2



• Molecule 1: Non-structural protein 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.04Å 192.31Å 105.75Å 90.00° 90.81° 90.00°	Depositor
Resolution (Å)	49.90 – 2.56 49.90 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.90-2.56) 92.1 (49.90-2.56)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.226 , 0.260 0.240 , 0.266	Depositor DCC
R_{free} test set	1997 reflections (2.73%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.932	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9717	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.66	0/4679	1.76	108/6320 (1.7%)
1	B	0.64	0/4679	1.83	115/6320 (1.8%)
All	All	0.65	0/9358	1.80	223/12640 (1.8%)

There are no bond length outliers.

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	423	SER	N-CA-C	31.00	154.34	111.56
1	B	317	LEU	N-CA-C	27.60	146.60	113.20
1	B	579	LEU	N-CA-C	27.21	151.23	112.04
1	B	418	LYS	N-CA-C	27.13	146.51	113.41
1	A	504	VAL	N-CA-C	27.10	140.84	113.47
1	A	423	SER	N-CA-C	26.91	150.88	112.94
1	A	569	CYS	N-CA-C	26.52	167.28	110.80
1	A	21	LYS	N-CA-C	-25.93	77.08	110.53
1	B	423	SER	CB-CA-C	-25.64	71.17	111.18
1	B	221	ALA	N-CA-C	-24.82	76.11	110.35
1	A	504	VAL	CB-CA-C	-23.61	85.12	110.62
1	A	222	ARG	N-CA-C	-22.05	77.81	108.23
1	A	569	CYS	CB-CA-C	-21.08	68.47	110.42
1	B	567	ARG	N-CA-C	21.05	147.11	108.17
1	B	587	LYS	N-CA-C	-20.29	75.36	109.24
1	A	223	SER	N-CA-C	19.68	139.17	110.24
1	A	579	LEU	CB-CA-C	-18.78	78.92	111.22
1	B	579	LEU	N-CA-CB	-18.77	81.11	110.19
1	A	423	SER	CB-CA-C	-17.80	80.02	110.64
1	B	420	ALA	N-CA-C	-17.60	87.63	110.33
1	A	61	GLN	CB-CA-C	-17.18	85.42	110.16
1	A	221	ALA	N-CA-C	17.14	133.58	113.19
1	A	577	ASP	N-CA-CB	-17.11	86.73	111.54
1	A	177	ASN	N-CA-C	-17.10	85.17	110.48
1	B	286	ASN	N-CA-CB	-16.97	89.83	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	GLY	N-CA-C	16.66	131.83	112.50
1	B	566	PHE	N-CA-C	16.55	134.05	111.54
1	B	578	LEU	CB-CA-C	-16.04	83.48	110.43
1	B	285	PRO	N-CA-C	15.92	139.56	113.78
1	A	76	VAL	CB-CA-C	-14.82	96.27	111.23
1	B	23	ILE	N-CA-C	-14.62	77.31	108.88
1	B	425	THR	N-CA-C	14.45	129.36	110.43
1	B	23	ILE	N-CA-CB	14.24	131.15	111.21
1	B	571	LEU	N-CA-C	-14.20	93.80	112.68
1	A	61	GLN	N-CA-C	14.05	130.90	109.96
1	A	578	LEU	CB-CA-C	-13.90	89.63	110.62
1	B	573	ARG	N-CA-C	13.51	128.72	110.35
1	B	567	ARG	CB-CA-C	-13.35	89.38	111.41
1	A	583	GLY	N-CA-C	-13.26	92.22	112.51
1	B	421	ALA	N-CA-C	13.05	138.59	110.80
1	A	58	THR	CB-CA-C	-13.00	83.73	109.33
1	B	498	TRP	N-CA-C	-13.00	97.89	113.88
1	B	421	ALA	N-CA-CB	-12.85	88.78	110.49
1	B	22	ASP	N-CA-C	-12.70	89.14	109.59
1	A	579	LEU	N-CA-CB	-12.38	89.54	110.46
1	B	564	LYS	N-CA-C	12.22	127.73	113.19
1	A	76	VAL	N-CA-C	11.82	124.27	106.42
1	B	504	VAL	N-CA-C	11.67	130.55	113.39
1	B	286	ASN	CB-CA-C	-11.65	94.65	112.12
1	B	580	PHE	N-CA-C	11.59	135.49	110.80
1	B	179	SER	N-CA-C	-11.51	99.77	114.04
1	B	571	LEU	CB-CA-C	11.41	129.30	110.24
1	A	449	VAL	CB-CA-C	11.37	121.79	110.65
1	B	497	ILE	CB-CA-C	-11.37	92.65	111.29
1	B	577	ASP	N-CA-C	11.21	126.87	111.74
1	A	21	LYS	CB-CA-C	11.09	133.36	110.40
1	A	58	THR	N-CA-C	-10.89	92.30	109.72
1	A	575	HIS	N-CA-C	-10.79	96.61	110.53
1	A	578	LEU	N-CA-C	-10.64	89.07	108.02
1	A	222	ARG	N-CA-CB	-10.58	95.48	110.51
1	B	426	LEU	CB-CA-C	10.53	129.11	110.36
1	B	418	LYS	CB-CA-C	-10.51	90.85	109.24
1	A	65	GLU	N-CA-C	-10.39	91.20	108.76
1	A	426	LEU	CB-CA-C	9.92	126.17	109.80
1	B	136	GLU	N-CA-C	-9.89	99.34	111.40
1	B	449	VAL	CB-CA-C	9.89	125.58	110.95
1	B	426	LEU	N-CA-C	-9.86	95.65	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	507	LYS	CB-CA-C	-9.81	95.13	111.02
1	A	222	ARG	CB-CA-C	-9.66	93.99	113.80
1	B	425	THR	N-CA-CB	-9.64	96.47	110.26
1	A	62	PHE	N-CA-CB	-9.64	95.52	110.46
1	B	569	CYS	N-CA-C	-9.61	88.92	107.57
1	A	569	CYS	CA-C-N	9.59	134.11	120.79
1	A	569	CYS	C-N-CA	9.59	134.11	120.79
1	A	422	VAL	N-CA-C	-9.49	95.91	108.06
1	A	576	GLY	N-CA-C	9.44	124.06	112.64
1	B	137	ILE	N-CA-CB	-9.43	99.34	112.35
1	A	426	LEU	N-CA-C	-9.37	95.89	110.42
1	B	508	VAL	N-CA-C	-9.29	93.63	107.37
1	A	423	SER	CA-C-N	9.02	135.67	122.41
1	A	423	SER	C-N-CA	9.02	135.67	122.41
1	B	427	ALA	N-CA-CB	8.87	126.47	111.57
1	A	60	LYS	CB-CA-C	-8.67	95.72	109.84
1	B	287	ALA	N-CA-C	8.67	115.93	108.13
1	B	318	ASP	N-CA-CB	8.63	128.43	114.27
1	A	595	ILE	N-CA-C	8.46	121.81	109.63
1	A	475	VAL	CB-CA-C	-8.39	99.56	111.31
1	A	427	ALA	N-CA-CB	8.34	123.98	110.97
1	B	226	VAL	CB-CA-C	8.30	122.94	111.49
1	B	450	TRP	N-CA-C	8.30	123.77	112.90
1	B	99	ASP	N-CA-C	-8.29	102.33	111.36
1	A	537	VAL	CB-CA-C	-8.27	100.89	110.73
1	B	468	VAL	N-CA-C	-8.26	95.83	107.80
1	A	320	LYS	N-CA-C	-8.22	97.68	110.42
1	B	495	GLU	N-CA-C	8.20	122.39	112.38
1	B	227	VAL	N-CA-CB	8.15	124.68	111.23
1	A	64	PHE	CB-CA-C	8.09	125.28	109.33
1	A	449	VAL	N-CA-C	-8.04	105.66	113.53
1	A	22	ASP	N-CA-C	8.01	124.69	113.56
1	A	582	LYS	N-CA-C	7.95	122.08	112.38
1	A	223	SER	CB-CA-C	-7.90	97.98	109.84
1	B	287	ALA	N-CA-CB	7.83	118.64	111.27
1	B	270	LEU	N-CA-C	7.83	122.77	110.32
1	A	64	PHE	N-CA-C	-7.81	97.22	109.72
1	B	417	ALA	CB-CA-C	7.77	125.19	110.51
1	B	272	PHE	N-CA-C	7.71	121.56	107.99
1	B	581	TRP	N-CA-C	7.71	120.27	110.33
1	A	537	VAL	N-CA-C	7.69	120.15	107.24
1	B	224	ILE	CB-CA-C	7.61	123.21	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	LEU	N-CA-C	7.58	120.61	108.41
1	A	319	GLN	N-CA-CB	-7.56	98.64	110.06
1	B	586	HIS	CB-CA-C	-7.56	96.57	110.62
1	A	476	LYS	N-CA-CB	-7.52	99.47	110.53
1	B	509	GLY	N-CA-C	-7.44	102.66	111.36
1	B	495	GLU	CB-CA-C	-7.44	94.63	110.32
1	B	317	LEU	CB-CA-C	-7.28	96.28	110.11
1	B	271	ALA	CB-CA-C	-7.24	98.15	110.16
1	A	65	GLU	N-CA-CB	7.23	123.30	110.80
1	A	575	HIS	CB-CA-C	7.20	125.29	110.40
1	B	574	ILE	N-CA-C	7.17	119.14	108.46
1	A	568	LYS	N-CA-C	-7.16	102.67	111.40
1	B	136	GLU	CB-CA-C	7.08	122.69	110.79
1	A	159	MET	N-CA-C	-6.98	104.50	112.87
1	A	581	TRP	N-CA-C	-6.91	99.12	108.86
1	A	428	LYS	CB-CA-C	-6.89	96.70	110.42
1	A	311	ARG	CB-CA-C	-6.85	97.30	109.70
1	A	505	ILE	N-CA-C	-6.83	102.55	111.09
1	A	422	VAL	CB-CA-C	6.77	122.23	111.80
1	A	429	ALA	N-CA-C	-6.76	103.34	112.26
1	B	100	ILE	N-CA-C	6.74	117.36	110.82
1	A	592	GLY	CA-C-N	6.72	134.38	121.54
1	A	592	GLY	C-N-CA	6.72	134.38	121.54
1	B	311	ARG	CB-CA-C	-6.64	96.69	109.37
1	B	408	LYS	N-CA-C	6.61	119.51	108.20
1	B	224	ILE	N-CA-C	-6.59	98.87	108.89
1	A	586	HIS	CB-CA-C	-6.57	95.95	109.94
1	B	271	ALA	N-CA-C	6.56	119.11	108.41
1	B	578	LEU	N-CA-C	-6.53	98.37	108.42
1	A	319	GLN	CB-CA-C	6.51	120.54	109.53
1	B	118	CYS	N-CA-C	6.45	119.31	111.82
1	B	222	ARG	N-CA-CB	6.45	121.40	110.49
1	A	450	TRP	N-CA-C	6.45	121.18	113.12
1	A	62	PHE	N-CA-C	6.39	119.92	110.46
1	A	579	LEU	N-CA-C	-6.38	95.05	107.62
1	B	92	SER	CB-CA-C	-6.38	98.75	109.53
1	A	220	CYS	CB-CA-C	-6.31	100.53	110.94
1	B	320	LYS	CB-CA-C	-6.31	98.87	109.53
1	A	551	CYS	N-CA-CB	-6.29	100.85	110.92
1	A	476	LYS	N-CA-C	6.29	121.24	113.50
1	B	77	ASP	CB-CA-C	-6.27	109.33	116.54
1	B	469	ARG	N-CA-C	-6.27	105.79	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	ASP	N-CA-CB	-6.24	100.64	110.69
1	B	505	ILE	CB-CA-C	-6.22	103.89	112.04
1	A	312	ASN	N-CA-C	6.21	120.45	112.26
1	A	415	VAL	CB-CA-C	-6.19	100.78	110.69
1	B	270	LEU	N-CA-CB	-6.17	100.35	110.41
1	B	119	GLN	N-CA-C	6.10	119.20	111.69
1	B	218	ALA	N-CA-C	-6.10	103.97	112.45
1	A	541	LEU	CB-CA-C	-6.08	100.78	110.81
1	B	178	LEU	N-CA-C	-6.07	94.38	107.49
1	B	503	GLN	CB-CA-C	6.03	121.50	110.11
1	B	576	GLY	N-CA-C	-6.03	98.89	113.18
1	B	583	GLY	N-CA-C	6.02	127.45	113.18
1	A	590	GLN	CA-C-N	5.99	132.97	121.54
1	A	590	GLN	C-N-CA	5.99	132.97	121.54
1	B	86	LYS	N-CA-C	-5.97	99.92	109.96
1	B	468	VAL	CB-CA-C	5.97	119.68	110.96
1	B	312	ASN	N-CA-C	5.96	119.86	112.59
1	B	567	ARG	N-CA-CB	-5.95	102.02	110.46
1	A	221	ALA	CB-CA-C	-5.94	98.75	110.27
1	A	579	LEU	CA-C-N	5.93	130.32	121.72
1	A	579	LEU	C-N-CA	5.93	130.32	121.72
1	A	351	ALA	CA-C-N	-5.91	113.85	119.76
1	A	351	ALA	C-N-CA	-5.91	113.85	119.76
1	A	268	THR	CB-CA-C	-5.90	109.20	117.23
1	B	408	LYS	CB-CA-C	-5.88	101.37	110.78
1	B	16	VAL	N-CA-C	-5.87	97.13	109.34
1	A	420	ALA	N-CA-C	-5.85	103.39	110.88
1	B	15	ASP	N-CA-C	-5.82	101.93	110.42
1	B	450	TRP	N-CA-CB	-5.79	101.64	110.33
1	B	93	LYS	N-CA-C	5.78	118.28	109.95
1	B	586	HIS	N-CA-C	5.77	117.62	108.79
1	B	574	ILE	N-CA-CB	-5.75	102.01	111.44
1	B	417	ALA	N-CA-C	-5.75	102.26	110.59
1	B	424	PHE	N-CA-C	5.74	120.08	111.81
1	B	225	THR	N-CA-CB	5.66	119.93	110.59
1	B	580	PHE	CB-CA-C	-5.63	99.21	110.42
1	A	223	SER	N-CA-CB	-5.62	100.77	109.48
1	B	572	GLY	N-CA-C	-5.61	101.25	110.56
1	A	110	TYR	CA-C-N	-5.59	112.95	122.56
1	A	110	TYR	C-N-CA	-5.59	112.95	122.56
1	A	589	ILE	CA-C-N	5.55	132.13	121.54
1	A	589	ILE	C-N-CA	5.55	132.13	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	VAL	CB-CA-C	5.49	118.72	110.98
1	A	542	CYS	N-CA-C	5.49	118.43	107.62
1	B	132	GLN	N-CA-C	-5.46	106.46	113.23
1	B	103	VAL	N-CA-C	5.42	115.66	107.80
1	B	587	LYS	CB-CA-C	-5.38	98.69	109.35
1	A	492	VAL	CB-CA-C	-5.37	101.22	110.94
1	B	217	PHE	CB-CA-C	-5.37	99.91	110.11
1	A	361	ASP	N-CA-C	-5.36	100.36	108.67
1	B	84	PRO	N-CA-C	-5.34	101.47	112.47
1	A	423	SER	O-C-N	5.33	128.64	122.19
1	B	272	PHE	N-CA-CB	-5.32	102.42	110.35
1	A	88	LEU	CB-CA-C	5.31	121.86	110.45
1	A	149	ALA	N-CA-C	5.30	117.38	110.43
1	A	490	ALA	N-CA-C	-5.29	105.97	112.90
1	A	318	ASP	N-CA-C	5.28	119.56	113.18
1	A	593	ASP	N-CA-CB	5.27	119.40	110.49
1	A	98	GLU	CB-CA-C	5.27	119.53	110.79
1	B	91	THR	N-CA-CB	-5.26	103.18	111.39
1	B	573	ARG	CB-CA-C	-5.22	100.27	109.62
1	A	497	ILE	N-CA-C	-5.21	105.42	110.42
1	A	550	HIS	CB-CA-C	-5.20	101.59	110.95
1	A	474	PHE	CB-CA-C	-5.17	101.00	109.99
1	B	566	PHE	CB-CA-C	-5.15	104.28	111.80
1	B	320	LYS	N-CA-C	5.11	118.28	110.20
1	B	472	GLU	N-CA-C	5.08	118.25	111.75
1	A	577	ASP	CA-C-N	-5.06	115.67	122.86
1	A	577	ASP	C-N-CA	-5.06	115.67	122.86
1	B	427	ALA	N-CA-C	-5.04	100.48	108.14
1	B	222	ARG	N-CA-C	5.02	121.50	110.80
1	B	285	PRO	CB-CA-C	-5.00	104.75	113.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4584	0	4703	224	0
1	B	4584	0	4704	360	0
2	A	291	0	0	66	0
2	B	258	0	0	119	0
All	All	9717	0	9407	584	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 31.

All (584) 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:B:579:LEU:HD11	1:B:581:TRP:CD1	1.21	1.65
1:B:579:LEU:CD1	1:B:581:TRP:HD1	0.95	1.58
1:B:578:LEU:HD22	1:B:579:LEU:CA	1.35	1.55
1:B:579:LEU:CD1	1:B:581:TRP:CD1	1.87	1.31
1:B:265:LYS:HD3	2:B:725:HOH:O	1.18	1.31
1:B:418:LYS:NZ	2:B:701:HOH:O	1.57	1.31
1:B:578:LEU:HD22	1:B:579:LEU:N	1.41	1.31
1:B:578:LEU:CD2	1:B:579:LEU:CA	2.09	1.30
1:B:570:ALA:HB2	2:B:840:HOH:O	1.27	1.28
1:B:61:GLN:OE1	1:B:74:LYS:NZ	1.66	1.28
1:B:578:LEU:O	1:B:578:LEU:CD1	1.83	1.26
1:A:581:TRP:CH2	1:A:583:GLY:HA3	1.72	1.23
1:B:79:ILE:HG23	2:B:807:HOH:O	1.38	1.23
1:B:575:HIS:O	1:B:578:LEU:HD12	1.37	1.23
1:B:578:LEU:O	1:B:578:LEU:HD13	1.10	1.22
1:B:568:LYS:O	1:B:574:ILE:HD11	1.36	1.21
1:B:367:ARG:NH2	1:B:424:PHE:HE2	1.39	1.20
1:B:575:HIS:H	1:B:578:LEU:CD1	1.56	1.17
1:A:538:THR:O	1:A:560:GLN:NE2	1.78	1.15
1:B:578:LEU:HD22	1:B:579:LEU:HA	1.22	1.14
1:A:420:ALA:HB1	2:A:862:HOH:O	1.45	1.13
1:B:15:ASP:OD1	1:B:86:LYS:NZ	1.80	1.13
1:B:594:GLU:HG3	2:B:945:HOH:O	1.47	1.12
1:A:83:VAL:HG22	1:A:84:PRO:CD	1.80	1.12
1:A:581:TRP:CZ2	1:A:583:GLY:HA3	1.83	1.12
1:A:419:ASP:OD2	2:A:705:HOH:O	1.65	1.12
1:A:504:VAL:HG12	1:A:504:VAL:O	1.36	1.12
1:A:83:VAL:HG21	2:A:991:HOH:O	1.46	1.12
1:B:578:LEU:HD22	1:B:578:LEU:C	1.72	1.12
1:B:88:LEU:HD21	1:B:97:LEU:HD13	1.21	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:LYS:O	1:B:574:ILE:CD1	1.98	1.11
1:B:15:ASP:CG	1:B:86:LYS:NZ	2.09	1.11
1:A:579:LEU:HG	1:A:579:LEU:O	1.44	1.10
1:B:575:HIS:H	1:B:578:LEU:HD11	0.96	1.09
1:B:85:ALA:HB3	2:B:885:HOH:O	0.92	1.09
1:B:578:LEU:CD2	1:B:579:LEU:N	2.15	1.09
1:B:575:HIS:N	1:B:578:LEU:HD11	1.65	1.08
1:B:83:VAL:HG12	2:B:885:HOH:O	1.50	1.08
1:A:581:TRP:CE3	1:A:583:GLY:N	2.22	1.07
1:B:565:SER:O	1:B:573:ARG:NH1	1.88	1.07
1:B:579:LEU:HD12	1:B:581:TRP:HD1	1.11	1.07
1:A:61:GLN:CG	1:A:61:GLN:O	1.97	1.07
1:B:567:ARG:O	1:B:567:ARG:CG	1.96	1.06
1:B:579:LEU:HD12	1:B:581:TRP:CD1	1.86	1.06
1:B:75:GLY:HA2	2:B:843:HOH:O	1.52	1.05
1:B:88:LEU:CD1	1:B:100:ILE:HD12	1.84	1.05
1:B:567:ARG:O	1:B:567:ARG:HG2	1.26	1.04
1:A:419:ASP:CB	2:A:705:HOH:O	2.04	1.04
1:A:368:VAL:HB	1:A:422:VAL:HG21	1.38	1.04
1:B:588:ILE:HD13	1:B:588:ILE:H	1.21	1.02
1:B:367:ARG:NH2	1:B:424:PHE:CE2	2.28	1.02
1:B:397:LEU:O	2:B:702:HOH:O	1.77	1.01
1:A:504:VAL:O	1:A:504:VAL:CG1	2.04	1.01
1:A:581:TRP:O	1:A:583:GLY:O	1.79	1.00
1:B:579:LEU:HD13	1:B:581:TRP:H	1.25	1.00
1:A:83:VAL:HG22	1:A:84:PRO:HD2	1.34	1.00
1:B:14:ARG:HD2	1:B:15:ASP:H	1.22	1.00
1:B:497:ILE:O	1:B:497:ILE:HG22	1.63	0.98
1:B:578:LEU:HD23	1:B:580:PHE:CD1	1.99	0.98
1:A:84:PRO:HB2	2:A:930:HOH:O	1.62	0.97
1:B:579:LEU:CD1	1:B:581:TRP:H	1.77	0.97
1:B:579:LEU:HD11	1:B:581:TRP:CG	1.98	0.97
1:A:58:THR:O	2:A:706:HOH:O	1.83	0.97
1:B:418:LYS:O	2:B:703:HOH:O	1.81	0.95
1:A:541:LEU:O	1:A:541:LEU:HD23	1.65	0.95
1:A:579:LEU:O	1:A:579:LEU:CG	1.96	0.94
1:A:574:ILE:HG12	1:A:579:LEU:HA	1.48	0.93
1:B:569:CYS:SG	2:B:925:HOH:O	2.26	0.93
1:B:253:PHE:O	2:B:704:HOH:O	1.86	0.92
1:A:419:ASP:HB2	2:A:705:HOH:O	1.62	0.92
1:B:574:ILE:HD12	1:B:574:ILE:N	1.83	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ARG:HH21	1:B:424:PHE:HE2	1.16	0.92
1:B:578:LEU:CD2	1:B:580:PHE:HD1	1.83	0.91
1:A:61:GLN:O	1:A:61:GLN:HG2	1.70	0.91
1:B:578:LEU:CD2	1:B:578:LEU:C	2.25	0.90
1:B:15:ASP:CG	1:B:86:LYS:HZ1	1.74	0.90
1:B:578:LEU:HD13	1:B:578:LEU:C	1.96	0.90
1:B:567:ARG:HD2	2:B:925:HOH:O	1.71	0.89
1:B:88:LEU:HD21	1:B:97:LEU:CD1	2.01	0.89
1:B:594:GLU:CG	2:B:945:HOH:O	2.12	0.89
1:A:425:THR:HG22	2:A:703:HOH:O	1.72	0.89
1:B:420:ALA:O	2:B:705:HOH:O	1.89	0.89
1:B:497:ILE:O	1:B:497:ILE:CG2	2.20	0.89
1:B:15:ASP:CB	1:B:86:LYS:NZ	2.37	0.88
1:B:575:HIS:O	1:B:578:LEU:CD1	2.20	0.88
1:B:565:SER:O	1:B:573:ARG:NH2	2.06	0.87
1:A:489:LEU:O	1:A:493:LEU:HD22	1.75	0.87
1:B:565:SER:O	1:B:573:ARG:CZ	2.23	0.86
1:A:419:ASP:CG	2:A:705:HOH:O	2.05	0.86
1:B:578:LEU:CD2	1:B:579:LEU:C	2.48	0.86
1:B:220:CYS:C	1:B:221:ALA:O	2.00	0.85
1:B:159:MET:HE1	1:B:210:ILE:HG23	1.57	0.85
1:B:365:CYS:SG	2:B:717:HOH:O	2.35	0.85
1:A:581:TRP:CZ3	1:A:583:GLY:HA3	2.12	0.84
1:B:477:THR:HG22	1:B:480:CYS:H	1.41	0.83
1:B:88:LEU:CD1	1:B:100:ILE:CD1	2.56	0.83
1:B:15:ASP:CB	1:B:86:LYS:HZ2	1.92	0.82
1:A:581:TRP:CH2	1:A:583:GLY:CA	2.60	0.82
1:A:74:LYS:NZ	1:A:75:GLY:O	2.13	0.81
1:A:581:TRP:CZ3	1:A:583:GLY:CA	2.63	0.81
1:B:27:LEU:HD22	1:B:92:SER:O	1.80	0.81
1:B:418:LYS:O	1:B:418:LYS:HG2	1.79	0.81
1:B:15:ASP:HB3	1:B:86:LYS:HZ2	1.45	0.81
1:A:368:VAL:HB	1:A:422:VAL:CG2	2.11	0.81
1:B:578:LEU:CD2	1:B:579:LEU:HA	1.97	0.81
1:B:495:GLU:O	2:B:706:HOH:O	1.98	0.81
1:B:578:LEU:CD2	1:B:580:PHE:CD1	2.62	0.81
1:A:64:PHE:O	1:A:70:LEU:HD12	1.81	0.80
1:A:61:GLN:O	1:A:61:GLN:HG3	1.81	0.80
1:B:466:GLY:O	1:B:469:ARG:NH1	2.15	0.80
1:B:286:ASN:H	1:B:286:ASN:ND2	1.76	0.79
1:B:61:GLN:CB	1:B:74:LYS:HD2	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:SER:OG	1:A:210:ILE:CD1	2.30	0.79
1:A:514:LYS:O	2:A:707:HOH:O	2.00	0.79
1:B:500:LEU:O	2:B:707:HOH:O	1.99	0.79
1:B:367:ARG:CZ	1:B:424:PHE:HE2	1.95	0.79
1:B:76:VAL:O	1:B:76:VAL:HG22	1.81	0.79
1:B:61:GLN:HB3	1:B:74:LYS:HD2	1.64	0.78
1:B:575:HIS:O	1:B:576:GLY:C	2.26	0.78
1:A:536:ILE:HD11	1:A:582:LYS:HA	1.63	0.78
1:B:83:VAL:CG1	2:B:885:HOH:O	2.18	0.78
1:B:170:VAL:O	2:B:709:HOH:O	2.00	0.78
1:B:590:GLN:HG2	2:B:917:HOH:O	1.82	0.78
1:B:570:ALA:HB3	2:B:791:HOH:O	1.82	0.78
1:B:15:ASP:HB3	1:B:86:LYS:NZ	1.98	0.77
1:B:590:GLN:HB3	2:B:915:HOH:O	1.85	0.77
1:B:14:ARG:HD2	1:B:15:ASP:N	2.00	0.77
1:B:79:ILE:HD12	1:B:79:ILE:H	1.49	0.77
1:B:575:HIS:N	1:B:578:LEU:CD1	2.35	0.77
1:B:416:TYR:OH	2:B:708:HOH:O	2.00	0.77
1:B:61:GLN:HB3	1:B:74:LYS:HZ2	1.50	0.76
1:A:89:LYS:HG3	1:A:90:ALA:H	1.49	0.76
1:B:497:ILE:O	1:B:501:VAL:HG23	1.85	0.76
1:B:567:ARG:HG3	1:B:569:CYS:SG	2.26	0.76
1:B:16:VAL:HG13	1:B:74:LYS:HE3	1.66	0.76
1:B:579:LEU:HD13	1:B:581:TRP:N	2.01	0.75
1:B:126:ALA:HB3	2:B:728:HOH:O	1.85	0.75
1:B:89:LYS:NZ	2:B:722:HOH:O	2.20	0.75
1:B:574:ILE:HD12	1:B:574:ILE:H	1.51	0.75
1:A:419:ASP:HB2	2:A:704:HOH:O	1.86	0.75
1:B:419:ASP:C	1:B:420:ALA:O	2.20	0.74
1:A:83:VAL:HG22	1:A:84:PRO:HD3	1.66	0.74
1:A:83:VAL:CG2	1:A:84:PRO:CD	2.64	0.74
1:A:400:ALA:HA	1:A:403:LYS:HE2	1.70	0.74
1:B:566:PHE:C	1:B:573:ARG:NH2	2.45	0.74
1:B:221:ALA:O	2:B:710:HOH:O	2.05	0.74
1:A:581:TRP:CZ3	1:A:583:GLY:N	2.56	0.73
1:B:79:ILE:HD12	1:B:79:ILE:N	2.04	0.73
1:B:578:LEU:HD23	1:B:579:LEU:CA	2.18	0.73
1:B:222:ARG:HG3	1:B:222:ARG:HH11	1.53	0.73
1:B:88:LEU:CD2	1:B:97:LEU:HD13	2.12	0.72
1:B:446:VAL:HG12	1:B:446:VAL:O	1.89	0.72
1:B:272:PHE:O	2:B:712:HOH:O	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:LYS:NZ	2:A:720:HOH:O	2.21	0.72
1:A:80:THR:OG1	1:A:81:PRO:HD2	1.90	0.72
1:B:483:GLN:OE1	2:B:711:HOH:O	2.06	0.72
1:A:581:TRP:CE2	1:A:583:GLY:HA3	2.25	0.72
1:A:321:ALA:O	2:A:709:HOH:O	2.07	0.71
1:B:588:ILE:H	1:B:588:ILE:CD1	2.00	0.71
1:A:578:LEU:HB2	1:A:580:PHE:CE1	2.25	0.71
1:A:378:GLU:O	2:A:711:HOH:O	2.08	0.71
1:A:142:GLU:OE2	2:A:712:HOH:O	2.09	0.71
1:A:196:ALA:O	2:A:710:HOH:O	2.07	0.71
1:B:178:LEU:HB2	2:B:732:HOH:O	1.90	0.71
1:B:88:LEU:HD13	1:B:100:ILE:HD12	1.73	0.70
1:B:495:GLU:O	1:B:495:GLU:HG3	1.91	0.70
1:B:259:ASN:ND2	2:B:725:HOH:O	2.23	0.70
1:A:20:SER:C	1:A:21:LYS:O	2.11	0.70
1:B:88:LEU:HD11	1:B:100:ILE:HD12	1.71	0.70
1:B:61:GLN:CD	1:B:74:LYS:HZ3	2.01	0.69
1:A:40:LYS:N	2:A:714:HOH:O	2.10	0.69
1:A:76:VAL:O	1:A:76:VAL:HG23	1.91	0.69
1:A:175:GLY:O	2:A:713:HOH:O	2.09	0.69
1:B:518:PHE:O	2:B:713:HOH:O	2.11	0.69
1:B:257:LEU:N	2:B:704:HOH:O	2.24	0.69
1:B:15:ASP:CG	1:B:86:LYS:HZ3	2.00	0.68
1:A:111:ARG:HA	1:A:114:LEU:HB2	1.76	0.68
1:A:114:LEU:HD21	1:A:151:LYS:HD3	1.76	0.68
1:A:259:ASN:OD1	2:A:715:HOH:O	2.12	0.68
1:B:567:ARG:HA	1:B:573:ARG:NE	2.09	0.68
1:B:63:LYS:HG3	1:B:70:LEU:HD11	1.76	0.68
1:A:533:ALA:HB1	1:A:544:LEU:HD22	1.76	0.67
1:B:121:SER:N	2:B:724:HOH:O	2.23	0.67
1:B:566:PHE:CA	1:B:573:ARG:NH2	2.57	0.67
1:B:575:HIS:C	1:B:578:LEU:HD12	2.19	0.67
1:A:541:LEU:O	1:A:541:LEU:CD2	2.42	0.67
1:A:578:LEU:CB	1:A:580:PHE:CE1	2.78	0.67
1:B:596:TRP:C	2:B:803:HOH:O	2.38	0.67
1:A:536:ILE:HD13	1:A:583:GLY:O	1.95	0.66
1:B:591:GLU:OE1	1:B:591:GLU:HA	1.92	0.66
1:A:56:LEU:HD12	1:A:62:PHE:HZ	1.60	0.66
1:B:396:GLU:OE1	2:B:715:HOH:O	2.14	0.66
1:B:208:GLN:HG3	2:B:810:HOH:O	1.96	0.66
1:A:83:VAL:CG2	1:A:84:PRO:HD3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LEU:HB2	1:A:580:PHE:HE1	1.60	0.66
1:B:132:GLN:O	1:B:132:GLN:HG3	1.96	0.66
1:A:94:LEU:HD21	1:A:108:ARG:HG2	1.76	0.66
1:A:536:ILE:HD13	1:A:584:GLY:HA2	1.78	0.66
1:A:89:LYS:HG3	1:A:90:ALA:N	2.11	0.66
1:B:178:LEU:HB3	1:B:181:LEU:HD12	1.77	0.66
1:A:451:SER:HA	1:A:479:PHE:HD2	1.60	0.65
1:B:122:LEU:N	2:B:728:HOH:O	2.28	0.65
1:B:369:VAL:HG13	1:B:424:PHE:O	1.96	0.65
1:B:364:CYS:O	2:B:717:HOH:O	2.15	0.65
1:B:574:ILE:CD1	1:B:574:ILE:N	2.51	0.65
1:A:77:ASP:OD1	1:A:77:ASP:O	2.14	0.65
1:B:566:PHE:C	1:B:573:ARG:CZ	2.69	0.65
1:A:24:PRO:HD3	1:A:90:ALA:HA	1.77	0.65
1:A:518:PHE:HB3	2:A:707:HOH:O	1.97	0.65
1:B:578:LEU:HD13	1:B:578:LEU:H	1.61	0.65
1:B:578:LEU:HD23	1:B:580:PHE:HD1	1.39	0.65
1:B:579:LEU:HD13	1:B:579:LEU:C	2.22	0.65
1:B:454:THR:HG23	2:B:736:HOH:O	1.97	0.65
1:B:118:CYS:SG	2:B:836:HOH:O	2.54	0.65
1:B:578:LEU:CD2	1:B:578:LEU:O	2.43	0.65
1:B:88:LEU:HD12	1:B:100:ILE:CD1	2.25	0.65
1:A:176:SER:OG	2:A:716:HOH:O	2.15	0.64
1:A:44:ASP:HB3	2:A:714:HOH:O	1.98	0.64
1:B:233:LEU:O	2:B:716:HOH:O	2.14	0.64
1:A:259:ASN:HA	2:A:715:HOH:O	1.97	0.64
1:A:580:PHE:CD2	1:A:585:VAL:HG22	2.33	0.63
1:A:580:PHE:HD1	1:A:580:PHE:H	1.44	0.63
1:B:130:ARG:O	1:B:134:LEU:HD12	1.97	0.63
1:B:498:TRP:O	1:B:502:SER:OG	2.16	0.63
1:A:209:ARG:NH1	2:A:710:HOH:O	2.31	0.63
1:A:431:THR:HG22	1:A:433:ALA:H	1.64	0.63
1:B:422:VAL:O	2:B:705:HOH:O	2.15	0.63
1:A:551:CYS:HB2	2:A:707:HOH:O	1.97	0.62
1:B:19:VAL:O	1:B:75:GLY:HA3	1.99	0.62
1:A:581:TRP:CE3	1:A:583:GLY:CA	2.82	0.62
1:B:573:ARG:HA	1:B:574:ILE:HD12	1.82	0.62
1:B:594:GLU:OE2	1:B:594:GLU:HA	1.99	0.62
1:A:562:MET:O	1:A:562:MET:HG2	1.99	0.62
1:A:581:TRP:CD2	1:A:583:GLY:N	2.62	0.62
1:B:465:TYR:O	1:B:468:VAL:O	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LEU:HB2	1:B:87:VAL:HG22	1.82	0.62
1:B:188:GLN:NE2	2:B:731:HOH:O	2.32	0.61
1:B:423:SER:O	1:B:423:SER:OG	1.81	0.61
1:B:130:ARG:O	1:B:134:LEU:CD1	2.49	0.61
1:B:316:LEU:HA	2:B:717:HOH:O	2.00	0.61
1:A:147:GLN:HA	2:A:753:HOH:O	2.01	0.61
1:A:560:GLN:HA	1:A:563:TYR:HB3	1.81	0.61
1:B:60:LYS:HD2	1:B:61:GLN:H	1.64	0.61
1:B:578:LEU:HD22	1:B:578:LEU:O	1.97	0.61
1:A:156:SER:OG	1:A:210:ILE:HD12	2.01	0.61
1:B:532:ARG:HG3	2:B:811:HOH:O	1.99	0.61
1:B:433:ALA:O	1:B:437:ARG:HG3	2.01	0.60
1:B:578:LEU:HD23	1:B:579:LEU:C	2.26	0.60
1:A:156:SER:OG	1:A:210:ILE:HD11	2.01	0.60
1:A:58:THR:O	1:A:58:THR:OG1	2.13	0.60
1:A:376:THR:HG22	1:A:379:ILE:H	1.66	0.60
1:A:354:SER:HB3	2:A:817:HOH:O	2.01	0.60
1:B:184:ILE:H	1:B:184:ILE:HD12	1.67	0.60
1:B:161:ARG:HG2	2:B:849:HOH:O	2.02	0.60
1:B:504:VAL:HG13	2:B:707:HOH:O	2.02	0.60
1:B:568:LYS:O	1:B:574:ILE:HD13	1.97	0.60
1:B:594:GLU:CB	2:B:945:HOH:O	2.45	0.60
1:B:21:LYS:HD3	1:B:76:VAL:HA	1.84	0.60
1:B:569:CYS:HB2	2:B:745:HOH:O	2.01	0.59
1:B:574:ILE:HG23	1:B:578:LEU:O	2.02	0.59
1:A:471:LEU:HB2	2:A:733:HOH:O	2.01	0.59
1:A:475:VAL:HG23	1:A:475:VAL:O	2.01	0.59
1:B:549:GLN:HG2	2:B:921:HOH:O	2.02	0.59
1:B:578:LEU:HD21	1:B:580:PHE:HD1	1.62	0.59
1:A:59:GLY:O	1:A:74:LYS:HE2	2.01	0.59
1:B:22:ASP:OD1	1:B:22:ASP:O	2.21	0.59
1:B:495:GLU:O	1:B:495:GLU:CG	2.49	0.59
1:B:64:PHE:HB3	2:B:821:HOH:O	2.03	0.59
1:B:61:GLN:HB3	1:B:74:LYS:NZ	2.17	0.58
1:B:518:PHE:CE1	1:B:522:TYR:HD2	2.21	0.58
1:B:538:THR:O	1:B:560:GLN:NE2	2.30	0.58
1:A:352:PRO:HD3	1:A:361:ASP:O	2.03	0.58
1:B:588:ILE:HD13	1:B:588:ILE:N	2.04	0.58
1:A:426:LEU:HD13	1:A:435:VAL:HG22	1.84	0.58
1:B:376:THR:HG22	1:B:379:ILE:H	1.69	0.58
1:B:127:LEU:HD22	2:B:874:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ILE:H	1:B:17:ILE:HD12	1.68	0.58
1:B:446:VAL:O	1:B:446:VAL:CG1	2.52	0.58
1:B:270:LEU:HD21	2:B:848:HOH:O	2.04	0.57
1:A:468:VAL:HB	2:A:733:HOH:O	2.04	0.57
1:B:56:LEU:HB3	2:B:928:HOH:O	2.04	0.57
1:B:259:ASN:HA	2:B:725:HOH:O	2.05	0.57
1:B:27:LEU:HB3	2:B:730:HOH:O	2.03	0.57
1:B:120:TRP:N	2:B:724:HOH:O	2.37	0.57
1:B:566:PHE:CB	1:B:573:ARG:NH2	2.68	0.57
1:B:574:ILE:HA	1:B:578:LEU:HD11	1.85	0.57
1:A:21:LYS:O	1:A:22:ASP:OD1	2.22	0.57
1:B:315:THR:OG1	1:B:422:VAL:HG21	2.04	0.57
1:A:101:PHE:HB3	2:A:972:HOH:O	2.03	0.57
1:A:580:PHE:N	1:A:580:PHE:CD1	2.72	0.57
1:B:152:ILE:HD12	1:B:153:HIS:H	1.69	0.57
1:B:381:ASP:OD2	1:B:477:THR:HB	2.05	0.57
1:A:492:VAL:HG22	1:A:492:VAL:O	2.05	0.56
1:A:270:LEU:HD11	2:A:952:HOH:O	2.04	0.56
1:A:536:ILE:O	2:A:718:HOH:O	2.18	0.56
1:A:541:LEU:HD23	1:A:541:LEU:C	2.30	0.56
1:B:151:LYS:NZ	2:B:739:HOH:O	2.38	0.56
1:B:270:LEU:O	2:B:718:HOH:O	2.18	0.56
1:B:195:LYS:HD2	1:B:195:LYS:O	2.06	0.56
1:B:367:ARG:CZ	1:B:424:PHE:CE2	2.83	0.56
1:A:139:ASP:N	2:A:712:HOH:O	2.11	0.55
1:A:23:ILE:HB	1:A:27:LEU:HD23	1.88	0.55
1:A:574:ILE:HG22	1:A:574:ILE:O	2.05	0.55
1:B:282:GLU:OE2	1:B:292:LYS:NZ	2.39	0.55
1:B:156:SER:HA	1:B:159:MET:HE3	1.87	0.55
1:B:580:PHE:O	2:B:719:HOH:O	2.18	0.55
1:A:477:THR:O	1:A:481:LYS:HD2	2.07	0.55
1:B:257:LEU:HG	2:B:704:HOH:O	2.07	0.55
1:B:574:ILE:CA	1:B:578:LEU:HD11	2.36	0.55
1:A:398:VAL:HA	2:A:941:HOH:O	2.05	0.55
1:A:581:TRP:CE2	1:A:583:GLY:CA	2.90	0.55
1:B:318:ASP:OD1	1:B:318:ASP:O	2.25	0.54
1:B:588:ILE:O	1:B:588:ILE:HG12	2.07	0.54
1:B:88:LEU:HD12	1:B:100:ILE:HD11	1.89	0.54
1:A:54:ARG:NH1	2:A:739:HOH:O	2.40	0.54
1:B:61:GLN:CB	1:B:74:LYS:NZ	2.70	0.54
1:B:547:VAL:HB	2:B:871:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:LEU:HD12	2:B:717:HOH:O	2.07	0.54
1:B:578:LEU:HG	1:B:580:PHE:HE1	1.73	0.54
1:A:80:THR:OG1	1:A:81:PRO:CD	2.56	0.53
1:B:14:ARG:NH1	1:B:15:ASP:O	2.41	0.53
1:B:63:LYS:HE2	1:B:70:LEU:HD11	1.89	0.53
1:B:451:SER:HA	1:B:479:PHE:CD2	2.43	0.53
1:A:46:PHE:O	1:A:50:GLN:HG2	2.09	0.53
1:B:232:THR:HG23	2:B:716:HOH:O	2.08	0.53
1:A:401:ILE:HD12	2:A:941:HOH:O	2.08	0.53
1:A:540:THR:OG1	2:A:717:HOH:O	2.17	0.53
1:B:461:TRP:CD1	2:B:767:HOH:O	2.61	0.53
1:B:21:LYS:NZ	2:B:743:HOH:O	2.41	0.53
1:A:24:PRO:HD2	1:A:27:LEU:HB3	1.89	0.53
1:A:578:LEU:HB3	1:A:580:PHE:CE1	2.43	0.53
1:B:374:GLY:O	2:B:720:HOH:O	2.19	0.53
1:A:56:LEU:HD12	1:A:62:PHE:CZ	2.41	0.53
1:A:368:VAL:CB	1:A:422:VAL:HG21	2.27	0.53
1:B:14:ARG:HG3	1:B:14:ARG:HH11	1.74	0.53
1:A:581:TRP:C	1:A:583:GLY:O	2.52	0.53
1:B:14:ARG:O	1:B:15:ASP:C	2.51	0.53
1:B:14:ARG:NH1	1:B:14:ARG:HG3	2.24	0.53
1:A:549:GLN:NE2	2:A:737:HOH:O	2.40	0.52
1:B:544:LEU:HB2	2:B:871:HOH:O	2.08	0.52
1:B:580:PHE:CD1	1:B:580:PHE:N	2.78	0.52
1:A:587:LYS:HD3	1:A:589:ILE:HD11	1.91	0.52
1:A:459:GLU:OE1	1:A:462:ARG:NH2	2.35	0.52
1:A:466:GLY:O	1:A:469:ARG:HD2	2.09	0.52
1:A:542:CYS:HB3	2:A:756:HOH:O	2.09	0.52
1:B:36:SER:OG	1:B:65:GLU:HG2	2.10	0.52
1:B:220:CYS:HB3	1:B:224:ILE:HD11	1.92	0.52
1:B:544:LEU:HD12	1:B:556:LEU:HD11	1.92	0.52
1:B:578:LEU:O	1:B:578:LEU:CG	2.25	0.52
1:A:77:ASP:OD1	1:A:77:ASP:C	2.52	0.52
1:B:14:ARG:NH1	2:B:714:HOH:O	2.11	0.52
1:B:590:GLN:CG	2:B:915:HOH:O	2.58	0.51
1:B:375:VAL:HA	2:B:720:HOH:O	2.09	0.51
1:B:274:LYS:HD2	2:B:903:HOH:O	2.10	0.51
1:B:373:ASP:OD2	1:B:428:LYS:HG2	2.09	0.51
1:B:123:THR:N	2:B:728:HOH:O	2.34	0.51
1:B:234:VAL:HG22	2:B:716:HOH:O	2.10	0.51
1:B:270:LEU:HD11	2:B:848:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LYS:HZ3	1:A:554:LEU:HD11	1.76	0.51
1:B:590:GLN:HG2	2:B:915:HOH:O	2.10	0.51
1:A:262:MET:HE1	1:A:351:ALA:HA	1.93	0.50
1:A:582:LYS:C	1:A:583:GLY:O	2.47	0.50
1:A:451:SER:HA	1:A:479:PHE:CD2	2.45	0.50
1:A:581:TRP:CD2	1:A:583:GLY:CA	2.94	0.50
1:A:581:TRP:CD1	1:A:581:TRP:N	2.80	0.50
1:B:88:LEU:CD2	1:B:97:LEU:CD1	2.82	0.50
1:B:98:GLU:OE2	1:B:108:ARG:NH2	2.44	0.50
1:B:130:ARG:O	1:B:130:ARG:HD2	2.10	0.50
1:B:538:THR:HG22	2:B:719:HOH:O	2.10	0.50
1:B:575:HIS:H	1:B:578:LEU:HD12	1.66	0.50
1:A:572:GLY:HA2	2:A:947:HOH:O	2.10	0.50
1:B:567:ARG:HG3	2:B:925:HOH:O	2.11	0.50
1:B:566:PHE:HB2	1:B:573:ARG:NH2	2.27	0.50
1:B:265:LYS:CD	2:B:725:HOH:O	2.04	0.50
1:A:278:VAL:HG12	1:A:296:VAL:HG23	1.94	0.50
1:B:305:VAL:HB	2:B:721:HOH:O	2.12	0.50
1:A:529:GLN:O	1:A:532:ARG:HG2	2.12	0.50
1:B:401:ILE:N	2:B:702:HOH:O	1.96	0.50
1:B:61:GLN:CA	1:B:74:LYS:HD2	2.42	0.50
1:B:222:ARG:HG3	1:B:222:ARG:NH1	2.22	0.50
1:B:179:SER:HA	1:B:182:PHE:CE1	2.47	0.49
1:A:536:ILE:HD12	1:A:537:VAL:N	2.27	0.49
1:A:524:LYS:HE2	2:A:978:HOH:O	2.13	0.49
1:B:137:ILE:HD11	2:B:737:HOH:O	2.11	0.49
1:B:379:ILE:HA	1:B:435:VAL:HG21	1.94	0.49
1:B:306:VAL:O	2:B:721:HOH:O	2.19	0.49
1:B:61:GLN:CB	1:B:74:LYS:CD	2.86	0.49
1:B:573:ARG:C	1:B:574:ILE:HD12	2.36	0.49
1:A:89:LYS:HE3	2:A:724:HOH:O	2.13	0.49
1:A:452:SER:N	2:A:742:HOH:O	2.42	0.49
1:A:492:VAL:HG13	1:A:493:LEU:HD13	1.95	0.49
1:B:181:LEU:HA	1:B:184:ILE:HD13	1.94	0.49
1:B:398:VAL:HG13	2:B:904:HOH:O	2.12	0.49
1:A:511:LEU:O	1:A:514:LYS:HB2	2.12	0.49
1:A:273:PHE:HB3	1:A:361:ASP:OD1	2.13	0.49
1:A:578:LEU:O	1:A:580:PHE:CE1	2.66	0.49
1:B:469:ARG:HH11	1:B:469:ARG:HG2	1.77	0.49
1:B:577:ASP:CG	1:B:577:ASP:O	2.56	0.49
1:A:489:LEU:O	1:A:489:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:PHE:CE2	1:B:410:LEU:HD22	2.48	0.48
1:A:569:CYS:HB2	2:A:944:HOH:O	2.13	0.48
1:A:431:THR:HB	1:A:434:ASP:H	1.78	0.48
1:A:33:PHE:HB3	1:A:106:PHE:CD2	2.48	0.48
1:A:270:LEU:HD21	2:A:952:HOH:O	2.13	0.48
1:A:515:VAL:HA	2:A:707:HOH:O	2.14	0.48
1:B:174:LEU:HG	2:B:709:HOH:O	2.13	0.48
1:B:501:VAL:O	1:B:505:ILE:HG13	2.14	0.48
1:A:94:LEU:HB2	1:A:111:ARG:HD3	1.95	0.48
1:B:574:ILE:C	1:B:578:LEU:HD11	2.32	0.48
1:B:39:PRO:HG3	1:B:145:TRP:CZ2	2.48	0.48
1:A:536:ILE:CD1	1:A:581:TRP:O	2.61	0.48
1:B:114:LEU:O	2:B:723:HOH:O	2.20	0.47
1:A:367:ARG:HB3	1:A:412:HIS:CD2	2.49	0.47
1:A:55:ASN:HB3	1:A:62:PHE:CD1	2.50	0.47
1:B:378:GLU:OE1	1:B:378:GLU:N	2.45	0.47
1:B:578:LEU:CD1	1:B:578:LEU:N	2.77	0.47
1:A:175:GLY:O	1:A:177:ASN:O	2.32	0.47
1:B:117:ALA:C	2:B:724:HOH:O	2.56	0.47
1:B:501:VAL:O	1:B:501:VAL:HG12	2.15	0.47
1:B:573:ARG:O	1:B:579:LEU:O	2.33	0.47
1:B:579:LEU:HD13	1:B:580:PHE:N	2.29	0.47
1:B:408:LYS:HG2	2:B:776:HOH:O	2.15	0.47
1:B:578:LEU:HD13	1:B:578:LEU:N	2.26	0.47
1:B:418:LYS:O	1:B:418:LYS:CG	2.56	0.47
1:B:73:LEU:HG	2:B:821:HOH:O	2.15	0.47
1:B:371:LEU:HD22	2:B:720:HOH:O	2.14	0.47
1:A:34:TYR:CD1	1:A:104:SER:HB2	2.50	0.47
1:B:61:GLN:CD	1:B:74:LYS:NZ	2.60	0.47
1:B:327:SER:HB3	2:B:932:HOH:O	2.14	0.47
1:B:86:LYS:NZ	2:B:746:HOH:O	2.47	0.46
1:B:153:HIS:HB2	2:B:739:HOH:O	2.14	0.46
1:A:59:GLY:O	1:A:74:LYS:CE	2.63	0.46
1:B:274:LYS:HE3	2:B:794:HOH:O	2.14	0.46
1:B:536:ILE:HD11	1:B:582:LYS:O	2.15	0.46
1:A:40:LYS:HB2	2:A:917:HOH:O	2.16	0.46
1:A:477:THR:HG22	1:A:480:CYS:H	1.80	0.46
1:B:14:ARG:HH22	1:B:71:PHE:HA	1.80	0.46
1:A:55:ASN:HB3	1:A:62:PHE:CE1	2.50	0.46
1:B:222:ARG:NH1	2:B:747:HOH:O	2.48	0.46
1:B:286:ASN:H	1:B:286:ASN:HD22	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:ASP:O	1:B:577:ASP:OD1	2.32	0.46
1:B:589:ILE:HB	1:B:590:GLN:H	1.51	0.46
1:A:536:ILE:HD12	1:A:537:VAL:H	1.81	0.46
1:A:465:TYR:HA	2:A:733:HOH:O	2.15	0.46
1:B:567:ARG:CD	2:B:925:HOH:O	2.45	0.46
1:A:134:LEU:O	1:A:138:PHE:HB2	2.16	0.45
1:A:570:ALA:CB	1:A:571:LEU:HD12	2.46	0.45
1:B:399:ALA:O	1:B:403:LYS:HG3	2.16	0.45
1:A:29:ASP:HB3	1:A:33:PHE:CE2	2.52	0.45
1:A:311:ARG:HB2	2:A:809:HOH:O	2.16	0.45
1:B:134:LEU:HD13	2:B:909:HOH:O	2.15	0.45
1:A:219:LYS:NZ	1:A:239:ALA:O	2.41	0.45
1:B:565:SER:C	1:B:573:ARG:HH22	2.22	0.45
1:A:497:ILE:O	1:A:501:VAL:HG23	2.16	0.45
1:B:451:SER:HA	1:B:479:PHE:HD2	1.80	0.45
1:A:449:VAL:O	1:A:483:GLN:OE1	2.35	0.45
1:A:578:LEU:HD13	1:A:585:VAL:HG11	1.98	0.45
1:A:415:VAL:O	1:A:415:VAL:HG23	2.17	0.45
1:A:174:LEU:HB3	2:A:713:HOH:O	2.16	0.45
1:A:426:LEU:CD1	1:A:435:VAL:HG22	2.45	0.45
1:B:560:GLN:O	1:B:563:TYR:HB3	2.17	0.45
1:B:449:VAL:HG22	2:B:767:HOH:O	2.16	0.44
1:B:590:GLN:CB	2:B:915:HOH:O	2.53	0.44
1:A:179:SER:HA	1:A:182:PHE:CD1	2.52	0.44
1:A:254:PHE:O	1:A:265:LYS:HD2	2.17	0.44
1:A:561:PHE:O	1:A:561:PHE:CD1	2.70	0.44
1:A:134:LEU:HD12	1:A:134:LEU:HA	1.81	0.44
1:A:375:VAL:HG21	1:A:401:ILE:HG23	1.98	0.44
1:A:382:GLY:HA3	2:A:711:HOH:O	2.17	0.44
1:A:479:PHE:H	1:A:479:PHE:HD1	1.66	0.44
1:B:31:LEU:O	1:B:34:TYR:HD2	1.99	0.44
1:B:267:PHE:HB3	2:B:718:HOH:O	2.16	0.44
1:B:567:ARG:CG	1:B:569:CYS:SG	3.00	0.44
1:A:500:LEU:HA	2:A:729:HOH:O	2.17	0.44
1:B:265:LYS:N	2:B:712:HOH:O	2.51	0.44
1:B:448:ASP:OD1	1:B:448:ASP:C	2.59	0.44
1:B:21:LYS:HB2	1:B:77:ASP:H	1.82	0.44
1:B:496:GLY:O	1:B:497:ILE:HB	2.18	0.44
1:A:60:LYS:N	2:A:728:HOH:O	2.33	0.44
1:B:590:GLN:HE21	1:B:590:GLN:HB2	1.51	0.44
1:B:469:ARG:HH11	1:B:469:ARG:CG	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:ALA:CB	2:B:791:HOH:O	2.52	0.44
1:B:579:LEU:HB3	1:B:586:HIS:H	1.82	0.44
1:A:79:ILE:C	1:A:79:ILE:HD12	2.43	0.44
1:B:183:GLN:HB2	2:B:842:HOH:O	2.17	0.44
1:B:567:ARG:CA	1:B:573:ARG:CD	2.96	0.44
1:A:84:PRO:CB	2:A:930:HOH:O	2.39	0.43
1:A:477:THR:CG2	1:A:480:CYS:H	2.31	0.43
1:B:428:LYS:HD3	2:B:941:HOH:O	2.17	0.43
1:B:460:PHE:HB3	2:B:767:HOH:O	2.18	0.43
1:A:64:PHE:O	1:A:70:LEU:CD1	2.62	0.43
1:A:448:ASP:HA	1:A:450:TRP:CH2	2.53	0.43
1:A:574:ILE:HG23	1:A:575:HIS:O	2.18	0.43
1:B:578:LEU:CD1	1:B:578:LEU:H	2.29	0.43
1:B:588:ILE:CD1	1:B:588:ILE:N	2.73	0.43
1:A:117:ALA:C	2:A:708:HOH:O	2.61	0.43
1:B:152:ILE:HD12	1:B:153:HIS:N	2.33	0.43
1:B:490:ALA:HA	1:B:498:TRP:CE3	2.54	0.43
1:B:571:LEU:HD23	1:B:571:LEU:HA	1.64	0.43
1:B:579:LEU:CD1	1:B:579:LEU:C	2.89	0.43
1:A:63:LYS:HB3	1:A:70:LEU:HD11	2.00	0.43
1:A:556:LEU:HD23	1:A:556:LEU:HA	1.88	0.43
1:B:567:ARG:HA	1:B:573:ARG:CD	2.48	0.43
1:A:152:ILE:O	1:A:153:HIS:C	2.61	0.43
1:A:379:ILE:HA	1:A:435:VAL:HG21	1.99	0.43
1:B:459:GLU:HG2	2:B:788:HOH:O	2.18	0.43
1:B:484:MET:O	1:B:488:ILE:HG12	2.18	0.43
1:A:111:ARG:CA	1:A:114:LEU:HB2	2.47	0.43
1:B:60:LYS:HD2	1:B:61:GLN:N	2.33	0.43
1:B:36:SER:HB2	2:B:798:HOH:O	2.18	0.43
1:A:50:GLN:NE2	2:A:754:HOH:O	2.51	0.43
1:B:61:GLN:HA	1:B:74:LYS:HD2	2.01	0.43
1:A:533:ALA:O	1:A:534:LYS:HD3	2.19	0.42
1:A:110:TYR:O	1:A:113:LEU:HB3	2.19	0.42
1:A:534:LYS:HD2	1:A:534:LYS:HA	1.75	0.42
1:B:380:ASN:O	1:B:384:ILE:HG13	2.19	0.42
1:B:455:GLU:HG3	1:B:506:TYR:CE2	2.54	0.42
1:A:190:VAL:HG13	2:A:833:HOH:O	2.20	0.42
1:B:518:PHE:CE1	1:B:522:TYR:CD2	3.05	0.42
1:B:29:ASP:HB3	1:B:33:PHE:CE2	2.55	0.42
1:B:71:PHE:O	1:B:72:LEU:HD12	2.19	0.42
1:B:118:CYS:HB3	2:B:900:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:ASP:O	1:B:347:ARG:HD3	2.19	0.42
1:B:501:VAL:HG12	1:B:505:ILE:HG12	2.02	0.42
1:A:159:MET:N	2:A:753:HOH:O	2.52	0.42
1:A:438:LEU:HD23	1:A:438:LEU:HA	1.65	0.42
1:A:579:LEU:C	1:A:579:LEU:HD12	2.44	0.42
1:B:455:GLU:HG3	1:B:506:TYR:CZ	2.54	0.42
1:B:567:ARG:CG	2:B:925:HOH:O	2.65	0.42
1:B:112:GLU:HG3	2:B:835:HOH:O	2.18	0.42
1:B:292:LYS:HE2	2:B:930:HOH:O	2.18	0.42
1:A:158:ALA:C	1:A:160:ARG:N	2.75	0.42
1:A:510:GLY:N	2:A:745:HOH:O	2.46	0.42
1:B:222:ARG:NH1	1:B:222:ARG:CG	2.83	0.42
1:B:130:ARG:HB3	1:B:157:MET:HE1	2.02	0.42
1:B:544:LEU:CD1	1:B:556:LEU:HD11	2.49	0.42
1:A:178:LEU:HD23	1:A:233:LEU:HD11	2.02	0.42
1:A:463:LEU:HD23	1:A:463:LEU:HA	1.88	0.42
1:A:524:LYS:NZ	2:A:738:HOH:O	2.40	0.42
1:B:158:ALA:HA	2:B:849:HOH:O	2.19	0.42
1:B:160:ARG:HD2	2:B:874:HOH:O	2.20	0.42
1:B:568:LYS:HA	1:B:568:LYS:HD2	1.55	0.42
1:B:231:ARG:HD3	2:B:712:HOH:O	2.20	0.41
1:A:542:CYS:SG	2:A:718:HOH:O	2.62	0.41
1:A:567:ARG:HA	1:A:573:ARG:HD3	2.03	0.41
1:A:172:ASP:O	2:A:721:HOH:O	2.22	0.41
1:B:266:ILE:N	1:B:266:ILE:HD13	2.35	0.41
1:B:19:VAL:O	1:B:75:GLY:CA	2.68	0.41
1:B:108:ARG:HB3	2:B:783:HOH:O	2.19	0.41
1:B:465:TYR:CD1	1:B:484:MET:HE1	2.55	0.41
1:A:63:LYS:CD	1:A:63:LYS:H	2.33	0.41
1:A:179:SER:HA	1:A:182:PHE:CE1	2.55	0.41
1:A:406:PRO:HA	1:A:414:PHE:O	2.20	0.41
1:A:581:TRP:CD1	1:A:581:TRP:H	2.38	0.41
1:B:26:GLN:HG2	1:B:151:LYS:HE2	2.02	0.41
1:B:173:ALA:HB3	2:B:709:HOH:O	2.19	0.41
1:A:422:VAL:HG13	2:A:704:HOH:O	2.21	0.41
1:A:536:ILE:HD13	1:A:583:GLY:C	2.45	0.41
1:B:489:LEU:HA	1:B:492:VAL:HG12	2.03	0.41
1:B:157:MET:HB2	1:B:157:MET:HE2	1.68	0.41
1:A:120:TRP:N	2:A:708:HOH:O	2.54	0.41
1:B:579:LEU:HB2	1:B:586:HIS:O	2.19	0.41
1:A:70:LEU:HD12	1:A:71:PHE:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:CG1	1:A:74:LYS:HB2	2.51	0.41
1:A:428:LYS:O	1:A:428:LYS:HG2	2.21	0.41
1:B:79:ILE:N	1:B:79:ILE:CD1	2.73	0.41
1:B:79:ILE:CD1	1:B:79:ILE:O	2.69	0.41
1:B:131:ALA:HA	2:B:909:HOH:O	2.20	0.41
1:A:139:ASP:OD1	1:A:142:GLU:HG3	2.20	0.40
1:B:577:ASP:OD1	1:B:577:ASP:C	2.64	0.40
1:B:42:TYR:HE2	1:B:147:GLN:HB3	1.85	0.40
1:B:46:PHE:HA	1:B:148:VAL:HG21	2.02	0.40
1:A:436:LEU:N	2:A:760:HOH:O	2.55	0.40
1:B:130:ARG:O	1:B:134:LEU:HD13	2.22	0.40
1:B:512:PHE:O	1:B:516:VAL:HG23	2.21	0.40
1:B:575:HIS:O	1:B:577:ASP:N	2.54	0.40
1:A:107:ALA:O	1:A:110:TYR:HB3	2.21	0.40
1:A:536:ILE:CD1	1:A:583:GLY:O	2.67	0.40
1:B:152:ILE:HG13	2:B:866:HOH:O	2.21	0.40
1:A:279:ARG:HG3	2:A:731:HOH:O	2.21	0.40
1:A:489:LEU:O	1:A:489:LEU:CG	2.69	0.40
1:A:582:LYS:HB2	1:A:582:LYS:HE2	1.82	0.40
1:B:107:ALA:O	1:B:110:TYR:HB3	2.22	0.40
1:B:403:LYS:HE2	1:B:403:LYS:HB3	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	582/673 (86%)	550 (94%)	25 (4%)	7 (1%)	10	14
1	B	582/673 (86%)	560 (96%)	19 (3%)	3 (0%)	24	33
All	All	1164/1346 (86%)	1110 (95%)	44 (4%)	10 (1%)	14	20

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	591	GLU
1	A	593	ASP
1	B	497	ILE
1	A	84	PRO
1	A	590	GLN
1	B	76	VAL
1	A	588	ILE
1	B	589	ILE
1	A	589	ILE
1	A	592	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	A	485/565 (86%)	435 (90%)	50 (10%)	7	8
1	B	485/565 (86%)	429 (88%)	56 (12%)	5	6
All	All	970/1130 (86%)	864 (89%)	106 (11%)	6	7

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

Mol	Chain	Res	Type
1	A	14	ARG
1	A	22	ASP
1	A	61	GLN
1	A	72	LEU
1	A	79	ILE
1	A	80	THR
1	A	86	LYS
1	A	87	VAL
1	A	91	THR
1	A	92	SER
1	A	137	ILE
1	A	141	THR
1	A	148	VAL

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Mol	Chain	Res	Type
1	A	159	MET
1	A	178	LEU
1	A	183	GLN
1	A	184	ILE
1	A	222	ARG
1	A	223	SER
1	A	296	VAL
1	A	314	LEU
1	A	376	THR
1	A	394	VAL
1	A	413	LYS
1	A	418	LYS
1	A	425	THR
1	A	452	SER
1	A	457	SER
1	A	462	ARG
1	A	469	ARG
1	A	472	GLU
1	A	477	THR
1	A	493	LEU
1	A	495	GLU
1	A	497	ILE
1	A	536	ILE
1	A	541	LEU
1	A	543	VAL
1	A	554	LEU
1	A	566	PHE
1	A	568	LYS
1	A	574	ILE
1	A	575	HIS
1	A	579	LEU
1	A	580	PHE
1	A	587	LYS
1	A	588	ILE
1	A	589	ILE
1	A	591	GLU
1	A	594	GLU
1	B	14	ARG
1	B	16	VAL
1	B	23	ILE
1	B	26	GLN
1	B	74	LYS

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Mol	Chain	Res	Type
1	B	76	VAL
1	B	78	LYS
1	B	79	ILE
1	B	80	THR
1	B	83	VAL
1	B	86	LYS
1	B	88	LEU
1	B	91	THR
1	B	109	LYS
1	B	119	GLN
1	B	137	ILE
1	B	140	PRO
1	B	148	VAL
1	B	152	ILE
1	B	157	MET
1	B	222	ARG
1	B	223	SER
1	B	255	GLU
1	B	270	LEU
1	B	322	ASP
1	B	346	ASP
1	B	376	THR
1	B	410	LEU
1	B	413	LYS
1	B	418	LYS
1	B	419	ASP
1	B	422	VAL
1	B	423	SER
1	B	424	PHE
1	B	425	THR
1	B	444	VAL
1	B	445	LYS
1	B	469	ARG
1	B	472	GLU
1	B	477	THR
1	B	504	VAL
1	B	505	ILE
1	B	543	VAL
1	B	544	LEU
1	B	568	LYS
1	B	569	CYS
1	B	574	ILE

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Mol	Chain	Res	Type
1	B	577	ASP
1	B	578	LEU
1	B	579	LEU
1	B	588	ILE
1	B	589	ILE
1	B	590	GLN
1	B	591	GLU
1	B	594	GLU
1	B	595	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	183	GLN
1	A	259	ASN
1	A	319	GLN
1	B	57	GLN
1	B	283	ASN
1	B	286	ASN
1	B	319	GLN
1	B	380	ASN
1	B	590	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	A	584/673 (86%)	0.87	84 (14%) 6 6	41, 65, 115, 182	0
1	B	584/673 (86%)	0.99	93 (15%) 5 4	43, 65, 133, 161	0
All	All	1168/1346 (86%)	0.93	177 (15%) 5 5	41, 65, 126, 182	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	588	ILE	8.3
1	B	588	ILE	6.9
1	A	13	LEU	6.8
1	B	422	VAL	6.5
1	B	420	ALA	6.4
1	B	13	LEU	6.3
1	A	596	TRP	6.0
1	B	18	LEU	5.9
1	B	587	LYS	5.7
1	B	16	VAL	5.6
1	A	79	ILE	5.4
1	B	86	LYS	5.4
1	B	80	THR	5.3
1	B	596	TRP	5.3
1	B	582	LYS	5.2
1	A	589	ILE	5.2
1	B	84	PRO	5.2
1	B	424	PHE	5.1
1	A	81	PRO	5.1
1	B	426	LEU	5.1
1	B	103	VAL	4.9
1	B	421	ALA	4.9
1	A	87	VAL	4.7
1	A	421	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	536	ILE	4.5
1	A	489	LEU	4.4
1	A	578	LEU	4.4
1	B	595	ILE	4.3
1	A	587	LYS	4.3
1	B	79	ILE	4.3
1	A	566	PHE	4.2
1	A	178	LEU	4.2
1	A	595	ILE	4.0
1	B	81	PRO	4.0
1	A	177	ASN	4.0
1	A	423	SER	4.0
1	A	575	HIS	4.0
1	B	101	PHE	4.0
1	B	593	ASP	4.0
1	B	15	ASP	3.9
1	B	576	GLY	3.8
1	B	583	GLY	3.8
1	A	60	LYS	3.8
1	A	586	HIS	3.8
1	B	87	VAL	3.7
1	B	286	ASN	3.7
1	A	83	VAL	3.7
1	B	72	LEU	3.7
1	A	91	THR	3.7
1	B	423	SER	3.6
1	B	541	LEU	3.6
1	A	80	THR	3.5
1	B	90	ALA	3.5
1	B	178	LEU	3.5
1	B	554	LEU	3.5
1	A	84	PRO	3.5
1	B	74	LYS	3.5
1	A	579	LEU	3.4
1	A	570	ALA	3.4
1	B	589	ILE	3.4
1	B	83	VAL	3.3
1	B	34	TYR	3.3
1	A	90	ALA	3.3
1	B	425	THR	3.3
1	B	27	LEU	3.3
1	A	76	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	64	PHE	3.2
1	A	86	LYS	3.2
1	A	583	GLY	3.2
1	A	496	GLY	3.1
1	B	449	VAL	3.1
1	A	584	GLY	3.1
1	B	70	LEU	3.1
1	B	88	LEU	3.1
1	B	566	PHE	3.1
1	A	61	GLN	3.0
1	A	422	VAL	3.0
1	A	568	LYS	3.0
1	B	76	VAL	3.0
1	B	108	ARG	3.0
1	B	82	GLY	3.0
1	B	221	ALA	2.9
1	B	132	GLN	2.9
1	B	102	GLY	2.9
1	B	19	VAL	2.8
1	A	424	PHE	2.8
1	A	547	VAL	2.8
1	B	73	LEU	2.8
1	B	571	LEU	2.8
1	B	543	VAL	2.7
1	A	97	LEU	2.7
1	A	569	CYS	2.7
1	B	63	LYS	2.7
1	B	89	LYS	2.7
1	A	577	ASP	2.7
1	B	52	PHE	2.7
1	B	71	PHE	2.7
1	B	156	SER	2.7
1	A	157	MET	2.7
1	A	565	SER	2.7
1	A	82	GLY	2.6
1	A	559	ILE	2.6
1	B	78	LYS	2.6
1	A	504	VAL	2.6
1	A	580	PHE	2.6
1	A	88	LEU	2.6
1	B	497	ILE	2.6
1	B	97	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	78	LYS	2.6
1	A	108	ARG	2.6
1	B	17	ILE	2.6
1	B	106	PHE	2.6
1	A	449	VAL	2.5
1	B	14	ARG	2.5
1	A	118	CYS	2.5
1	B	540	THR	2.5
1	A	571	LEU	2.5
1	B	569	CYS	2.5
1	A	63	LYS	2.5
1	A	475	VAL	2.5
1	B	271	ALA	2.5
1	B	105	PRO	2.4
1	B	484	MET	2.4
1	A	28	CYS	2.4
1	B	419	ASP	2.4
1	B	577	ASP	2.4
1	B	535	LEU	2.4
1	B	590	GLN	2.4
1	B	586	HIS	2.4
1	B	85	ALA	2.4
1	A	85	ALA	2.4
1	B	91	THR	2.4
1	A	479	PHE	2.4
1	A	111	ARG	2.3
1	A	56	LEU	2.3
1	A	52	PHE	2.3
1	A	574	ILE	2.3
1	B	568	LYS	2.3
1	A	16	VAL	2.3
1	A	519	CYS	2.3
1	A	581	TRP	2.3
1	A	418	LYS	2.3
1	B	418	LYS	2.3
1	A	567	ARG	2.3
1	A	18	LEU	2.2
1	A	72	LEU	2.2
1	A	64	PHE	2.2
1	A	430	ALA	2.2
1	A	122	LEU	2.2
1	A	156	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	92	SER	2.2
1	A	361	ASP	2.2
1	B	417	ALA	2.2
1	B	69	GLY	2.2
1	A	497	ILE	2.2
1	B	23	ILE	2.2
1	A	106	PHE	2.2
1	B	122	LEU	2.1
1	A	582	LYS	2.1
1	A	103	VAL	2.1
1	B	500	LEU	2.1
1	A	563	TYR	2.1
1	A	15	ASP	2.1
1	A	585	VAL	2.1
1	A	14	ARG	2.1
1	B	255	GLU	2.1
1	B	539	GLU	2.1
1	B	110	TYR	2.1
1	A	364	CYS	2.1
1	A	67	VAL	2.1
1	A	101	PHE	2.1
1	B	317	LEU	2.0
1	B	67	VAL	2.0
1	B	561	PHE	2.0
1	B	430	ALA	2.0
1	A	576	GLY	2.0
1	B	96	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.