



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:32 PM UTC

PDB ID : 3FZ3 / pdb_00003fz3
Title : Crystal Structure of almond Pru1 protein
Authors : Jin, T.C.; Zhang, Y.Z.
Deposited on : 2009-01-23
Resolution : 2.40 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

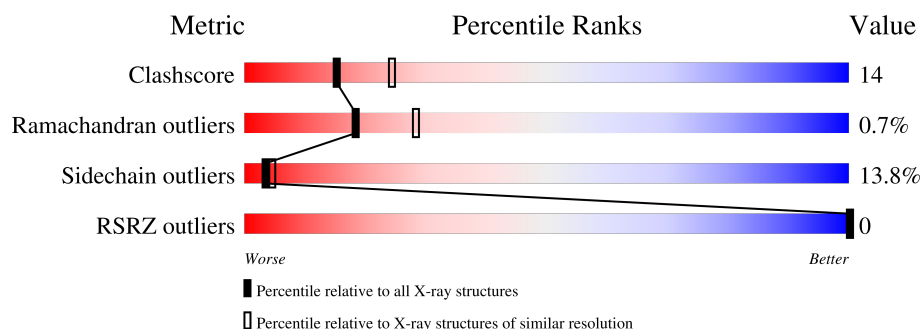
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	531	
1	B	531	
1	C	531	
1	D	531	
1	E	531	
1	F	531	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19957 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 Prunin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	2	0
			3104	1926	583	591	4			
1	B	410	Total	C	N	O	S	0	1	0
			3296	2034	626	632	4			
1	C	410	Total	C	N	O	S	0	1	0
			3298	2035	628	631	4			
1	D	388	Total	C	N	O	S	0	1	0
			3102	1924	583	591	4			
1	E	388	Total	C	N	O	S	0	1	0
			3097	1922	580	591	4			
1	F	410	Total	C	N	O	S	0	2	0
			3302	2038	627	633	4			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		
2	F	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Na 2 2	0	0
3	B	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	E	2	Total Na 2 2	0	0
3	F	2	Total Na 2 2	0	0

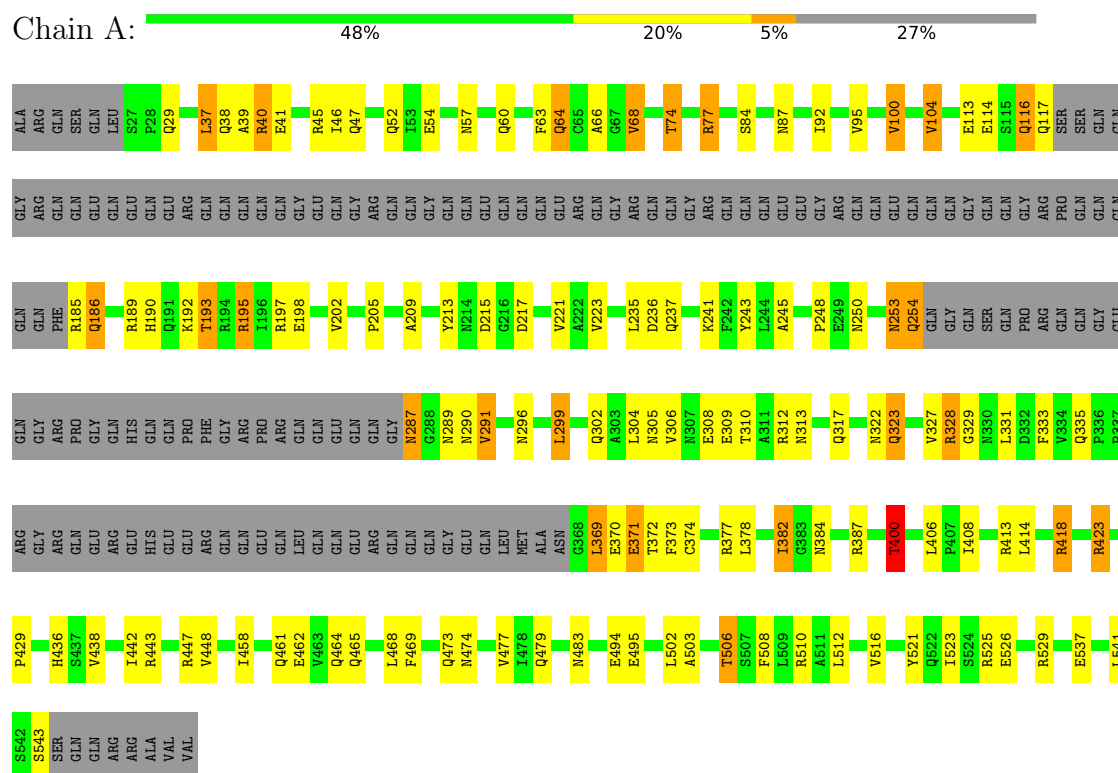
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	90	Total O 90 90	0	0
4	B	162	Total O 162 162	0	0
4	C	123	Total O 123 123	0	0
4	D	136	Total O 136 136	0	0
4	E	102	Total O 102 102	0	0
4	F	130	Total O 130 130	0	0

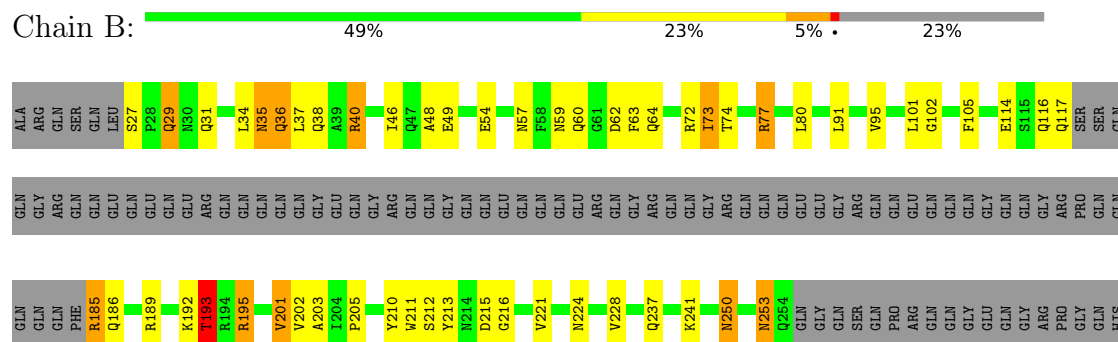
3 Residue-property plots

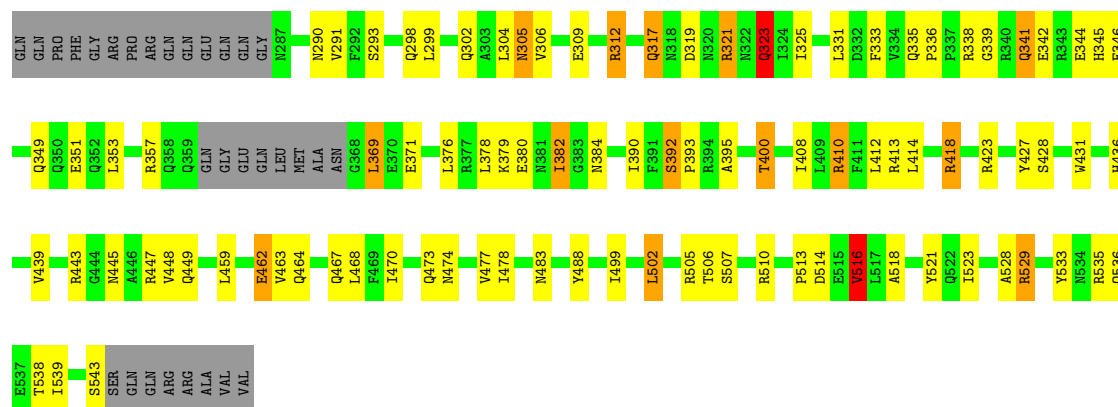
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



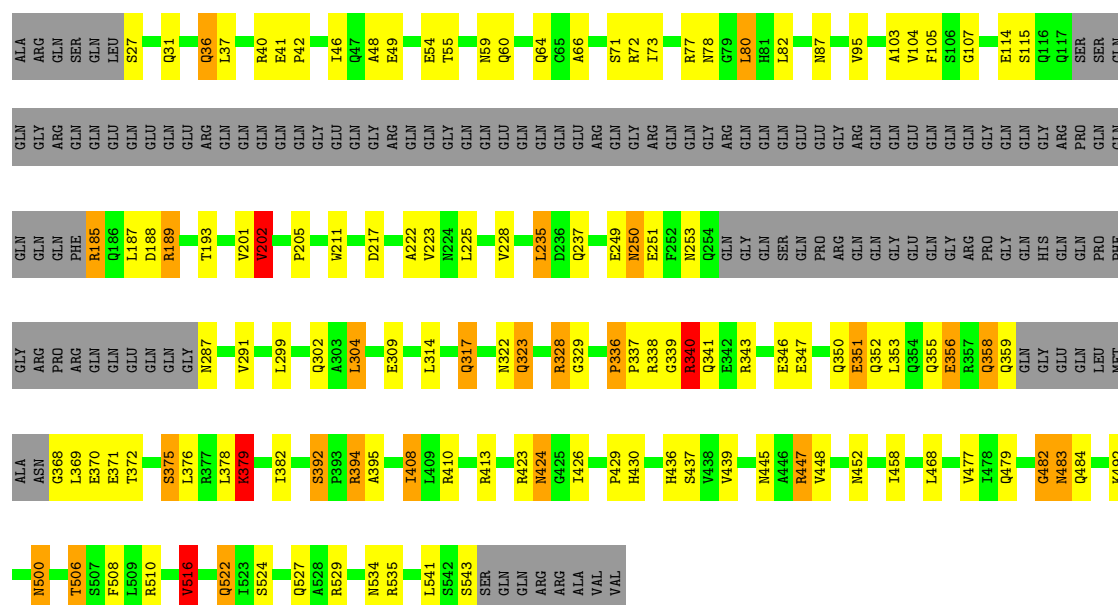
• Molecule 1: Prunin





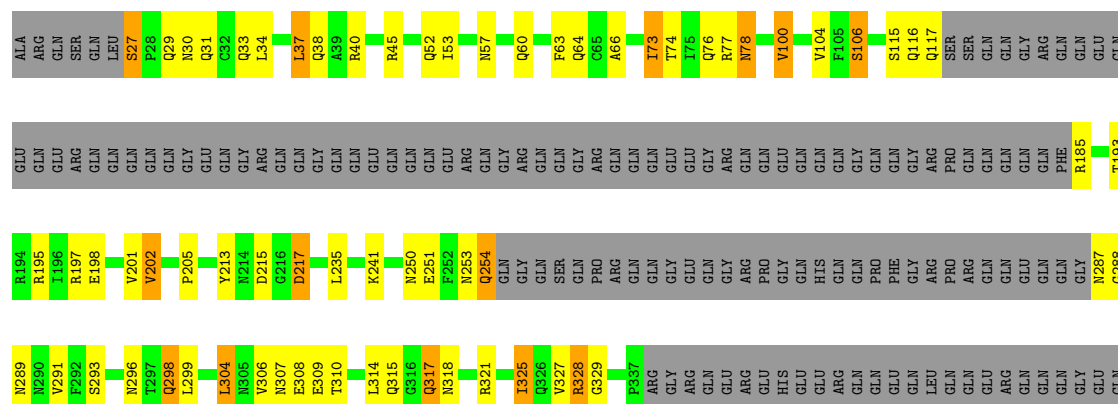
• Molecule 1: Prunin

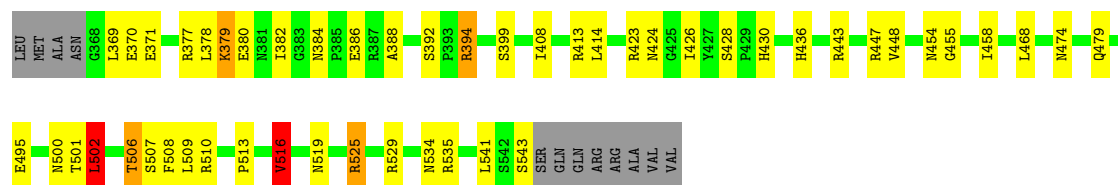
Chain C: 53% 19% 5% • 23%



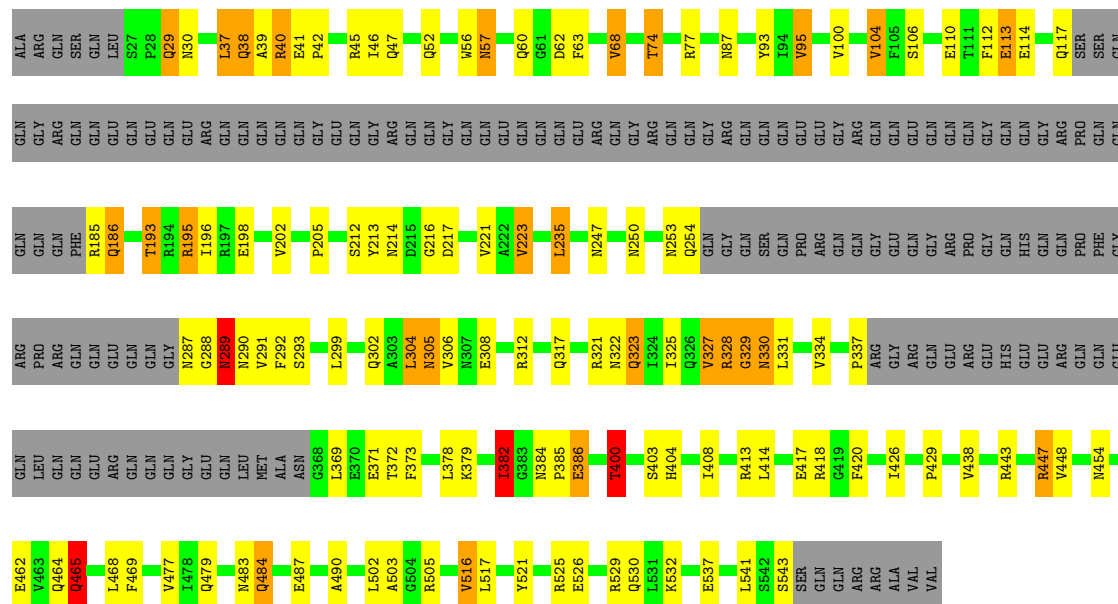
• Molecule 1: Prunin

Chain D: 51% 18% • 27%

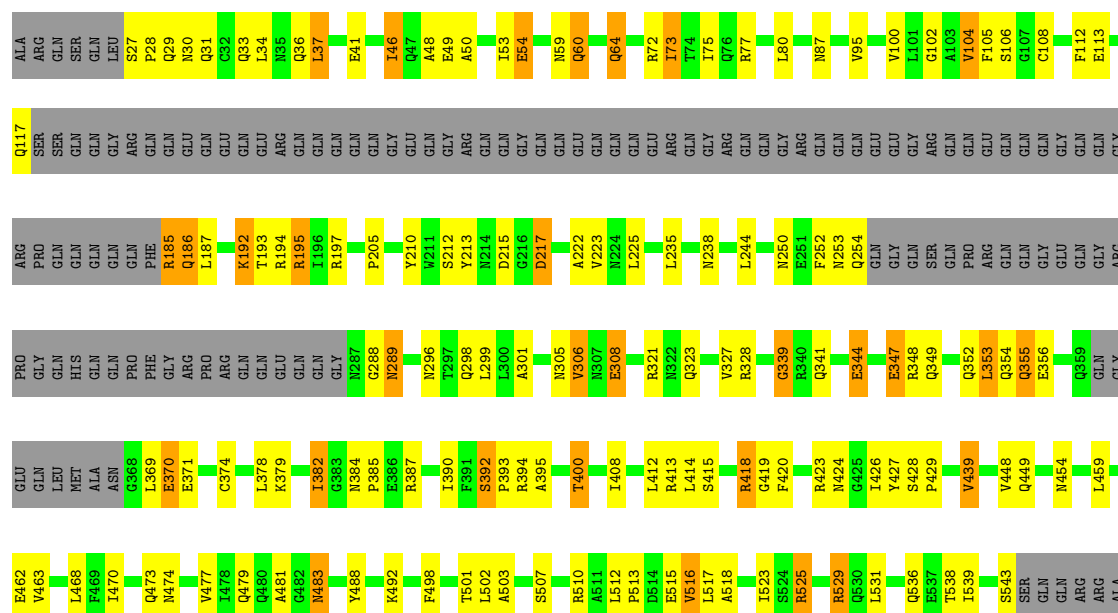




• Molecule 1: Prunin



• Molecule 1: Prunin



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4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	151.02Å 151.02Å 165.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.08 – 2.40 36.08 – 2.40	Depositor EDS
% Data completeness (in resolution range)	88.7 (36.08-2.40) 88.0 (36.08-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.229 0.175 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19957	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.83	1/3168 (0.0%)	1.18	7/4291 (0.2%)
1	B	0.93	0/3358	1.27	21/4542 (0.5%)
1	C	0.89	2/3360 (0.1%)	1.25	18/4544 (0.4%)
1	D	0.90	1/3163 (0.0%)	1.25	13/4284 (0.3%)
1	E	0.84	1/3158 (0.0%)	1.20	9/4278 (0.2%)
1	F	0.95	0/3367	1.30	19/4554 (0.4%)
All	All	0.89	5/19574 (0.0%)	1.24	87/26493 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	516	VAL	CA-CB	5.97	1.62	1.54
1	C	522	GLN	CA-C	-5.58	1.48	1.53
1	A	372	THR	CA-C	5.37	1.55	1.52
1	C	372	THR	CA-C	5.28	1.54	1.52
1	E	372	THR	CA-C	5.03	1.54	1.52

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	ASN	N-CA-C	8.22	120.80	109.54
1	C	251	GLU	N-CA-C	8.09	123.69	112.93
1	F	384	ASN	CA-C-N	7.97	127.26	118.97
1	F	384	ASN	C-N-CA	7.97	127.26	118.97
1	C	251	GLU	CA-C-N	7.22	134.69	121.70
1	C	251	GLU	C-N-CA	7.22	134.69	121.70
1	D	78	ASN	N-CA-C	6.93	121.32	112.86
1	F	238	ASN	CA-C-N	-6.79	113.00	119.85
1	F	238	ASN	C-N-CA	-6.79	113.00	119.85
1	F	289	ASN	N-CA-C	6.73	120.85	112.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	463	VAL	N-CA-C	-6.70	98.83	108.48
1	D	379	LYS	N-CA-C	6.65	120.00	109.50
1	D	516	VAL	N-CA-CB	6.61	120.49	110.58
1	F	339	GLY	N-CA-C	6.59	123.47	112.85
1	B	392	SER	CA-C-N	6.57	127.09	119.47
1	B	392	SER	C-N-CA	6.57	127.09	119.47
1	E	104	VAL	N-CA-C	6.53	117.31	108.17
1	C	351	GLU	N-CA-C	-6.52	105.19	113.01
1	F	46	ILE	N-CA-C	-6.46	98.83	108.46
1	F	501	THR	N-CA-C	6.30	118.84	110.53
1	A	104	VAL	N-CA-C	6.29	116.97	108.17
1	C	336	PRO	CA-C-N	6.26	127.66	119.84
1	C	336	PRO	C-N-CA	6.26	127.66	119.84
1	B	201	VAL	N-CA-C	-6.14	99.64	108.48
1	B	384	ASN	CA-C-N	6.04	125.26	118.97
1	B	384	ASN	C-N-CA	6.04	125.26	118.97
1	F	463	VAL	N-CA-C	-6.02	99.81	108.48
1	E	327	VAL	CA-C-N	6.01	132.52	121.70
1	E	327	VAL	C-N-CA	6.01	132.52	121.70
1	A	253	ASN	N-CA-C	5.95	118.14	110.65
1	B	510	ARG	N-CA-C	5.92	119.60	112.38
1	D	509	LEU	N-CA-C	5.90	117.71	111.28
1	B	101	LEU	O-C-N	-5.85	116.23	123.36
1	E	382	ILE	N-CA-CB	-5.84	105.78	112.21
1	C	107	GLY	N-CA-C	5.83	123.30	114.61
1	B	193	THR	CB-CA-C	5.80	120.45	109.37
1	C	424	ASN	N-CA-C	5.72	119.83	112.86
1	F	36	GLN	N-CA-C	5.69	118.64	109.83
1	F	41	GLU	N-CA-C	-5.68	101.87	110.39
1	E	56	TRP	N-CA-C	-5.62	101.12	110.17
1	C	379	LYS	N-CA-C	5.61	117.92	109.23
1	D	428	SER	CA-C-N	-5.60	113.99	119.76
1	D	428	SER	C-N-CA	-5.60	113.99	119.76
1	B	290	ASN	CB-CA-C	5.58	120.29	110.36
1	B	516	VAL	CB-CA-C	5.56	119.89	112.22
1	C	202	VAL	CB-CA-C	5.53	119.21	110.81
1	E	516	VAL	N-CA-CB	5.50	120.73	110.77
1	F	323	GLN	N-CA-C	5.50	119.61	113.01
1	A	331	LEU	N-CA-C	5.42	118.43	110.30
1	F	510	ARG	N-CA-C	5.40	118.97	112.38
1	C	516	VAL	N-CA-CB	5.35	120.45	110.77
1	B	323	GLN	N-CA-C	5.34	119.42	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	507	SER	N-CA-C	5.33	117.75	110.55
1	A	442	ILE	N-CA-C	5.33	116.11	110.72
1	F	108	CYS	CA-C-N	-5.28	114.80	120.03
1	F	108	CYS	C-N-CA	-5.28	114.80	120.03
1	B	336	PRO	CA-C-N	5.28	125.27	119.89
1	B	336	PRO	C-N-CA	5.28	125.27	119.89
1	F	507	SER	N-CA-C	5.27	117.49	110.53
1	D	455	GLY	N-CA-C	-5.26	108.02	115.43
1	E	400	THR	CB-CA-C	5.26	119.42	109.37
1	A	523	ILE	N-CA-C	-5.26	100.71	108.23
1	C	375	SER	CB-CA-C	-5.25	102.57	111.02
1	B	528	ALA	N-CA-C	-5.20	105.61	111.28
1	D	202	VAL	CB-CA-C	5.20	118.32	110.63
1	D	27	SER	CA-C-N	5.20	124.64	119.24
1	D	27	SER	C-N-CA	5.20	124.64	119.24
1	C	410	ARG	N-CA-C	-5.19	105.70	111.36
1	D	519	ASN	N-CA-C	5.19	116.94	111.28
1	C	103	ALA	CA-C-N	-5.18	116.36	123.14
1	C	103	ALA	C-N-CA	-5.18	116.36	123.14
1	F	50	ALA	N-CA-C	5.14	119.30	112.30
1	B	101	LEU	N-CA-CB	-5.13	102.20	110.81
1	E	289	ASN	N-CA-C	5.13	118.38	107.67
1	F	327	VAL	N-CA-C	-5.10	102.27	109.21
1	C	452	ASN	N-CA-C	5.10	117.74	109.79
1	B	335	GLN	CA-C-N	-5.10	115.13	120.38
1	B	335	GLN	C-N-CA	-5.10	115.13	120.38
1	C	340	ARG	CA-C-N	5.09	130.86	121.70
1	C	340	ARG	C-N-CA	5.09	130.86	121.70
1	A	400	THR	CB-CA-C	5.09	118.54	109.38
1	E	329	GLY	N-CA-C	-5.08	101.15	113.18
1	F	462	GLU	N-CA-C	-5.07	102.19	110.20
1	D	502	LEU	N-CA-C	-5.06	107.49	113.97
1	B	192	LYS	N-CA-C	5.04	117.40	110.35
1	B	462	GLU	N-CA-C	-5.04	102.83	110.28
1	D	106	SER	N-CA-C	5.01	117.57	110.10

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	3104	0	2974	97	0
1	B	3296	0	3143	99	0
1	C	3298	0	3148	90	0
1	D	3102	0	2972	69	0
1	E	3097	0	2963	103	0
1	F	3302	0	3151	113	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	90	0	0	7	0
4	B	162	0	0	11	0
4	C	123	0	0	5	0
4	D	136	0	0	4	0
4	E	102	0	0	5	0
4	F	130	0	0	4	0
All	All	19957	0	18351	510	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 14.

All (510) 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:250:ASN:HB3	1:B:253:ASN:ND2	1.43	1.30
1:B:250:ASN:CB	1:B:253:ASN:HD21	1.49	1.23
1:A:195:ARG:HH21	1:A:195:ARG:HG3	1.05	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:ARG:HH21	1:F:195:ARG:CG	1.67	1.08
1:F:195:ARG:NH2	1:F:195:ARG:HG3	1.53	1.05
1:E:195:ARG:HH21	1:E:195:ARG:CG	1.72	1.03
1:F:77:ARG:H	1:F:77:ARG:HD3	1.22	1.02
1:A:423:ARG:HH11	1:A:423:ARG:HB2	1.23	1.01
1:C:413:ARG:HD3	4:C:613:HOH:O	1.59	1.00
1:A:100:VAL:HG23	1:A:193:THR:HG23	1.42	0.98
1:B:390:ILE:HD13	1:B:539:ILE:HD12	1.44	0.97
1:E:327:VAL:HA	1:E:328:ARG:HB3	1.45	0.97
1:E:195:ARG:NH2	1:E:195:ARG:HG3	1.57	0.96
1:A:195:ARG:HH21	1:A:195:ARG:CG	1.79	0.94
1:E:195:ARG:HH21	1:E:195:ARG:HG3	0.79	0.94
1:E:331:LEU:HD12	1:F:515:GLU:HG2	1.51	0.93
1:C:447:ARG:HG2	1:C:447:ARG:HH11	1.33	0.92
1:C:340:ARG:H	1:C:341:GLN:CB	1.84	0.90
1:F:195:ARG:HH21	1:F:195:ARG:HG3	0.78	0.90
1:B:323:GLN:H	1:B:323:GLN:HE21	0.93	0.90
1:F:77:ARG:H	1:F:77:ARG:CD	1.86	0.88
1:A:195:ARG:HG3	1:A:195:ARG:NH2	1.77	0.88
1:D:53:ILE:HG12	1:D:73:ILE:HG13	1.56	0.87
1:A:423:ARG:HH11	1:A:423:ARG:CB	1.87	0.86
1:A:302:GLN:OE1	1:B:543:SER:HB2	1.75	0.85
1:F:34:LEU:HD13	1:F:37:LEU:HD21	1.57	0.85
1:E:328:ARG:HG3	1:E:328:ARG:O	1.75	0.84
1:D:287:ASN:HD22	1:D:317:GLN:HB3	1.41	0.84
1:F:339:GLY:HA2	4:F:752:HOH:O	1.76	0.84
1:A:100:VAL:CG2	1:A:193:THR:HG23	2.07	0.84
1:B:506:THR:HG22	4:B:941:HOH:O	1.78	0.83
1:D:30:ASN:HB3	1:D:33:GLN:HG3	1.60	0.83
1:F:77:ARG:HD3	1:F:77:ARG:N	1.94	0.82
1:B:323:GLN:H	1:B:323:GLN:NE2	1.74	0.82
1:C:339:GLY:HA2	1:C:340:ARG:HB3	1.61	0.81
1:A:37:LEU:HD22	1:A:458:ILE:HG13	1.60	0.81
1:F:390:ILE:CD1	1:F:539:ILE:HD12	2.11	0.81
1:B:323:GLN:HE21	1:B:323:GLN:N	1.77	0.81
1:B:529:ARG:HD2	4:B:1024:HOH:O	1.80	0.80
1:A:186:GLN:HA	4:B:1024:HOH:O	1.80	0.80
1:B:193:THR:HG23	4:B:952:HOH:O	1.81	0.79
1:E:331:LEU:CD1	1:F:515:GLU:HG2	2.12	0.79
1:A:423:ARG:HB2	1:A:423:ARG:NH1	1.97	0.79
1:E:447:ARG:NH1	1:E:462:GLU:HG2	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:GLN:H	1:E:323:GLN:HE21	1.30	0.79
1:D:454:ASN:O	1:F:289:ASN:HB2	1.81	0.79
1:B:445:ASN:HB2	1:B:462:GLU:OE1	1.85	0.77
1:E:185:ARG:HA	4:E:777:HOH:O	1.84	0.76
1:D:287:ASN:ND2	1:D:317:GLN:HB3	2.00	0.76
1:B:390:ILE:CD1	1:B:539:ILE:HD12	2.16	0.75
1:F:390:ILE:HD13	1:F:539:ILE:HD12	1.69	0.75
1:D:513:PRO:HD2	1:D:516:VAL:HG13	1.67	0.74
1:A:77:ARG:HD3	4:A:583:HOH:O	1.88	0.74
1:B:34:LEU:HD13	1:B:37:LEU:HD11	1.69	0.74
1:B:74:THR:HG23	1:B:221:VAL:HG22	1.70	0.74
1:B:185:ARG:O	1:C:529:ARG:HD2	1.88	0.73
1:A:377:ARG:HD3	4:A:1026:HOH:O	1.89	0.72
1:B:73:ILE:HG22	1:B:224:ASN:HD21	1.54	0.72
1:A:113:GLU:OE2	1:F:538:THR:HG23	1.90	0.71
1:E:328:ARG:O	1:E:328:ARG:CG	2.38	0.71
1:A:506:THR:HG22	4:A:577:HOH:O	1.91	0.71
1:A:423:ARG:HH11	1:A:423:ARG:CG	2.04	0.70
1:A:382:ILE:HD13	1:A:418:ARG:HB2	1.73	0.70
1:B:319:ASP:OD2	1:B:321:ARG:CD	2.39	0.70
1:A:309:GLU:HG2	1:A:312:ARG:HH22	1.56	0.70
1:C:448:VAL:HG22	1:C:479:GLN:HG2	1.74	0.70
1:E:250:ASN:HB3	1:E:253:ASN:OD1	1.92	0.69
1:C:185:ARG:HB2	1:C:189:ARG:HH21	1.57	0.69
1:E:186:GLN:HB2	1:F:529:ARG:NH1	2.07	0.69
1:B:412:LEU:O	1:B:413:ARG:HB2	1.93	0.69
1:C:250:ASN:HB3	1:C:253:ASN:HB2	1.75	0.69
1:C:340:ARG:N	1:C:341:GLN:CB	2.56	0.69
1:E:186:GLN:O	1:F:529:ARG:NH1	2.26	0.68
1:C:185:ARG:HB2	1:C:189:ARG:NH2	2.09	0.68
1:C:322:ASN:HB3	1:C:323:GLN:HE21	1.56	0.68
1:A:100:VAL:HG23	1:A:193:THR:CG2	2.20	0.67
1:C:338:ARG:HH11	1:C:343:ARG:HG3	1.59	0.67
1:D:304:LEU:HD13	1:E:503:ALA:HB2	1.77	0.67
1:E:74:THR:HB	1:E:221:VAL:HG22	1.76	0.66
1:E:77:ARG:CD	1:E:216:GLY:O	2.43	0.66
1:B:37:LEU:O	1:B:459:LEU:HD12	1.96	0.66
1:C:323:GLN:HE21	1:C:323:GLN:H	1.44	0.66
1:C:424:ASN:O	1:C:543:SER:HB3	1.95	0.66
1:C:340:ARG:HD3	1:C:343:ARG:HH21	1.61	0.66
1:F:513:PRO:HD2	1:F:516:VAL:HG13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:ARG:HD2	1:E:216:GLY:O	1.95	0.66
1:E:447:ARG:HH12	1:E:462:GLU:HG2	1.60	0.66
1:A:308:GLU:HG2	1:A:312:ARG:NH1	2.11	0.65
1:F:412:LEU:O	1:F:413:ARG:HB2	1.96	0.65
1:D:534:ASN:HB3	1:F:305:ASN:HB3	1.79	0.65
1:B:250:ASN:HB3	1:B:253:ASN:HD21	0.60	0.65
1:C:77:ARG:HD2	1:C:217:ASP:O	1.97	0.65
1:D:195:ARG:NH1	1:D:215:ASP:OD1	2.27	0.65
1:A:461:GLN:HG2	1:A:462:GLU:H	1.60	0.65
1:E:323:GLN:H	1:E:323:GLN:NE2	1.93	0.65
1:B:319:ASP:OD2	1:B:321:ARG:HD2	1.95	0.65
1:C:185:ARG:CB	1:C:189:ARG:NH2	2.60	0.64
1:E:526:GLU:HB3	4:E:582:HOH:O	1.97	0.64
1:B:464:GLN:O	1:B:467:GLN:HG3	1.97	0.64
1:B:305:ASN:HB3	1:C:534:ASN:HB3	1.79	0.64
1:B:533:TYR:O	1:B:536:GLN:NE2	2.29	0.64
1:A:84:SER:OG	1:A:241:LYS:HE3	1.98	0.63
1:E:443[A]:ARG:HA	1:E:465:GLN:HG2	1.80	0.63
1:D:185:ARG:O	1:E:529:ARG:HD3	1.99	0.63
1:F:104:VAL:HG22	4:F:584:HOH:O	1.99	0.63
1:F:518:ALA:HA	1:F:523:ILE:HG13	1.80	0.63
1:A:448:VAL:HG22	1:A:479:GLN:HG2	1.80	0.63
1:F:390:ILE:HD11	1:F:539:ILE:HD12	1.80	0.63
1:A:461:GLN:HG2	1:A:462:GLU:N	2.13	0.63
1:B:77:ARG:HG2	1:B:216:GLY:O	1.99	0.62
1:F:423:ARG:NH1	1:F:483:ASN:CG	2.56	0.62
1:A:185:ARG:HG2	4:B:1024:HOH:O	1.98	0.62
1:E:247:ASN:ND2	1:E:288:GLY:HA3	2.14	0.62
1:B:102:GLY:HA3	1:B:211:TRP:O	2.00	0.61
1:C:66:ALA:HA	1:C:436:HIS:CD2	2.35	0.61
1:A:310:THR:O	1:A:313:ASN:HB2	1.99	0.61
1:D:53:ILE:HG21	1:D:251:GLU:HG2	1.82	0.61
1:F:185:ARG:O	1:F:186:GLN:NE2	2.33	0.61
1:B:447:ARG:HD3	4:B:614:HOH:O	1.99	0.61
1:F:73:ILE:HD13	1:F:75:ILE:HG13	1.82	0.60
1:B:193:THR:CG2	4:B:952:HOH:O	2.43	0.60
1:E:443[B]:ARG:HA	1:E:465:GLN:HG2	1.83	0.60
1:E:448:VAL:HG22	1:E:479:GLN:HG2	1.82	0.60
1:A:197:ARG:NH1	4:A:582:HOH:O	2.34	0.60
1:A:100:VAL:CG2	1:A:193:THR:CG2	2.78	0.60
1:B:40[A]:ARG:NH1	1:B:62:ASP:OD1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:387:ARG:O	1:F:387:ARG:HG3	2.01	0.60
1:E:68:VAL:HG21	1:E:438:VAL:HG21	1.83	0.60
1:B:319:ASP:OD2	1:B:321:ARG:HD3	2.01	0.59
1:C:370:GLU:OE2	1:D:506:THR:HG21	2.01	0.59
1:E:195:ARG:CG	1:E:195:ARG:NH2	2.42	0.59
1:A:400:THR:HG21	1:F:371:GLU:O	2.01	0.59
1:B:195:ARG:HB3	1:B:195:ARG:HH21	1.68	0.59
1:C:413:ARG:NH1	4:C:620:HOH:O	2.35	0.59
1:C:41:GLU:HB3	1:C:42:PRO:CD	2.32	0.59
1:E:418:ARG:NH1	1:E:487:GLU:HB3	2.18	0.59
1:D:40:ARG:HH11	1:D:60:GLN:HG3	1.67	0.58
1:D:287:ASN:N	1:D:288:GLY:HA2	2.17	0.58
1:B:73:ILE:CG2	1:B:224:ASN:HD21	2.16	0.58
1:E:112:PHE:CD2	1:E:193:THR:HG22	2.38	0.58
1:E:186:GLN:HA	1:F:529:ARG:HD2	1.86	0.58
1:E:464:GLN:O	1:E:465:GLN:C	2.46	0.58
1:C:423:ARG:HD2	1:C:483:ASN:OD1	2.04	0.58
1:D:66:ALA:HA	1:D:436:HIS:CD2	2.38	0.58
1:C:40:ARG:HH11	1:C:60:GLN:HG3	1.68	0.58
1:F:423:ARG:HH12	1:F:483:ASN:CG	2.11	0.58
1:F:382:ILE:HD13	1:F:418:ARG:HB2	1.84	0.58
1:F:448:VAL:HG12	1:F:459:LEU:HD23	1.85	0.57
1:E:57:ASN:O	1:E:60:GLN:HG3	2.04	0.57
1:E:305:ASN:C	1:E:305:ASN:HD22	2.13	0.57
1:F:423:ARG:NH1	1:F:483:ASN:OD1	2.37	0.57
4:B:615:HOH:O	1:E:400:THR:HG22	2.05	0.57
1:F:205:PRO:HG3	1:F:408:ILE:HD11	1.85	0.57
1:A:296:ASN:HD22	1:A:299:LEU:H	1.51	0.57
1:C:249:GLU:H	1:C:323:GLN:HE22	1.53	0.57
1:F:195:ARG:CG	1:F:195:ARG:NH2	2.40	0.57
1:E:57:ASN:HA	1:E:254:GLN:NE2	2.20	0.56
1:F:473:GLN:O	1:F:474:ASN:HB2	2.03	0.56
1:F:348:ARG:HG3	1:F:352:GLN:HE21	1.70	0.56
1:B:513:PRO:HD2	1:B:516:VAL:HG13	1.86	0.56
1:F:393:PRO:C	1:F:394[B]:ARG:HD2	2.30	0.56
1:D:100:VAL:HG12	1:D:213:TYR:HB3	1.87	0.56
1:B:473:GLN:O	1:B:474:ASN:HB2	2.05	0.56
1:C:54:GLU:OE2	1:C:72:ARG:HD2	2.05	0.56
1:B:339:GLY:HA2	1:B:342:GLU:H	1.70	0.56
1:D:217:ASP:OD1	1:D:217:ASP:N	2.29	0.56
1:D:500:ASN:ND2	1:F:106:SER:HB2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:HG21	1:A:438:VAL:HG21	1.87	0.56
1:A:512:LEU:HD22	1:C:211:TRP:CD1	2.41	0.56
1:A:529:ARG:HD3	1:C:185:ARG:O	2.06	0.56
1:B:102:GLY:O	1:B:210:TYR:HA	2.06	0.56
1:F:223:VAL:HG12	1:F:225:LEU:CD2	2.36	0.56
1:C:205:PRO:HG3	1:C:408:ILE:HD11	1.88	0.55
1:E:302:GLN:HE21	1:F:543:SER:HA	1.71	0.55
1:B:341:GLN:N	4:B:717:HOH:O	2.37	0.55
1:C:392:SER:HB3	1:C:395:ALA:HB3	1.88	0.55
1:D:474:ASN:ND2	1:F:87:ASN:HA	2.21	0.55
1:A:189:ARG:HH22	1:F:536:GLN:HE21	1.53	0.55
1:B:205:PRO:HG3	1:B:408:ILE:HD11	1.89	0.54
1:A:198:GLU:HB3	1:F:341:GLN:HE22	1.72	0.54
1:B:400:THR:HG21	1:E:371:GLU:O	2.08	0.54
1:E:38:GLN:NE2	1:E:40:ARG:HG2	2.22	0.54
1:E:327:VAL:HA	1:E:328:ARG:CB	2.28	0.54
1:C:115:SER:CB	1:D:394[A]:ARG:HB2	2.37	0.54
1:D:474:ASN:HD21	1:F:87:ASN:HA	1.70	0.54
1:D:513:PRO:HD2	1:D:516:VAL:CG1	2.36	0.54
1:A:245:ALA:HB2	1:B:521:TYR:CE1	2.43	0.54
1:C:522:GLN:HG2	4:C:612:HOH:O	2.07	0.54
1:D:31:GLN:NE2	4:D:11:HOH:O	2.41	0.54
1:E:327:VAL:CA	1:E:328:ARG:HB3	2.28	0.54
1:F:59:ASN:HA	1:F:64:GLN:NE2	2.23	0.54
1:A:468:LEU:C	1:A:468:LEU:HD23	2.34	0.53
1:A:195:ARG:CG	1:A:195:ARG:NH2	2.49	0.53
1:F:30:ASN:HB3	1:F:33:GLN:NE2	2.23	0.53
1:B:418:ARG:HD3	1:B:488:TYR:O	2.09	0.53
1:A:100:VAL:HG13	1:A:213:TYR:HB3	1.89	0.53
1:B:427:TYR:O	1:B:428:SER:C	2.51	0.53
1:A:117:GLN:HG2	4:F:577:HOH:O	2.07	0.53
1:D:53:ILE:CG1	1:D:73:ILE:HG13	2.34	0.53
1:A:443[B]:ARG:HA	1:A:465:GLN:HG3	1.91	0.53
1:E:39:ALA:HB2	1:E:469:PHE:HB3	1.90	0.53
1:D:426:ILE:HB	1:D:541:LEU:HB2	1.91	0.53
1:F:213:TYR:CE2	1:F:215:ASP:HB3	2.44	0.53
1:F:427:TYR:O	1:F:428:SER:C	2.53	0.52
1:A:45:ARG:HD2	1:A:52:GLN:NE2	2.23	0.52
1:A:543:SER:HA	1:F:117:GLN:NE2	2.24	0.52
1:D:45:ARG:HD3	1:D:52:GLN:OE1	2.09	0.52
1:A:371:GLU:OE1	1:F:498:PHE:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:ARG:HH11	1:E:47:GLN:HB2	1.73	0.52
1:B:408:ILE:HG12	1:B:408:ILE:O	2.09	0.52
1:E:38:GLN:HG3	4:E:618:HOH:O	2.09	0.52
1:A:60:GLN:O	1:A:64:GLN:HG2	2.10	0.52
1:B:193:THR:HG21	1:B:333:PHE:HE2	1.74	0.52
1:F:355:GLN:HG3	1:F:356:GLU:N	2.25	0.52
1:A:377:ARG:NE	4:A:1026:HOH:O	2.42	0.52
1:C:228:VAL:HG11	1:C:237:GLN:O	2.10	0.51
1:D:29:GLN:CD	1:D:29:GLN:H	2.18	0.51
1:E:186:GLN:H	1:E:186:GLN:CD	2.18	0.51
1:A:369:LEU:HD23	1:E:369:LEU:HD23	1.91	0.51
1:C:202:VAL:HB	1:C:379:LYS:HB3	1.91	0.51
1:C:350:GLN:HE22	1:C:353:LEU:HD23	1.76	0.51
1:D:289:ASN:HB3	1:E:454:ASN:O	2.11	0.51
1:E:305:ASN:O	1:E:305:ASN:ND2	2.40	0.51
1:C:37:LEU:HD22	1:C:458:ILE:HD12	1.93	0.51
1:F:418:ARG:HD3	1:F:488:TYR:O	2.10	0.51
1:C:77:ARG:CD	1:C:217:ASP:O	2.58	0.51
1:D:63:PHE:CZ	1:D:468:LEU:HD22	2.46	0.51
1:F:48:ALA:O	1:F:49:GLU:C	2.52	0.51
1:A:74:THR:HB	1:A:221:VAL:HG22	1.91	0.51
1:F:185:ARG:C	1:F:186:GLN:NE2	2.68	0.51
1:B:338:ARG:HA	1:E:386:GLU:OE1	2.11	0.51
1:C:445:ASN:ND2	1:C:482:GLY:HA3	2.26	0.51
1:F:296:ASN:OD1	1:F:298[B]:GLN:HB2	2.11	0.51
4:B:950:HOH:O	1:E:337:PRO:CG	2.58	0.51
1:E:205:PRO:HG3	1:E:408:ILE:HD11	1.93	0.50
1:B:48:ALA:O	1:B:49:GLU:C	2.53	0.50
1:C:114:GLU:HB2	1:C:187:LEU:HB3	1.94	0.50
1:C:447:ARG:HG2	1:C:447:ARG:NH1	2.11	0.50
1:A:537:GLU:OE1	1:A:541:LEU:HA	2.11	0.50
1:B:73:ILE:HG22	1:B:224:ASN:ND2	2.25	0.50
1:C:201:VAL:HG23	1:C:382:ILE:CG2	2.41	0.50
1:F:301:ALA:HB1	1:F:306:VAL:O	2.11	0.50
1:B:447:ARG:HG3	1:B:448:VAL:N	2.25	0.50
1:D:502:LEU:HD11	1:F:244:LEU:HD22	1.94	0.50
1:E:77:ARG:HD3	1:E:216:GLY:O	2.10	0.50
1:E:213:TYR:CD2	1:E:331:LEU:HD23	2.46	0.50
1:F:449:GLN:HA	1:F:459:LEU:O	2.10	0.50
1:B:448:VAL:HG12	1:B:459:LEU:HD23	1.93	0.50
1:D:501:THR:OG1	1:D:507:SER:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:GLN:HB3	4:B:611:HOH:O	2.11	0.50
1:B:213:TYR:CE2	1:B:215:ASP:HB3	2.47	0.50
1:B:321:ARG:HB2	1:B:325:ILE:HG22	1.93	0.50
1:D:63:PHE:HZ	1:D:468:LEU:HD22	1.77	0.50
1:F:513:PRO:HD2	1:F:516:VAL:CG1	2.42	0.50
1:E:37:LEU:HD11	1:E:62:ASP:HB3	1.93	0.49
1:E:382:ILE:HD13	1:E:418:ARG:HB2	1.94	0.49
1:E:429:PRO:HA	1:E:477:VAL:O	2.11	0.49
1:F:195:ARG:O	1:F:379:LYS:HE2	2.12	0.49
1:C:355:GLN:HG3	1:C:356:GLU:N	2.26	0.49
1:B:228:VAL:HG11	1:B:237:GLN:O	2.13	0.49
1:F:250:ASN:ND2	1:F:253:ASN:OD1	2.46	0.49
1:A:287:ASN:HB3	4:A:1017:HOH:O	2.13	0.49
1:A:305:ASN:C	1:A:305:ASN:HD22	2.21	0.49
1:D:201:VAL:HG23	1:D:382:ILE:CG2	2.41	0.49
1:A:84:SER:O	1:A:209:ALA:HA	2.13	0.49
1:A:443[A]:ARG:HA	1:A:465:GLN:HG3	1.95	0.49
1:B:49:GLU:HB3	1:B:321:ARG:HB3	1.95	0.49
1:B:59:ASN:O	1:B:64:GLN:NE2	2.46	0.49
1:C:408:ILE:HG12	1:C:408:ILE:O	2.13	0.49
1:B:40[A]:ARG:HE	1:B:63:PHE:HE2	1.61	0.49
1:B:505:ARG:NH2	1:E:110:GLU:O	2.45	0.49
1:F:252:PHE:HE1	4:F:942:HOH:O	1.96	0.49
1:F:525:ARG:HB2	1:F:529:ARG:HH21	1.77	0.49
1:D:27:SER:OG	1:D:29:GLN:NE2	2.46	0.48
1:F:53:ILE:HG12	1:F:73:ILE:HG12	1.96	0.48
1:F:77:ARG:CG	1:F:217:ASP:O	2.61	0.48
1:A:52:GLN:HG2	1:A:74:THR:HG23	1.95	0.48
1:A:370:GLU:HA	1:A:374:CYS:HB2	1.96	0.48
1:B:54:GLU:CD	1:B:72:ARG:HH11	2.20	0.48
1:C:394[A]:ARG:HB2	1:D:115:SER:CB	2.43	0.48
1:C:524:SER:H	1:C:527:GLN:NE2	2.11	0.48
1:E:95:VAL:O	1:E:198:GLU:HG3	2.14	0.48
1:F:344:GLU:HA	1:F:347:GLU:HB2	1.94	0.48
1:C:468:LEU:C	1:C:468:LEU:HD23	2.39	0.48
1:A:40:ARG:NH1	1:A:63:PHE:HE2	2.11	0.48
1:A:423:ARG:NH1	1:A:423:ARG:CG	2.71	0.48
1:F:73:ILE:HG22	1:F:222:ALA:HB3	1.95	0.48
1:A:494:GLU:HG3	1:A:495:GLU:N	2.28	0.48
1:D:424:ASN:O	1:D:543:SER:HB3	2.14	0.48
1:C:426:ILE:HB	1:C:541:LEU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:LEU:HD13	1:F:503:ALA:HB2	1.96	0.47
1:A:429:PRO:HA	1:A:477:VAL:O	2.14	0.47
1:B:392:SER:HB3	1:B:395:ALA:HB3	1.97	0.47
1:A:377:ARG:CD	4:A:1026:HOH:O	2.53	0.47
1:B:185:ARG:HG2	1:B:189:ARG:HH12	1.79	0.47
1:B:431:TRP:HZ3	1:B:502:LEU:CD1	2.28	0.47
1:F:197:ARG:HH22	1:F:349:GLN:HE21	1.63	0.47
1:B:357:ARG:HE	1:B:443:ARG:CD	2.27	0.47
1:D:296:ASN:OD1	1:D:298:GLN:HG2	2.14	0.47
1:F:423:ARG:HH12	1:F:483:ASN:ND2	2.12	0.47
1:B:250:ASN:HB3	1:B:253:ASN:CG	2.30	0.47
1:A:213:TYR:CE2	1:A:215:ASP:HB3	2.50	0.47
1:D:201:VAL:HG23	1:D:382:ILE:HG22	1.96	0.47
1:F:370:GLU:HA	1:F:374:CYS:HB2	1.97	0.47
1:C:41:GLU:HB3	1:C:42:PRO:HD2	1.95	0.46
1:D:205:PRO:HG3	1:D:408:ILE:HD11	1.96	0.46
1:E:63:PHE:HD1	1:E:68:VAL:O	1.98	0.46
1:E:413:ARG:HG2	1:E:413:ARG:HH11	1.80	0.46
1:E:321:ARG:CB	1:E:325:ILE:HG22	2.44	0.46
1:F:353:LEU:HD12	1:F:385:PRO:HD3	1.96	0.46
1:C:185:ARG:CB	1:C:189:ARG:HH22	2.29	0.46
1:D:34:LEU:HD13	1:D:37:LEU:HD11	1.97	0.46
1:F:420:PHE:CD1	1:F:420:PHE:C	2.93	0.46
1:B:410:ARG:HD3	1:B:410:ARG:C	2.41	0.46
1:E:289:ASN:HB3	1:F:454:ASN:O	2.16	0.46
1:D:448:VAL:HG22	1:D:479:GLN:HG2	1.97	0.46
1:E:186:GLN:HB2	1:F:529:ARG:HH11	1.79	0.46
1:F:429:PRO:HA	1:F:477:VAL:O	2.16	0.46
1:F:513:PRO:CD	1:F:516:VAL:HG13	2.44	0.46
1:A:309:GLU:HG2	1:A:312:ARG:NH2	2.25	0.46
1:C:37:LEU:HD22	1:C:458:ILE:CD1	2.46	0.46
1:C:201:VAL:HG23	1:C:382:ILE:HG22	1.98	0.46
1:D:377:ARG:NH2	1:D:380:GLU:OE1	2.44	0.46
1:E:331:LEU:HD12	1:F:515:GLU:CG	2.36	0.46
1:E:186:GLN:CD	1:E:186:GLN:N	2.74	0.46
1:F:112:PHE:CE1	1:F:192:LYS:HB2	2.51	0.46
1:C:87:ASN:HB3	1:C:235:LEU:HD12	1.98	0.45
1:F:37:LEU:O	1:F:459:LEU:HD12	2.16	0.45
1:B:513:PRO:HD2	1:B:516:VAL:CG1	2.47	0.45
1:C:73:ILE:HG22	1:C:222:ALA:HB3	1.97	0.45
1:D:423:ARG:HG2	1:D:424:ASN:ND2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:448:VAL:CG1	1:F:459:LEU:HD23	2.45	0.45
1:C:317:GLN:H	1:C:317:GLN:HG2	1.41	0.45
1:D:413:ARG:HA	1:D:495:GLU:HB2	1.97	0.45
1:F:195:ARG:NH1	1:F:215:ASP:OD2	2.50	0.45
1:F:525:ARG:HB2	1:F:529:ARG:NH2	2.32	0.45
1:C:114:GLU:HG3	1:C:188:ASP:N	2.31	0.45
1:F:54:GLU:CD	1:F:72:ARG:HH11	2.24	0.45
1:B:102:GLY:HA2	1:B:211:TRP:CE2	2.51	0.45
1:E:186:GLN:C	1:F:529:ARG:HH11	2.23	0.45
1:F:448:VAL:HG22	1:F:479:GLN:HG2	1.98	0.45
1:A:84:SER:HG	1:A:241:LYS:HE3	1.81	0.45
1:D:321:ARG:HH12	1:D:325:ILE:HD13	1.82	0.45
1:B:357:ARG:HE	1:B:443:ARG:HD3	1.82	0.45
1:B:449:GLN:O	1:B:477:VAL:HA	2.16	0.45
1:C:413:ARG:CD	4:C:613:HOH:O	2.39	0.45
1:D:37:LEU:HD22	1:D:458:ILE:HG13	1.99	0.45
1:E:195:ARG:O	1:E:379:LYS:HE2	2.17	0.45
1:C:105:PHE:CZ	1:C:376:LEU:HD21	2.52	0.45
1:C:323:GLN:HE21	1:C:323:GLN:N	2.11	0.45
1:C:368:GLY:N	1:C:371:GLU:OE1	2.49	0.45
1:C:322:ASN:HB3	1:C:323:GLN:NE2	2.30	0.45
1:C:336:PRO:HA	1:C:337:PRO:HD2	1.70	0.45
1:C:358:GLN:HE21	1:C:358:GLN:HA	1.81	0.45
1:C:382:ILE:HG21	1:C:382:ILE:HD13	1.59	0.45
1:E:484:GLN:N	1:E:484:GLN:CD	2.75	0.45
1:C:36:GLN:HA	1:C:36:GLN:NE2	2.31	0.45
1:C:445:ASN:HD21	1:C:482:GLY:HA3	1.82	0.45
1:D:293:SER:HA	1:D:315:GLN:HG2	1.99	0.45
1:C:223:VAL:HG12	1:C:225:LEU:CD2	2.48	0.44
1:B:345:HIS:O	1:B:349:GLN:HG2	2.17	0.44
1:E:418:ARG:HH12	1:E:487:GLU:HB3	1.83	0.44
1:F:392:SER:HB3	1:F:395:ALA:HB3	2.00	0.44
1:A:461:GLN:CG	1:A:462:GLU:H	2.28	0.44
1:E:329:GLY:CA	1:E:330:ASN:HB2	2.46	0.44
1:F:298[B]:GLN:HE21	1:F:308:GLU:CD	2.26	0.44
1:F:513:PRO:O	1:F:516:VAL:N	2.49	0.44
1:A:464:GLN:O	1:A:465:GLN:C	2.58	0.44
1:A:473:GLN:O	1:A:474:ASN:HB2	2.16	0.44
1:B:369:LEU:HD12	1:B:369:LEU:HA	1.74	0.44
1:D:525:ARG:HH11	1:D:525:ARG:HB2	1.82	0.44
1:A:40:ARG:NH1	1:A:63:PHE:CE2	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:GLN:NE2	1:E:30:ASN:OD1	2.50	0.44
1:F:288:GLY:O	1:F:289:ASN:HB3	2.17	0.44
1:A:302:GLN:O	1:B:535:ARG:NH2	2.48	0.44
1:A:327:VAL:O	1:A:329:GLY:N	2.51	0.44
1:A:205:PRO:HG3	1:A:408:ILE:HD11	1.98	0.44
1:C:31:GLN:NE2	4:C:874:HOH:O	2.51	0.44
1:D:328:ARG:HD2	1:D:328:ARG:HA	1.71	0.44
1:E:87:ASN:HA	1:F:474:ASN:HD21	1.82	0.44
1:E:214:ASN:C	1:E:214:ASN:OD1	2.60	0.44
1:B:518:ALA:HA	1:B:523:ILE:HG13	2.00	0.44
1:D:195:ARG:HH12	1:D:215:ASP:CG	2.20	0.43
1:B:54:GLU:OE2	1:B:72:ARG:HD2	2.17	0.43
1:D:382:ILE:HG21	1:D:382:ILE:HD13	1.65	0.43
1:E:304:LEU:HD12	1:E:304:LEU:HA	1.85	0.43
1:A:406:LEU:HG	1:A:408:ILE:HG22	2.00	0.43
1:A:521:TYR:CD1	1:C:314:LEU:HA	2.53	0.43
1:C:114:GLU:HG3	1:C:188:ASP:H	1.84	0.43
1:E:290:ASN:OD1	1:E:292:PHE:HB2	2.18	0.43
1:F:387:ARG:O	1:F:387:ARG:CG	2.67	0.43
1:F:525:ARG:H	1:F:525:ARG:NH2	2.17	0.43
1:B:57:ASN:O	1:B:60:GLN:HG3	2.18	0.43
1:C:80:LEU:HD13	1:C:82:LEU:HD23	2.00	0.43
1:D:529:ARG:HD2	1:F:186:GLN:HB3	1.99	0.43
1:E:308:GLU:HG2	1:E:312:ARG:HH11	1.84	0.43
1:C:437:SER:OG	1:C:492:LYS:HE2	2.18	0.43
1:E:321:ARG:HB3	1:E:325:ILE:HG22	2.00	0.43
1:F:28:PRO:O	1:F:31:GLN:HG2	2.19	0.43
1:A:87:ASN:HA	1:B:474:ASN:ND2	2.33	0.43
1:C:439:VAL:O	1:C:468:LEU:HA	2.19	0.43
1:A:92:ILE:HD12	1:A:202:VAL:HG13	2.00	0.43
1:A:186:GLN:O	1:B:529:ARG:NH2	2.52	0.43
1:A:236:ASP:HB2	1:B:29:GLN:O	2.18	0.43
1:A:243:TYR:HB2	1:A:248:PRO:HG3	2.01	0.43
1:F:49:GLU:OE2	1:F:321:ARG:HD2	2.19	0.43
1:A:299:LEU:HD13	1:B:478:ILE:HG12	2.01	0.43
1:B:371:GLU:O	1:E:400:THR:HG21	2.18	0.43
1:C:115:SER:OG	1:D:394[A]:ARG:HB2	2.19	0.43
1:C:375:SER:HB3	4:D:939:HOH:O	2.19	0.43
1:F:419:GLY:HA3	1:F:488:TYR:CZ	2.54	0.43
1:A:39:ALA:HB2	1:A:469:PHE:HB3	2.01	0.43
1:B:538:THR:HG23	1:E:113:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ARG:HD2	1:C:328:ARG:HA	1.77	0.43
1:D:321:ARG:NH1	1:D:325:ILE:HD13	2.34	0.43
1:D:388:ALA:HA	1:D:399:SER:OG	2.19	0.43
1:B:36:GLN:O	1:B:37:LEU:HD12	2.19	0.43
1:E:87:ASN:HA	1:F:474:ASN:ND2	2.33	0.43
1:E:114:GLU:HG3	1:E:334:VAL:HG22	2.00	0.43
1:E:369:LEU:HD12	4:E:588:HOH:O	2.19	0.43
1:C:48:ALA:O	1:C:49:GLU:C	2.62	0.42
1:C:328:ARG:CZ	1:C:329:GLY:H	2.32	0.42
1:D:78:ASN:ND2	1:D:329:GLY:O	2.52	0.42
1:F:223:VAL:HG12	1:F:225:LEU:HD22	2.00	0.42
1:A:461:GLN:CG	1:A:462:GLU:N	2.81	0.42
1:A:371:GLU:O	1:F:400:THR:HG21	2.19	0.42
1:B:201:VAL:CG2	1:B:382:ILE:HG21	2.50	0.42
1:D:304:LEU:CD1	1:E:503:ALA:HB2	2.48	0.42
1:D:430:HIS:HB2	1:D:500:ASN:O	2.19	0.42
1:B:392:SER:HA	1:B:393:PRO:HD3	1.89	0.42
1:E:41:GLU:HB3	1:E:42:PRO:HD2	2.01	0.42
1:A:308:GLU:O	1:A:308:GLU:HG3	2.19	0.42
1:E:417:GLU:HB3	1:E:490:ALA:HB3	2.02	0.42
1:A:189:ARG:HH22	1:F:536:GLN:NE2	2.16	0.42
1:A:190:HIS:ND1	1:B:513:PRO:HG3	2.35	0.42
1:E:404:HIS:HE1	4:E:601:HOH:O	2.02	0.42
1:E:517:LEU:HD11	1:E:532:LYS:HE3	2.02	0.42
1:F:105:PHE:HE1	1:F:194:ARG:NH1	2.18	0.42
1:F:185:ARG:HH21	1:F:185:ARG:HG2	1.85	0.42
1:A:290:ASN:O	1:A:291:VAL:C	2.61	0.42
1:A:503:ALA:HB2	1:C:304:LEU:HD13	2.02	0.42
1:B:105:PHE:CZ	1:B:376:LEU:HD21	2.54	0.42
1:C:287:ASN:CB	1:C:317:GLN:HE21	2.33	0.42
1:D:314:LEU:HA	1:E:521:TYR:CD1	2.54	0.42
1:E:235:LEU:HA	1:E:235:LEU:HD23	1.73	0.42
1:F:102:GLY:O	1:F:210:TYR:HA	2.20	0.42
1:A:235:LEU:HD23	1:B:436:HIS:HE1	1.85	0.42
1:A:510:ARG:HE	1:A:510:ARG:HB3	1.63	0.42
1:B:513:PRO:O	1:B:514:ASP:C	2.63	0.42
1:C:350:GLN:C	1:C:352:GLN:H	2.27	0.42
1:A:66:ALA:HA	1:A:436:HIS:CD2	2.55	0.42
1:D:116:GLN:O	1:D:117:GLN:HB3	2.19	0.42
1:D:197:ARG:O	1:D:198:GLU:C	2.62	0.42
1:D:307:ASN:OD1	1:D:309:GLU:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:PHE:CD2	1:A:335:GLN:HB2	2.55	0.41
1:A:423:ARG:HH11	1:A:423:ARG:HG3	1.81	0.41
1:C:506:THR:HG21	1:D:370:GLU:OE2	2.20	0.41
1:B:423:ARG:HD3	1:B:483:ASN:HD22	1.85	0.41
1:B:505:ARG:HB2	1:B:538:THR:HG22	2.03	0.41
1:E:112:PHE:CE2	1:E:193:THR:HG22	2.54	0.41
1:F:439:VAL:O	1:F:468:LEU:HA	2.20	0.41
1:B:323:GLN:NE2	1:B:323:GLN:N	2.51	0.41
1:C:429:PRO:HA	1:C:477:VAL:O	2.20	0.41
1:C:535:ARG:HD3	1:C:535:ARG:HA	1.76	0.41
1:E:322:ASN:HB3	1:E:323:GLN:NE2	2.36	0.41
1:A:116:GLN:H	1:A:116:GLN:HG3	1.66	0.41
1:A:193:THR:HG21	1:A:333:PHE:CE2	2.55	0.41
1:B:331:LEU:HD21	1:C:516:VAL:HG12	2.02	0.41
1:D:384:ASN:HB2	4:D:757:HOH:O	2.20	0.41
1:E:484:GLN:CD	1:E:484:GLN:H	2.29	0.41
1:C:59:ASN:HA	1:C:64:GLN:NE2	2.35	0.41
1:D:298:GLN:HB3	1:D:308:GLU:OE1	2.21	0.41
1:E:420:PHE:C	1:E:420:PHE:CD1	2.98	0.41
1:B:35:ASN:HD22	1:B:35:ASN:HA	1.56	0.41
1:D:535:ARG:HA	1:D:535:ARG:HD3	1.66	0.41
1:E:93:TYR:HB3	1:E:223:VAL:HG23	2.02	0.41
1:F:60:GLN:H	1:F:60:GLN:HG2	1.56	0.41
1:F:77:ARG:HG3	1:F:217:ASP:O	2.21	0.41
1:F:424:ASN:HA	1:F:481:ALA:O	2.21	0.41
1:A:57:ASN:HA	1:A:254:GLN:NE2	2.35	0.41
1:B:193:THR:HG21	1:B:333:PHE:CE2	2.53	0.41
1:B:449:GLN:HA	1:B:459:LEU:O	2.21	0.41
1:B:513:PRO:CD	1:B:516:VAL:HG13	2.50	0.41
1:C:78:ASN:ND2	1:C:329:GLY:O	2.53	0.41
1:D:57:ASN:HD21	1:D:254:GLN:HB2	1.86	0.41
1:E:39:ALA:HA	1:E:468:LEU:O	2.21	0.41
1:E:384:ASN:HA	1:E:385:PRO:HD2	1.96	0.41
1:F:449:GLN:O	1:F:477:VAL:HA	2.21	0.41
1:F:531:LEU:HD23	1:F:531:LEU:HA	1.87	0.41
1:C:338:ARG:NH1	1:C:343:ARG:HG3	2.30	0.41
1:E:112:PHE:CE2	1:E:193:THR:CG2	3.04	0.41
1:F:423:ARG:NH1	1:F:483:ASN:ND2	2.68	0.41
1:A:373:PHE:CZ	1:E:373:PHE:CE1	3.09	0.40
1:E:426:ILE:HB	1:E:541:LEU:HB2	2.02	0.40
1:A:384:ASN:O	1:A:387:ARG:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LEU:HD23	1:B:203:ALA:HA	2.03	0.40
1:E:100:VAL:CG2	1:E:193:THR:OG1	2.69	0.40
1:E:505:ARG:HG3	1:E:537:GLU:O	2.21	0.40
1:A:322:ASN:HB3	1:A:323:GLN:H	1.75	0.40
1:B:410:ARG:O	1:B:413:ARG:NH1	2.54	0.40
1:C:55:THR:HG22	1:C:71:SER:HB2	2.03	0.40
1:F:426:ILE:HG22	1:F:427:TYR:N	2.36	0.40
1:B:317:GLN:HE21	1:B:317:GLN:HB3	1.75	0.40
1:C:340:ARG:HB2	1:C:343:ARG:HE	1.87	0.40
1:C:430:HIS:HB2	1:C:500:ASN:O	2.21	0.40
1:D:76:GLN:O	1:D:77:ARG:C	2.65	0.40
1:D:443:ARG:HD3	4:D:933:HOH:O	2.20	0.40
1:B:312:ARG:HG3	1:B:317:GLN:OE1	2.21	0.40
1:E:420:PHE:C	1:E:420:PHE:HD1	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	382/531 (72%)	342 (90%)	36 (9%)	4 (1%)	12	20
1	B	403/531 (76%)	371 (92%)	32 (8%)	0	100	100
1	C	403/531 (76%)	375 (93%)	24 (6%)	4 (1%)	12	20
1	D	381/531 (72%)	356 (93%)	23 (6%)	2 (0%)	24	37
1	E	381/531 (72%)	354 (93%)	22 (6%)	5 (1%)	9	14
1	F	404/531 (76%)	372 (92%)	30 (7%)	2 (0%)	24	37
All	All	2354/3186 (74%)	2170 (92%)	167 (7%)	17 (1%)	18	28

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328[A]	ARG
1	A	328[B]	ARG
1	C	340	ARG
1	E	328	ARG
1	E	330	ASN
1	F	37	LEU
1	A	237	GLN
1	D	235	LEU
1	E	235	LEU
1	E	465	GLN
1	A	192	LYS
1	C	250	ASN
1	D	318	ASN
1	E	106	SER
1	C	235	LEU
1	F	235	LEU
1	C	482	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	330/452 (73%)	279 (84%)	51 (16%)	2	3
1	B	349/452 (77%)	290 (83%)	59 (17%)	2	3
1	C	349/452 (77%)	310 (89%)	39 (11%)	6	9
1	D	330/452 (73%)	289 (88%)	41 (12%)	4	6
1	E	329/452 (73%)	283 (86%)	46 (14%)	3	4
1	F	350/452 (77%)	301 (86%)	49 (14%)	3	4
All	All	2037/2712 (75%)	1752 (86%)	285 (14%)	3	4

All (285) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	37	LEU

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Mol	Chain	Res	Type
1	A	38	GLN
1	A	40	ARG
1	A	41	GLU
1	A	46	ILE
1	A	47	GLN
1	A	54	GLU
1	A	64	GLN
1	A	68	VAL
1	A	74	THR
1	A	77	ARG
1	A	95	VAL
1	A	100	VAL
1	A	104	VAL
1	A	114	GLU
1	A	116	GLN
1	A	186	GLN
1	A	193	THR
1	A	195	ARG
1	A	217	ASP
1	A	223	VAL
1	A	250	ASN
1	A	253	ASN
1	A	254	GLN
1	A	287	ASN
1	A	291	VAL
1	A	299	LEU
1	A	304	LEU
1	A	306	VAL
1	A	317	GLN
1	A	323	GLN
1	A	328[A]	ARG
1	A	328[B]	ARG
1	A	369	LEU
1	A	371	GLU
1	A	378	LEU
1	A	382	ILE
1	A	400	THR
1	A	413	ARG
1	A	414	LEU
1	A	418	ARG
1	A	423	ARG
1	A	447	ARG

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Mol	Chain	Res	Type
1	A	483	ASN
1	A	502	LEU
1	A	506	THR
1	A	508	PHE
1	A	516	VAL
1	A	525	ARG
1	A	526	GLU
1	B	27	SER
1	B	29	GLN
1	B	31	GLN
1	B	35	ASN
1	B	36	GLN
1	B	38	GLN
1	B	40[A]	ARG
1	B	40[B]	ARG
1	B	46	ILE
1	B	73	ILE
1	B	77	ARG
1	B	80	LEU
1	B	95	VAL
1	B	114	GLU
1	B	116	GLN
1	B	117	GLN
1	B	185	ARG
1	B	186	GLN
1	B	193	THR
1	B	195	ARG
1	B	202	VAL
1	B	212	SER
1	B	241	LYS
1	B	250	ASN
1	B	253	ASN
1	B	291	VAL
1	B	293	SER
1	B	298	GLN
1	B	299	LEU
1	B	302	GLN
1	B	304	LEU
1	B	305	ASN
1	B	306	VAL
1	B	309	GLU
1	B	312	ARG

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Mol	Chain	Res	Type
1	B	317	GLN
1	B	321	ARG
1	B	323	GLN
1	B	341	GLN
1	B	344	GLU
1	B	346	GLU
1	B	351	GLU
1	B	353	LEU
1	B	369	LEU
1	B	378	LEU
1	B	379	LYS
1	B	380	GLU
1	B	382	ILE
1	B	400	THR
1	B	410	ARG
1	B	414	LEU
1	B	418	ARG
1	B	439	VAL
1	B	468	LEU
1	B	470	ILE
1	B	499	ILE
1	B	502	LEU
1	B	516	VAL
1	B	529	ARG
1	C	27	SER
1	C	36	GLN
1	C	46	ILE
1	C	80	LEU
1	C	95	VAL
1	C	104	VAL
1	C	185	ARG
1	C	189	ARG
1	C	193	THR
1	C	202	VAL
1	C	291	VAL
1	C	299	LEU
1	C	302	GLN
1	C	304	LEU
1	C	309	GLU
1	C	317	GLN
1	C	323	GLN
1	C	328	ARG

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Mol	Chain	Res	Type
1	C	346	GLU
1	C	347	GLU
1	C	351	GLU
1	C	356	GLU
1	C	358	GLN
1	C	359	GLN
1	C	369	LEU
1	C	378	LEU
1	C	379	LYS
1	C	392	SER
1	C	394[A]	ARG
1	C	394[B]	ARG
1	C	408	ILE
1	C	447	ARG
1	C	483	ASN
1	C	484	GLN
1	C	500	ASN
1	C	506	THR
1	C	508	PHE
1	C	510	ARG
1	C	516	VAL
1	D	37	LEU
1	D	38	GLN
1	D	64	GLN
1	D	73	ILE
1	D	74	THR
1	D	100	VAL
1	D	104	VAL
1	D	106	SER
1	D	193	THR
1	D	202	VAL
1	D	217	ASP
1	D	241	LYS
1	D	250	ASN
1	D	253	ASN
1	D	254	GLN
1	D	291	VAL
1	D	298	GLN
1	D	299	LEU
1	D	304	LEU
1	D	306	VAL
1	D	310	THR

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Mol	Chain	Res	Type
1	D	317	GLN
1	D	325	ILE
1	D	327	VAL
1	D	328	ARG
1	D	369	LEU
1	D	371	GLU
1	D	378	LEU
1	D	379	LYS
1	D	386	GLU
1	D	392	SER
1	D	394[A]	ARG
1	D	394[B]	ARG
1	D	414	LEU
1	D	447	ARG
1	D	502	LEU
1	D	506	THR
1	D	508	PHE
1	D	510	ARG
1	D	516	VAL
1	D	525	ARG
1	E	29	GLN
1	E	37	LEU
1	E	38	GLN
1	E	40	ARG
1	E	46	ILE
1	E	52	GLN
1	E	57	ASN
1	E	68	VAL
1	E	74	THR
1	E	95	VAL
1	E	104	VAL
1	E	113	GLU
1	E	117	GLN
1	E	186	GLN
1	E	193	THR
1	E	195	ARG
1	E	196	ILE
1	E	202	VAL
1	E	212	SER
1	E	217	ASP
1	E	223	VAL
1	E	287	ASN

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Mol	Chain	Res	Type
1	E	289	ASN
1	E	291	VAL
1	E	293	SER
1	E	299	LEU
1	E	304	LEU
1	E	305	ASN
1	E	306	VAL
1	E	317	GLN
1	E	323	GLN
1	E	378	LEU
1	E	382	ILE
1	E	386	GLU
1	E	400	THR
1	E	403	SER
1	E	414	LEU
1	E	447	ARG
1	E	465	GLN
1	E	483	ASN
1	E	484	GLN
1	E	502	LEU
1	E	516	VAL
1	E	525	ARG
1	E	530	GLN
1	E	543	SER
1	F	27	SER
1	F	29	GLN
1	F	46	ILE
1	F	54	GLU
1	F	60	GLN
1	F	64	GLN
1	F	73	ILE
1	F	80	LEU
1	F	95	VAL
1	F	100	VAL
1	F	104	VAL
1	F	113	GLU
1	F	185	ARG
1	F	186	GLN
1	F	187	LEU
1	F	192	LYS
1	F	193	THR
1	F	195	ARG

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Mol	Chain	Res	Type
1	F	212	SER
1	F	217	ASP
1	F	254	GLN
1	F	299	LEU
1	F	306	VAL
1	F	308	GLU
1	F	328	ARG
1	F	344	GLU
1	F	347	GLU
1	F	353	LEU
1	F	354	GLN
1	F	355	GLN
1	F	369	LEU
1	F	370	GLU
1	F	378	LEU
1	F	382	ILE
1	F	392	SER
1	F	400	THR
1	F	414	LEU
1	F	415	SER
1	F	418	ARG
1	F	439	VAL
1	F	470	ILE
1	F	483	ASN
1	F	492	LYS
1	F	502	LEU
1	F	512	LEU
1	F	516	VAL
1	F	517	LEU
1	F	525	ARG
1	F	529	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	47	GLN
1	A	52	GLN
1	A	57	ASN
1	A	59	ASN
1	A	76	GLN
1	A	90	GLN

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Mol	Chain	Res	Type
1	A	254	GLN
1	A	289	ASN
1	A	296	ASN
1	A	313	ASN
1	A	317	GLN
1	A	323	GLN
1	A	326	GLN
1	A	424	ASN
1	A	479	GLN
1	A	519	ASN
1	A	527	GLN
1	A	530	GLN
1	B	35	ASN
1	B	36	GLN
1	B	59	ASN
1	B	81	HIS
1	B	116	GLN
1	B	117	GLN
1	B	224	ASN
1	B	237	GLN
1	B	238	ASN
1	B	253	ASN
1	B	289	ASN
1	B	313	ASN
1	B	323	GLN
1	B	341	GLN
1	B	381	ASN
1	B	474	ASN
1	B	480	GLN
1	B	483	ASN
1	B	530	GLN
1	C	31	GLN
1	C	36	GLN
1	C	47	GLN
1	C	57	ASN
1	C	59	ASN
1	C	64	GLN
1	C	78	ASN
1	C	218	GLN
1	C	224	ASN
1	C	237	GLN
1	C	238	ASN

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Mol	Chain	Res	Type
1	C	247	ASN
1	C	298	GLN
1	C	317	GLN
1	C	323	GLN
1	C	326	GLN
1	C	335	GLN
1	C	350	GLN
1	C	355	GLN
1	C	358	GLN
1	C	359	GLN
1	C	445	ASN
1	C	500	ASN
1	C	527	GLN
1	D	29	GLN
1	D	31	GLN
1	D	44	ASN
1	D	78	ASN
1	D	237	GLN
1	D	253	ASN
1	D	287	ASN
1	D	302	GLN
1	D	305	ASN
1	D	313	ASN
1	D	326	GLN
1	D	335	GLN
1	D	404	HIS
1	D	424	ASN
1	D	454	ASN
1	D	464	GLN
1	D	474	ASN
1	D	479	GLN
1	D	480	GLN
1	D	500	ASN
1	D	530	GLN
1	D	536	GLN
1	E	29	GLN
1	E	35	ASN
1	E	38	GLN
1	E	52	GLN
1	E	117	GLN
1	E	224	ASN
1	E	250	ASN

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Mol	Chain	Res	Type
1	E	254	GLN
1	E	302	GLN
1	E	313	ASN
1	E	315	GLN
1	E	323	GLN
1	E	424	ASN
1	E	465	GLN
1	E	522	GLN
1	E	536	GLN
1	F	33	GLN
1	F	36	GLN
1	F	57	ASN
1	F	64	GLN
1	F	76	GLN
1	F	81	HIS
1	F	96	GLN
1	F	117	GLN
1	F	186	GLN
1	F	224	ASN
1	F	237	GLN
1	F	238	ASN
1	F	250	ASN
1	F	302	GLN
1	F	313	ASN
1	F	341	GLN
1	F	350	GLN
1	F	352	GLN
1	F	355	GLN
1	F	465	GLN
1	F	474	ASN
1	F	500	ASN
1	F	522	GLN
1	F	530	GLN
1	F	536	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](#)

Of 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	A	388/531 (73%)	-1.65	0 100 100	24, 44, 66, 84	2 (0%)
1	B	410/531 (77%)	-1.67	0 100 100	21, 39, 81, 96	1 (0%)
1	C	410/531 (77%)	-1.69	0 100 100	20, 38, 80, 103	1 (0%)
1	D	388/531 (73%)	-1.70	0 100 100	21, 37, 61, 87	1 (0%)
1	E	388/531 (73%)	-1.66	0 100 100	25, 45, 67, 80	1 (0%)
1	F	410/531 (77%)	-1.69	0 100 100	21, 38, 75, 86	2 (0%)
All	All	2394/3186 (75%)	-1.68	0 100 100	20, 40, 68, 103	8 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	CA	C	3	1/1	0.99	0.04	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	D	4	1/1	0.99	0.03	45,45,45,45	0
3	NA	A	9	1/1	0.99	0.09	50,50,50,50	0
3	NA	F	7	1/1	0.99	0.12	53,53,53,53	0
2	CA	E	5	1/1	1.00	0.05	51,51,51,51	0
2	CA	F	6	1/1	1.00	0.02	51,51,51,51	0
3	NA	A	552	1/1	1.00	0.14	53,53,53,53	0
2	CA	A	1	1/1	1.00	0.05	52,52,52,52	0
3	NA	B	552	1/1	1.00	0.12	40,40,40,40	0
3	NA	C	552	1/1	1.00	0.14	51,51,51,51	0
3	NA	D	552	1/1	1.00	0.17	58,58,58,58	0
3	NA	E	552	1/1	1.00	0.15	67,67,67,67	0
3	NA	E	8	1/1	1.00	0.09	44,44,44,44	0
3	NA	F	552	1/1	1.00	0.10	43,43,43,43	0
2	CA	B	2	1/1	1.00	0.03	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.