



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:39 AM UTC

PDB ID : 3MKQ / pdb_00003mkq
Title : Crystal structure of yeast alpha/betaprime-COP subcomplex of the COPI vesicular coat
Authors : Lee, C.; Goldberg, J.
Deposited on : 2010-04-15
Resolution : 2.50 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

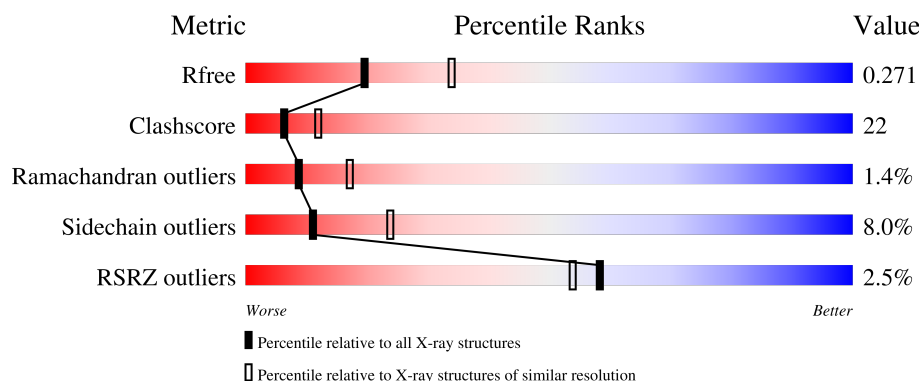
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

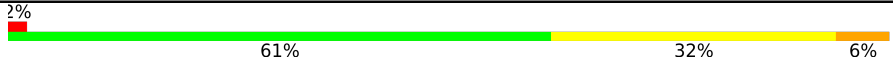
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	814	
1	C	814	
1	E	814	
2	B	177	
2	D	177	

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Mol	Chain	Length	Quality of chain
2	F	177	4% 59% 35% . ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23730 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 Coatomer beta'-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	811	Total	C	N	O	S	0	0	0
			6438	4110	1063	1252	13			
1	C	811	Total	C	N	O	S	0	0	0
			6437	4109	1063	1252	13			
1	E	810	Total	C	N	O	S	0	0	0
			6430	4107	1061	1248	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	701	ILE	VAL	variant	UNP A6ZU46
C	701	ILE	VAL	variant	UNP A6ZU46
E	701	ILE	VAL	variant	UNP A6ZU46

- Molecule 2 is a protein called Coatomer subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	0	0
			1390	877	230	279	4			
2	D	177	Total	C	N	O	S	0	0	0
			1390	877	230	279	4			
2	F	175	Total	C	N	O	S	0	0	0
			1375	869	228	274	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	664	ALA	VAL	variant	UNP P53622
B	676	ILE	SER	variant	UNP P53622
D	664	ALA	VAL	variant	UNP P53622
D	676	ILE	SER	variant	UNP P53622
F	664	ALA	VAL	variant	UNP P53622

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Chain	Residue	Modelled	Actual	Comment	Reference
F	676	ILE	SER	variant	UNP P53622

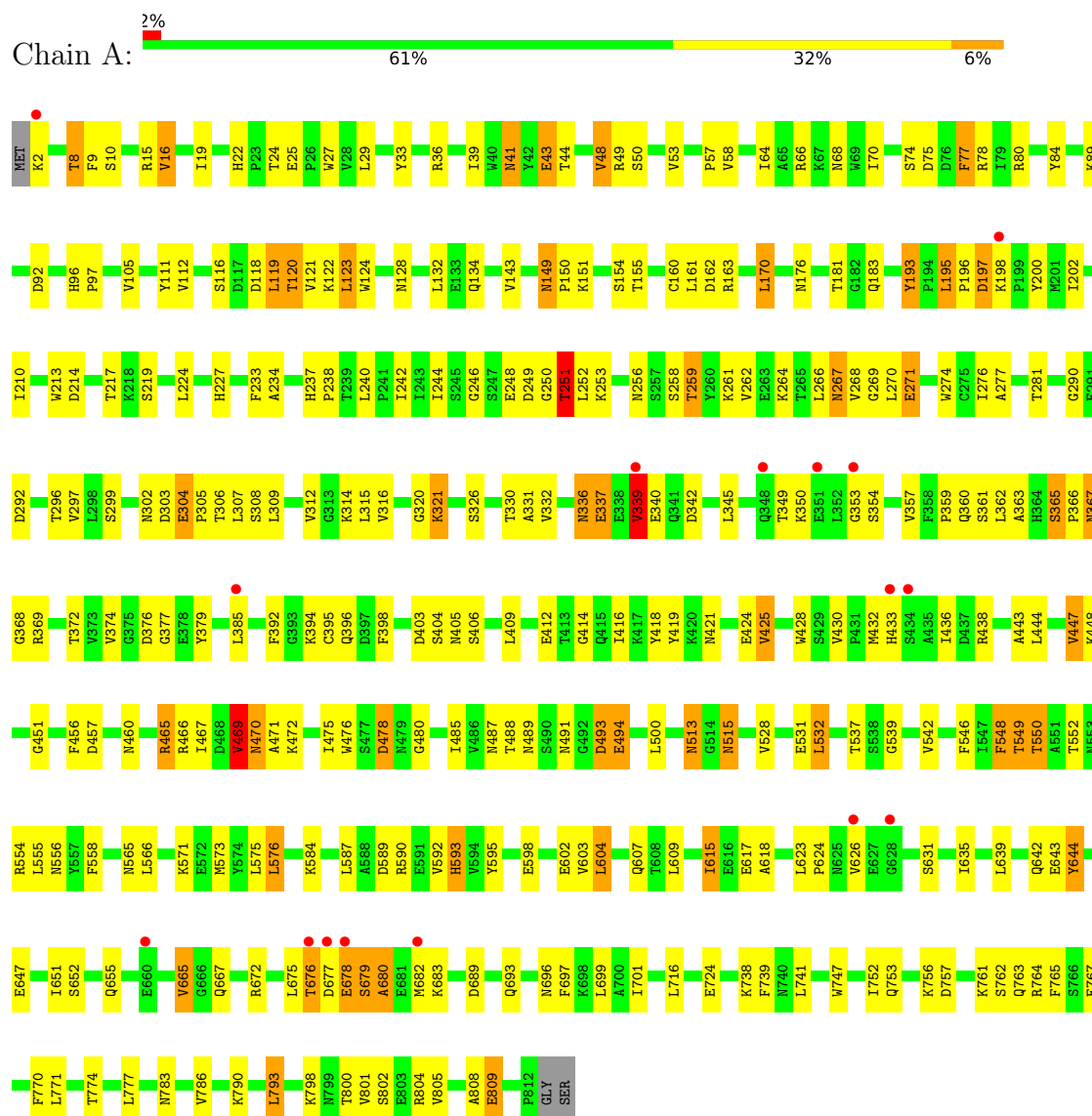
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total 100	O 100	0	0
3	B	17	Total 17	O 17	0	0
3	C	76	Total 76	O 76	0	0
3	D	5	Total 5	O 5	0	0
3	E	66	Total 66	O 66	0	0
3	F	6	Total 6	O 6	0	0

3 Residue-property plots

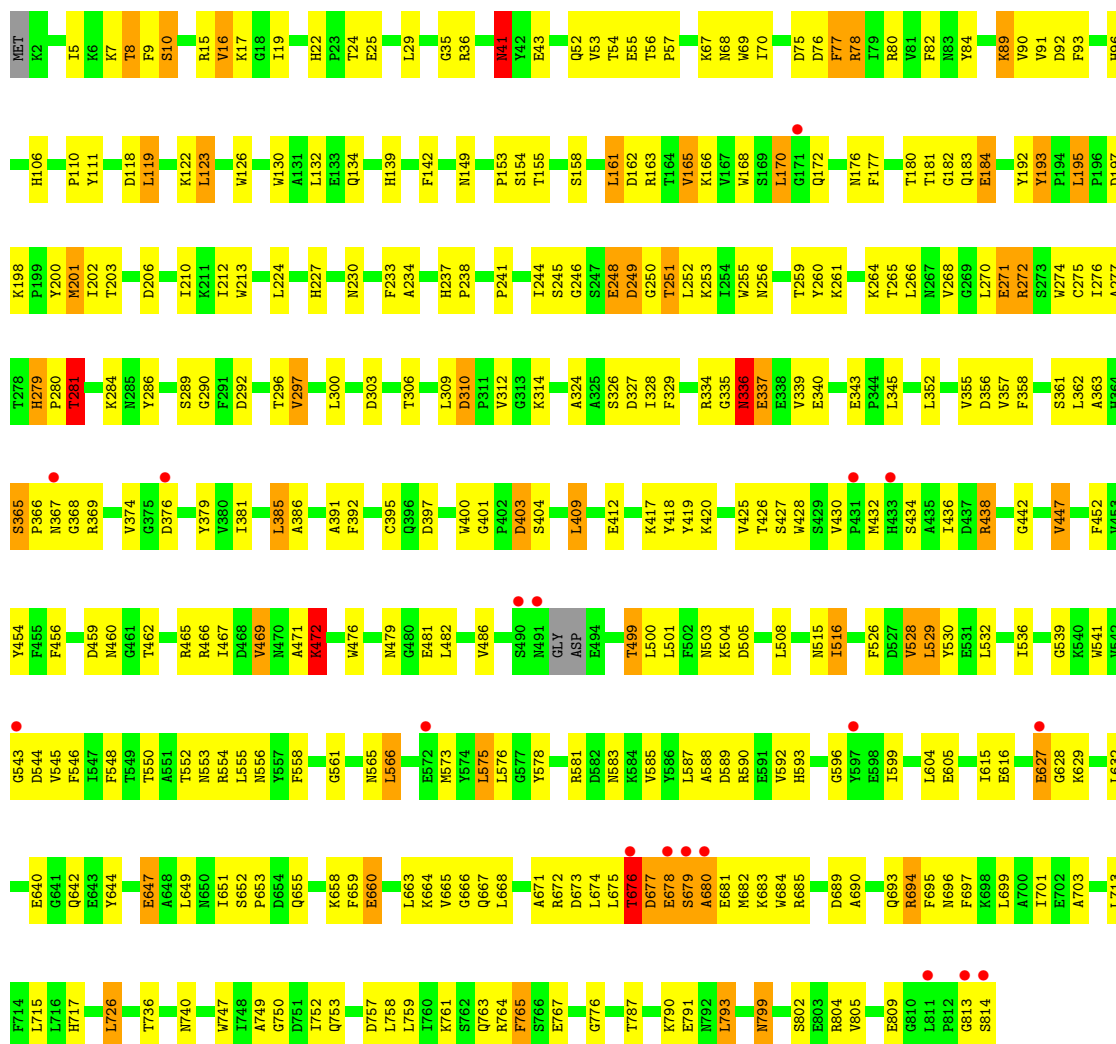
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

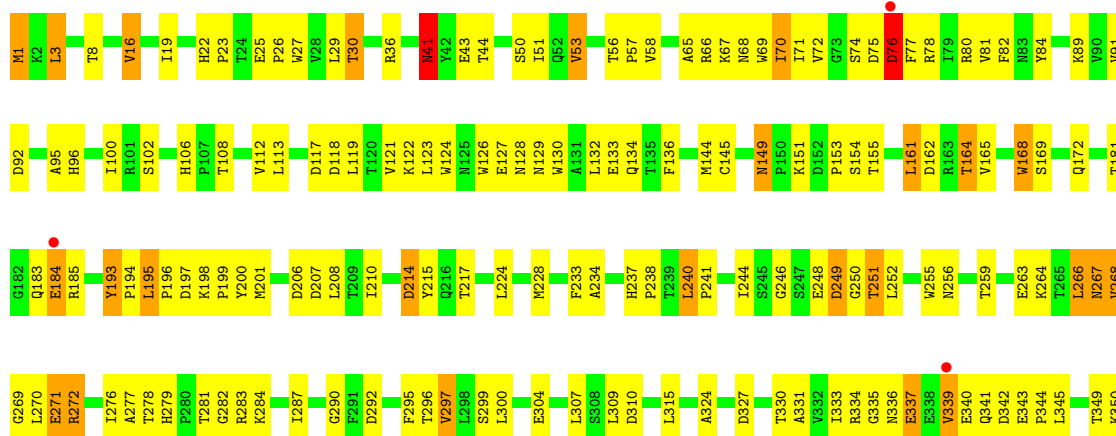


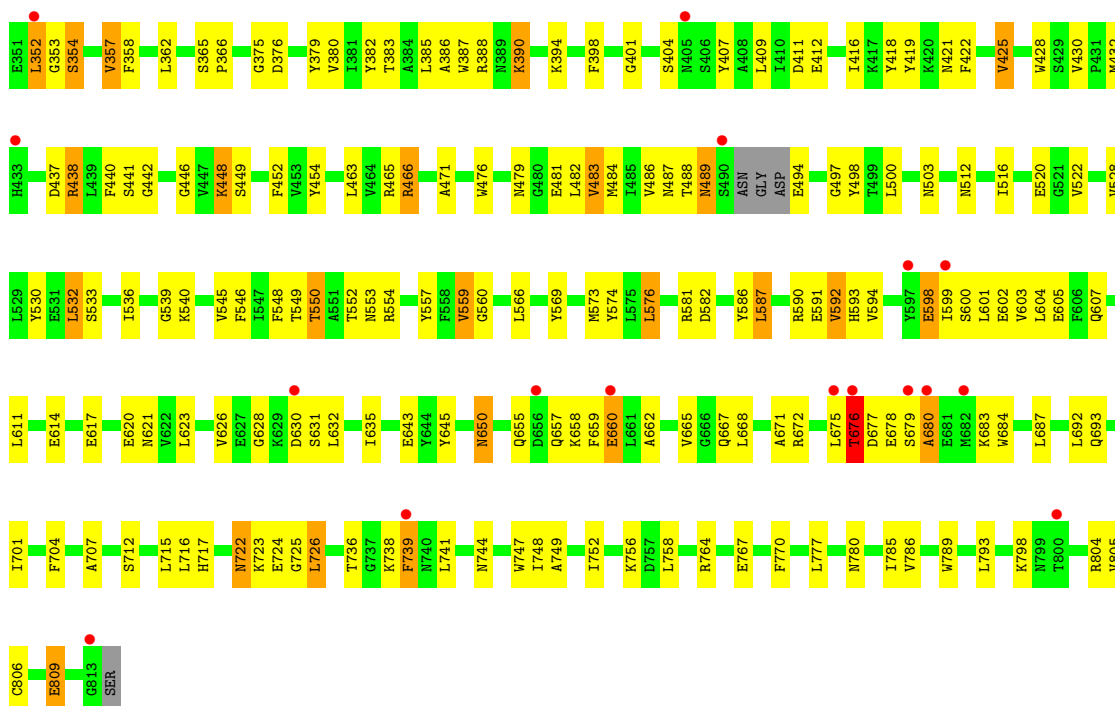
• Molecule 1: Coatomer beta'-subunit



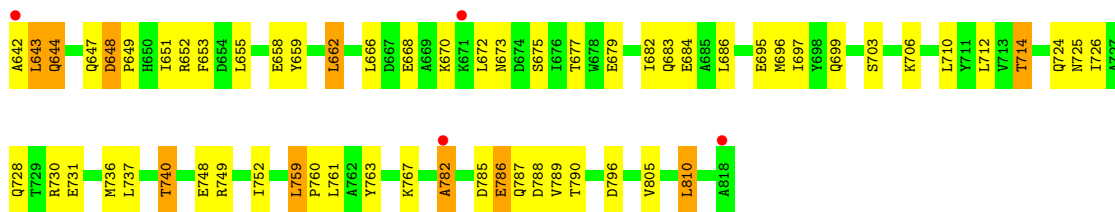


• Molecule 1: Coatomer beta'-subunit

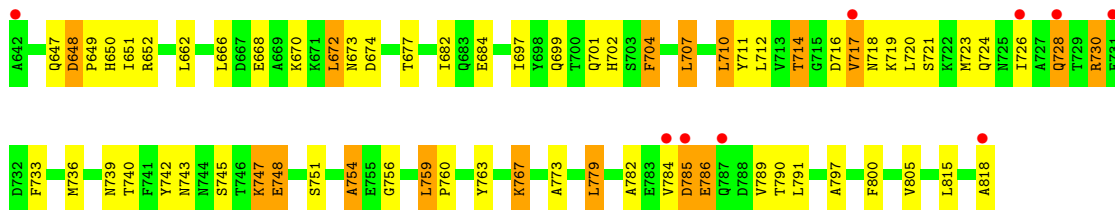




• Molecule 2: Coatomer subunit alpha

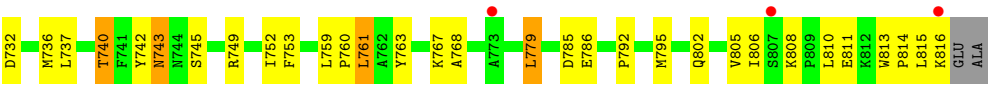


• Molecule 2: Coatomer subunit alpha



• Molecule 2: Coatomer subunit alpha





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.64Å 152.64Å 294.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.98 – 2.50 24.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.9 (24.98-2.50) 90.9 (24.98-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.272 0.219 , 0.271	Depositor DCC
R_{free} test set	6381 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23730	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.16% 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

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	0.45	0/6591	0.99	28/8960 (0.3%)
1	C	0.43	0/6589	0.99	33/8954 (0.4%)
1	E	0.44	0/6582	0.95	23/8945 (0.3%)
2	B	0.42	0/1415	0.94	4/1915 (0.2%)
2	D	0.41	0/1415	0.95	5/1915 (0.3%)
2	F	0.42	0/1400	0.91	7/1896 (0.4%)
All	All	0.44	0/23992	0.97	100/32585 (0.3%)

There are no bond length outliers.

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	677	ASP	N-CA-C	-13.67	98.48	112.97
2	D	647	GLN	N-CA-C	12.01	124.06	110.97
2	B	647	GLN	N-CA-C	9.57	121.31	111.07
2	B	782	ALA	N-CA-C	-9.14	96.33	109.31
1	C	154	SER	N-CA-C	-8.42	103.00	113.28
1	E	195	LEU	CA-C-N	8.03	127.67	119.56
1	E	195	LEU	C-N-CA	8.03	127.67	119.56
1	C	676	THR	CB-CA-C	-8.01	105.54	117.07
1	A	472	LYS	N-CA-C	-8.00	103.32	113.72
1	C	368	GLY	N-CA-C	-7.90	104.18	114.85
1	C	652	SER	N-CA-C	7.83	119.20	109.57
1	A	193	TYR	N-CA-C	-7.64	98.61	109.24
1	C	365	SER	N-CA-C	-7.35	99.61	110.20
1	E	70	ILE	N-CA-C	-7.31	97.59	108.12
1	C	676	THR	CA-C-O	7.16	122.09	117.94
1	A	593	HIS	N-CA-C	-6.99	98.22	109.96
1	C	681	GLU	N-CA-C	-6.94	103.77	111.82
1	E	365	SER	N-CA-C	-6.85	100.34	110.20
1	E	471	ALA	N-CA-C	6.84	121.01	110.20
1	E	154	SER	N-CA-C	-6.76	105.03	113.28
1	A	548	PHE	N-CA-C	6.74	119.09	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	652	SER	N-CA-C	6.73	117.85	109.57
1	A	70	ILE	N-CA-C	-6.71	97.92	108.86
2	F	647	GLN	N-CA-C	6.70	125.06	110.80
1	E	127	GLU	N-CA-C	-6.68	105.01	113.02
1	E	251	THR	N-CA-C	6.65	120.23	109.40
2	B	675	SER	N-CA-C	6.60	118.27	111.14
2	F	648	ASP	N-CA-C	6.45	118.97	109.62
1	C	279	HIS	CA-C-N	6.45	127.90	119.84
1	C	279	HIS	C-N-CA	6.45	127.90	119.84
1	E	193	TYR	CA-C-N	6.42	126.11	119.56
1	E	193	TYR	C-N-CA	6.42	126.11	119.56
1	C	472	LYS	N-CA-C	-6.28	105.78	113.50
1	C	403	ASP	N-CA-C	6.22	118.06	111.28
1	C	193	TYR	N-CA-C	-6.22	100.36	109.50
1	A	365	SER	N-CA-C	-6.16	101.14	110.39
1	C	182	GLY	N-CA-C	-6.11	106.81	115.30
1	A	299	SER	N-CA-C	-6.08	99.28	109.07
1	C	312	VAL	N-CA-C	6.04	118.81	112.83
1	C	516	ILE	N-CA-C	6.03	117.20	109.30
1	C	765	PHE	N-CA-C	6.00	117.82	111.28
1	A	478	ASP	N-CA-C	5.98	117.47	111.07
1	A	195	LEU	CA-C-N	5.93	125.80	119.28
1	A	195	LEU	C-N-CA	5.93	125.80	119.28
1	E	401	GLY	N-CA-C	-5.89	104.86	112.10
1	A	396	GLN	N-CA-C	-5.87	106.45	113.97
1	C	195	LEU	CA-C-N	5.87	125.49	119.56
1	C	195	LEU	C-N-CA	5.87	125.49	119.56
2	D	702	HIS	N-CA-C	5.86	119.26	111.30
1	C	459	ASP	N-CA-C	5.85	117.33	111.07
1	C	248	GLU	N-CA-C	-5.85	106.19	113.15
1	E	739	PHE	N-CA-C	5.83	117.71	111.36
2	B	648	ASP	N-CA-C	5.83	117.00	109.72
1	E	41	ASN	N-CA-C	-5.73	99.19	108.41
1	C	70	ILE	N-CA-C	-5.69	100.03	108.45
1	E	76	ASP	N-CA-C	-5.69	105.60	112.54
1	E	194	PRO	N-CA-C	5.67	121.22	113.84
1	A	97	PRO	N-CA-C	-5.62	107.32	114.35
1	A	154	SER	N-CA-C	-5.57	106.46	113.20
1	A	739	PHE	N-CA-C	5.57	117.44	111.36
1	A	128	ASN	N-CA-C	-5.57	103.87	111.56
1	A	251	THR	N-CA-C	5.55	118.78	109.95
1	E	78	ARG	N-CA-C	5.54	118.75	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	566	LEU	N-CA-C	-5.50	106.62	113.55
1	C	41	ASN	N-CA-C	-5.49	98.33	107.99
1	C	363	ALA	N-CA-C	5.47	118.33	108.48
1	A	197	ASP	N-CA-C	5.42	119.37	112.87
1	A	304	GLU	N-CA-C	5.41	116.51	109.64
2	D	648	ASP	N-CA-C	5.40	117.25	109.04
2	D	704	PHE	N-CA-C	5.39	117.86	111.33
1	E	593	HIS	N-CA-C	-5.39	101.68	110.20
1	E	299	SER	N-CA-C	-5.38	99.74	108.52
1	A	339	VAL	N-CA-C	5.33	120.44	109.34
1	E	249	ASP	N-CA-C	-5.32	106.81	113.15
2	F	717	VAL	N-CA-C	5.29	116.07	110.72
1	A	78	ARG	N-CA-C	5.28	118.34	109.95
1	A	513	ASN	N-CA-C	-5.25	105.61	112.23
1	C	471	ALA	N-CA-C	5.25	117.85	110.23
1	A	676	THR	N-CA-C	-5.25	99.89	108.67
1	A	363	ALA	N-CA-C	5.22	117.93	108.69
1	C	78	ARG	N-CA-C	5.20	118.53	110.17
1	A	631	SER	N-CA-C	-5.18	105.64	111.28
1	A	64	ILE	N-CA-C	-5.16	98.60	109.34
1	E	196	PRO	N-CA-C	5.14	120.28	113.86
2	F	704	PHE	N-CA-C	5.13	116.88	111.28
1	C	249	ASP	N-CA-C	-5.13	106.86	113.02
1	A	312	VAL	N-CA-C	5.13	117.50	111.09
1	E	252	LEU	N-CA-C	-5.12	100.83	109.07
2	F	648	ASP	CA-C-N	5.10	126.22	119.84
2	F	648	ASP	C-N-CA	5.10	126.22	119.84
1	E	106	HIS	N-CA-C	-5.09	103.36	109.83
1	C	201	MET	N-CA-C	-5.09	101.55	109.24
1	C	356	ASP	N-CA-C	5.08	117.71	111.82
2	D	797	ALA	N-CA-C	-5.07	103.98	110.53
1	E	200	TYR	N-CA-C	5.07	118.02	109.95
1	C	252	LEU	N-CA-C	-5.04	100.68	108.90
2	F	792	PRO	N-CA-C	-5.03	103.86	111.41
1	C	165	VAL	N-CA-C	-5.01	101.10	108.11
1	A	644	TYR	N-CA-C	-5.01	104.34	110.65
1	C	272	ARG	N-CA-C	5.00	117.55	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	6438	0	6225	284	0
1	C	6437	0	6225	296	0
1	E	6430	0	6226	290	0
2	B	1390	0	1349	51	0
2	D	1390	0	1349	61	0
2	F	1375	0	1338	70	0
3	A	100	0	0	3	0
3	B	17	0	0	0	0
3	C	76	0	0	5	0
3	D	5	0	0	0	0
3	E	66	0	0	2	0
3	F	6	0	0	0	0
All	All	23730	0	22712	1021	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 22.

All (1021) 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:A:550:THR:HG22	1:A:554:ARG:H	1.11	1.12
1:C:334:ARG:HA	1:C:581:ARG:HH22	1.06	1.10
1:A:615:ILE:HD12	1:A:615:ILE:H	1.22	1.04
1:A:111:TYR:HB3	1:A:123:LEU:HD11	1.41	1.03
2:B:810:LEU:HD23	2:B:810:LEU:H	1.23	1.03
1:C:550:THR:HG22	1:C:554:ARG:H	1.25	1.01
1:A:550:THR:HG23	1:A:552:THR:H	1.27	0.99
1:A:675:LEU:HA	1:A:678:GLU:HG3	1.40	0.98
1:C:556:ASN:HD21	1:C:565:ASN:HD22	1.08	0.97
1:C:799:ASN:HD22	1:C:799:ASN:H	1.03	0.97
1:A:366:PRO:HD2	1:A:404:SER:HA	1.49	0.95
1:E:96:HIS:CE1	1:E:122:LYS:HD2	2.02	0.94
1:E:390:LYS:HA	1:E:390:LYS:HE2	1.49	0.94
1:A:256:ASN:HD22	1:A:259:THR:H	1.05	0.94
1:E:550:THR:HG22	1:E:554:ARG:H	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:THR:HB	1:A:549:THR:HG22	1.48	0.93
1:E:22:HIS:HD2	1:E:25:GLU:H	1.05	0.93
1:E:550:THR:HG23	1:E:552:THR:H	1.33	0.92
2:F:682:ILE:HD11	2:F:697:ILE:HB	1.51	0.92
1:E:256:ASN:HD22	1:E:259:THR:H	0.98	0.92
2:B:728:GLN:HG2	2:B:736:MET:HE3	1.52	0.91
2:D:759:LEU:HD23	2:D:782:ALA:HB2	1.52	0.91
1:C:334:ARG:HA	1:C:581:ARG:NH2	1.86	0.91
1:C:556:ASN:ND2	1:C:565:ASN:HD22	1.70	0.90
1:E:267:ASN:HD22	1:E:269:GLY:H	1.19	0.89
1:C:253:LYS:HG2	1:C:265:THR:HG22	1.56	0.88
2:F:740:THR:CG2	2:F:749:ARG:HE	1.86	0.88
1:E:22:HIS:CD2	1:E:25:GLU:H	1.92	0.87
1:E:16:VAL:HG22	1:E:290:GLY:HA3	1.56	0.87
1:C:328:ILE:HG22	1:C:352:LEU:HB3	1.56	0.87
1:A:303:ASP:OD1	1:A:590:ARG:HD3	1.74	0.85
2:F:740:THR:HG23	2:F:749:ARG:HE	1.38	0.85
1:E:197:ASP:OD1	1:E:198:LYS:HD3	1.76	0.85
2:F:768:ALA:HA	2:F:795:MET:HE3	1.56	0.85
1:E:256:ASN:ND2	1:E:259:THR:H	1.74	0.85
1:A:256:ASN:ND2	1:A:259:THR:H	1.73	0.85
1:A:783:ASN:ND2	1:A:808:ALA:H	1.75	0.84
1:E:89:LYS:HD3	1:E:92:ASP:HB2	1.57	0.84
2:B:740:THR:CG2	2:B:749:ARG:HE	1.91	0.83
1:E:809:GLU:CD	1:E:809:GLU:H	1.84	0.82
1:C:467:ILE:HG22	1:C:469:VAL:HG13	1.61	0.81
1:C:799:ASN:HD22	1:C:799:ASN:N	1.78	0.81
2:F:728:GLN:HG2	2:F:736:MET:HE3	1.62	0.81
1:E:717:HIS:HB3	1:E:726:LEU:HD13	1.63	0.81
1:C:334:ARG:CA	1:C:581:ARG:HH22	1.90	0.81
1:E:454:TYR:CZ	1:E:466:ARG:HD2	2.15	0.80
1:C:16:VAL:HG22	1:C:290:GLY:HA3	1.64	0.80
1:A:281:THR:HG22	1:A:590:ARG:HH12	1.45	0.80
1:A:149:ASN:ND2	1:A:151:LYS:H	1.80	0.80
1:C:689:ASP:O	1:C:693:GLN:HG3	1.82	0.80
2:D:710:LEU:O	2:D:714:THR:HB	1.82	0.79
1:A:302:ASN:OD1	1:A:304:GLU:HG2	1.83	0.79
1:A:550:THR:HG23	1:A:552:THR:N	1.98	0.78
1:A:2:LYS:NZ	1:A:360:GLN:HE22	1.81	0.78
1:E:41:ASN:ND2	1:E:44:THR:H	1.80	0.78
1:C:676:THR:C	1:C:678:GLU:H	1.90	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:740:THR:HG23	2:B:749:ARG:HE	1.49	0.78
1:E:659:PHE:CE1	1:E:675:LEU:HG	2.18	0.78
2:F:649:PRO:HB3	2:F:672:LEU:HD21	1.65	0.78
1:C:90:VAL:HG12	1:C:91:VAL:HG13	1.67	0.77
2:D:747:LYS:H	2:D:747:LYS:HD3	1.50	0.77
1:C:36:ARG:HG2	1:C:52:GLN:HE22	1.50	0.76
1:C:573:MET:HE1	1:C:589:ASP:HB3	1.68	0.76
2:D:747:LYS:HD3	2:D:747:LYS:N	2.00	0.76
2:B:810:LEU:H	2:B:810:LEU:CD2	1.99	0.76
1:A:493:ASP:CG	1:A:494:GLU:H	1.91	0.76
1:A:487:ASN:HD22	1:A:488:THR:H	1.34	0.75
1:A:432:MET:HG2	1:A:436:ILE:CD1	2.17	0.75
1:A:149:ASN:C	1:A:149:ASN:HD22	1.93	0.75
1:A:111:TYR:HB3	1:A:123:LEU:CD1	2.15	0.75
1:A:550:THR:CG2	1:A:554:ARG:H	1.96	0.74
1:A:57:PRO:HG2	1:A:75:ASP:OD2	1.88	0.74
1:A:451:GLY:HA2	1:A:470:ASN:HB3	1.69	0.74
1:A:556:ASN:HD21	1:A:565:ASN:HD22	1.32	0.74
1:A:467:ILE:HG22	1:A:469:VAL:HG12	1.68	0.74
1:A:118:ASP:OD1	1:A:120:THR:HB	1.87	0.74
1:C:550:THR:HG23	1:C:552:THR:H	1.51	0.74
1:E:675:LEU:HD23	1:E:678:GLU:HG3	1.69	0.73
1:A:15:ARG:HD3	1:A:292:ASP:OD1	1.89	0.73
2:F:644:GLN:CD	2:F:644:GLN:H	1.97	0.73
1:A:256:ASN:HB3	1:A:259:THR:HG22	1.71	0.72
1:A:432:MET:HG2	1:A:436:ILE:HD11	1.71	0.72
1:E:155:THR:HG22	1:E:169:SER:HB3	1.70	0.72
1:C:337:GLU:HG2	1:C:345:LEU:HD23	1.70	0.71
1:C:550:THR:HG22	1:C:554:ARG:N	2.04	0.71
1:A:470:ASN:HD22	1:A:470:ASN:H	1.38	0.71
1:A:680:ALA:HB3	1:A:683:LYS:HG3	1.72	0.71
1:A:432:MET:HE3	1:A:447:VAL:HG21	1.71	0.71
1:E:549:THR:HG21	1:E:573:MET:O	1.90	0.71
1:E:438:ARG:HH11	1:E:438:ARG:HB2	1.55	0.70
1:E:41:ASN:C	1:E:41:ASN:HD22	1.99	0.70
1:E:601:LEU:O	1:E:605:GLU:HG3	1.91	0.70
1:A:405:ASN:ND2	1:A:421:ASN:HA	2.06	0.70
1:A:487:ASN:HD22	1:A:488:THR:N	1.89	0.70
1:A:214:ASP:CG	1:A:217:THR:HG22	2.17	0.70
1:C:253:LYS:HZ3	1:C:265:THR:HG21	1.57	0.70
1:A:701:ILE:HD13	1:A:716:LEU:HD13	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:PHE:CE1	2:D:784:VAL:HG21	2.27	0.69
1:E:267:ASN:ND2	1:E:269:GLY:H	1.91	0.69
1:C:556:ASN:ND2	1:C:565:ASN:HA	2.08	0.69
1:A:675:LEU:HA	1:A:678:GLU:CG	2.20	0.69
1:E:675:LEU:HA	1:E:678:GLU:CG	2.23	0.69
1:C:550:THR:CG2	1:C:554:ARG:H	2.05	0.69
1:E:256:ASN:HD22	1:E:259:THR:N	1.83	0.69
1:E:756:LYS:HD2	1:E:785:ILE:HD11	1.72	0.69
1:C:499:THR:HG22	1:C:529:LEU:HB2	1.73	0.69
1:A:550:THR:HG22	1:A:554:ARG:N	1.96	0.68
1:C:764:ARG:HD2	1:C:767:GLU:OE2	1.91	0.68
1:A:89:LYS:HD3	1:A:92:ASP:HB2	1.75	0.68
1:C:91:VAL:HG11	1:C:130:TRP:CD1	2.28	0.68
1:E:123:LEU:HD12	1:E:133:GLU:HB3	1.76	0.68
1:E:722:ASN:ND2	1:E:725:GLY:H	1.91	0.68
1:A:315:LEU:O	1:A:330:THR:HG23	1.94	0.68
1:C:647:GLU:CD	1:C:647:GLU:H	2.01	0.68
1:E:267:ASN:HD22	1:E:267:ASN:C	2.01	0.68
1:A:783:ASN:HD21	1:A:808:ALA:H	1.42	0.68
2:B:668:GLU:O	2:B:672:LEU:HD13	1.94	0.67
1:C:253:LYS:NZ	1:C:265:THR:HG21	2.08	0.67
1:A:66:ARG:HD3	3:A:823:HOH:O	1.94	0.67
1:A:16:VAL:HG22	1:A:290:GLY:HA3	1.77	0.67
2:D:707:LEU:HD22	2:D:711:TYR:CZ	2.29	0.67
1:A:679:SER:O	1:A:680:ALA:C	2.35	0.67
1:E:77:PHE:HB3	1:E:96:HIS:O	1.94	0.67
1:C:409:LEU:HD21	1:C:417:LYS:HB2	1.76	0.67
1:A:134:GLN:NE2	1:A:170:LEU:O	2.23	0.67
1:A:697:PHE:O	1:A:701:ILE:HG12	1.94	0.67
1:C:89:LYS:HE3	1:C:92:ASP:HB2	1.76	0.67
1:C:281:THR:HG23	1:C:590:ARG:HH22	1.59	0.67
1:C:799:ASN:H	1:C:799:ASN:ND2	1.81	0.67
1:E:770:PHE:HB2	2:F:713:VAL:HG12	1.77	0.67
1:C:809:GLU:CD	1:C:809:GLU:H	2.03	0.67
1:C:412:GLU:CD	1:C:412:GLU:H	2.03	0.66
1:E:484:MET:HE1	1:E:498:TYR:N	2.10	0.66
1:E:675:LEU:O	1:E:677:ASP:N	2.28	0.66
1:E:675:LEU:HD12	1:E:687:LEU:HD12	1.77	0.66
1:C:5:ILE:HD12	1:C:300:LEU:CD2	2.25	0.66
1:A:256:ASN:HD22	1:A:259:THR:N	1.88	0.66
1:A:774:THR:O	2:B:805:VAL:HG12	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:627:GLU:H	1:C:627:GLU:CD	2.02	0.66
1:E:256:ASN:ND2	1:E:259:THR:HG23	2.10	0.66
2:F:718:ASN:OD1	2:F:722:LYS:HE3	1.96	0.66
1:C:41:ASN:HD22	1:C:43:GLU:H	1.44	0.66
1:C:139:HIS:HE1	1:C:158:SER:OG	1.78	0.66
2:F:698:TYR:HB2	2:F:707:LEU:HD13	1.77	0.66
1:C:336:ASN:N	1:C:336:ASN:HD22	1.91	0.66
1:A:281:THR:HG22	1:A:590:ARG:NH1	2.11	0.65
1:A:555:LEU:HD22	1:A:587:LEU:HD11	1.78	0.65
1:A:68:ASN:HA	1:A:84:TYR:CZ	2.31	0.65
1:A:556:ASN:ND2	1:A:565:ASN:HD22	1.94	0.65
1:C:420:LYS:HG3	1:C:425:VAL:HG21	1.78	0.65
2:D:747:LYS:H	2:D:747:LYS:CD	2.08	0.65
1:A:267:ASN:C	1:A:267:ASN:HD22	2.04	0.65
2:F:743:ASN:ND2	2:F:745:SER:HB2	2.11	0.65
1:E:770:PHE:CB	2:F:713:VAL:HG12	2.26	0.65
1:E:550:THR:HG23	1:E:552:THR:N	2.09	0.65
1:A:647:GLU:O	1:A:651:ILE:HG12	1.96	0.65
1:E:394:LYS:HE2	1:E:412:GLU:OE2	1.95	0.65
1:E:599:ILE:HG21	1:E:604:LEU:HD11	1.78	0.65
1:A:271:GLU:HB2	1:A:292:ASP:HB2	1.79	0.65
1:E:650:ASN:HD22	1:E:650:ASN:N	1.93	0.65
1:A:757:ASP:O	1:A:761:LYS:HG3	1.96	0.64
1:A:149:ASN:HD22	1:A:151:LYS:H	1.45	0.64
1:C:41:ASN:HD22	1:C:41:ASN:C	2.05	0.64
1:A:336:ASN:C	1:A:336:ASN:HD22	2.05	0.64
1:A:489:ASN:OD1	1:A:494:GLU:HB2	1.98	0.64
1:C:54:THR:HG21	1:C:76:ASP:OD2	1.97	0.64
1:E:752:ILE:CG1	2:F:802:GLN:HG3	2.28	0.64
1:A:677:ASP:C	1:A:679:SER:H	2.05	0.64
1:E:786:VAL:O	1:E:789:TRP:HB3	1.98	0.64
1:E:165:VAL:HG11	1:E:201:MET:HE1	1.79	0.64
1:C:68:ASN:HA	1:C:84:TYR:CZ	2.33	0.64
1:E:249:ASP:OD1	1:E:251:THR:HB	1.98	0.64
1:A:465:ARG:HG3	1:A:466:ARG:N	2.13	0.63
1:C:736:THR:HG22	1:C:736:THR:O	1.96	0.63
1:E:722:ASN:C	1:E:722:ASN:HD22	2.05	0.63
1:A:592:VAL:HG12	1:A:592:VAL:O	1.97	0.63
1:A:22:HIS:HD2	1:A:25:GLU:H	1.45	0.63
1:C:438:ARG:HH11	1:C:438:ARG:HB2	1.64	0.63
2:D:779:LEU:HD23	2:D:786:GLU:HG3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:MET:HE3	1:E:358:PHE:CD2	2.34	0.63
1:E:8:THR:HB	1:E:297:VAL:HG22	1.79	0.63
2:B:736:MET:HB3	2:B:752:ILE:HD12	1.80	0.63
1:C:501:LEU:HB2	1:C:529:LEU:HD21	1.80	0.63
1:A:111:TYR:CB	1:A:123:LEU:HD11	2.24	0.63
1:A:470:ASN:HD22	1:A:470:ASN:N	1.93	0.63
1:E:672:ARG:HD3	1:E:672:ARG:C	2.24	0.63
1:A:267:ASN:HD22	1:A:269:GLY:H	1.47	0.63
1:E:723:LYS:HE2	1:E:749:ALA:O	1.99	0.63
2:F:642:ALA:HA	2:F:644:GLN:HE22	1.63	0.63
1:A:314:LYS:HG2	1:A:332:VAL:HG22	1.81	0.62
1:A:515:ASN:H	1:A:515:ASN:HD22	1.45	0.62
1:E:25:GLU:HG3	1:E:26:PRO:HD2	1.81	0.62
1:A:584:LYS:HG2	1:A:598:GLU:HA	1.80	0.62
1:C:629:LYS:HD3	1:C:653:PRO:HB2	1.80	0.62
1:A:339:VAL:HG21	1:A:345:LEU:HA	1.80	0.62
1:A:2:LYS:HZ2	1:A:360:GLN:HE22	1.48	0.62
1:C:339:VAL:HG12	1:C:340:GLU:H	1.65	0.62
1:C:385:LEU:HD22	1:C:386:ALA:N	2.15	0.62
1:C:676:THR:H	1:C:678:GLU:HG3	1.64	0.62
1:E:675:LEU:HA	1:E:678:GLU:HG3	1.82	0.62
1:C:672:ARG:C	1:C:674:LEU:H	2.08	0.62
2:D:728:GLN:HG3	2:D:736:MET:HE3	1.81	0.62
1:E:339:VAL:HG21	1:E:345:LEU:HA	1.82	0.62
1:C:668:LEU:HD11	1:C:694:ARG:HG3	1.81	0.62
1:E:747:TRP:CZ2	2:F:712:LEU:HD11	2.34	0.62
1:C:403:ASP:O	1:C:404:SER:HB2	1.97	0.62
1:C:666:GLY:HA3	1:C:694:ARG:HH11	1.65	0.62
1:A:116:SER:O	1:A:143:VAL:HG22	1.99	0.61
1:A:256:ASN:HD22	1:A:258:SER:H	1.47	0.61
2:B:728:GLN:HG2	2:B:736:MET:CE	2.29	0.61
2:B:695:GLU:O	2:B:699:GLN:HG3	2.00	0.61
1:C:757:ASP:O	1:C:761:LYS:HG3	2.01	0.61
1:A:556:ASN:ND2	1:A:565:ASN:HA	2.15	0.61
1:A:309:LEU:HD22	1:A:576:LEU:HB3	1.83	0.61
1:A:360:GLN:HG2	1:A:374:VAL:O	1.99	0.61
2:B:662:LEU:HD11	2:B:684:GLU:HG3	1.83	0.61
1:C:22:HIS:HD2	1:C:24:THR:H	1.47	0.61
1:A:251:THR:HG21	1:A:253:LYS:HE2	1.83	0.61
1:C:644:TYR:HB3	1:C:647:GLU:HG2	1.83	0.61
1:A:770:PHE:HD2	2:B:810:LEU:HD11	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:ASP:O	1:A:693:GLN:HG3	2.00	0.61
2:D:785:ASP:O	2:D:786:GLU:HB2	2.00	0.61
2:D:648:ASP:HB3	2:D:651:ILE:HG12	1.83	0.60
1:E:70:ILE:HG13	1:E:70:ILE:O	2.00	0.60
1:C:717:HIS:HB3	1:C:726:LEU:HD13	1.82	0.60
1:E:1:MET:HB2	1:E:263:GLU:OE2	2.00	0.60
1:C:198:LYS:HD2	1:C:200:TYR:CE2	2.36	0.60
1:C:804:ARG:CD	2:D:818:ALA:OXT	2.49	0.60
1:C:15:ARG:HD2	1:C:274:TRP:NE1	2.16	0.60
2:D:716:ASP:OD1	2:D:719:LYS:HD3	2.01	0.60
1:E:121:VAL:HB	1:E:136:PHE:HB2	1.83	0.60
1:E:672:ARG:HD3	1:E:672:ARG:O	1.99	0.60
2:B:759:LEU:N	2:B:760:PRO:CD	2.64	0.60
1:C:447:VAL:HG13	1:C:454:TYR:HB2	1.82	0.60
1:C:272:ARG:HB2	1:C:292:ASP:OD2	2.01	0.60
2:D:662:LEU:HD21	2:D:684:GLU:HG3	1.84	0.60
1:E:675:LEU:O	1:E:676:THR:C	2.44	0.60
1:E:268:VAL:HG11	1:E:296:THR:HG21	1.83	0.60
1:E:466:ARG:NH1	1:E:520:GLU:HG2	2.17	0.60
2:B:759:LEU:HD23	2:B:782:ALA:HB2	1.84	0.60
1:A:623:LEU:HD21	1:A:651:ILE:HD12	1.83	0.60
1:A:2:LYS:HZ1	1:A:360:GLN:HE22	1.49	0.59
1:C:678:GLU:O	1:C:679:SER:C	2.45	0.59
1:E:592:VAL:HG12	1:E:592:VAL:O	2.02	0.59
1:E:112:VAL:CG1	1:E:124:TRP:HB2	2.32	0.59
1:C:249:ASP:OD1	1:C:251:THR:HB	2.01	0.59
1:C:430:VAL:O	1:C:430:VAL:HG23	2.03	0.59
2:B:649:PRO:HB3	2:B:652:ARG:HH21	1.67	0.59
1:C:336:ASN:H	1:C:336:ASN:ND2	2.00	0.59
1:C:339:VAL:CG1	1:C:343:GLU:HB2	2.33	0.59
1:E:550:THR:HG22	1:E:554:ARG:N	2.14	0.59
2:B:810:LEU:HD23	2:B:810:LEU:N	2.06	0.59
1:E:352:LEU:HD22	1:E:387:TRP:HB2	1.84	0.59
1:A:267:ASN:ND2	1:A:269:GLY:H	2.00	0.59
1:C:5:ILE:HD12	1:C:300:LEU:HD22	1.84	0.59
1:C:310:ASP:OD1	1:C:314:LYS:HD2	2.03	0.59
1:E:271:GLU:HB2	1:E:292:ASP:HB2	1.84	0.59
1:E:770:PHE:HB2	2:F:713:VAL:CG1	2.33	0.59
1:E:144:MET:HG3	1:E:161:LEU:HD13	1.84	0.58
1:E:352:LEU:CD2	1:E:387:TRP:HB2	2.33	0.58
2:B:649:PRO:HA	2:B:652:ARG:HE	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:438:ARG:HB2	1:E:438:ARG:NH1	2.17	0.58
1:A:77:PHE:HB3	1:A:96:HIS:O	2.02	0.58
1:A:256:ASN:HD21	1:A:258:SER:HB2	1.69	0.58
1:C:676:THR:HG22	1:C:677:ASP:OD1	2.03	0.58
1:E:386:ALA:HB3	1:E:388:ARG:HG3	1.84	0.58
2:F:728:GLN:CG	2:F:736:MET:HE3	2.33	0.58
1:A:532:LEU:HD11	1:A:558:PHE:CD1	2.39	0.58
1:C:552:THR:O	1:C:553:ASN:HB2	2.03	0.58
1:E:798:LYS:NZ	1:E:798:LYS:HB3	2.18	0.58
2:B:710:LEU:O	2:B:714:THR:HB	2.03	0.58
1:C:776:GLY:HA3	2:D:805:VAL:HG21	1.85	0.58
1:A:412:GLU:CD	1:A:412:GLU:H	2.11	0.58
1:A:575:LEU:HA	1:A:587:LEU:HD23	1.85	0.58
1:E:425:VAL:O	1:E:425:VAL:HG22	2.02	0.58
1:C:339:VAL:HG12	1:C:340:GLU:N	2.19	0.58
2:F:724:GLN:HE22	2:F:736:MET:HA	1.69	0.58
1:C:306:THR:HG22	1:C:362:LEU:HB2	1.86	0.57
1:C:659:PHE:O	1:C:663:LEU:HD13	2.04	0.57
2:F:688:GLN:HB3	2:F:815:LEU:HD11	1.87	0.57
2:F:726:ILE:O	2:F:730:ARG:HB2	2.04	0.57
2:F:753:PHE:CE1	2:F:761:LEU:HD23	2.39	0.57
1:A:200:TYR:HA	1:A:213:TRP:O	2.03	0.57
2:F:759:LEU:N	2:F:760:PRO:CD	2.67	0.57
1:C:499:THR:O	1:C:500:LEU:HD23	2.04	0.57
1:E:193:TYR:CZ	1:E:195:LEU:HB2	2.40	0.57
1:E:586:TYR:C	1:E:587:LEU:HD12	2.29	0.57
1:A:493:ASP:CG	1:A:494:GLU:N	2.61	0.57
1:C:550:THR:HG23	1:C:552:THR:N	2.18	0.57
1:A:123:LEU:HD12	1:A:124:TRP:N	2.19	0.57
1:E:201:MET:HG3	1:E:215:TYR:HD1	1.69	0.57
1:A:763:GLN:HA	1:A:765:PHE:CE1	2.40	0.57
1:A:367:ASN:HD22	1:A:368:GLY:N	2.03	0.57
1:E:210:ILE:HB	1:E:224:LEU:HB2	1.87	0.57
1:C:573:MET:CE	1:C:589:ASP:HB3	2.34	0.56
2:D:763:TYR:CD1	2:D:779:LEU:HD13	2.40	0.56
1:A:124:TRP:CZ3	1:A:132:LEU:HB2	2.40	0.56
1:C:77:PHE:HB3	1:C:96:HIS:O	2.05	0.56
1:A:36:ARG:HD3	1:A:50:SER:OG	2.05	0.56
1:A:573:MET:HE1	1:A:595:TYR:CD1	2.40	0.56
1:A:804:ARG:HG3	1:A:804:ARG:HH11	1.71	0.56
1:C:8:THR:HG23	1:C:297:VAL:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:GLU:O	1:C:501:LEU:HD12	2.05	0.56
2:D:745:SER:HA	2:D:747:LYS:HE2	1.88	0.56
1:E:36:ARG:HD3	1:E:50:SER:OG	2.04	0.56
1:E:149:ASN:C	1:E:149:ASN:HD22	2.14	0.56
2:B:724:GLN:O	2:B:728:GLN:HG3	2.05	0.56
1:C:666:GLY:CA	1:C:694:ARG:HH11	2.18	0.56
1:A:8:THR:HG23	1:A:297:VAL:O	2.05	0.56
1:C:210:ILE:HB	1:C:224:LEU:HB2	1.86	0.56
1:C:500:LEU:HD22	1:C:528:VAL:HG12	1.88	0.56
2:D:728:GLN:HG3	2:D:736:MET:CE	2.36	0.56
1:E:41:ASN:ND2	1:E:43:GLU:H	2.02	0.56
2:F:711:TYR:HA	2:F:714:THR:HG22	1.88	0.56
1:A:367:ASN:CG	1:A:404:SER:OG	2.48	0.56
1:E:65:ALA:C	1:E:67:LYS:H	2.14	0.56
1:E:71:ILE:HD13	1:E:112:VAL:HG21	1.87	0.56
1:E:418:TYR:HB2	1:E:428:TRP:CD2	2.41	0.56
1:A:615:ILE:HD12	1:A:615:ILE:N	2.07	0.56
1:C:432:MET:HG2	1:C:436:ILE:CD1	2.36	0.56
1:A:2:LYS:HZ2	1:A:360:GLN:NE2	2.04	0.56
1:C:592:VAL:HG12	1:C:592:VAL:O	2.06	0.56
1:A:214:ASP:HB3	1:A:217:THR:HG22	1.86	0.56
1:C:339:VAL:HG12	1:C:343:GLU:HB2	1.87	0.56
1:A:210:ILE:HB	1:A:224:LEU:HB2	1.88	0.55
1:C:165:VAL:HG21	1:C:203:THR:HG21	1.88	0.55
2:D:751:SER:O	2:D:754:ALA:HB3	2.06	0.55
2:D:763:TYR:CE2	2:D:789:VAL:HG11	2.41	0.55
1:A:118:ASP:O	1:A:119:LEU:HB2	2.06	0.55
1:A:281:THR:HG22	1:A:281:THR:O	2.06	0.55
1:A:602:GLU:HB3	1:A:626:VAL:HG22	1.89	0.55
1:A:798:LYS:HB3	1:A:801:VAL:HG22	1.87	0.55
1:C:587:LEU:N	1:C:587:LEU:HD12	2.22	0.55
1:C:799:ASN:N	1:C:799:ASN:ND2	2.46	0.55
2:F:720:LEU:HD11	2:F:742:TYR:HB3	1.88	0.55
1:A:22:HIS:CD2	1:A:25:GLU:H	2.24	0.55
1:C:181:THR:HB	1:C:183:GLN:HE21	1.71	0.55
1:E:41:ASN:HD22	1:E:43:GLU:H	1.55	0.55
1:A:330:THR:HG22	1:A:331:ALA:N	2.22	0.55
1:E:805:VAL:HA	2:F:815:LEU:HD23	1.88	0.55
1:A:143:VAL:O	1:A:143:VAL:HG23	2.05	0.55
2:B:728:GLN:CG	2:B:736:MET:HE3	2.32	0.55
1:E:339:VAL:HG12	1:E:340:GLU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:LEU:HD23	1:A:802:SER:HA	1.88	0.55
1:C:41:ASN:ND2	1:C:43:GLU:H	2.03	0.55
1:A:432:MET:HE1	1:A:456:PHE:CE1	2.42	0.55
1:A:677:ASP:C	1:A:679:SER:N	2.64	0.55
1:C:674:LEU:O	1:C:675:LEU:HD12	2.07	0.55
2:F:743:ASN:HD21	2:F:745:SER:HB2	1.71	0.55
1:A:753:GLN:NE2	1:A:756:LYS:NZ	2.55	0.55
1:E:181:THR:HB	1:E:183:GLN:HE21	1.72	0.55
1:A:15:ARG:HD2	1:A:274:TRP:NE1	2.22	0.54
2:F:740:THR:HG21	2:F:749:ARG:HE	1.70	0.54
1:A:25:GLU:HG2	1:A:27:TRP:CE2	2.42	0.54
2:B:763:TYR:CZ	2:B:767:LYS:HG3	2.42	0.54
2:B:658:GLU:HG2	2:B:659:TYR:CD2	2.42	0.54
1:C:747:TRP:CZ2	2:D:712:LEU:HD11	2.43	0.54
2:D:724:GLN:NE2	2:D:739:ASN:HB2	2.23	0.54
1:C:193:TYR:CE1	1:C:195:LEU:HB2	2.43	0.54
1:C:335:GLY:N	1:C:581:ARG:NH2	2.56	0.54
1:C:550:THR:HG21	1:C:552:THR:OG1	2.08	0.54
1:E:603:VAL:O	1:E:607:GLN:HG3	2.06	0.54
1:C:335:GLY:H	1:C:581:ARG:NH2	2.05	0.54
1:C:787:THR:O	1:C:791:GLU:HG3	2.08	0.54
2:F:732:ASP:O	2:F:736:MET:HG3	2.08	0.54
1:A:336:ASN:HD22	1:A:337:GLU:N	2.05	0.54
1:C:256:ASN:C	1:C:256:ASN:HD22	2.16	0.54
1:A:281:THR:O	1:A:281:THR:CG2	2.56	0.54
1:A:41:ASN:ND2	1:A:44:THR:H	2.06	0.54
1:A:162:ASP:O	1:A:163:ARG:HB2	2.07	0.54
2:B:670:LYS:O	2:B:673:ASN:HB2	2.07	0.54
1:C:409:LEU:CD2	1:C:417:LYS:HB2	2.38	0.54
1:A:41:ASN:C	1:A:41:ASN:HD22	2.16	0.53
1:C:233:PHE:CE1	1:C:276:ILE:HB	2.43	0.53
2:D:739:ASN:O	2:D:743:ASN:HB2	2.08	0.53
1:E:276:ILE:HG13	1:E:277:ALA:N	2.23	0.53
1:E:409:LEU:O	1:E:416:ILE:HA	2.08	0.53
1:A:532:LEU:N	1:A:532:LEU:HD22	2.24	0.53
1:A:677:ASP:CG	1:A:677:ASP:O	2.48	0.53
1:C:7:LYS:HE2	1:C:10:SER:OG	2.08	0.53
1:E:744:ASN:O	1:E:748:ILE:HG12	2.08	0.53
1:A:22:HIS:HD2	1:A:24:THR:H	1.54	0.53
1:A:242:ILE:HD12	1:A:244:ILE:HD11	1.90	0.53
1:C:409:LEU:HD21	1:C:419:TYR:HE2	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:ASN:C	1:C:503:ASN:HD22	2.16	0.53
1:C:790:LYS:HE3	1:C:802:SER:O	2.08	0.53
1:E:279:HIS:HD2	1:E:281:THR:H	1.56	0.53
1:E:304:GLU:HG2	1:E:574:TYR:CE1	2.43	0.53
2:F:740:THR:HG23	2:F:749:ARG:NE	2.17	0.53
1:E:81:VAL:HB	1:E:91:VAL:HG12	1.89	0.53
1:C:176:ASN:ND2	3:C:815:HOH:O	2.42	0.53
1:E:162:ASP:OD2	1:E:164:THR:HB	2.07	0.53
1:E:337:GLU:HG3	1:E:345:LEU:HD22	1.90	0.53
1:A:249:ASP:OD2	1:A:251:THR:HB	2.08	0.53
1:A:276:ILE:HG13	1:A:277:ALA:N	2.22	0.53
1:A:349:THR:HG22	1:A:350:LYS:N	2.23	0.53
1:C:361:SER:OG	1:C:374:VAL:HB	2.08	0.53
1:A:786:VAL:O	1:A:790:LYS:HG3	2.09	0.53
1:E:476:TRP:CE3	1:E:483:VAL:HG22	2.44	0.53
1:E:587:LEU:HD12	1:E:587:LEU:N	2.24	0.53
1:A:116:SER:N	1:A:143:VAL:CG2	2.72	0.53
1:C:550:THR:CG2	1:C:552:THR:OG1	2.57	0.53
1:C:695:PHE:CZ	2:D:784:VAL:HG21	2.44	0.53
1:E:487:ASN:ND2	1:E:488:THR:H	2.06	0.53
1:A:256:ASN:ND2	1:A:258:SER:H	2.07	0.53
1:C:500:LEU:CD2	1:C:528:VAL:HG12	2.39	0.53
1:A:515:ASN:H	1:A:515:ASN:ND2	2.06	0.52
1:C:281:THR:HG23	1:C:281:THR:O	2.08	0.52
1:C:336:ASN:HD22	1:C:336:ASN:H	1.53	0.52
1:C:750:GLY:HA3	2:D:800:PHE:O	2.09	0.52
1:E:214:ASP:OD2	1:E:217:THR:HG23	2.09	0.52
1:E:489:ASN:HD22	1:E:494:GLU:HB2	1.74	0.52
1:E:503:ASN:C	1:E:503:ASN:HD22	2.17	0.52
1:A:542:VAL:HG11	1:A:604:LEU:HD23	1.90	0.52
1:C:465:ARG:HD3	1:C:466:ARG:N	2.24	0.52
2:F:743:ASN:C	2:F:743:ASN:HD22	2.16	0.52
1:C:53:VAL:O	1:C:54:THR:HG23	2.08	0.52
1:E:270:LEU:O	1:E:271:GLU:HB2	2.07	0.52
1:A:96:HIS:CE1	1:A:122:LYS:HD2	2.44	0.52
1:C:616:GLU:CD	1:C:616:GLU:H	2.16	0.52
1:E:16:VAL:CG2	1:E:290:GLY:HA3	2.34	0.52
1:A:149:ASN:HD22	1:A:150:PRO:N	2.06	0.52
1:E:3:LEU:O	1:E:3:LEU:HD12	2.10	0.52
1:E:324:ALA:HB3	1:E:327:ASP:OD2	2.10	0.52
1:C:82:PHE:CE2	1:C:89:LYS:HG2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ASP:CB	1:A:217:THR:HG22	2.39	0.52
2:B:740:THR:HG21	2:B:749:ARG:HE	1.74	0.52
1:A:233:PHE:CE1	1:A:276:ILE:HB	2.45	0.52
1:A:58:VAL:HG22	1:A:74:SER:HB3	1.92	0.52
1:A:160:CYS:HB3	1:A:162:ASP:OD1	2.10	0.52
2:B:648:ASP:HB3	2:B:651:ILE:HG13	1.92	0.52
1:C:310:ASP:OD2	1:C:310:ASP:C	2.52	0.52
1:E:599:ILE:CG2	1:E:604:LEU:HD11	2.40	0.52
1:A:361:SER:HB3	1:A:374:VAL:HB	1.92	0.51
1:A:753:GLN:HE22	1:A:756:LYS:HZ3	1.59	0.51
1:C:644:TYR:HB3	1:C:647:GLU:CG	2.41	0.51
1:E:704:PHE:CE1	1:E:712:SER:HB3	2.45	0.51
2:F:644:GLN:H	2:F:644:GLN:NE2	2.08	0.51
2:F:711:TYR:O	2:F:714:THR:HG22	2.09	0.51
1:A:251:THR:CG2	1:A:253:LYS:HG3	2.40	0.51
1:C:696:ASN:OD1	2:D:790:THR:HB	2.11	0.51
1:E:437:ASP:HB2	1:E:448:LYS:HB3	1.93	0.51
2:F:806:ILE:HD12	2:F:808:LYS:O	2.09	0.51
2:F:759:LEU:HD22	2:F:759:LEU:H	1.74	0.51
1:A:214:ASP:HB3	1:A:217:THR:CG2	2.41	0.51
1:C:35:GLY:HA3	1:C:54:THR:O	2.11	0.51
1:C:752:ILE:HG23	1:C:753:GLN:N	2.25	0.51
1:A:198:LYS:HD2	1:A:200:TYR:CE2	2.44	0.51
1:A:217:THR:HG23	1:A:219:SER:H	1.74	0.51
1:A:430:VAL:HG12	1:A:430:VAL:O	2.10	0.51
1:C:233:PHE:CZ	1:C:246:GLY:HA3	2.46	0.51
1:C:677:ASP:O	1:C:679:SER:N	2.43	0.51
1:E:479:ASN:HD21	1:E:481:GLU:HB2	1.76	0.51
1:C:193:TYR:HE1	1:C:195:LEU:HB2	1.75	0.51
1:C:279:HIS:CD2	1:C:281:THR:HG22	2.45	0.51
1:C:366:PRO:HG2	1:C:404:SER:OG	2.10	0.51
1:C:503:ASN:HD21	1:C:505:ASP:HB2	1.75	0.51
1:C:671:ALA:O	1:C:674:LEU:HB3	2.11	0.51
1:A:22:HIS:CD2	1:A:24:THR:H	2.27	0.51
1:A:418:TYR:HB2	1:A:428:TRP:CD2	2.46	0.51
1:C:253:LYS:HG2	1:C:265:THR:CG2	2.35	0.51
1:C:764:ARG:CD	1:C:767:GLU:OE2	2.58	0.51
1:A:365:SER:OG	1:A:367:ASN:ND2	2.44	0.51
1:A:696:ASN:OD1	1:A:699:LEU:HB2	2.11	0.51
1:C:134:GLN:NE2	1:C:170:LEU:O	2.34	0.51
2:B:651:ILE:O	2:B:655:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:484:MET:HE1	1:E:497:GLY:C	2.35	0.51
1:A:783:ASN:HD21	1:A:808:ALA:N	2.05	0.50
1:C:250:GLY:HA2	1:C:271:GLU:O	2.11	0.50
1:E:233:PHE:CE1	1:E:276:ILE:HB	2.46	0.50
1:A:39:ILE:HG22	1:A:48:VAL:HG13	1.94	0.50
1:A:701:ILE:CD1	1:A:716:LEU:HB3	2.41	0.50
2:B:672:LEU:N	2:B:672:LEU:HD12	2.26	0.50
1:C:53:VAL:HG13	1:C:80:ARG:HD2	1.93	0.50
1:C:259:THR:HG22	1:C:261:LYS:HG3	1.93	0.50
1:C:482:LEU:HD23	1:C:541:TRP:CZ3	2.47	0.50
1:C:679:SER:O	1:C:680:ALA:C	2.54	0.50
1:A:409:LEU:O	1:A:416:ILE:HA	2.11	0.50
1:C:15:ARG:HG2	1:C:17:LYS:HD2	1.93	0.50
1:C:504:LYS:O	1:C:508:LEU:HG	2.10	0.50
1:E:701:ILE:HG13	1:E:716:LEU:HD13	1.93	0.50
1:A:237:HIS:HB2	1:A:242:ILE:HG13	1.93	0.50
1:A:256:ASN:ND2	1:A:259:THR:N	2.52	0.50
1:A:642:GLN:O	1:A:643:GLU:HB2	2.11	0.50
1:A:770:PHE:CD2	2:B:810:LEU:HD11	2.46	0.50
1:C:57:PRO:HG2	1:C:75:ASP:OD2	2.12	0.50
1:C:227:HIS:HE1	1:C:245:SER:OG	1.94	0.50
1:C:676:THR:C	1:C:678:GLU:N	2.59	0.50
2:D:789:VAL:HG12	2:D:791:LEU:CD1	2.41	0.50
1:E:149:ASN:ND2	1:E:151:LYS:H	2.09	0.50
1:E:234:ALA:HA	1:E:244:ILE:O	2.11	0.50
1:E:602:GLU:H	1:E:602:GLU:CD	2.19	0.50
1:E:770:PHE:CD2	2:F:810:LEU:HD23	2.46	0.50
2:F:695:GLU:O	2:F:699:GLN:HG3	2.12	0.50
2:F:740:THR:CG2	2:F:749:ARG:NE	2.66	0.50
1:A:584:LYS:HG2	1:A:598:GLU:CA	2.41	0.50
1:C:432:MET:HG2	1:C:436:ILE:HD13	1.93	0.50
2:F:666:LEU:HG	2:F:670:LYS:HE3	1.92	0.50
2:F:707:LEU:HB3	2:F:723:MET:HE2	1.92	0.50
2:B:785:ASP:HB3	2:B:788:ASP:OD1	2.11	0.50
1:C:442:GLY:HA3	1:C:476:TRP:CD1	2.46	0.50
1:C:539:GLY:HA2	1:C:575:LEU:HD12	1.94	0.50
2:D:674:ASP:HB3	2:D:677:THR:HB	1.94	0.50
1:E:553:ASN:N	1:E:553:ASN:HD22	2.10	0.50
1:C:418:TYR:HB2	1:C:428:TRP:CE3	2.47	0.50
1:C:804:ARG:NE	2:D:818:ALA:OXT	2.45	0.49
1:E:736:THR:HG22	1:E:736:THR:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:ASP:OD2	1:A:593:HIS:HB2	2.12	0.49
1:C:19:ILE:HA	1:C:29:LEU:O	2.12	0.49
1:C:36:ARG:HG2	1:C:52:GLN:NE2	2.24	0.49
1:E:717:HIS:CB	1:E:726:LEU:HD13	2.40	0.49
1:A:793:LEU:HG	1:A:801:VAL:HG23	1.94	0.49
1:C:259:THR:O	1:C:260:TYR:HB2	2.13	0.49
1:C:447:VAL:HG11	1:C:456:PHE:HE1	1.76	0.49
1:E:379:TYR:CE2	1:E:409:LEU:HD21	2.47	0.49
1:C:224:LEU:HD12	1:C:224:LEU:N	2.27	0.49
1:C:578:TYR:CE1	1:C:599:ILE:HD11	2.47	0.49
1:E:56:THR:OG1	1:E:76:ASP:OD2	2.30	0.49
1:E:344:PRO:HA	1:E:594:VAL:O	2.12	0.49
1:E:479:ASN:ND2	1:E:481:GLU:HB2	2.27	0.49
1:A:532:LEU:N	1:A:532:LEU:CD2	2.76	0.49
1:A:767:GLU:HG3	3:A:869:HOH:O	2.12	0.49
1:C:15:ARG:HG2	1:C:17:LYS:CD	2.42	0.49
1:C:324:ALA:O	1:C:327:ASP:HB2	2.13	0.49
2:D:704:PHE:CE2	2:D:726:ILE:HG21	2.47	0.49
1:E:19:ILE:HA	1:E:29:LEU:O	2.12	0.49
1:E:113:LEU:CD2	1:E:123:LEU:HD23	2.43	0.49
1:E:484:MET:CE	1:E:498:TYR:N	2.76	0.49
1:E:798:LYS:HB3	1:E:798:LYS:HZ2	1.78	0.49
1:A:19:ILE:HA	1:A:29:LEU:O	2.11	0.49
1:A:418:TYR:HB2	1:A:428:TRP:CE3	2.47	0.49
1:E:550:THR:CG2	1:E:554:ARG:HB3	2.43	0.49
1:E:617:GLU:OE1	1:E:621:ASN:ND2	2.46	0.49
1:E:770:PHE:CE2	2:F:810:LEU:HD23	2.47	0.49
1:C:5:ILE:HD12	1:C:300:LEU:HD23	1.94	0.49
1:C:367:ASN:HB3	1:C:369:ARG:H	1.77	0.49
1:E:228:MET:HE2	1:E:228:MET:HA	1.94	0.49
1:A:181:THR:HB	1:A:183:GLN:HE21	1.78	0.49
1:A:264:LYS:HD3	1:A:266:LEU:HD21	1.95	0.49
1:C:682:MET:O	1:C:682:MET:HG2	2.12	0.49
2:D:747:LYS:N	2:D:747:LYS:CD	2.70	0.49
1:A:767:GLU:HA	1:A:770:PHE:HD1	1.78	0.49
2:B:649:PRO:HB3	2:B:652:ARG:NH2	2.28	0.49
1:E:185:ARG:HD2	1:E:206:ASP:HB3	1.95	0.49
1:E:600:SER:OG	1:E:603:VAL:HG23	2.13	0.49
1:A:176:ASN:ND2	3:A:830:HOH:O	2.45	0.48
1:A:451:GLY:CA	1:A:470:ASN:HB3	2.42	0.48
1:A:615:ILE:HG12	1:A:644:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:GLU:CD	1:C:664:LYS:HZ2	2.20	0.48
1:E:330:THR:OG1	1:E:352:LEU:HD12	2.13	0.48
1:E:614:GLU:HA	3:E:849:HOH:O	2.13	0.48
2:F:768:ALA:HA	2:F:795:MET:CE	2.36	0.48
1:A:197:ASP:OD1	1:A:198:LYS:HG3	2.13	0.48
1:A:532:LEU:CD2	1:A:532:LEU:H	2.26	0.48
1:C:426:THR:O	1:C:427:SER:CB	2.61	0.48
1:C:460:ASN:OD1	1:C:462:THR:HG23	2.13	0.48
1:C:672:ARG:C	1:C:674:LEU:N	2.71	0.48
1:E:398:PHE:CD1	1:E:409:LEU:HD11	2.48	0.48
1:A:41:ASN:HD22	1:A:43:GLU:H	1.60	0.48
1:A:339:VAL:HG12	1:A:340:GLU:N	2.29	0.48
1:C:426:THR:O	1:C:427:SER:OG	2.29	0.48
1:C:696:ASN:ND2	1:C:699:LEU:HD12	2.28	0.48
1:A:337:GLU:HG3	1:A:345:LEU:CD2	2.43	0.48
1:C:336:ASN:O	1:C:337:GLU:C	2.55	0.48
2:D:668:GLU:O	2:D:672:LEU:HB2	2.14	0.48
1:E:333:ILE:HG21	1:E:586:TYR:CZ	2.47	0.48
1:E:530:TYR:CE1	1:E:560:GLY:HA2	2.48	0.48
1:A:193:TYR:CZ	1:A:195:LEU:HB2	2.48	0.48
1:C:465:ARG:HD2	1:C:467:ILE:HD13	1.95	0.48
1:C:628:GLY:O	1:C:632:LEU:HD13	2.14	0.48
1:E:112:VAL:HG12	1:E:124:TRP:HB2	1.96	0.48
1:E:199:PRO:HG2	1:E:214:ASP:OD1	2.13	0.48
1:E:380:VAL:HG23	1:E:382:TYR:HE1	1.77	0.48
1:A:406:SER:HB2	1:A:419:TYR:O	2.13	0.48
1:A:665:VAL:CG1	1:A:667:GLN:HG3	2.44	0.48
1:C:452:PHE:CD2	1:C:466:ARG:HD3	2.48	0.48
2:F:668:GLU:O	2:F:672:LEU:HG	2.14	0.48
2:F:710:LEU:O	2:F:714:THR:HB	2.13	0.48
1:A:268:VAL:HG11	1:A:296:THR:HG21	1.96	0.48
1:C:516:ILE:HG21	3:C:889:HOH:O	2.13	0.48
1:C:655:GLN:NE2	1:C:658:LYS:HE2	2.29	0.48
1:E:149:ASN:HD22	1:E:151:LYS:H	1.62	0.48
1:E:484:MET:HG2	1:E:546:PHE:CZ	2.48	0.48
1:C:447:VAL:HG11	1:C:456:PHE:CE1	2.48	0.48
1:C:813:GLY:O	1:C:814:SER:C	2.56	0.48
2:F:691:ALA:HB3	2:F:811:GLU:O	2.14	0.48
1:A:403:ASP:O	1:A:404:SER:HB3	2.13	0.48
1:C:9:PHE:HB3	1:C:297:VAL:CG1	2.44	0.48
2:F:743:ASN:HD21	2:F:745:SER:CB	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ASN:ND2	1:A:369:ARG:H	2.12	0.47
1:E:81:VAL:HG21	1:E:130:TRP:CZ2	2.49	0.47
1:E:122:LYS:HD3	1:E:124:TRP:CZ2	2.48	0.47
1:E:224:LEU:HD13	1:E:255:TRP:CD2	2.49	0.47
1:E:546:PHE:O	1:E:557:TYR:HA	2.14	0.47
1:E:598:GLU:O	1:E:599:ILE:HD13	2.13	0.47
1:E:679:SER:O	1:E:680:ALA:C	2.56	0.47
1:A:405:ASN:HD21	1:A:421:ASN:HA	1.75	0.47
2:F:729:THR:C	2:F:731:GLU:H	2.22	0.47
1:A:412:GLU:C	1:A:414:GLY:H	2.22	0.47
1:A:549:THR:HG21	1:A:573:MET:O	2.15	0.47
1:E:41:ASN:ND2	1:E:41:ASN:C	2.69	0.47
1:E:207:ASP:OD2	1:E:207:ASP:C	2.56	0.47
1:E:722:ASN:HD22	1:E:725:GLY:H	1.60	0.47
1:A:432:MET:HE1	1:A:456:PHE:CZ	2.49	0.47
1:A:752:ILE:HD13	1:A:777:LEU:HD21	1.96	0.47
1:C:397:ASP:OD2	1:C:438:ARG:HB2	2.14	0.47
1:E:466:ARG:HH11	1:E:466:ARG:CG	2.27	0.47
1:E:516:ILE:HG12	1:E:522:VAL:HG22	1.96	0.47
1:E:539:GLY:O	1:E:540:LYS:HD2	2.14	0.47
1:C:647:GLU:O	1:C:651:ILE:HG12	2.14	0.47
1:A:281:THR:HG22	1:A:590:ARG:HH22	1.79	0.47
1:A:337:GLU:HG3	1:A:345:LEU:HD23	1.95	0.47
1:C:326:SER:HB3	1:C:355:VAL:O	2.14	0.47
1:C:684:TRP:O	1:C:703:ALA:HB1	2.13	0.47
1:E:1:MET:HE2	1:E:1:MET:C	2.39	0.47
1:A:432:MET:CG	1:A:436:ILE:HD11	2.42	0.47
1:A:489:ASN:OD1	1:A:493:ASP:O	2.32	0.47
1:C:52:GLN:NE2	1:C:52:GLN:HA	2.30	0.47
1:E:30:THR:HG21	3:E:838:HOH:O	2.15	0.47
1:E:272:ARG:CD	1:E:292:ASP:OD2	2.62	0.47
1:E:628:GLY:C	1:E:630:ASP:N	2.72	0.47
1:E:687:LEU:O	1:E:687:LEU:HD23	2.15	0.47
2:F:737:LEU:O	2:F:740:THR:HG22	2.14	0.47
1:C:91:VAL:HG11	1:C:130:TRP:NE1	2.29	0.47
1:C:499:THR:C	1:C:500:LEU:HD23	2.40	0.47
1:E:335:GLY:HA3	1:E:582:ASP:OD1	2.15	0.47
1:E:449:SER:O	1:E:452:PHE:HB2	2.15	0.47
1:C:142:PHE:HB2	1:C:161:LEU:HD22	1.96	0.47
2:D:666:LEU:O	2:D:670:LYS:HG3	2.15	0.47
1:E:144:MET:CG	1:E:161:LEU:HD13	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:440:PHE:HB2	1:E:446:GLY:HA3	1.95	0.47
1:E:603:VAL:CG2	1:E:631:SER:HB3	2.45	0.47
1:E:736:THR:O	1:E:736:THR:CG2	2.63	0.47
1:A:678:GLU:HB3	1:A:683:LYS:HE3	1.97	0.47
1:C:381:ILE:HD12	1:C:391:ALA:HB3	1.96	0.47
1:C:615:ILE:HD11	1:C:647:GLU:HG3	1.97	0.47
1:E:310:ASP:OD2	1:E:310:ASP:C	2.58	0.47
1:E:357:VAL:HG13	1:E:375:GLY:HA3	1.97	0.47
2:B:643:LEU:HD13	2:B:643:LEU:O	2.14	0.46
1:C:251:THR:HG21	1:C:253:LYS:HE2	1.97	0.46
1:E:58:VAL:HG22	1:E:74:SER:HB3	1.97	0.46
1:E:118:ASP:O	1:E:119:LEU:HB2	2.15	0.46
1:E:267:ASN:C	1:E:269:GLY:H	2.23	0.46
1:A:696:ASN:CG	1:A:699:LEU:HB2	2.40	0.46
2:B:748:GLU:O	2:B:752:ILE:HG12	2.14	0.46
1:C:695:PHE:CE1	2:D:760:PRO:HG3	2.50	0.46
2:D:721:SER:O	2:D:724:GLN:HB3	2.15	0.46
1:E:736:THR:HG22	1:E:738:LYS:HG3	1.96	0.46
1:A:25:GLU:HG2	1:A:27:TRP:CZ2	2.50	0.46
1:A:515:ASN:ND2	1:A:515:ASN:N	2.63	0.46
1:A:677:ASP:O	1:A:679:SER:N	2.48	0.46
1:A:793:LEU:HG	1:A:801:VAL:CG2	2.46	0.46
1:E:390:LYS:HE2	1:E:390:LYS:CA	2.35	0.46
1:A:457:ASP:HB3	1:A:460:ASN:OD1	2.15	0.46
1:C:96:HIS:CE1	1:C:122:LYS:HD2	2.50	0.46
1:C:454:TYR:CE2	1:C:466:ARG:HG3	2.50	0.46
2:F:743:ASN:ND2	2:F:745:SER:H	2.12	0.46
1:E:237:HIS:CG	1:E:238:PRO:HD2	2.50	0.46
1:E:266:LEU:N	1:E:266:LEU:HD23	2.30	0.46
1:E:341:GLN:C	1:E:343:GLU:H	2.23	0.46
1:E:770:PHE:HB3	2:F:713:VAL:HG12	1.95	0.46
1:A:262:VAL:HG13	1:A:262:VAL:O	2.15	0.46
1:A:626:VAL:HG12	1:A:626:VAL:O	2.15	0.46
1:E:532:LEU:HD11	1:E:548:PHE:CZ	2.51	0.46
1:E:752:ILE:HG12	2:F:802:GLN:HG3	1.97	0.46
1:A:77:PHE:N	1:A:77:PHE:CD1	2.79	0.46
1:A:357:VAL:HB	1:A:376:ASP:OD2	2.16	0.46
1:C:425:VAL:HG12	1:C:425:VAL:O	2.14	0.46
1:C:726:LEU:HB3	1:C:749:ALA:HB2	1.98	0.46
2:F:698:TYR:CB	2:F:707:LEU:HD13	2.45	0.46
1:A:270:LEU:O	1:A:271:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:ILE:H	1:A:615:ILE:CD1	2.00	0.46
1:C:355:VAL:HG12	1:C:357:VAL:H	1.81	0.46
1:E:272:ARG:HD3	1:E:292:ASP:OD2	2.15	0.46
1:E:337:GLU:HG3	1:E:345:LEU:HD13	1.97	0.46
1:C:172:GLN:HG2	3:C:815:HOH:O	2.15	0.46
1:C:804:ARG:HG2	2:D:818:ALA:OXT	2.16	0.46
2:D:723:MET:CE	2:D:726:ILE:HD12	2.46	0.46
1:A:116:SER:H	1:A:143:VAL:CG2	2.28	0.46
1:C:234:ALA:HA	1:C:244:ILE:O	2.16	0.46
1:C:241:PRO:HD3	1:C:358:PHE:CZ	2.51	0.46
1:C:327:ASP:HB3	1:C:329:PHE:CZ	2.51	0.46
1:E:569:TYR:CD2	1:E:573:MET:HE2	2.51	0.46
2:F:813:TRP:CG	2:F:814:PRO:HD2	2.51	0.46
1:A:419:TYR:CZ	1:A:424:GLU:HB2	2.50	0.45
1:C:111:TYR:HB3	1:C:123:LEU:HD21	1.98	0.45
1:C:680:ALA:HB1	1:C:683:LYS:HG3	1.97	0.45
2:D:704:PHE:CD2	2:D:726:ILE:HG21	2.51	0.45
2:D:779:LEU:HD23	2:D:786:GLU:CG	2.45	0.45
1:E:65:ALA:C	1:E:67:LYS:N	2.73	0.45
1:E:233:PHE:CD1	1:E:233:PHE:C	2.95	0.45
1:E:287:ILE:HG21	1:E:300:LEU:HD11	1.97	0.45
1:E:675:LEU:HD21	1:E:683:LYS:HB3	1.98	0.45
1:A:471:ALA:HB2	1:A:485:ILE:CG2	2.46	0.45
1:A:675:LEU:O	1:A:678:GLU:HG2	2.15	0.45
2:B:666:LEU:HD11	2:B:696:MET:HE1	1.97	0.45
2:B:726:ILE:O	2:B:730:ARG:HG3	2.16	0.45
1:C:78:ARG:HH12	1:C:93:PHE:HA	1.80	0.45
1:E:398:PHE:C	1:E:398:PHE:CD2	2.94	0.45
1:E:454:TYR:CE2	1:E:466:ARG:HD2	2.49	0.45
1:E:665:VAL:HG23	1:E:667:GLN:HG3	1.98	0.45
1:E:806:CYS:HB2	2:F:814:PRO:HG2	1.98	0.45
1:A:259:THR:CG2	1:A:261:LYS:H	2.29	0.45
1:A:747:TRP:CZ2	2:B:712:LEU:HD11	2.52	0.45
2:B:703:SER:CB	2:B:706:LYS:HD2	2.46	0.45
1:C:276:ILE:HG13	1:C:277:ALA:N	2.31	0.45
1:C:809:GLU:CD	1:C:809:GLU:N	2.73	0.45
1:E:96:HIS:ND1	1:E:122:LYS:HD2	2.31	0.45
1:E:240:LEU:HA	1:E:241:PRO:HD3	1.83	0.45
1:E:333:ILE:HD13	1:E:586:TYR:CD2	2.50	0.45
1:E:366:PRO:HG2	1:E:404:SER:OG	2.16	0.45
1:A:377:GLY:O	1:A:394:LYS:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:SER:HA	1:C:400:TRP:CD1	2.51	0.45
1:C:615:ILE:CD1	1:C:647:GLU:HG3	2.46	0.45
1:C:56:THR:OG1	1:C:75:ASP:HB2	2.17	0.45
1:C:56:THR:HG21	1:C:76:ASP:H	1.81	0.45
1:C:69:TRP:NE1	1:C:90:VAL:HG21	2.31	0.45
1:C:200:TYR:HA	1:C:213:TRP:O	2.16	0.45
1:C:543:GLY:O	1:C:544:ASP:HB2	2.16	0.45
1:C:672:ARG:O	1:C:674:LEU:N	2.44	0.45
1:E:57:PRO:HG2	1:E:75:ASP:OD2	2.17	0.45
1:E:476:TRP:CZ3	1:E:483:VAL:HG22	2.52	0.45
1:E:657:GLN:O	1:E:658:LYS:C	2.59	0.45
1:A:22:HIS:HE1	1:A:84:TYR:OH	2.00	0.45
1:C:197:ASP:O	1:C:198:LYS:HG2	2.16	0.45
1:A:626:VAL:HG11	1:A:635:ILE:CD1	2.46	0.45
1:A:809:GLU:H	1:A:809:GLU:HG3	1.36	0.45
2:B:648:ASP:HB3	2:B:651:ILE:CG1	2.46	0.45
1:C:22:HIS:CD2	1:C:25:GLU:H	2.35	0.45
1:C:149:ASN:HA	1:C:192:TYR:CD1	2.52	0.45
1:C:206:ASP:OD1	1:C:230:ASN:HB3	2.17	0.45
1:C:420:LYS:HE2	3:C:851:HOH:O	2.16	0.45
1:E:68:ASN:HA	1:E:84:TYR:CE2	2.52	0.45
1:E:69:TRP:HA	1:E:82:PHE:O	2.17	0.45
1:E:412:GLU:OE1	1:E:412:GLU:N	2.41	0.45
1:A:320:GLY:O	1:A:321:LYS:C	2.60	0.45
1:A:487:ASN:ND2	1:A:488:THR:N	2.60	0.45
1:A:556:ASN:HD22	1:A:565:ASN:HA	1.79	0.45
2:B:703:SER:HB3	2:B:706:LYS:HD2	1.98	0.45
1:C:275:CYS:O	1:C:289:SER:HA	2.17	0.45
1:E:566:LEU:HD13	1:E:599:ILE:HD11	1.98	0.45
2:F:662:LEU:HD11	2:F:688:GLN:OE1	2.17	0.45
1:C:327:ASP:HB3	1:C:329:PHE:CE1	2.52	0.45
1:E:76:ASP:O	1:E:77:PHE:CB	2.65	0.45
1:C:665:VAL:HG23	1:C:667:GLN:HG3	1.99	0.45
2:D:672:LEU:HD22	2:D:674:ASP:HB2	1.99	0.45
1:E:334:ARG:HB2	1:E:336:ASN:OD1	2.17	0.45
1:E:349:THR:HG22	1:E:350:LYS:N	2.32	0.45
1:A:623:LEU:HB3	1:A:624:PRO:HD3	1.98	0.44
1:C:585:VAL:O	1:C:596:GLY:HA2	2.17	0.44
1:E:330:THR:HG22	1:E:331:ALA:N	2.31	0.44
1:E:333:ILE:HG21	1:E:586:TYR:CE2	2.52	0.44
1:E:425:VAL:HG22	1:E:428:TRP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:736:MET:HB3	2:F:752:ILE:HD13	1.98	0.44
1:A:379:TYR:HB3	1:A:395:CYS:SG	2.57	0.44
1:A:425:VAL:HG22	1:A:428:TRP:HB2	2.00	0.44
1:C:303:ASP:CG	1:C:590:ARG:HD2	2.42	0.44
1:C:555:LEU:HD13	1:C:587:LEU:HD21	1.99	0.44
2:D:759:LEU:N	2:D:760:PRO:CD	2.80	0.44
1:E:19:ILE:HG23	1:E:277:ALA:HB2	1.99	0.44
1:A:448:LYS:HE2	1:A:470:ASN:HB2	1.99	0.44
2:D:736:MET:O	2:D:740:THR:HG23	2.17	0.44
1:E:333:ILE:O	1:E:581:ARG:NH2	2.43	0.44
1:E:486:VAL:CG1	1:E:536:ILE:HB	2.47	0.44
1:E:692:LEU:HD13	1:E:716:LEU:HD21	1.99	0.44
1:A:197:ASP:OD1	1:A:198:LYS:HE2	2.17	0.44
1:C:5:ILE:CD1	1:C:300:LEU:HD22	2.47	0.44
1:C:266:LEU:HD12	1:C:266:LEU:N	2.32	0.44
1:C:499:THR:HG22	1:C:529:LEU:HD23	1.99	0.44
1:C:690:ALA:O	1:C:694:ARG:HG2	2.18	0.44
1:E:68:ASN:HA	1:E:84:TYR:CZ	2.52	0.44
1:A:259:THR:HG22	1:A:261:LYS:H	1.81	0.44
1:A:513:ASN:HB2	1:A:515:ASN:ND2	2.32	0.44
1:A:531:GLU:O	1:A:531:GLU:HG3	2.18	0.44
1:C:54:THR:OG1	1:C:56:THR:HG22	2.17	0.44
1:C:589:ASP:OD2	1:C:593:HIS:HB2	2.18	0.44
1:E:418:TYR:HB2	1:E:428:TRP:CE3	2.53	0.44
1:E:488:THR:O	1:E:489:ASN:C	2.60	0.44
1:A:398:PHE:CD2	1:A:398:PHE:C	2.95	0.44
1:A:500:LEU:CD2	1:A:528:VAL:HG22	2.47	0.44
1:A:515:ASN:HD22	1:A:515:ASN:N	2.07	0.44
1:C:281:THR:HG23	1:C:590:ARG:NH2	2.31	0.44
1:E:279:HIS:CD2	1:E:281:THR:H	2.33	0.44
1:E:550:THR:HG21	1:E:554:ARG:HB3	1.99	0.44
1:E:643:GLU:HG2	1:E:645:TYR:OH	2.18	0.44
1:C:17:LYS:HE2	1:C:17:LYS:HA	1.99	0.44
1:C:118:ASP:O	1:C:119:LEU:HB2	2.18	0.44
2:D:733:PHE:CE2	2:D:756:GLY:HA2	2.53	0.44
2:F:682:ILE:HD13	2:F:697:ILE:HD12	2.00	0.44
2:F:759:LEU:N	2:F:759:LEU:HD22	2.33	0.44
1:E:532:LEU:CD2	1:E:533:SER:H	2.30	0.44
1:E:545:VAL:HG13	1:E:559:VAL:HG22	1.99	0.44
1:A:149:ASN:ND2	1:A:149:ASN:C	2.64	0.44
1:A:281:THR:CG2	1:A:590:ARG:HH22	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:ARG:CZ	1:E:284:LYS:HZ3	2.30	0.44
1:E:438:ARG:HH11	1:E:438:ARG:CB	2.29	0.44
1:C:365:SER:HA	1:C:400:TRP:CG	2.53	0.43
2:D:674:ASP:HB3	2:D:677:THR:CB	2.47	0.43
1:E:25:GLU:HG2	1:E:27:TRP:CE2	2.53	0.43
1:A:603:VAL:O	1:A:607:GLN:HG3	2.18	0.43
2:B:653:PHE:CZ	2:B:677:THR:HG23	2.53	0.43
1:C:22:HIS:HD2	1:C:25:GLU:H	1.64	0.43
1:C:676:THR:HB	1:C:677:ASP:H	1.48	0.43
1:E:36:ARG:HG3	1:E:51:ILE:C	2.43	0.43
2:F:682:ILE:HD11	2:F:697:ILE:CB	2.35	0.43
1:A:227:HIS:HE1	1:A:251:THR:HG22	1.84	0.43
1:A:336:ASN:C	1:A:336:ASN:ND2	2.75	0.43
2:B:649:PRO:CB	2:B:652:ARG:HH21	2.31	0.43
1:C:89:LYS:HE3	1:C:92:ASP:CB	2.44	0.43
1:C:588:ALA:HA	1:C:593:HIS:O	2.19	0.43
1:C:695:PHE:CD1	1:C:695:PHE:N	2.86	0.43
1:C:736:THR:O	1:C:736:THR:CG2	2.64	0.43
1:E:134:GLN:NE2	1:E:172:GLN:O	2.51	0.43
1:E:315:LEU:O	1:E:330:THR:HG23	2.17	0.43
1:A:315:LEU:O	1:A:330:THR:HA	2.19	0.43
1:C:22:HIS:CD2	1:C:24:THR:H	2.33	0.43
1:E:309:LEU:HD22	1:E:576:LEU:HB3	2.01	0.43
2:F:724:GLN:HG3	2:F:728:GLN:HE21	1.84	0.43
1:A:227:HIS:CE1	1:A:253:LYS:HD2	2.53	0.43
1:A:308:SER:O	1:A:315:LEU:HD12	2.18	0.43
1:C:202:ILE:HD12	1:C:212:ILE:CD1	2.49	0.43
1:E:124:TRP:CZ3	1:E:132:LEU:HB2	2.54	0.43
1:E:201:MET:HG3	1:E:215:TYR:CD1	2.52	0.43
1:E:278:THR:HG22	1:E:287:ILE:HG22	2.01	0.43
1:E:553:ASN:N	1:E:553:ASN:ND2	2.67	0.43
1:E:804:ARG:HA	2:F:816:LYS:HB2	2.00	0.43
2:B:740:THR:HG21	2:B:749:ARG:HB2	2.00	0.43
1:C:67:LYS:O	1:C:68:ASN:HB2	2.18	0.43
1:E:282:GLY:O	1:E:283:ARG:C	2.62	0.43
1:E:660:GLU:O	1:E:660:GLU:HG2	2.19	0.43
1:A:357:VAL:O	1:A:359:PRO:HD3	2.18	0.43
1:C:472:LYS:HE2	1:C:486:VAL:CG1	2.48	0.43
1:C:696:ASN:ND2	1:C:699:LEU:HB2	2.33	0.43
1:E:281:THR:HG22	1:E:281:THR:O	2.18	0.43
1:E:345:LEU:HD11	1:E:586:TYR:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:650:ASN:N	1:E:650:ASN:ND2	2.62	0.43
1:E:662:ALA:HB3	1:E:671:ALA:HB2	2.00	0.43
1:A:672:ARG:HG3	1:A:699:LEU:HD21	2.01	0.43
1:C:237:HIS:ND1	1:C:238:PRO:HD2	2.34	0.43
2:D:728:GLN:O	2:D:730:ARG:N	2.41	0.43
1:E:248:GLU:C	1:E:250:GLY:H	2.26	0.43
2:F:696:MET:HA	2:F:699:GLN:OE1	2.18	0.43
1:A:626:VAL:HG11	1:A:635:ILE:HD11	2.01	0.43
1:C:515:ASN:N	1:C:515:ASN:HD22	2.16	0.43
1:E:25:GLU:HG2	1:E:27:TRP:CZ2	2.54	0.43
1:E:602:GLU:CD	1:E:602:GLU:N	2.77	0.43
1:E:739:PHE:HD2	1:E:758:LEU:HD11	1.84	0.43
1:A:53:VAL:HG13	1:A:80:ARG:HD2	2.01	0.43
1:A:326:SER:O	1:A:354:SER:HB2	2.19	0.43
1:E:53:VAL:HG23	1:E:80:ARG:HD2	2.00	0.43
1:E:626:VAL:HG21	1:E:635:ILE:CD1	2.47	0.43
2:F:724:GLN:HE22	2:F:736:MET:CA	2.31	0.43
1:A:233:PHE:CZ	1:A:246:GLY:HA3	2.54	0.42
1:C:367:ASN:ND2	3:C:824:HOH:O	2.52	0.42
1:E:128:ASN:O	1:E:129:ASN:HB3	2.19	0.42
1:E:442:GLY:HA3	1:E:476:TRP:CD1	2.53	0.42
1:E:675:LEU:HA	1:E:678:GLU:HB2	2.01	0.42
2:F:779:LEU:HD12	2:F:779:LEU:HA	1.89	0.42
2:B:682:ILE:HG13	2:B:697:ILE:HG21	2.01	0.42
1:C:168:TRP:CD1	1:C:168:TRP:N	2.87	0.42
1:C:409:LEU:CD2	1:C:409:LEU:N	2.82	0.42
1:C:465:ARG:HG3	1:C:526:PHE:HD1	1.84	0.42
1:C:804:ARG:HD2	2:D:818:ALA:OXT	2.19	0.42
1:E:466:ARG:HH11	1:E:466:ARG:HB3	1.84	0.42
1:E:591:GLU:O	1:E:592:VAL:HB	2.18	0.42
1:A:195:LEU:HA	1:A:196:PRO:HD3	1.83	0.42
1:A:470:ASN:CG	1:A:470:ASN:O	2.62	0.42
1:C:503:ASN:C	1:C:503:ASN:ND2	2.78	0.42
1:C:529:LEU:HB3	1:C:530:TYR:CD1	2.54	0.42
2:D:701:GLN:O	2:D:701:GLN:HG2	2.20	0.42
1:E:407:TYR:CE1	1:E:419:TYR:HB2	2.53	0.42
1:A:237:HIS:CG	1:A:238:PRO:HD2	2.55	0.42
1:A:237:HIS:ND1	1:A:238:PRO:HD2	2.35	0.42
1:A:804:ARG:HG3	1:A:804:ARG:NH1	2.34	0.42
1:C:77:PHE:CD1	1:C:77:PHE:N	2.87	0.42
1:C:165:VAL:HG11	1:C:201:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:VAL:HG11	1:C:296:THR:HG21	2.01	0.42
1:C:685:ARG:HH11	1:C:685:ARG:HB2	1.83	0.42
1:C:697:PHE:O	1:C:701:ILE:HG13	2.19	0.42
2:D:699:GLN:HG2	2:D:707:LEU:HD11	2.02	0.42
1:E:76:ASP:O	1:E:77:PHE:HB2	2.19	0.42
1:A:234:ALA:HA	1:A:244:ILE:O	2.20	0.42
1:C:805:VAL:HA	2:D:815:LEU:HD23	2.01	0.42
1:E:379:TYR:CD1	1:E:379:TYR:C	2.98	0.42
1:E:603:VAL:HG21	1:E:631:SER:HB3	2.01	0.42
1:A:120:THR:CG2	1:A:121:VAL:N	2.82	0.42
1:A:306:THR:HG22	1:A:362:LEU:CB	2.50	0.42
1:A:609:LEU:HB2	1:A:618:ALA:HB2	2.01	0.42
1:C:41:ASN:C	1:C:41:ASN:ND2	2.76	0.42
1:C:163:ARG:NH1	1:C:184:GLU:HG3	2.35	0.42
2:D:650:HIS:CE1	2:D:672:LEU:HD21	2.54	0.42
2:D:714:THR:CG2	2:D:716:ASP:HB2	2.50	0.42
2:D:789:VAL:HG12	2:D:791:LEU:HD12	2.01	0.42
1:E:678:GLU:O	1:E:679:SER:C	2.61	0.42
2:B:725:ASN:HA	2:B:728:GLN:OE1	2.18	0.42
1:C:106:HIS:NE2	1:C:153:PRO:HB2	2.35	0.42
1:C:385:LEU:HD22	1:C:386:ALA:H	1.83	0.42
1:C:479:ASN:OD1	1:C:479:ASN:C	2.63	0.42
2:D:720:LEU:HD21	2:D:742:TYR:HB3	2.02	0.42
1:A:392:PHE:CD1	1:A:392:PHE:C	2.97	0.42
1:A:475:ILE:HD13	1:A:539:GLY:O	2.20	0.42
1:C:56:THR:HG21	1:C:76:ASP:N	2.35	0.42
2:D:649:PRO:HA	2:D:652:ARG:NH1	2.35	0.42
1:A:478:ASP:C	1:A:480:GLY:H	2.28	0.42
2:B:666:LEU:HG	2:B:670:LYS:HE3	2.01	0.42
1:C:271:GLU:HB2	1:C:292:ASP:HB2	2.02	0.42
1:C:546:PHE:CE1	1:C:548:PHE:HB3	2.55	0.42
1:E:233:PHE:CZ	1:E:246:GLY:HA3	2.55	0.42
1:E:532:LEU:HD23	1:E:533:SER:H	1.85	0.42
1:A:267:ASN:C	1:A:267:ASN:ND2	2.72	0.42
1:A:337:GLU:CD	1:A:337:GLU:H	2.28	0.42
2:B:737:LEU:HD12	2:B:737:LEU:HA	1.86	0.42
1:E:102:SER:CB	1:E:145:CYS:HA	2.50	0.42
1:E:430:VAL:HG12	1:E:432:MET:HG2	2.02	0.42
1:A:120:THR:HG23	1:A:121:VAL:N	2.35	0.41
1:C:19:ILE:HG23	1:C:277:ALA:HB2	2.02	0.41
1:C:224:LEU:HD23	1:C:255:TRP:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:TRP:CD1	1:E:126:TRP:C	2.98	0.41
1:E:655:GLN:OE1	1:E:655:GLN:HA	2.20	0.41
1:A:330:THR:CG2	1:A:331:ALA:N	2.82	0.41
1:C:804:ARG:O	2:D:815:LEU:HA	2.21	0.41
1:E:532:LEU:HD13	1:E:536:ILE:HD11	2.01	0.41
1:E:741:LEU:HD12	1:E:741:LEU:HA	1.90	0.41
1:A:248:GLU:C	1:A:250:GLY:H	2.27	0.41
1:A:764:ARG:HD3	1:A:767:GLU:OE2	2.21	0.41
2:F:648:ASP:HA	2:F:649:PRO:HD3	1.90	0.41
1:C:110:PRO:HA	1:C:126:TRP:CZ2	2.55	0.41
1:C:161:LEU:HD12	1:C:161:LEU:HA	1.94	0.41
1:C:532:LEU:HD22	1:C:536:ILE:HD11	2.01	0.41
1:C:660:GLU:CD	1:C:664:LYS:NZ	2.78	0.41
1:E:545:VAL:HG11	1:E:604:LEU:HD22	2.01	0.41
2:F:763:TYR:CZ	2:F:767:LYS:HG3	2.55	0.41
1:A:762:SER:O	1:A:763:GLN:HB2	2.19	0.41
2:D:717:VAL:HG22	2:D:718:ASN:N	2.33	0.41
1:E:380:VAL:CG2	1:E:382:TYR:HE1	2.34	0.41
1:C:401:GLY:C	1:C:403:ASP:N	2.78	0.41
1:E:684:TRP:HB2	1:E:707:ALA:HB2	2.03	0.41
1:E:704:PHE:CD1	1:E:712:SER:HB3	2.55	0.41
1:E:752:ILE:HG13	2:F:802:GLN:HG3	2.02	0.41
1:A:448:LYS:HE3	1:A:471:ALA:O	2.21	0.41
1:C:248:GLU:O	1:C:272:ARG:HG2	2.20	0.41
1:C:379:TYR:O	1:C:392:PHE:HA	2.21	0.41
2:D:763:TYR:CZ	2:D:767:LYS:HG3	2.56	0.41
1:E:777:LEU:HD23	1:E:777:LEU:HA	1.85	0.41
1:A:316:VAL:HG22	1:A:330:THR:OG1	2.20	0.41
1:A:589:ASP:OD1	1:A:589:ASP:C	2.63	0.41
1:A:790:LYS:HE3	1:A:802:SER:O	2.21	0.41
2:B:730:ARG:O	2:B:731:GLU:CG	2.69	0.41
1:C:436:ILE:HG23	1:C:447:VAL:HG23	2.01	0.41
1:C:482:LEU:CD2	1:C:544:ASP:HA	2.50	0.41
2:D:745:SER:OG	2:D:748:GLU:HB2	2.21	0.41
1:E:155:THR:HA	1:E:168:TRP:O	2.20	0.41
2:F:729:THR:C	2:F:731:GLU:N	2.78	0.41
1:A:412:GLU:C	1:A:414:GLY:N	2.78	0.41
1:A:432:MET:CB	1:A:436:ILE:HD11	2.51	0.41
1:A:675:LEU:HD22	1:A:678:GLU:HB2	2.03	0.41
2:B:642:ALA:N	2:B:644:GLN:HE22	2.19	0.41
2:B:786:GLU:OE1	2:B:786:GLU:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:THR:HG21	1:C:286:TYR:HE2	1.85	0.41
1:C:162:ASP:O	1:C:163:ARG:HB2	2.21	0.41
1:C:640:GLU:C	1:C:642:GLN:H	2.29	0.41
2:D:648:ASP:HB3	2:D:651:ILE:CG1	2.50	0.41
1:E:41:ASN:HD22	1:E:43:GLU:N	2.17	0.41
1:E:91:VAL:HG22	1:E:92:ASP:N	2.36	0.41
1:E:123:LEU:CD1	1:E:133:GLU:HB3	2.46	0.41
1:E:207:ASP:O	1:E:208:LEU:HB2	2.21	0.41
1:A:120:THR:HG21	1:A:122:LYS:HE3	2.03	0.41
1:A:305:PRO:HD3	1:A:590:ARG:HA	2.03	0.41
1:A:362:LEU:HA	1:A:372:THR:O	2.20	0.41
2:B:740:THR:CG2	2:B:749:ARG:NE	2.72	0.41
1:C:334:ARG:HH11	1:C:334:ARG:HG2	1.86	0.41
1:E:117:ASP:C	1:E:119:LEU:H	2.28	0.41
1:E:201:MET:HE3	1:E:201:MET:HB3	1.85	0.41
1:E:357:VAL:HG22	1:E:376:ASP:HB2	2.03	0.41
1:A:33:TYR:HA	1:A:57:PRO:HB3	2.03	0.40
2:B:785:ASP:C	2:B:787:GLN:N	2.77	0.40
1:E:95:ALA:HB3	1:E:100:ILE:HD11	2.03	0.40
1:E:281:THR:O	1:E:590:ARG:NH2	2.53	0.40
1:E:454:TYR:OH	1:E:466:ARG:HD2	2.21	0.40
1:E:500:LEU:HD22	1:E:528:VAL:HG22	2.04	0.40
1:A:9:PHE:CD2	1:A:10:SER:N	2.90	0.40
1:A:281:THR:HG22	1:A:590:ARG:NH2	2.36	0.40
1:A:470:ASN:O	1:A:470:ASN:ND2	2.54	0.40
1:A:546:PHE:CE2	1:A:548:PHE:HB3	2.56	0.40
1:A:615:ILE:HD11	1:A:644:TYR:OH	2.21	0.40
2:B:789:VAL:HG12	2:B:790:THR:N	2.36	0.40
1:C:139:HIS:CE1	1:C:166:LYS:HD2	2.56	0.40
1:C:284:LYS:HD2	1:C:286:TYR:CZ	2.56	0.40
2:D:759:LEU:HA	2:D:759:LEU:HD12	1.81	0.40
1:E:353:GLY:O	1:E:354:SER:HB3	2.21	0.40
1:E:362:LEU:C	1:E:362:LEU:HD23	2.46	0.40
1:E:512:ASN:HD22	1:E:512:ASN:HA	1.68	0.40
2:F:743:ASN:HD22	2:F:745:SER:N	2.20	0.40
1:A:259:THR:HG23	1:A:261:LYS:CG	2.51	0.40
1:A:418:TYR:CB	1:A:428:TRP:CD2	3.04	0.40
1:A:676:THR:HG22	1:A:677:ASP:H	1.86	0.40
1:C:224:LEU:N	1:C:224:LEU:CD1	2.84	0.40
1:C:465:ARG:HD2	1:C:467:ILE:CD1	2.51	0.40
1:C:532:LEU:HD12	1:C:532:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:LEU:HD21	1:C:585:VAL:CG1	2.52	0.40
1:C:763:GLN:HA	1:C:765:PHE:CE1	2.57	0.40
1:E:185:ARG:HD2	1:E:206:ASP:CB	2.51	0.40
1:E:295:PHE:CD2	1:E:295:PHE:C	3.00	0.40
1:A:202:ILE:HD11	1:A:210:ILE:CG2	2.51	0.40
1:A:240:LEU:HB2	1:A:242:ILE:HG12	2.03	0.40
1:C:176:ASN:O	1:C:177:PHE:HB3	2.20	0.40
1:C:270:LEU:O	1:C:271:GLU:HB2	2.21	0.40
1:C:556:ASN:HD22	1:C:565:ASN:HA	1.85	0.40
1:C:793:LEU:HD23	1:C:802:SER:HA	2.04	0.40
2:D:682:ILE:HD11	2:D:697:ILE:CG2	2.52	0.40
1:E:383:THR:O	1:E:387:TRP:HA	2.22	0.40
1:E:692:LEU:HD11	2:F:761:LEU:CD1	2.52	0.40
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.85	0.40
1:A:443:ALA:HB3	1:A:476:TRP:CZ3	2.57	0.40
1:C:158:SER:O	1:C:165:VAL:HA	2.21	0.40
1:C:558:PHE:CZ	1:C:561:GLY:HA2	2.57	0.40
1:C:713:LEU:HG	1:C:717:HIS:CD2	2.56	0.40
1:E:421:ASN:O	1:E:422:PHE:HB2	2.21	0.40
1:E:668:LEU:O	1:E:672:ARG:HB2	2.22	0.40
1:E:764:ARG:HB3	1:E:767:GLU:OE1	2.22	0.40
2:F:648:ASP:OD1	2:F:651:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	809/814 (99%)	755 (93%)	43 (5%)	11 (1%)	9	17
1	C	807/814 (99%)	741 (92%)	55 (7%)	11 (1%)	9	17
1	E	806/814 (99%)	749 (93%)	43 (5%)	14 (2%)	7	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
2	D	175/177 (99%)	153 (87%)	17 (10%)	5 (3%)	3	5
2	F	173/177 (98%)	166 (96%)	7 (4%)	0	100	100
All	All	2945/2973 (99%)	2732 (93%)	172 (6%)	41 (1%)	9	17

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	VAL
1	A	493	ASP
1	A	494	GLU
1	C	336	ASN
1	C	679	SER
1	C	680	ALA
1	E	354	SER
1	E	592	VAL
1	E	676	THR
1	A	321	LYS
1	A	353	GLY
1	A	385	LEU
1	A	680	ALA
1	C	337	GLU
1	C	678	GLU
1	E	339	VAL
1	E	411	ASP
1	E	680	ALA
1	A	271	GLU
1	A	433	HIS
1	C	376	ASP
2	D	673	ASN
2	D	730	ARG
1	E	271	GLU
1	E	489	ASN
1	A	678	GLU
1	C	264	LYS
1	C	271	GLU
1	C	281	THR
1	C	673	ASP
2	D	773	ALA
1	E	66	ARG
1	E	184	GLU

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Mol	Chain	Res	Type
1	C	280	PRO
2	D	785	ASP
2	D	754	ALA
1	E	342	ASP
1	A	469	VAL
1	E	153	PRO
1	E	268	VAL
1	E	23	PRO

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	698/700 (100%)	643 (92%)	55 (8%)	11	24
1	C	698/700 (100%)	646 (93%)	52 (7%)	13	27
1	E	697/700 (100%)	640 (92%)	57 (8%)	10	23
2	B	148/148 (100%)	135 (91%)	13 (9%)	9	20
2	D	148/148 (100%)	136 (92%)	12 (8%)	11	23
2	F	147/148 (99%)	134 (91%)	13 (9%)	9	20
All	All	2536/2544 (100%)	2334 (92%)	202 (8%)	11	24

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	16	VAL
1	A	41	ASN
1	A	43	GLU
1	A	48	VAL
1	A	49	ARG
1	A	77	PHE
1	A	105	VAL
1	A	112	VAL
1	A	119	LEU

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Mol	Chain	Res	Type
1	A	120	THR
1	A	123	LEU
1	A	149	ASN
1	A	155	THR
1	A	170	LEU
1	A	251	THR
1	A	252	LEU
1	A	259	THR
1	A	267	ASN
1	A	307	LEU
1	A	336	ASN
1	A	337	GLU
1	A	342	ASP
1	A	367	ASN
1	A	425	VAL
1	A	438	ARG
1	A	444	LEU
1	A	447	VAL
1	A	465	ARG
1	A	469	VAL
1	A	470	ASN
1	A	491	ASN
1	A	515	ASN
1	A	532	LEU
1	A	549	THR
1	A	550	THR
1	A	566	LEU
1	A	571	LYS
1	A	576	LEU
1	A	604	LEU
1	A	615	ILE
1	A	617	GLU
1	A	639	LEU
1	A	655	GLN
1	A	665	VAL
1	A	679	SER
1	A	682	MET
1	A	724	GLU
1	A	738	LYS
1	A	741	LEU
1	A	771	LEU
1	A	793	LEU

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Mol	Chain	Res	Type
1	A	800	THR
1	A	805	VAL
1	A	809	GLU
2	B	643	LEU
2	B	644	GLN
2	B	662	LEU
2	B	679	GLU
2	B	683	GLN
2	B	686	LEU
2	B	714	THR
2	B	740	THR
2	B	759	LEU
2	B	761	LEU
2	B	786	GLU
2	B	796	ASP
2	B	810	LEU
1	C	8	THR
1	C	10	SER
1	C	16	VAL
1	C	41	ASN
1	C	55	GLU
1	C	77	PHE
1	C	89	LYS
1	C	119	LEU
1	C	123	LEU
1	C	132	LEU
1	C	155	THR
1	C	161	LEU
1	C	170	LEU
1	C	180	THR
1	C	184	GLU
1	C	251	THR
1	C	281	THR
1	C	297	VAL
1	C	309	LEU
1	C	310	ASP
1	C	336	ASN
1	C	385	LEU
1	C	395	CYS
1	C	409	LEU
1	C	434	SER
1	C	438	ARG

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Mol	Chain	Res	Type
1	C	447	VAL
1	C	469	VAL
1	C	472	LYS
1	C	499	THR
1	C	528	VAL
1	C	529	LEU
1	C	545	VAL
1	C	566	LEU
1	C	575	LEU
1	C	576	LEU
1	C	583	ASN
1	C	604	LEU
1	C	605	GLU
1	C	627	GLU
1	C	647	GLU
1	C	649	LEU
1	C	660	GLU
1	C	676	THR
1	C	694	ARG
1	C	715	LEU
1	C	726	LEU
1	C	740	ASN
1	C	758	LEU
1	C	759	LEU
1	C	793	LEU
1	C	799	ASN
2	D	672	LEU
2	D	707	LEU
2	D	710	LEU
2	D	714	THR
2	D	717	VAL
2	D	728	GLN
2	D	747	LYS
2	D	748	GLU
2	D	759	LEU
2	D	767	LYS
2	D	779	LEU
2	D	786	GLU
1	E	1	MET
1	E	3	LEU
1	E	16	VAL
1	E	30	THR

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Mol	Chain	Res	Type
1	E	41	ASN
1	E	53	VAL
1	E	72	VAL
1	E	76	ASP
1	E	108	THR
1	E	149	ASN
1	E	161	LEU
1	E	164	THR
1	E	168	TRP
1	E	184	GLU
1	E	214	ASP
1	E	240	LEU
1	E	264	LYS
1	E	266	LEU
1	E	267	ASN
1	E	272	ARG
1	E	297	VAL
1	E	307	LEU
1	E	337	GLU
1	E	352	LEU
1	E	357	VAL
1	E	385	LEU
1	E	390	LYS
1	E	425	VAL
1	E	438	ARG
1	E	441	SER
1	E	448	LYS
1	E	463	LEU
1	E	465	ARG
1	E	466	ARG
1	E	482	LEU
1	E	483	VAL
1	E	532	LEU
1	E	550	THR
1	E	559	VAL
1	E	576	LEU
1	E	587	LEU
1	E	598	GLU
1	E	611	LEU
1	E	620	GLU
1	E	623	LEU
1	E	632	LEU

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Mol	Chain	Res	Type
1	E	650	ASN
1	E	660	GLU
1	E	676	THR
1	E	693	GLN
1	E	715	LEU
1	E	722	ASN
1	E	724	GLU
1	E	726	LEU
1	E	780	ASN
1	E	793	LEU
1	E	809	GLU
2	F	648	ASP
2	F	667	ASP
2	F	675	SER
2	F	696	MET
2	F	714	THR
2	F	720	LEU
2	F	740	THR
2	F	743	ASN
2	F	761	LEU
2	F	779	LEU
2	F	785	ASP
2	F	786	GLU
2	F	805	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	41	ASN
1	A	68	ASN
1	A	149	ASN
1	A	172	GLN
1	A	176	ASN
1	A	183	GLN
1	A	256	ASN
1	A	267	ASN
1	A	285	ASN
1	A	293	ASN
1	A	336	ASN
1	A	341	GLN
1	A	360	GLN

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Mol	Chain	Res	Type
1	A	367	ASN
1	A	405	ASN
1	A	470	ASN
1	A	487	ASN
1	A	515	ASN
1	A	556	ASN
1	A	593	HIS
1	A	655	GLN
1	A	667	GLN
1	A	708	HIS
1	A	744	ASN
1	A	753	GLN
1	A	783	ASN
1	A	799	ASN
2	B	718	ASN
2	B	739	ASN
2	B	781	GLN
2	B	794	GLN
1	C	11	ASN
1	C	22	HIS
1	C	41	ASN
1	C	52	GLN
1	C	68	ASN
1	C	139	HIS
1	C	176	ASN
1	C	183	GLN
1	C	227	HIS
1	C	256	ASN
1	C	279	HIS
1	C	336	ASN
1	C	360	GLN
1	C	396	GLN
1	C	405	ASN
1	C	421	ASN
1	C	487	ASN
1	C	503	ASN
1	C	512	ASN
1	C	515	ASN
1	C	556	ASN
1	C	583	ASN
1	C	655	GLN
1	C	796	ASN

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Mol	Chain	Res	Type
1	C	799	ASN
2	D	644	GLN
2	D	647	GLN
2	D	650	HIS
2	D	683	GLN
2	D	699	GLN
2	D	701	GLN
2	D	702	HIS
2	D	725	ASN
2	D	744	ASN
2	D	781	GLN
1	E	22	HIS
1	E	41	ASN
1	E	128	ASN
1	E	129	ASN
1	E	149	ASN
1	E	176	ASN
1	E	183	GLN
1	E	256	ASN
1	E	267	ASN
1	E	279	HIS
1	E	285	ASN
1	E	341	GLN
1	E	405	ASN
1	E	415	GLN
1	E	421	ASN
1	E	487	ASN
1	E	489	ASN
1	E	512	ASN
1	E	513	ASN
1	E	553	ASN
1	E	565	ASN
1	E	607	GLN
1	E	642	GLN
1	E	650	ASN
1	E	708	HIS
1	E	717	HIS
1	E	722	ASN
1	E	753	GLN
1	E	763	GLN
1	E	792	ASN
2	F	644	GLN

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Mol	Chain	Res	Type
2	F	673	ASN
2	F	724	GLN
2	F	728	GLN
2	F	739	ASN
2	F	743	ASN

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	811/814 (99%)	0.02	16 (1%) 65 61	17, 39, 62, 84	0
1	C	811/814 (99%)	0.16	18 (2%) 62 58	20, 43, 66, 89	0
1	E	810/814 (99%)	0.19	20 (2%) 58 54	19, 42, 67, 89	0
2	B	177/177 (100%)	0.29	4 (2%) 61 57	29, 44, 68, 74	0
2	D	177/177 (100%)	0.74	9 (5%) 33 29	32, 55, 77, 83	0
2	F	175/177 (98%)	0.62	7 (4%) 42 38	30, 53, 73, 80	0
All	All	2961/2973 (99%)	0.20	74 (2%) 58 54	17, 43, 68, 89	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	642	ALA	6.6
2	D	818	ALA	6.0
2	F	642	ALA	5.9
1	E	676	THR	5.0
1	A	676	THR	4.6
2	D	642	ALA	3.9
1	C	676	THR	3.9
1	C	679	SER	3.8
1	C	814	SER	3.8
1	A	682	MET	3.6
1	A	678	GLU	3.6
1	A	353	GLY	3.6
1	C	811	LEU	3.4
1	E	597	TYR	3.2
1	C	678	GLU	3.1
1	C	433	HIS	3.1
1	C	490	SER	3.0
1	E	599	ILE	2.9
1	C	627	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	352	LEU	2.8
1	C	543	GLY	2.7
1	E	739	PHE	2.7
1	A	660	GLU	2.7
1	E	433	HIS	2.7
1	A	339	VAL	2.7
1	E	679	SER	2.7
2	B	818	ALA	2.7
1	A	626	VAL	2.6
1	C	491	ASN	2.6
1	E	184	GLU	2.6
1	C	680	ALA	2.6
1	A	348	GLN	2.5
2	D	785	ASP	2.5
1	A	433	HIS	2.5
1	E	339	VAL	2.5
2	B	782	ALA	2.5
1	E	656	ASP	2.5
2	F	816	LYS	2.4
1	A	198	LYS	2.4
1	C	376	ASP	2.4
1	C	171	GLY	2.4
1	C	431	PRO	2.3
1	C	597	TYR	2.3
2	F	674	ASP	2.3
2	B	671	LYS	2.3
1	E	490	SER	2.3
1	E	675	LEU	2.3
2	D	726	ILE	2.3
1	E	800	THR	2.3
1	E	630	ASP	2.3
1	E	680	ALA	2.2
2	F	722	LYS	2.2
1	C	367	ASN	2.2
1	A	351	GLU	2.2
2	D	728	GLN	2.2
1	C	813	GLY	2.2
1	A	677	ASP	2.2
2	D	787	GLN	2.1
2	D	731	GLU	2.1
1	C	572	GLU	2.1
2	F	807	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	773	ALA	2.1
1	A	628	GLY	2.1
1	E	813	GLY	2.1
1	E	660	GLU	2.1
1	E	76	ASP	2.1
2	D	784	VAL	2.1
1	A	385	LEU	2.1
1	A	434	SER	2.1
1	E	405	ASN	2.0
2	F	672	LEU	2.0
1	A	2	LYS	2.0
1	E	682	MET	2.0
2	D	717	VAL	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.