



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:17 PM UTC

PDB ID : 2NPP / pdb_00002npp
Title : Structure of the Protein Phosphatase 2A Holoenzyme
Authors : Xu, Y.; Chen, Y.; Xing, Y.; Chao, Y.; Shi, Y.
Deposited on : 2006-10-28
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

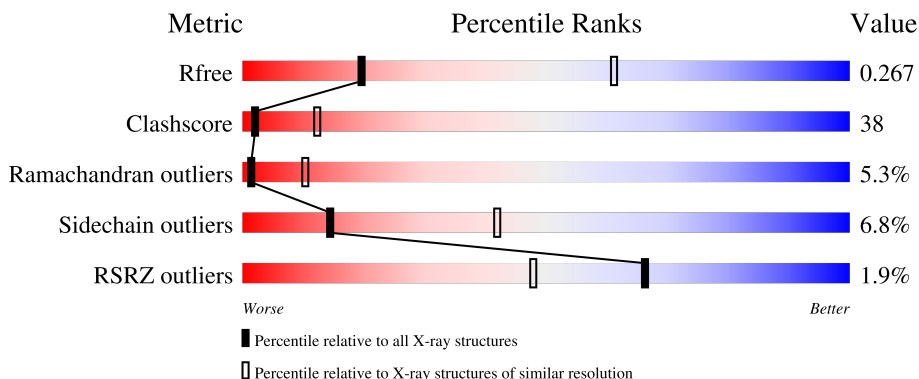
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

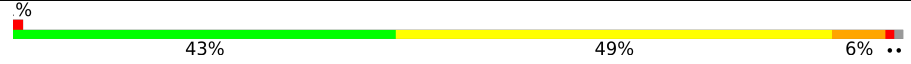

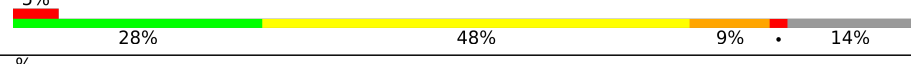
The reported resolution of this entry is 3.30 Å.

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.



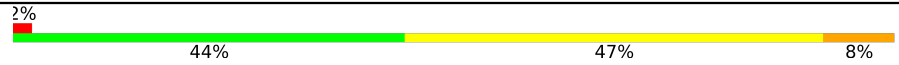
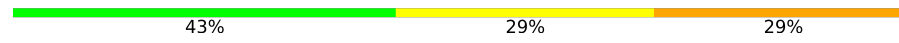

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	589	
1	D	589	
2	B	449	
2	E	449	
3	C	309	

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Mol	Chain	Length	Quality of chain
3	F	309	 <p>2% 44% 47% 8%</p>
4	X	7	 <p>43% 29% 29%</p>
4	Y	7	 <p>14% 43% 29% 14%</p>

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 20466 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 Protein Phosphatase 2, regulatory subunit A (PR 65), alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	582	4535	2881	764	863	27	0	0	0
1	D	582	4535	2881	764	863	27	0	0	0

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	388	3130	2043	513	560	14	0	0	0
2	E	388	3130	2043	513	560	14	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	433	VAL	-	cloning artifact	UNP Q13362
B	434	LEU	-	cloning artifact	UNP Q13362
B	435	LYS	-	cloning artifact	UNP Q13362
B	436	LYS	-	cloning artifact	UNP Q13362
B	437	ARG	-	cloning artifact	UNP Q13362
B	438	ILE	-	cloning artifact	UNP Q13362
B	439	THR	-	cloning artifact	UNP Q13362
E	433	VAL	-	cloning artifact	UNP Q13362
E	434	LEU	-	cloning artifact	UNP Q13362
E	435	LYS	-	cloning artifact	UNP Q13362
E	436	LYS	-	cloning artifact	UNP Q13362
E	437	ARG	-	cloning artifact	UNP Q13362
E	438	ILE	-	cloning artifact	UNP Q13362
E	439	THR	-	cloning artifact	UNP Q13362

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	308	2497	1579	431	472	15	0	0	0
3	F	308	2497	1579	431	472	15	0	0	0

- Molecule 4 is a protein called microcystin LR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	X	7	69	49	10	10	0	0	0
4	Y	7	69	49	10	10	0	0	0

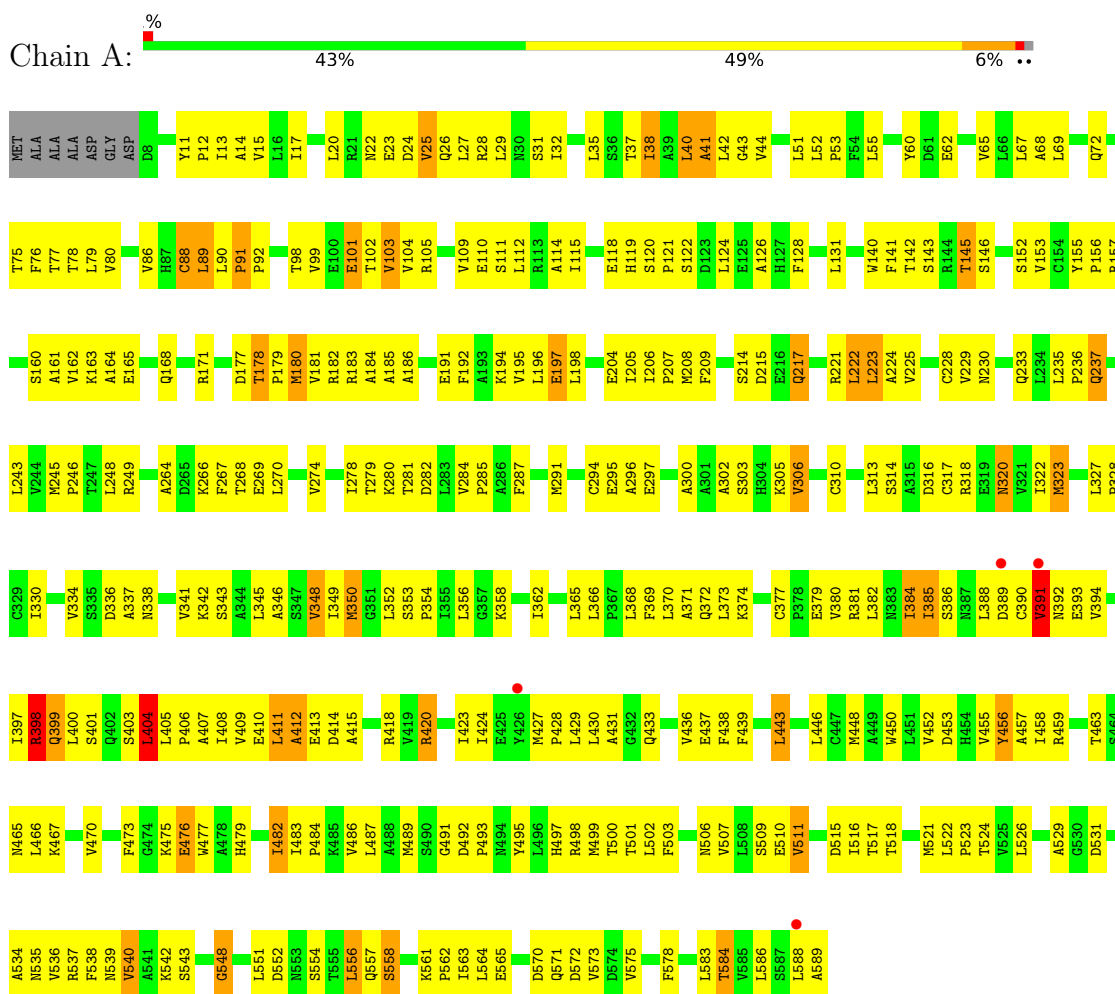
- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
5	C	2	2	2	0	0
5	F	2	2	2	0	0

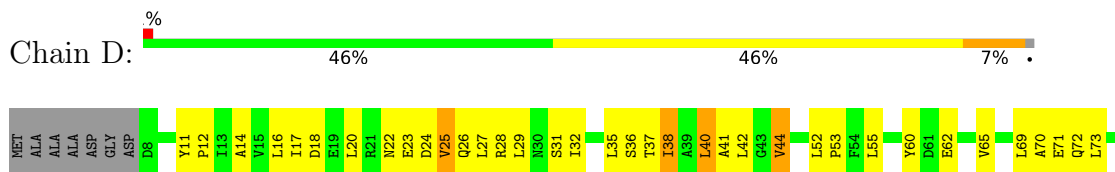
3 Residue-property plots

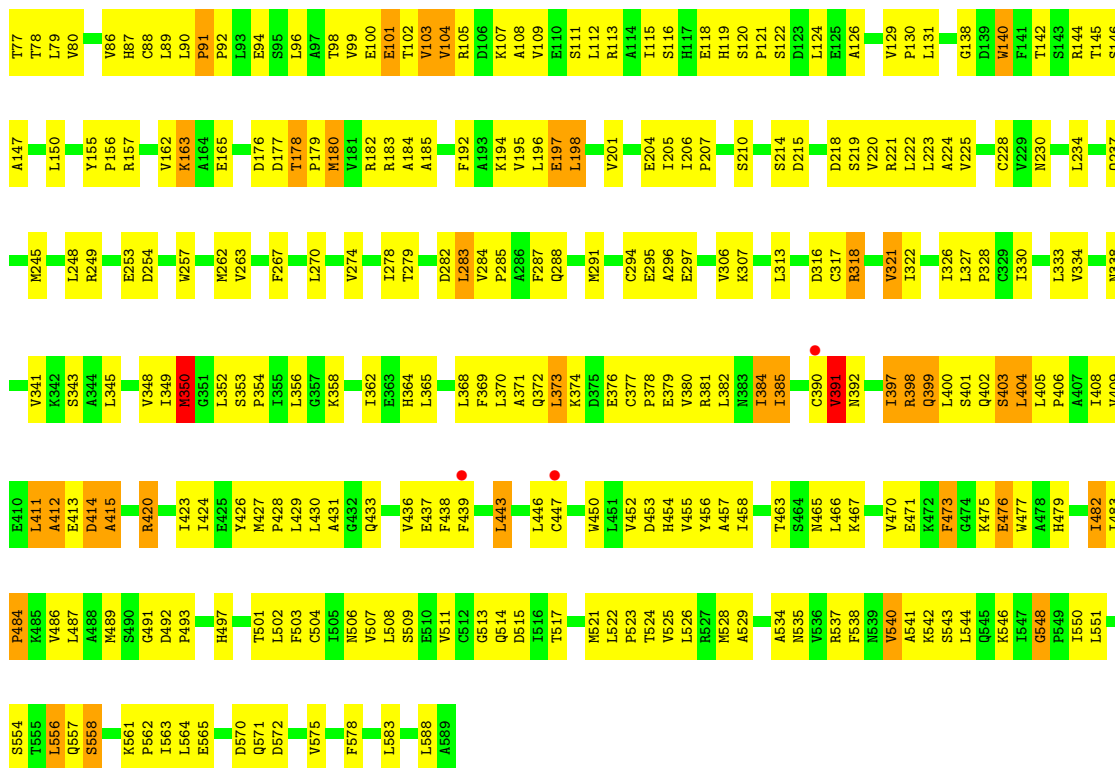
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Protein Phosphatase 2, regulatory subunit A (PR 65), alpha isoform

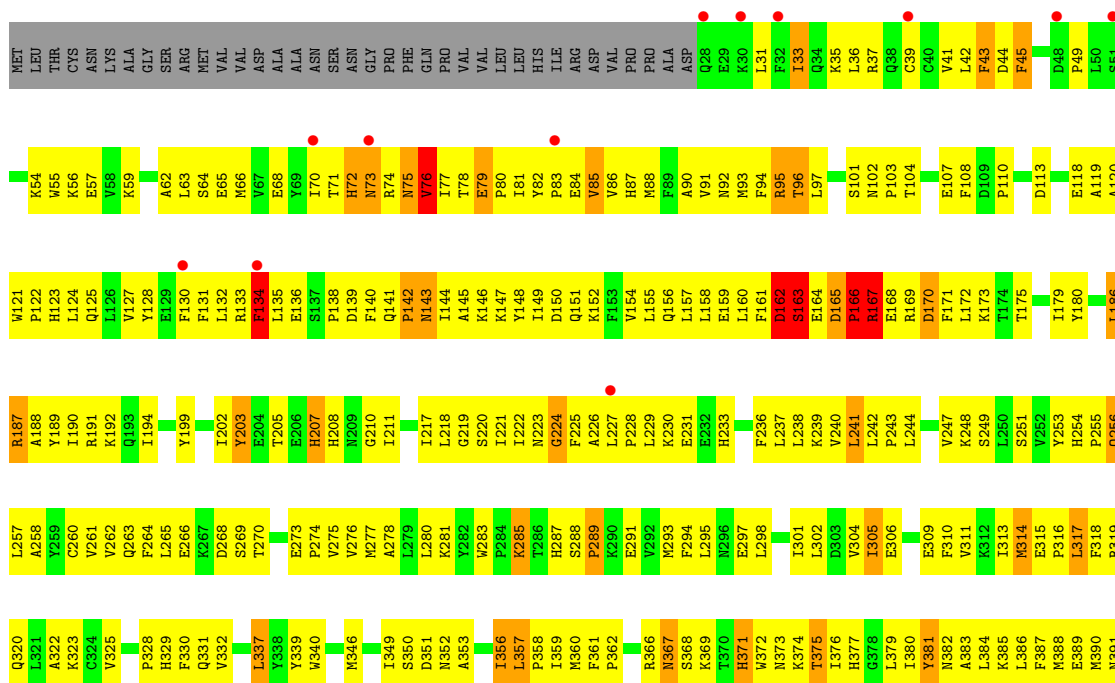


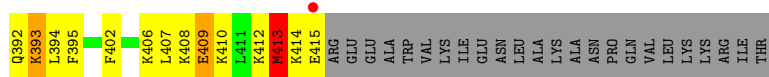
- Molecule 1: Protein Phosphatase 2, regulatory subunit A (PR 65), alpha isoform



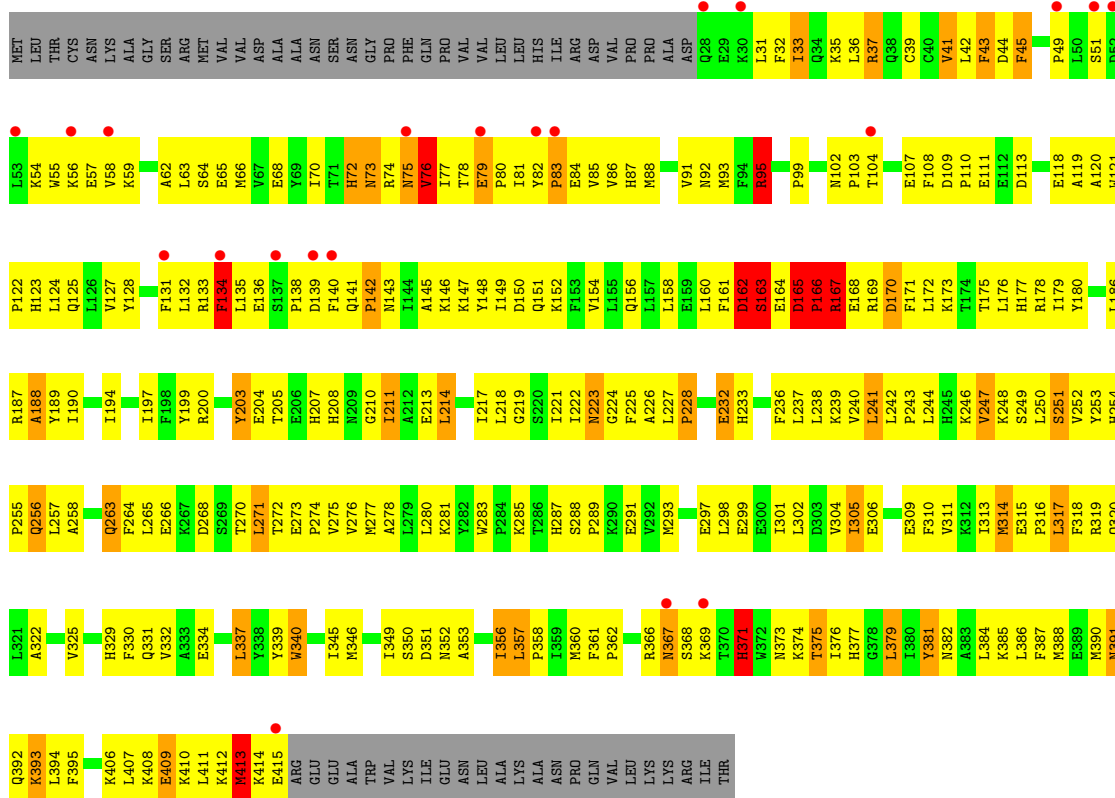


• Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

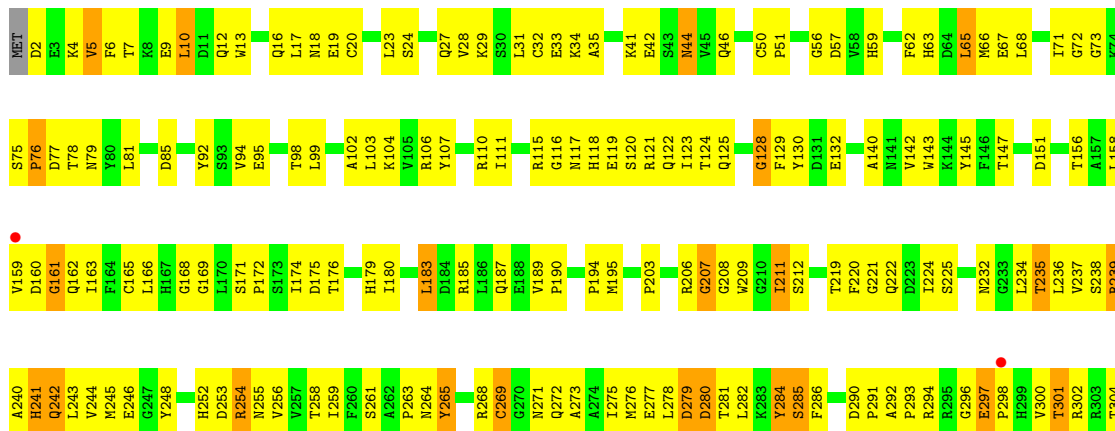


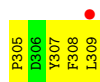


• Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

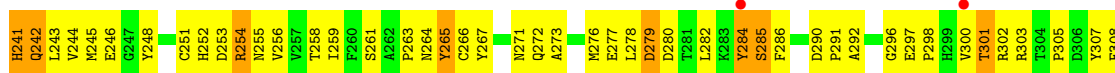
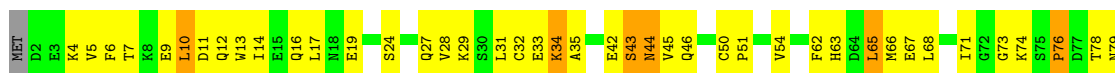


• Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform





- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform



- Molecule 4: microcystin LR



- Molecule 4: microcystin LR



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.26Å 159.05Å 269.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.30 100.00 – 3.31	Depositor EDS
% Data completeness (in resolution range)	98.4 (100.00-3.30) 99.2 (100.00-3.31)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.33Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.255 , 0.299 0.225 , 0.267	Depositor DCC
R_{free} test set	3549 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	93.9	Xtrriage
Anisotropy	0.381	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 100.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20466	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: DAM, FGA, DAL, ACB, MN, 1ZN

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	0.52	0/4609	1.01	18/6257 (0.3%)
1	D	0.62	1/4609 (0.0%)	1.02	23/6257 (0.4%)
2	B	0.50	0/3212	0.99	16/4359 (0.4%)
2	E	0.53	0/3212	1.01	18/4359 (0.4%)
3	C	0.48	0/2559	0.94	5/3469 (0.1%)
3	F	0.51	0/2559	0.96	7/3469 (0.2%)
4	X	0.39	0/17	0.87	0/19
4	Y	0.49	0/17	0.85	0/19
All	All	0.54	1/20794 (0.0%)	0.99	87/28208 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	X	0	3
4	Y	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	350	MET	SD-CE	-6.46	1.63	1.79

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	49	PRO	N-CA-CB	10.39	109.65	102.79
1	A	38	ILE	N-CA-C	-9.37	101.61	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	162	ASP	N-CA-C	8.82	127.77	114.09
1	D	38	ILE	N-CA-C	-8.71	101.85	110.30
2	B	162	ASP	N-CA-C	8.55	127.41	113.89
2	B	356	ILE	N-CA-C	8.43	118.46	110.53
3	C	65	LEU	N-CA-C	-7.65	103.02	111.36
2	E	84	GLU	N-CA-C	-7.64	103.68	113.16
3	C	19	GLU	N-CA-C	-7.62	104.08	113.15
2	E	37	ARG	N-CA-C	-7.46	106.12	114.62
1	D	397	ILE	N-CA-C	-7.37	103.04	113.07
1	A	386	SER	N-CA-C	7.32	121.65	112.87
1	A	153	VAL	N-CA-C	7.28	120.15	111.05
1	D	473	PHE	N-CA-C	7.10	121.94	113.28
3	F	272	GLN	N-CA-C	-6.79	100.42	110.46
3	C	272	GLN	N-CA-C	-6.78	99.63	110.14
2	B	84	GLU	N-CA-C	-6.77	104.90	113.02
2	E	283	TRP	CA-C-N	6.57	126.92	119.83
2	E	283	TRP	C-N-CA	6.57	126.92	119.83
2	E	163	SER	N-CA-C	6.54	124.73	110.80
2	E	75	ASN	N-CA-C	6.48	117.01	107.88
1	D	283	LEU	N-CA-C	6.36	118.00	111.14
2	B	85	VAL	N-CA-C	-6.33	104.68	110.82
1	A	482	ILE	N-CA-C	6.32	117.42	111.48
1	A	223	LEU	N-CA-C	-6.30	104.33	111.14
1	D	316	ASP	N-CA-C	6.28	120.19	112.54
1	D	44	VAL	N-CA-C	-6.24	104.97	111.58
2	B	75	ASN	N-CA-C	6.08	116.44	107.88
2	E	356	ILE	N-CA-C	6.01	116.65	110.82
2	B	163	SER	N-CA-C	5.98	123.54	110.80
2	E	241	LEU	N-CA-C	5.95	117.57	111.14
2	E	49	PRO	N-CA-CB	5.95	109.50	103.25
3	F	65	LEU	N-CA-C	-5.91	104.91	111.36
1	A	51	LEU	N-CA-C	5.91	118.23	111.02
2	E	211	ILE	N-CA-C	-5.90	104.57	111.00
2	E	203	TYR	N-CA-C	5.88	121.36	113.72
1	A	342	LYS	N-CA-C	-5.86	104.58	110.97
1	A	43	GLY	N-CA-C	-5.86	102.33	111.00
1	A	511	VAL	N-CA-C	5.84	117.80	112.43
1	D	163	LYS	N-CA-C	-5.83	104.11	111.11
1	D	126	ALA	N-CA-C	5.81	117.69	111.36
1	A	397	ILE	N-CA-C	-5.78	103.95	112.04
1	D	385	ILE	CB-CA-C	-5.70	104.59	111.88
1	A	316	ASP	N-CA-C	5.69	118.25	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	140	TRP	N-CA-C	5.62	118.40	109.24
3	F	19	GLU	N-CA-C	-5.62	106.40	113.20
1	D	420	ARG	N-CA-C	-5.60	105.25	111.36
3	F	303	ARG	N-CA-C	5.60	117.52	110.24
1	A	126	ALA	N-CA-C	5.59	117.17	111.14
2	E	371	HIS	N-CA-C	5.58	117.49	110.24
1	D	541	ALA	N-CA-C	-5.57	104.61	111.40
1	D	364	HIS	N-CA-C	5.56	120.32	112.93
2	E	340	TRP	N-CA-C	5.48	119.81	113.18
2	B	203	TYR	N-CA-C	5.48	120.84	113.72
2	B	102	ASN	CA-C-N	5.47	126.67	119.84
2	B	102	ASN	C-N-CA	5.47	126.67	119.84
1	A	385	ILE	CB-CA-C	-5.44	104.91	112.04
2	E	85	VAL	N-CA-C	-5.42	105.09	111.00
3	C	128	GLY	N-CA-C	5.41	126.01	113.18
1	D	220	VAL	N-CA-C	-5.38	106.93	111.56
3	C	279	ASP	N-CA-C	5.38	117.83	109.60
2	E	95	ARG	N-CA-C	-5.38	102.24	110.14
2	B	229	LEU	N-CA-C	5.37	118.26	110.42
1	D	306	VAL	N-CA-C	5.37	116.00	110.36
2	B	372	TRP	N-CA-C	-5.36	106.24	112.89
1	D	511	VAL	N-CA-C	5.36	117.56	111.88
3	F	279	ASP	N-CA-C	5.32	117.74	109.60
1	A	420	ARG	N-CA-C	-5.30	105.50	111.28
2	B	328	PRO	N-CA-C	-5.29	107.14	114.27
1	D	513	GLY	N-CA-C	5.27	119.24	112.18
1	A	573	VAL	N-CA-C	5.27	116.62	110.62
2	B	241	LEU	N-CA-C	5.22	116.78	111.14
1	D	548	GLY	CA-C-N	5.22	125.53	119.47
1	D	548	GLY	C-N-CA	5.22	125.53	119.47
1	D	358	LYS	N-CA-C	5.20	117.36	111.02
1	D	482	ILE	N-CA-C	5.20	116.36	111.48
1	D	138	GLY	N-CA-C	5.19	118.04	112.33
3	F	236	LEU	N-CA-C	5.17	116.92	108.55
1	D	326	ILE	N-CA-C	5.15	115.37	110.53
1	A	398	ARG	N-CA-C	-5.14	105.13	111.40
2	B	207	HIS	N-CA-C	5.10	117.47	108.75
2	B	202	ILE	N-CA-C	5.09	115.86	110.72
2	E	247	VAL	N-CA-C	5.07	117.80	109.78
1	A	323	MET	N-CA-C	5.07	116.89	111.36
2	E	41	VAL	N-CA-C	-5.04	105.80	110.53
1	A	348	VAL	N-CA-C	5.02	118.16	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	172	PRO	N-CA-C	-5.01	107.33	113.84

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	X	4	ARG	Peptide
4	X	5	1ZN	Mainchain,Peptide
4	Y	4	ARG	Peptide
4	Y	5	1ZN	Mainchain,Peptide

5.2 Too-close contacts [i](#)

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	4535	0	4637	318	0
1	D	4535	0	4637	311	0
2	B	3130	0	3050	300	0
2	E	3130	0	3050	288	0
3	C	2497	0	2393	179	0
3	F	2497	0	2393	170	0
4	X	69	0	62	2	0
4	Y	69	0	62	5	0
5	C	2	0	0	0	0
5	F	2	0	0	0	0
All	All	20466	0	20284	1543	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 38.

All (1543) 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)
3:C:276:MET:HE3	3:C:278:LEU:HD21	1.36	1.08
2:E:388:MET:HE2	2:E:392:GLN:HE22	1.19	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:301:THR:HG22	3:C:302:ARG:H	1.27	0.99
2:B:251:SER:HA	2:B:293:MET:HE1	1.44	0.99
1:D:427:MET:HE3	1:D:427:MET:HA	1.45	0.96
3:F:174:ILE:HD13	3:F:180:ILE:HG12	1.48	0.96
3:F:301:THR:HG22	3:F:302:ARG:H	1.30	0.95
3:C:190:PRO:HD3	3:C:195:MET:HE2	1.48	0.94
2:E:273:GLU:HA	2:E:313:ILE:HD11	1.46	0.93
2:B:208:HIS:HD2	2:B:210:GLY:H	1.14	0.92
1:A:455:VAL:HG23	3:C:71:ILE:HA	1.51	0.91
1:A:278:ILE:HD12	1:A:278:ILE:H	1.34	0.91
2:B:340:TRP:HA	2:B:346:MET:HE3	1.52	0.91
1:A:102:THR:HG22	1:A:105:ARG:NH2	1.87	0.90
2:B:329:HIS:CD2	2:B:332:VAL:HG23	2.06	0.90
3:C:174:ILE:HD13	3:C:180:ILE:HG12	1.52	0.90
1:D:455:VAL:HG23	3:F:71:ILE:HA	1.54	0.88
3:C:237:VAL:HB	3:C:256:VAL:HG22	1.54	0.88
1:A:427:MET:HE3	1:A:427:MET:HA	1.55	0.88
1:A:178:THR:HB	1:A:180:MET:HG2	1.55	0.87
1:D:537:ARG:O	1:D:540:VAL:HG12	1.74	0.87
2:E:208:HIS:HD2	2:E:210:GLY:H	1.18	0.87
1:A:77:THR:HG21	1:A:118:GLU:HG3	1.57	0.86
1:D:401:SER:HA	1:D:405:LEU:HB2	1.57	0.86
3:F:276:MET:HE3	3:F:278:LEU:HD21	1.56	0.86
2:E:131:PHE:O	2:E:134:PHE:HB3	1.76	0.86
1:A:561:LYS:HB2	1:A:588:LEU:HD13	1.58	0.86
2:B:121:TRP:N	2:B:122:PRO:HD2	1.90	0.85
1:D:535:ASN:HA	1:D:538:PHE:CE2	2.11	0.85
2:E:133:ARG:HA	2:E:136:GLU:HG2	1.56	0.85
1:A:537:ARG:O	1:A:540:VAL:HG12	1.77	0.84
2:E:381:TYR:HE2	2:E:385:LYS:HD2	1.42	0.84
3:C:162:GLN:HB3	3:C:235:THR:CG2	2.07	0.84
1:D:99:VAL:HG21	1:D:104:VAL:HG11	1.59	0.84
2:E:121:TRP:N	2:E:122:PRO:HD2	1.92	0.84
1:D:35:LEU:HD21	1:D:55:LEU:HD11	1.58	0.83
2:B:133:ARG:HA	2:B:136:GLU:HG2	1.60	0.83
3:F:190:PRO:HD3	3:F:195:MET:HE2	1.59	0.83
2:B:164:GLU:HB3	2:B:168:GLU:HB3	1.60	0.83
1:D:428:PRO:HD3	1:D:465:ASN:HD21	1.43	0.82
2:E:208:HIS:CD2	2:E:210:GLY:H	1.96	0.82
2:B:237:LEU:HA	2:B:241:LEU:HB2	1.62	0.82
2:B:330:PHE:CE2	3:C:122:GLN:HG3	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:ILE:HD13	1:D:399:GLN:HG3	1.61	0.82
1:A:385:ILE:HD12	1:A:423:ILE:HD11	1.61	0.81
2:B:131:PHE:O	2:B:134:PHE:HB3	1.79	0.81
2:E:78:THR:C	2:E:80:PRO:HD2	2.05	0.81
2:B:208:HIS:CD2	2:B:210:GLY:H	1.98	0.81
1:A:428:PRO:HD3	1:A:465:ASN:ND2	1.95	0.81
2:B:152:LYS:HG2	2:B:156:GLN:HE21	1.45	0.80
1:D:162:VAL:HA	1:D:165:GLU:OE1	1.80	0.80
1:D:467:LYS:HB2	1:D:507:VAL:HG12	1.63	0.79
2:E:208:HIS:HB3	2:E:211:ILE:CD1	2.13	0.79
1:D:350:MET:HE3	1:D:369:PHE:CZ	2.17	0.79
1:D:278:ILE:HD12	1:D:278:ILE:H	1.45	0.79
2:E:208:HIS:HB3	2:E:211:ILE:HD11	1.64	0.79
1:A:155:TYR:HB3	1:A:156:PRO:HD3	1.65	0.78
2:B:199:TYR:CE2	2:B:240:VAL:HG22	2.19	0.78
1:D:22:ASN:ND2	1:D:27:LEU:HD12	1.97	0.78
2:E:175:THR:O	2:E:179:ILE:HG13	1.82	0.78
1:D:77:THR:HG21	1:D:118:GLU:HG3	1.63	0.78
1:D:517:THR:HA	1:D:521:MET:HE2	1.66	0.78
2:E:244:LEU:HD23	2:E:244:LEU:O	1.83	0.78
3:F:54:VAL:HG13	3:F:81:LEU:HD22	1.64	0.78
3:C:162:GLN:HB3	3:C:235:THR:HG22	1.64	0.78
1:D:398:ARG:HH11	1:D:398:ARG:HB3	1.49	0.78
2:E:93:MET:HE2	2:E:128:TYR:CZ	2.19	0.77
2:E:164:GLU:HB3	2:E:168:GLU:HB3	1.66	0.77
2:B:75:ASN:O	2:B:76:VAL:HG23	1.84	0.77
1:D:467:LYS:HB2	1:D:507:VAL:CG1	2.15	0.77
1:D:428:PRO:HD3	1:D:465:ASN:ND2	1.99	0.76
2:B:175:THR:HG22	2:B:179:ILE:HD11	1.66	0.76
1:D:561:LYS:HB2	1:D:588:LEU:HD13	1.67	0.76
3:F:175:ASP:H	3:F:179:HIS:HD2	1.34	0.76
3:F:237:VAL:HB	3:F:256:VAL:HG22	1.68	0.76
2:B:118:GLU:H	2:B:164:GLU:HG2	1.50	0.76
1:D:206:ILE:HB	1:D:207:PRO:HD3	1.66	0.76
1:D:267:PHE:CE2	1:D:287:PHE:HB2	2.20	0.76
3:C:44:ASN:N	3:C:44:ASN:HD22	1.81	0.76
2:E:83:PRO:HG3	2:E:148:TYR:CD2	2.20	0.76
2:E:88:MET:HE2	2:E:92:ASN:ND2	2.00	0.76
2:E:35:LYS:C	2:E:37:ARG:H	1.94	0.75
2:E:330:PHE:CE1	2:E:331:GLN:HG2	2.21	0.75
2:B:190:ILE:H	2:B:190:ILE:HD12	1.48	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:SER:HB2	2:B:289:PRO:HD3	1.68	0.75
2:B:208:HIS:HB3	2:B:211:ILE:CD1	2.16	0.75
2:E:95:ARG:H	2:E:95:ARG:HD2	1.50	0.75
1:D:179:PRO:HD2	1:D:180:MET:HE3	1.67	0.75
2:B:164:GLU:O	2:B:165:ASP:O	2.04	0.75
2:E:310:PHE:O	2:E:314:MET:HB2	1.87	0.75
1:D:405:LEU:HD21	1:D:430:LEU:HD11	1.69	0.75
1:D:452:VAL:HG12	1:D:452:VAL:O	1.86	0.75
2:E:75:ASN:O	2:E:76:VAL:HG23	1.87	0.75
2:E:164:GLU:O	2:E:165:ASP:O	2.04	0.74
3:C:104:LYS:N	3:C:111:ILE:HD11	2.01	0.74
2:B:78:THR:C	2:B:80:PRO:HD2	2.12	0.74
2:B:217:ILE:HG22	2:B:221:ILE:HD11	1.70	0.74
1:D:350:MET:SD	1:D:391:VAL:HG13	2.27	0.74
2:E:128:TYR:HB3	2:E:171:PHE:CD2	2.22	0.74
2:E:251:SER:HA	2:E:293:MET:HE1	1.69	0.74
2:B:349:ILE:HG22	2:B:390:MET:HE1	1.69	0.74
1:D:492:ASP:OD2	1:D:493:PRO:HD2	1.88	0.74
2:B:273:GLU:HA	2:B:313:ILE:HD11	1.69	0.74
3:F:209:TRP:N	3:F:224:ILE:HD11	2.02	0.74
2:B:79:GLU:O	2:B:79:GLU:HG2	1.87	0.73
2:B:83:PRO:HG3	2:B:148:TYR:CD2	2.23	0.73
1:D:487:LEU:C	1:D:489:MET:H	1.96	0.73
1:D:334:VAL:HG21	1:D:368:LEU:HD22	1.68	0.73
1:A:222:LEU:HD23	1:A:223:LEU:N	2.04	0.73
3:C:76:PRO:HB2	3:C:110:ARG:HG3	1.69	0.73
3:C:209:TRP:N	3:C:224:ILE:HD11	2.04	0.73
3:F:162:GLN:HB3	3:F:235:THR:HG22	1.68	0.73
3:C:160:ASP:HB3	3:C:282:LEU:HD11	1.70	0.73
3:C:175:ASP:H	3:C:179:HIS:HD2	1.36	0.73
1:D:197:GLU:H	1:D:197:GLU:CD	1.97	0.73
3:F:252:HIS:O	3:F:255:ASN:HB2	1.89	0.73
3:F:290:ASP:HB3	3:F:291:PRO:HD2	1.70	0.73
3:F:44:ASN:N	3:F:44:ASN:HD22	1.86	0.72
1:A:282:ASP:O	1:A:285:PRO:HD2	1.89	0.72
1:A:467:LYS:HB2	1:A:507:VAL:HG12	1.70	0.72
2:B:277:MET:HE2	2:B:277:MET:HA	1.72	0.72
1:A:330:ILE:O	1:A:334:VAL:HG23	1.87	0.72
2:E:118:GLU:H	2:E:164:GLU:HG2	1.52	0.72
3:C:120:SER:O	3:C:124:THR:HG23	1.89	0.72
1:A:334:VAL:HG21	1:A:368:LEU:HD22	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ASP:O	2:B:166:PRO:C	2.33	0.72
3:F:243:LEU:HD11	3:F:271:ASN:CG	2.15	0.72
3:F:171:SER:OG	3:F:174:ILE:HB	1.89	0.71
1:A:392:ASN:HB3	1:A:400:LEU:HD22	1.70	0.71
2:E:123:HIS:O	2:E:127:VAL:HG23	1.90	0.71
1:A:381:ARG:NH1	1:A:414:ASP:OD2	2.22	0.71
1:A:526:LEU:HD22	1:A:563:ILE:HG21	1.70	0.71
2:B:325:VAL:HG22	2:B:337:LEU:HD13	1.73	0.71
2:B:175:THR:O	2:B:179:ILE:HG13	1.90	0.71
2:B:208:HIS:HB3	2:B:211:ILE:HD11	1.72	0.71
1:A:161:ALA:O	1:A:164:ALA:HB3	1.91	0.71
3:C:28:VAL:HG11	3:C:142:VAL:HG13	1.71	0.71
2:E:329:HIS:CD2	2:E:332:VAL:HG23	2.25	0.71
1:A:401:SER:HA	1:A:405:LEU:HB2	1.72	0.70
1:D:105:ARG:NH1	1:D:142:THR:HG22	2.06	0.70
1:A:385:ILE:HD11	1:A:411:LEU:HG	1.71	0.70
1:D:526:LEU:HD22	1:D:563:ILE:HG21	1.73	0.70
2:B:165:ASP:O	2:B:167:ARG:N	2.24	0.70
3:C:17:LEU:HD21	3:C:23:LEU:HG	1.74	0.70
1:D:109:VAL:HG13	1:D:150:LEU:HD21	1.73	0.70
3:F:17:LEU:HD11	3:F:98:THR:HG22	1.73	0.70
3:F:120:SER:O	3:F:124:THR:HG23	1.92	0.70
3:F:162:GLN:HB3	3:F:235:THR:CG2	2.21	0.70
3:C:308:PHE:O	3:C:309:LEU:HG	1.91	0.69
2:E:165:ASP:O	2:E:166:PRO:C	2.35	0.69
1:D:408:ILE:HD13	1:D:426:TYR:HE2	1.57	0.69
1:A:535:ASN:HA	1:A:538:PHE:CE2	2.27	0.69
2:E:165:ASP:O	2:E:167:ARG:N	2.25	0.69
2:E:242:LEU:N	2:E:243:PRO:HD2	2.07	0.69
2:E:381:TYR:CE2	2:E:385:LYS:HD2	2.27	0.69
2:B:381:TYR:HD2	2:B:381:TYR:C	2.01	0.69
1:A:452:VAL:HG12	1:A:452:VAL:O	1.92	0.68
2:E:59:LYS:HD3	2:E:123:HIS:CD2	2.27	0.68
1:A:487:LEU:C	1:A:489:MET:H	1.99	0.68
2:B:35:LYS:C	2:B:37:ARG:H	1.99	0.68
3:C:76:PRO:HD3	3:C:107:TYR:CE2	2.27	0.68
2:E:79:GLU:O	2:E:79:GLU:HG2	1.92	0.68
2:B:93:MET:HE2	2:B:128:TYR:CZ	2.28	0.68
2:B:244:LEU:HD23	2:B:244:LEU:O	1.92	0.68
1:A:467:LYS:HB2	1:A:507:VAL:CG1	2.23	0.68
3:F:76:PRO:HB2	3:F:110:ARG:HG3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:GLU:HA	1:D:28:ARG:HH21	1.58	0.68
3:F:115:ARG:NH1	3:F:151:ASP:HA	2.09	0.68
3:C:296:GLY:C	3:C:298:PRO:HD2	2.18	0.68
1:D:377:CYS:SG	1:D:379:GLU:HG2	2.34	0.68
1:A:428:PRO:HD3	1:A:465:ASN:HD21	1.56	0.68
2:E:388:MET:HE2	2:E:392:GLN:NE2	2.03	0.68
1:D:385:ILE:HD12	1:D:423:ILE:HD11	1.75	0.68
2:E:152:LYS:HG2	2:E:156:GLN:HE21	1.58	0.68
2:B:277:MET:HE2	2:B:280:LEU:HD12	1.75	0.67
2:B:222:ILE:HA	2:B:225:PHE:CE1	2.29	0.67
2:B:310:PHE:O	2:B:314:MET:HB2	1.94	0.67
3:C:244:VAL:O	3:C:246:GLU:N	2.27	0.67
3:F:180:ILE:HA	3:F:183:LEU:HD12	1.76	0.67
1:A:390:CYS:O	1:A:392:ASN:N	2.26	0.67
2:E:346:MET:CE	2:E:349:ILE:HD12	2.25	0.67
2:E:409:GLU:O	2:E:413:MET:HB2	1.95	0.67
1:D:350:MET:HE3	1:D:369:PHE:CE1	2.29	0.67
2:B:80:PRO:HG2	2:B:82:TYR:CD2	2.29	0.67
2:B:83:PRO:HG3	2:B:148:TYR:CE2	2.30	0.67
3:F:296:GLY:C	3:F:298:PRO:HD2	2.18	0.67
1:A:140:TRP:CZ2	2:B:239:LYS:HD2	2.30	0.67
2:B:59:LYS:HD3	2:B:123:HIS:CD2	2.30	0.67
2:E:217:ILE:HG22	2:E:221:ILE:HD11	1.77	0.66
1:D:330:ILE:O	1:D:334:VAL:HG23	1.96	0.66
1:A:390:CYS:SG	1:A:391:VAL:N	2.68	0.66
2:B:318:PHE:HB3	2:B:360:MET:HE3	1.77	0.66
3:C:244:VAL:O	3:C:244:VAL:HG23	1.95	0.66
2:B:123:HIS:O	2:B:127:VAL:HG23	1.96	0.66
2:B:353:ALA:HB2	2:B:390:MET:HE3	1.77	0.66
1:D:24:ASP:O	1:D:25:VAL:C	2.39	0.66
1:D:390:CYS:O	1:D:392:ASN:N	2.28	0.66
1:A:152:SER:HB2	1:A:191:GLU:HG3	1.78	0.66
2:B:141:GLN:HB3	2:B:142:PRO:HD2	1.77	0.66
2:B:218:LEU:HA	2:B:221:ILE:HD12	1.78	0.66
3:F:194:PRO:HG2	3:F:195:MET:H	1.59	0.66
1:A:22:ASN:ND2	1:A:27:LEU:HD12	2.11	0.66
2:B:169:ARG:HA	2:B:172:LEU:HD12	1.77	0.66
1:D:338:ASN:HD22	1:D:341:VAL:HG23	1.59	0.66
1:D:381:ARG:NH1	1:D:414:ASP:OD2	2.29	0.66
2:B:381:TYR:C	2:B:381:TYR:CD2	2.73	0.66
2:E:79:GLU:N	2:E:80:PRO:CD	2.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:141:GLN:HB3	2:E:142:PRO:HD2	1.76	0.65
2:B:242:LEU:N	2:B:243:PRO:HD2	2.11	0.65
1:D:22:ASN:ND2	1:D:24:ASP:HB3	2.11	0.65
2:E:340:TRP:HE1	2:E:387:PHE:HE1	1.42	0.65
1:A:350:MET:HE1	1:A:391:VAL:CG1	2.27	0.65
3:C:252:HIS:O	3:C:255:ASN:HB2	1.96	0.65
2:E:317:LEU:HD12	2:E:317:LEU:C	2.22	0.65
1:A:214:SER:HA	1:A:221:ARG:HD2	1.78	0.65
1:A:437:GLU:CD	1:A:438:PHE:H	2.04	0.65
3:C:62:PHE:CZ	3:C:66:MET:HE3	2.31	0.65
1:D:529:ALA:HA	1:D:540:VAL:HG11	1.79	0.65
1:D:529:ALA:HB3	1:D:563:ILE:HD11	1.78	0.65
2:E:254:HIS:CD2	2:E:293:MET:HB3	2.31	0.65
3:C:62:PHE:O	3:C:65:LEU:HB3	1.97	0.65
3:C:243:LEU:HD11	3:C:271:ASN:CG	2.22	0.65
2:B:107:GLU:HG3	2:B:108:PHE:CE1	2.31	0.65
2:B:134:PHE:C	2:B:134:PHE:CD2	2.75	0.65
1:D:20:LEU:HD23	1:D:31:SER:HB2	1.79	0.65
3:C:180:ILE:HA	3:C:183:LEU:HD12	1.78	0.64
2:E:93:MET:HE2	2:E:128:TYR:OH	1.97	0.64
2:E:119:ALA:O	2:E:120:ALA:HB3	1.97	0.64
2:E:322:ALA:N	2:E:360:MET:HE1	2.12	0.64
2:B:152:LYS:O	2:B:156:GLN:HG3	1.97	0.64
2:B:254:HIS:CD2	2:B:293:MET:HB3	2.32	0.64
2:E:322:ALA:HB2	2:E:360:MET:HE2	1.80	0.64
3:C:301:THR:HG22	3:C:302:ARG:N	2.07	0.64
2:E:237:LEU:HA	2:E:241:LEU:HB2	1.79	0.64
1:A:24:ASP:O	1:A:25:VAL:C	2.41	0.64
2:B:222:ILE:HA	2:B:225:PHE:CZ	2.33	0.64
2:E:340:TRP:HA	2:E:346:MET:HE3	1.80	0.64
3:C:117:ASN:CG	3:C:241:HIS:HE1	2.05	0.64
1:D:70:ALA:HB2	1:D:96:LEU:HD13	1.78	0.64
1:A:403:SER:O	1:A:404:LEU:HD13	1.97	0.64
2:B:287:HIS:CE1	2:B:289:PRO:HB2	2.33	0.64
3:C:243:LEU:HD22	4:X:7:DAM:HM3	1.78	0.64
1:A:35:LEU:HB3	1:A:72:GLN:HG2	1.80	0.64
1:A:280:LYS:HA	1:A:284:VAL:CG2	2.28	0.64
1:A:338:ASN:HD22	1:A:341:VAL:HG23	1.61	0.64
1:A:381:ARG:O	1:A:385:ILE:HG12	1.98	0.64
2:B:128:TYR:HB3	2:B:171:PHE:CD2	2.33	0.64
2:B:318:PHE:O	2:B:360:MET:HE1	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:104:LYS:N	3:F:111:ILE:HD11	2.12	0.64
1:A:350:MET:HE3	1:A:369:PHE:CZ	2.33	0.64
2:B:346:MET:HE1	2:B:349:ILE:HD12	1.80	0.64
2:E:169:ARG:HA	2:E:172:LEU:HD12	1.80	0.64
2:E:298:LEU:HB3	2:E:339:TYR:OH	1.98	0.64
1:A:436:VAL:HB	1:A:473:PHE:CD1	2.32	0.63
1:D:446:LEU:HD12	1:D:446:LEU:H	1.62	0.63
3:F:284:TYR:N	3:F:284:TYR:CD2	2.65	0.63
1:D:284:VAL:HB	1:D:285:PRO:HD3	1.79	0.63
2:E:325:VAL:HG22	2:E:337:LEU:HD13	1.79	0.63
3:F:244:VAL:O	3:F:246:GLU:N	2.31	0.63
2:B:273:GLU:N	2:B:274:PRO:HD2	2.14	0.63
2:B:297:GLU:O	2:B:301:ILE:HG13	1.98	0.63
1:D:392:ASN:ND2	1:D:433:GLN:HE22	1.96	0.63
1:D:405:LEU:CD2	1:D:430:LEU:HD11	2.27	0.63
1:A:52:LEU:HD11	1:A:89:LEU:HD12	1.80	0.63
2:B:218:LEU:O	2:B:222:ILE:HG13	1.99	0.63
2:B:247:VAL:HG12	2:B:249:SER:H	1.64	0.63
2:B:79:GLU:N	2:B:80:PRO:CD	2.62	0.63
2:B:88:MET:HE2	2:B:92:ASN:ND2	2.14	0.63
3:F:172:PRO:HG3	3:F:209:TRP:CE3	2.33	0.63
1:D:452:VAL:HG13	1:D:497:HIS:CD2	2.33	0.62
1:A:52:LEU:HB2	1:A:53:PRO:HD3	1.81	0.62
3:C:17:LEU:HD11	3:C:98:THR:HG22	1.81	0.62
3:F:221:GLY:H	3:F:224:ILE:HD12	1.63	0.62
1:A:350:MET:HE1	1:A:391:VAL:HG11	1.80	0.62
3:C:56:GLY:N	3:C:261:SER:OG	2.32	0.62
3:C:175:ASP:H	3:C:179:HIS:CD2	2.17	0.62
1:D:274:VAL:CG1	1:D:278:ILE:HB	2.29	0.62
1:D:62:GLU:CD	1:D:62:GLU:H	2.07	0.62
1:D:156:PRO:HG3	1:D:195:VAL:HB	1.81	0.62
3:F:172:PRO:HG3	3:F:209:TRP:CD2	2.35	0.62
1:D:427:MET:HE1	1:D:430:LEU:HD12	1.81	0.62
2:E:254:HIS:CD2	2:E:293:MET:HE2	2.35	0.62
3:F:50:CYS:HB2	3:F:51:PRO:HA	1.81	0.62
2:B:164:GLU:OE2	2:B:167:ARG:HB2	2.00	0.62
3:C:29:LYS:HB2	3:C:145:TYR:CE1	2.34	0.62
1:D:52:LEU:HB2	1:D:53:PRO:HD3	1.80	0.62
3:F:14:ILE:HD13	3:F:103:LEU:HD23	1.81	0.62
1:A:564:LEU:HD22	1:A:583:LEU:HD21	1.81	0.62
3:C:290:ASP:HB3	3:C:291:PRO:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:152:LYS:O	2:E:156:GLN:HG3	1.99	0.62
1:D:561:LYS:HB3	1:D:562:PRO:HD3	1.82	0.62
2:E:42:LEU:O	2:E:59:LYS:HE3	2.00	0.62
2:E:190:ILE:HD12	2:E:190:ILE:H	1.64	0.62
1:A:155:TYR:CZ	1:A:196:LEU:HD23	2.34	0.62
1:A:156:PRO:HG3	1:A:195:VAL:HB	1.80	0.62
1:D:561:LYS:O	1:D:565:GLU:HG2	1.99	0.62
1:A:179:PRO:HD2	1:A:180:MET:HE3	1.81	0.62
2:E:346:MET:HE1	2:E:349:ILE:HD12	1.82	0.62
1:A:282:ASP:C	1:A:285:PRO:HD2	2.24	0.61
1:A:502:LEU:HD13	1:A:540:VAL:HA	1.82	0.61
2:E:134:PHE:C	2:E:134:PHE:CD2	2.74	0.61
2:B:166:PRO:O	2:B:167:ARG:C	2.42	0.61
1:D:483:ILE:HB	1:D:484:PRO:HD3	1.82	0.61
1:D:222:LEU:HD23	1:D:223:LEU:H	1.64	0.61
3:F:174:ILE:HD13	3:F:180:ILE:CG1	2.27	0.61
1:A:300:ALA:HB2	1:A:341:VAL:HG22	1.81	0.61
1:A:529:ALA:HA	1:A:540:VAL:HG11	1.83	0.61
2:B:409:GLU:O	2:B:413:MET:HB2	1.99	0.61
1:D:427:MET:HA	1:D:427:MET:CE	2.26	0.61
2:E:164:GLU:O	2:E:165:ASP:C	2.44	0.61
3:F:67:GLU:HB2	3:F:292:ALA:HB2	1.80	0.61
3:F:244:VAL:O	3:F:244:VAL:HG23	1.99	0.61
1:D:392:ASN:HD21	1:D:433:GLN:HE22	1.48	0.61
2:E:83:PRO:HG3	2:E:148:TYR:CE2	2.35	0.61
1:D:101:GLU:HG2	2:E:246:LYS:NZ	2.16	0.61
1:D:506:ASN:HD21	1:D:543:SER:HA	1.66	0.61
1:A:287:PHE:CD2	1:A:291:MET:HE2	2.36	0.61
3:F:80:TYR:HB2	3:F:111:ILE:HG22	1.82	0.61
1:A:572:ASP:OD2	3:C:110:ARG:NH2	2.34	0.61
2:B:164:GLU:O	2:B:165:ASP:C	2.43	0.61
3:F:251:CYS:SG	3:F:256:VAL:HB	2.40	0.61
2:B:373:ASN:HD22	2:B:376:ILE:HG23	1.66	0.61
1:D:214:SER:HA	1:D:221:ARG:HD2	1.81	0.61
2:E:166:PRO:O	2:E:167:ARG:C	2.44	0.61
1:D:40:LEU:C	1:D:40:LEU:HD12	2.26	0.60
2:E:227:LEU:HB2	2:E:228:PRO:HD3	1.81	0.60
2:E:381:TYR:C	2:E:381:TYR:CD2	2.79	0.60
1:A:215:ASP:H	1:A:221:ARG:HG2	1.66	0.60
3:C:284:TYR:CD2	3:C:284:TYR:N	2.69	0.60
2:E:199:TYR:CE2	2:E:240:VAL:HG22	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ALA:HB3	1:A:563:ILE:HD11	1.84	0.60
3:F:117:ASN:CG	3:F:241:HIS:HE1	2.09	0.60
3:C:239:ARG:HD3	3:C:239:ARG:C	2.26	0.60
3:C:239:ARG:HH11	3:C:258:THR:HG23	1.67	0.60
1:D:102:THR:HG22	1:D:105:ARG:NH2	2.17	0.60
1:D:538:PHE:HB2	1:D:578:PHE:HD2	1.65	0.60
3:F:239:ARG:C	3:F:239:ARG:HD3	2.25	0.60
1:A:162:VAL:HA	1:A:165:GLU:OE1	2.01	0.60
3:F:174:ILE:CD1	3:F:180:ILE:HG12	2.29	0.60
1:A:517:THR:HA	1:A:521:MET:HE2	1.84	0.60
2:B:59:LYS:HD3	2:B:123:HIS:HD2	1.67	0.60
1:D:225:VAL:O	1:D:228:CYS:HB3	2.02	0.60
2:B:133:ARG:HA	2:B:136:GLU:CG	2.31	0.60
2:B:119:ALA:O	2:B:120:ALA:HB3	2.02	0.60
2:B:384:LEU:HD22	2:B:395:PHE:HZ	1.66	0.59
1:D:115:ILE:O	1:D:119:HIS:HD2	1.85	0.59
1:D:399:GLN:HE21	1:D:399:GLN:CA	2.15	0.59
3:F:308:PHE:O	3:F:309:LEU:HG	2.01	0.59
1:A:477:TRP:CH2	1:A:482:ILE:HD11	2.37	0.59
3:C:57:ASP:O	3:C:261:SER:HB2	2.01	0.59
3:C:42:GLU:HB3	3:C:46:GLN:OE1	2.02	0.59
1:D:427:MET:O	1:D:428:PRO:C	2.45	0.59
2:E:149:ILE:O	2:E:149:ILE:HG22	2.01	0.59
2:E:376:ILE:HG13	2:E:377:HIS:N	2.17	0.59
1:A:197:GLU:CD	1:A:197:GLU:H	2.11	0.59
2:B:149:ILE:HG22	2:B:149:ILE:O	2.01	0.59
2:E:222:ILE:HA	2:E:225:PHE:CE1	2.37	0.59
3:C:162:GLN:HB3	3:C:235:THR:HG21	1.85	0.59
2:E:255:PRO:HG2	2:E:256:GLN:NE2	2.17	0.59
3:F:243:LEU:HD22	4:Y:7:DAM:HM3	1.84	0.59
2:B:388:MET:HE2	2:B:392:GLN:HE22	1.67	0.59
3:C:50:CYS:HB2	3:C:51:PRO:HA	1.85	0.59
3:C:156:THR:HG22	3:C:166:LEU:CB	2.33	0.59
3:C:176:THR:H	3:C:179:HIS:CD2	2.21	0.59
1:D:100:GLU:O	1:D:105:ARG:NH1	2.36	0.59
1:D:564:LEU:HD13	1:D:583:LEU:HD23	1.84	0.59
3:F:301:THR:HG22	3:F:302:ARG:N	2.08	0.59
1:A:23:GLU:O	1:A:23:GLU:HG2	2.03	0.59
1:A:446:LEU:N	1:A:446:LEU:HD12	2.18	0.59
2:B:121:TRP:N	2:B:122:PRO:CD	2.65	0.59
2:B:317:LEU:HD12	2:B:317:LEU:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:ARG:HH11	1:D:398:ARG:CB	2.14	0.59
2:E:250:LEU:C	2:E:252:VAL:H	2.11	0.59
2:E:373:ASN:HD21	2:E:375:THR:HG22	1.67	0.59
1:A:358:LYS:O	1:A:362:ILE:HG13	2.03	0.58
1:A:437:GLU:CD	1:A:438:PHE:N	2.61	0.58
1:A:564:LEU:HD22	1:A:583:LEU:CD2	2.32	0.58
3:C:115:ARG:NH1	3:C:151:ASP:HA	2.18	0.58
2:E:87:HIS:O	2:E:91:VAL:HG23	2.03	0.58
2:E:170:ASP:O	2:E:173:LYS:HB3	2.01	0.58
2:E:62:ALA:O	2:E:66:MET:HG3	2.03	0.58
2:B:266:GLU:HG2	2:B:304:VAL:HG11	1.85	0.58
1:D:399:GLN:NE2	1:D:399:GLN:HA	2.18	0.58
2:B:95:ARG:H	2:B:95:ARG:HD2	1.67	0.58
1:D:400:LEU:HD12	1:D:404:LEU:HD23	1.85	0.58
2:B:80:PRO:O	2:B:82:TYR:HD2	1.87	0.58
2:B:93:MET:HE2	2:B:128:TYR:OH	2.04	0.58
2:B:237:LEU:HG	2:B:238:LEU:HD23	1.85	0.58
2:B:43:PHE:O	2:B:44:ASP:C	2.47	0.58
2:B:190:ILE:HD12	2:B:190:ILE:N	2.16	0.58
2:B:346:MET:CE	2:B:349:ILE:HD12	2.34	0.58
2:E:88:MET:HE2	2:E:92:ASN:HD21	1.66	0.58
2:B:166:PRO:O	2:B:170:ASP:N	2.35	0.58
2:B:254:HIS:N	2:B:255:PRO:HD2	2.19	0.58
1:D:564:LEU:HD22	1:D:583:LEU:HD21	1.85	0.58
2:E:128:TYR:HB3	2:E:171:PHE:HD2	1.67	0.58
1:A:115:ILE:O	1:A:119:HIS:HD2	1.87	0.58
1:D:28:ARG:HD3	1:D:60:TYR:CE2	2.39	0.58
3:F:124:THR:HB	3:F:129:PHE:HB3	1.84	0.58
3:F:165:CYS:HA	3:F:238:SER:O	2.04	0.58
3:F:240:ALA:CB	3:F:259:ILE:O	2.52	0.58
3:F:297:GLU:N	3:F:298:PRO:HD2	2.18	0.58
1:A:77:THR:HG21	1:A:118:GLU:CG	2.32	0.57
1:A:368:LEU:O	1:A:371:ALA:HB3	2.04	0.57
2:E:59:LYS:HD3	2:E:123:HIS:HD2	1.70	0.57
1:A:412:ALA:HB1	1:A:450:TRP:HZ2	1.69	0.57
2:B:128:TYR:HB3	2:B:171:PHE:HD2	1.68	0.57
2:E:218:LEU:HA	2:E:221:ILE:HD12	1.86	0.57
1:A:225:VAL:O	1:A:228:CYS:HB3	2.05	0.57
1:D:376:GLU:N	1:D:376:GLU:OE2	2.36	0.57
2:E:223:ASN:ND2	2:E:263:GLN:HE21	2.02	0.57
1:A:32:ILE:O	1:A:35:LEU:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:C	1:A:42:LEU:H	2.13	0.57
2:B:376:ILE:HG13	2:B:377:HIS:N	2.18	0.57
2:E:82:TYR:O	2:E:82:TYR:CG	2.57	0.57
2:E:118:GLU:N	2:E:164:GLU:HG2	2.18	0.57
1:A:411:LEU:C	1:A:413:GLU:H	2.13	0.57
3:C:12:GLN:NE2	3:C:16:GLN:HB2	2.19	0.57
1:D:20:LEU:HD23	1:D:31:SER:CB	2.34	0.57
3:F:183:LEU:HD21	3:F:194:PRO:CG	2.34	0.57
1:A:280:LYS:HA	1:A:284:VAL:HG21	1.86	0.57
2:B:160:LEU:O	2:B:162:ASP:N	2.35	0.57
1:A:184:ALA:O	1:A:185:ALA:C	2.47	0.57
1:A:495:TYR:HE2	1:A:535:ASN:ND2	2.02	0.57
1:A:229:VAL:O	1:A:233:GLN:HG3	2.05	0.57
2:B:93:MET:HA	2:B:93:MET:HE3	1.86	0.57
1:A:284:VAL:HB	1:A:285:PRO:HD3	1.85	0.57
2:B:413:MET:O	2:B:414:LYS:HG3	2.05	0.57
3:C:121:ARG:HG3	3:C:121:ARG:HH11	1.70	0.57
1:D:564:LEU:HD22	1:D:583:LEU:CD2	2.35	0.57
2:E:254:HIS:N	2:E:255:PRO:HD2	2.19	0.57
3:F:94:VAL:HG23	3:F:132:GLU:OE2	2.04	0.57
1:A:99:VAL:O	1:A:105:ARG:HD3	2.04	0.57
1:A:487:LEU:C	1:A:489:MET:N	2.61	0.57
3:C:169:GLY:HA3	3:C:220:PHE:HE2	1.70	0.57
3:C:297:GLU:N	3:C:298:PRO:HD2	2.20	0.57
3:F:284:TYR:N	3:F:284:TYR:HD2	2.01	0.57
1:A:356:LEU:HD12	1:A:365:LEU:HD11	1.87	0.56
2:E:80:PRO:HG2	2:E:82:TYR:CD2	2.39	0.56
2:E:160:LEU:O	2:E:162:ASP:N	2.34	0.56
3:F:63:HIS:O	3:F:66:MET:HB2	2.05	0.56
2:B:265:LEU:CD1	2:B:301:ILE:HG23	2.34	0.56
1:D:349:ILE:HG23	1:D:350:MET:N	2.19	0.56
1:D:437:GLU:CD	1:D:438:PHE:H	2.13	0.56
1:A:40:LEU:C	1:A:40:LEU:HD12	2.29	0.56
3:C:24:SER:OG	3:C:27:GLN:HG3	2.05	0.56
3:C:221:GLY:H	3:C:224:ILE:HD12	1.70	0.56
1:D:508:LEU:HD22	1:D:508:LEU:H	1.71	0.56
2:E:72:HIS:O	2:E:74:ARG:N	2.38	0.56
2:E:190:ILE:O	2:E:194:ILE:HG13	2.06	0.56
3:F:160:ASP:HB3	3:F:282:LEU:HD11	1.86	0.56
2:B:376:ILE:HA	2:B:379:LEU:HB2	1.86	0.56
2:E:80:PRO:O	2:E:82:TYR:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:TYR:CD1	1:A:456:TYR:C	2.84	0.56
3:C:68:LEU:HD23	3:C:68:LEU:C	2.30	0.56
1:D:23:GLU:HA	1:D:28:ARG:NH2	2.20	0.56
2:E:164:GLU:OE2	2:E:167:ARG:HB2	2.05	0.56
1:A:492:ASP:OD2	1:A:493:PRO:HD2	2.03	0.56
3:C:44:ASN:N	3:C:44:ASN:ND2	2.51	0.56
3:C:243:LEU:CD2	4:X:7:DAM:HM3	2.36	0.56
1:D:29:LEU:CD1	1:D:65:VAL:HA	2.36	0.56
2:B:152:LYS:HG2	2:B:156:GLN:NE2	2.17	0.56
2:B:190:ILE:O	2:B:194:ILE:HG13	2.05	0.56
1:A:178:THR:HB	1:A:180:MET:CG	2.34	0.56
1:A:181:VAL:O	1:A:184:ALA:HB3	2.06	0.56
2:B:77:ILE:HG22	2:B:77:ILE:O	2.06	0.56
1:D:120:SER:O	1:D:121:PRO:C	2.48	0.56
2:E:317:LEU:HD12	2:E:317:LEU:O	2.04	0.56
2:B:227:LEU:HB2	2:B:228:PRO:HD3	1.87	0.56
1:D:452:VAL:O	1:D:452:VAL:CG1	2.53	0.56
1:D:477:TRP:CH2	1:D:482:ILE:HD11	2.41	0.56
3:F:209:TRP:H	3:F:224:ILE:HD11	1.67	0.56
1:A:483:ILE:HB	1:A:484:PRO:HD3	1.88	0.56
2:B:222:ILE:CD1	2:B:260:CYS:HB3	2.36	0.56
3:C:103:LEU:HB3	3:C:111:ILE:HD13	1.88	0.56
1:D:489:MET:HB3	1:D:501:THR:OG1	2.06	0.56
2:E:208:HIS:HD2	2:E:210:GLY:N	1.98	0.56
2:E:277:MET:HE2	2:E:277:MET:HA	1.86	0.56
2:E:298:LEU:HD21	2:E:317:LEU:HD13	1.88	0.56
1:D:467:LYS:O	1:D:471:GLU:HG3	2.06	0.55
1:A:538:PHE:HB2	1:A:578:PHE:HD2	1.71	0.55
1:D:403:SER:O	1:D:404:LEU:HB2	2.04	0.55
1:D:405:LEU:N	1:D:406:PRO:CD	2.70	0.55
2:E:43:PHE:O	2:E:44:ASP:C	2.48	0.55
2:E:288:SER:O	2:E:291:GLU:HB3	2.05	0.55
1:A:322:ILE:HG21	1:A:356:LEU:HD21	1.87	0.55
2:B:247:VAL:HG12	2:B:248:LYS:N	2.20	0.55
3:C:209:TRP:H	3:C:224:ILE:HD11	1.70	0.55
1:D:554:SER:O	1:D:558:SER:HB3	2.07	0.55
3:F:203:PRO:HD2	3:F:242:GLN:OE1	2.06	0.55
1:D:446:LEU:HD12	1:D:446:LEU:N	2.20	0.55
2:E:133:ARG:HA	2:E:136:GLU:CG	2.35	0.55
2:E:350:SER:C	2:E:352:ASN:H	2.13	0.55
2:E:353:ALA:HB2	2:E:390:MET:HE3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ILE:HD13	1:A:399:GLN:HG3	1.88	0.55
3:C:67:GLU:HB2	3:C:292:ALA:HB2	1.89	0.55
3:C:79:ASN:OD1	3:C:110:ARG:HD3	2.07	0.55
1:A:206:ILE:HB	1:A:207:PRO:HD3	1.88	0.55
3:C:190:PRO:CD	3:C:195:MET:HE2	2.29	0.55
3:F:62:PHE:O	3:F:65:LEU:HB3	2.06	0.55
1:A:327:LEU:HD12	1:A:327:LEU:O	2.06	0.55
2:B:162:ASP:O	2:B:163:SER:HB2	2.06	0.55
3:C:51:PRO:HB3	3:C:279:ASP:C	2.31	0.55
3:C:124:THR:HB	3:C:129:PHE:HB3	1.88	0.55
2:E:302:LEU:HA	2:E:305:ILE:HB	1.89	0.55
2:E:357:LEU:HD22	2:E:387:PHE:HD2	1.72	0.55
1:A:310:CYS:HA	1:A:313:LEU:HD12	1.88	0.55
2:B:254:HIS:CD2	2:B:293:MET:HE2	2.42	0.55
3:C:172:PRO:HG3	3:C:209:TRP:CD2	2.42	0.55
1:D:99:VAL:HG21	1:D:104:VAL:CG1	2.35	0.55
3:C:71:ILE:HG22	3:C:275:ILE:HD11	1.87	0.55
1:A:105:ARG:HH12	1:A:142:THR:HG22	1.72	0.55
2:B:118:GLU:N	2:B:164:GLU:HG2	2.22	0.55
2:B:180:TYR:CE1	2:B:187:ARG:HA	2.42	0.55
3:C:163:ILE:HD13	3:C:236:LEU:HD23	1.88	0.55
1:D:155:TYR:CZ	1:D:196:LEU:HD23	2.42	0.55
1:A:557:GLN:HG2	1:A:588:LEU:HD22	1.90	0.54
2:B:205:THR:C	2:B:207:HIS:H	2.15	0.54
2:E:44:ASP:O	2:E:45:PHE:C	2.49	0.54
2:E:246:LYS:HG3	3:F:307:TYR:HE2	1.73	0.54
1:A:20:LEU:HD23	1:A:31:SER:HB2	1.90	0.54
2:E:265:LEU:CD1	2:E:301:ILE:HG23	2.37	0.54
2:E:322:ALA:HB2	2:E:360:MET:CE	2.36	0.54
1:A:405:LEU:CD2	1:A:430:LEU:HD11	2.37	0.54
1:A:522:LEU:O	1:A:526:LEU:HG	2.07	0.54
2:B:317:LEU:HD12	2:B:317:LEU:C	2.32	0.54
1:D:40:LEU:C	1:D:42:LEU:H	2.16	0.54
2:E:373:ASN:HD22	2:E:376:ILE:HG23	1.72	0.54
2:E:381:TYR:C	2:E:381:TYR:HD2	2.14	0.54
3:F:103:LEU:C	3:F:111:ILE:HD11	2.32	0.54
1:D:222:LEU:HD23	1:D:223:LEU:N	2.22	0.54
1:D:373:LEU:HD13	1:D:384:ILE:CG2	2.37	0.54
2:E:302:LEU:O	2:E:305:ILE:HG22	2.08	0.54
1:A:194:LYS:HD2	1:A:230:ASN:HD22	1.72	0.54
1:A:405:LEU:N	1:A:406:PRO:CD	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:THR:CG2	2:E:203:TYR:HB3	2.37	0.54
2:E:79:GLU:N	2:E:80:PRO:HD2	2.21	0.54
2:E:107:GLU:HG3	2:E:108:PHE:CE1	2.42	0.54
1:A:206:ILE:HD11	1:A:235:LEU:HD11	1.90	0.54
1:A:489:MET:C	1:A:491:GLY:H	2.14	0.54
3:C:284:TYR:N	3:C:284:TYR:HD2	2.06	0.54
1:D:11:TYR:O	1:D:14:ALA:HB3	2.07	0.54
1:D:538:PHE:O	1:D:542:LYS:HG3	2.08	0.54
2:E:72:HIS:O	2:E:74:ARG:HG2	2.08	0.54
2:E:138:PRO:O	2:E:140:PHE:HD1	1.91	0.54
1:A:385:ILE:HD12	1:A:423:ILE:CD1	2.37	0.54
2:B:35:LYS:C	2:B:37:ARG:N	2.65	0.54
2:B:133:ARG:CA	2:B:136:GLU:HG2	2.35	0.54
2:B:375:THR:O	2:B:379:LEU:HD12	2.08	0.54
2:B:388:MET:C	2:B:390:MET:H	2.16	0.54
1:A:538:PHE:HB3	1:A:575:VAL:HA	1.90	0.54
1:A:564:LEU:HD23	1:A:564:LEU:O	2.08	0.54
2:B:154:VAL:O	2:B:157:LEU:HB3	2.07	0.54
2:B:251:SER:HA	2:B:293:MET:CE	2.29	0.54
2:B:359:ILE:HG22	2:B:360:MET:HE2	1.90	0.54
3:C:176:THR:H	3:C:179:HIS:HD2	1.55	0.54
3:F:51:PRO:HB3	3:F:279:ASP:C	2.33	0.54
2:B:88:MET:HE1	2:B:127:VAL:HG22	1.89	0.54
1:D:94:GLU:HB2	1:D:131:LEU:CD1	2.38	0.54
2:E:35:LYS:C	2:E:37:ARG:N	2.62	0.54
2:B:62:ALA:O	2:B:66:MET:HG3	2.08	0.53
1:D:274:VAL:HG12	1:D:278:ILE:HB	1.90	0.53
1:D:437:GLU:CD	1:D:438:PHE:N	2.66	0.53
2:E:31:LEU:C	2:E:33:ILE:H	2.15	0.53
2:E:167:ARG:CB	2:E:167:ARG:HH11	2.20	0.53
2:E:237:LEU:HD23	2:E:271:LEU:HD13	1.90	0.53
2:B:381:TYR:CE2	2:B:385:LYS:HD2	2.44	0.53
1:D:452:VAL:HG13	1:D:497:HIS:HD2	1.73	0.53
2:E:305:ILE:HD13	2:E:306:GLU:N	2.23	0.53
1:A:278:ILE:H	1:A:278:ILE:CD1	2.12	0.53
3:C:29:LYS:O	3:C:33:GLU:HG2	2.09	0.53
3:C:208:GLY:HA2	3:C:224:ILE:HD11	1.89	0.53
2:E:376:ILE:HA	2:E:379:LEU:HB2	1.90	0.53
3:F:305:PRO:HB3	3:F:307:TYR:CE2	2.43	0.53
1:A:145:THR:HG22	1:A:146:SER:N	2.22	0.53
2:E:255:PRO:HG2	2:E:256:GLN:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:TYR:O	1:A:14:ALA:HB3	2.07	0.53
1:A:407:ALA:O	1:A:410:GLU:N	2.41	0.53
2:B:87:HIS:O	2:B:91:VAL:HG23	2.09	0.53
2:B:190:ILE:H	2:B:190:ILE:CD1	2.20	0.53
2:B:287:HIS:HE1	2:B:289:PRO:HB2	1.74	0.53
3:C:171:SER:OG	3:C:174:ILE:HB	2.08	0.53
3:C:263:PRO:HD3	3:C:273:ALA:HB2	1.90	0.53
1:D:116:SER:O	1:D:119:HIS:HB2	2.09	0.53
1:D:404:LEU:H	1:D:406:PRO:HD2	1.74	0.53
1:A:222:LEU:HD23	1:A:223:LEU:H	1.70	0.53
1:A:561:LYS:O	1:A:565:GLU:HG2	2.08	0.53
1:D:384:ILE:CG2	1:D:385:ILE:N	2.71	0.53
2:E:121:TRP:N	2:E:122:PRO:CD	2.66	0.53
2:E:297:GLU:O	2:E:301:ILE:HG13	2.09	0.53
3:F:297:GLU:N	3:F:298:PRO:CD	2.72	0.53
1:A:111:SER:O	1:A:112:LEU:C	2.52	0.53
1:A:482:ILE:O	1:A:486:VAL:HG23	2.09	0.53
2:B:44:ASP:O	2:B:45:PHE:C	2.51	0.53
3:F:156:THR:HG22	3:F:166:LEU:CB	2.38	0.53
2:B:236:PHE:O	2:B:240:VAL:HB	2.09	0.53
2:B:291:GLU:HG2	2:B:332:VAL:HG13	1.91	0.53
3:C:85:ASP:H	3:C:116:GLY:HA3	1.72	0.53
1:D:192:PHE:O	1:D:195:VAL:HG22	2.09	0.53
1:D:524:THR:O	1:D:528:MET:HG3	2.08	0.53
2:E:218:LEU:HD13	2:E:236:PHE:HZ	1.74	0.53
1:A:40:LEU:O	1:A:42:LEU:N	2.42	0.53
2:B:322:ALA:HB2	2:B:360:MET:CE	2.39	0.53
1:D:155:TYR:CE2	1:D:196:LEU:HD23	2.43	0.53
1:D:267:PHE:HE2	1:D:287:PHE:HB2	1.71	0.53
2:E:371:HIS:ND1	2:E:376:ILE:HD13	2.24	0.53
3:F:76:PRO:HD3	3:F:107:TYR:CE2	2.43	0.53
3:F:240:ALA:HB1	3:F:259:ILE:O	2.09	0.53
1:A:400:LEU:HD12	1:A:404:LEU:HD23	1.91	0.53
2:B:138:PRO:O	2:B:140:PHE:HD1	1.92	0.53
2:B:330:PHE:CE1	2:B:331:GLN:HG2	2.44	0.53
3:C:165:CYS:SG	3:C:238:SER:HB3	2.49	0.53
1:D:287:PHE:CD2	1:D:291:MET:HE2	2.44	0.53
2:E:247:VAL:HG12	2:E:249:SER:H	1.74	0.53
3:F:169:GLY:HA3	3:F:220:PHE:HE2	1.74	0.53
1:A:98:THR:O	1:A:98:THR:HG22	2.09	0.52
1:D:102:THR:OG1	1:D:103:VAL:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:10:LEU:HD11	3:F:105:VAL:HG12	1.90	0.52
1:D:307:LYS:HB2	1:D:348:VAL:HB	1.91	0.52
1:D:522:LEU:HD22	1:D:551:LEU:CD2	2.39	0.52
1:A:35:LEU:HD21	1:A:55:LEU:HD11	1.90	0.52
1:A:369:PHE:O	1:A:373:LEU:HD23	2.10	0.52
2:B:78:THR:HG22	2:B:82:TYR:OH	2.10	0.52
1:D:184:ALA:O	1:D:185:ALA:C	2.52	0.52
1:D:420:ARG:O	1:D:424:ILE:HG13	2.09	0.52
3:C:12:GLN:HE22	3:C:16:GLN:HB2	1.73	0.52
3:C:263:PRO:HD3	3:C:273:ALA:CB	2.38	0.52
1:D:178:THR:HG22	1:D:180:MET:SD	2.50	0.52
1:D:381:ARG:O	1:D:385:ILE:HG12	2.09	0.52
1:D:399:GLN:CA	1:D:399:GLN:NE2	2.72	0.52
1:D:466:LEU:O	1:D:470:VAL:HG23	2.10	0.52
1:D:487:LEU:C	1:D:489:MET:N	2.60	0.52
2:E:330:PHE:CE2	3:F:122:GLN:HG3	2.43	0.52
2:E:375:THR:O	2:E:379:LEU:HD12	2.08	0.52
1:D:25:VAL:O	1:D:26:GLN:C	2.53	0.52
1:D:194:LYS:HD2	1:D:230:ASN:HD22	1.75	0.52
3:F:143:TRP:CE2	3:F:147:THR:HG21	2.45	0.52
1:A:152:SER:HB3	1:A:191:GLU:OE1	2.09	0.52
3:C:156:THR:HG22	3:C:166:LEU:HB3	1.92	0.52
3:C:297:GLU:N	3:C:298:PRO:CD	2.73	0.52
1:D:99:VAL:O	1:D:105:ARG:HD3	2.10	0.52
1:D:572:ASP:OD2	3:F:110:ARG:NH2	2.40	0.52
2:E:150:ASP:CG	2:E:151:GLN:N	2.68	0.52
3:F:243:LEU:CD2	4:Y:7:DAM:HM3	2.40	0.52
3:F:244:VAL:C	3:F:246:GLU:H	2.17	0.52
1:A:420:ARG:O	1:A:424:ILE:HG13	2.09	0.52
1:A:489:MET:C	1:A:491:GLY:N	2.64	0.52
2:B:255:PRO:HG2	2:B:256:GLN:NE2	2.24	0.52
1:D:345:LEU:HD23	1:D:345:LEU:C	2.35	0.52
2:E:150:ASP:CG	2:E:151:GLN:H	2.18	0.52
2:E:384:LEU:HD22	2:E:395:PHE:HZ	1.75	0.52
1:A:128:PHE:O	1:A:131:LEU:HB3	2.10	0.52
3:C:276:MET:HB2	3:C:286:PHE:CE1	2.44	0.52
1:D:322:ILE:HG21	1:D:356:LEU:HD21	1.91	0.52
1:A:452:VAL:O	1:A:452:VAL:CG1	2.57	0.52
1:A:470:VAL:HG11	1:A:511:VAL:HG23	1.92	0.52
2:B:167:ARG:CB	2:B:167:ARG:HH11	2.22	0.52
2:B:169:ARG:O	2:B:172:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:143:TRP:CE2	3:C:147:THR:HG21	2.45	0.52
2:B:208:HIS:HD2	2:B:210:GLY:N	1.96	0.52
2:B:371:HIS:ND1	2:B:376:ILE:HD13	2.25	0.52
3:C:240:ALA:CB	3:C:259:ILE:O	2.57	0.52
1:A:446:LEU:HD12	1:A:446:LEU:H	1.74	0.51
1:A:554:SER:O	1:A:558:SER:HB3	2.10	0.51
2:B:42:LEU:O	2:B:59:LYS:HE3	2.10	0.51
3:F:185:ARG:O	3:F:187:GLN:N	2.43	0.51
1:A:427:MET:HA	1:A:427:MET:CE	2.36	0.51
3:F:261:SER:HA	3:F:273:ALA:HB1	1.91	0.51
1:A:438:PHE:O	1:A:439:PHE:C	2.52	0.51
2:B:244:LEU:CD2	2:B:253:TYR:CE1	2.93	0.51
3:C:165:CYS:HA	3:C:238:SER:O	2.11	0.51
1:D:77:THR:HG21	1:D:118:GLU:CG	2.36	0.51
2:E:189:TYR:O	2:E:190:ILE:C	2.53	0.51
2:E:350:SER:C	2:E:352:ASN:N	2.68	0.51
1:A:345:LEU:HD21	1:A:349:ILE:HD12	1.90	0.51
1:D:405:LEU:HD13	1:D:405:LEU:O	2.09	0.51
2:E:164:GLU:OE2	2:E:164:GLU:C	2.54	0.51
2:E:247:VAL:HG12	2:E:248:LYS:N	2.25	0.51
2:E:289:PRO:O	2:E:293:MET:HG3	2.11	0.51
1:A:40:LEU:C	1:A:42:LEU:N	2.63	0.51
1:A:287:PHE:CE2	1:A:291:MET:HE2	2.45	0.51
2:B:320:GLN:O	2:B:323:LYS:N	2.43	0.51
1:D:11:TYR:O	1:D:14:ALA:N	2.43	0.51
3:C:305:PRO:HB3	3:C:307:TYR:CE2	2.45	0.51
1:D:109:VAL:HG13	1:D:150:LEU:CD2	2.38	0.51
2:B:108:PHE:HB3	3:C:268:ARG:NH2	2.26	0.51
2:B:373:ASN:HD21	2:B:375:THR:HG22	1.76	0.51
1:D:397:ILE:HD11	1:D:433:GLN:HB3	1.92	0.51
2:E:124:LEU:O	2:E:125:GLN:C	2.53	0.51
2:E:340:TRP:NE1	2:E:387:PHE:HE1	2.09	0.51
2:E:406:LYS:HD3	2:E:406:LYS:O	2.11	0.51
1:A:529:ALA:CB	1:A:563:ILE:HD11	2.41	0.51
3:C:31:LEU:HD11	3:C:102:ALA:HA	1.93	0.51
3:F:42:GLU:HB3	3:F:46:GLN:OE1	2.09	0.51
1:A:407:ALA:O	1:A:408:ILE:C	2.54	0.51
1:A:502:LEU:HD21	1:A:540:VAL:HG23	1.92	0.51
2:B:366:ARG:O	2:B:367:ASN:C	2.54	0.51
1:D:411:LEU:C	1:D:413:GLU:H	2.18	0.51
2:E:91:VAL:HG12	2:E:91:VAL:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:373:ASN:ND2	2:E:375:THR:HG22	2.26	0.51
3:F:24:SER:O	3:F:28:VAL:HG23	2.11	0.51
3:F:263:PRO:HD3	3:F:273:ALA:HB2	1.92	0.51
1:A:105:ARG:NH1	1:A:142:THR:HG22	2.24	0.51
1:A:192:PHE:O	1:A:195:VAL:HG22	2.11	0.51
1:A:280:LYS:HA	1:A:284:VAL:HG23	1.93	0.51
1:A:506:ASN:HD21	1:A:543:SER:CB	2.24	0.51
1:A:556:LEU:O	1:A:558:SER:N	2.43	0.51
2:B:373:ASN:ND2	2:B:375:THR:HG22	2.26	0.51
2:B:31:LEU:C	2:B:33:ILE:H	2.19	0.50
3:C:63:HIS:O	3:C:66:MET:HB2	2.11	0.50
3:C:103:LEU:C	3:C:111:ILE:HD11	2.36	0.50
1:D:412:ALA:HB1	1:D:450:TRP:HZ2	1.75	0.50
1:A:165:GLU:O	1:A:168:GLN:HB3	2.11	0.50
1:A:456:TYR:HA	1:A:459:ARG:NH1	2.26	0.50
2:B:175:THR:HG22	2:B:179:ILE:CD1	2.39	0.50
2:B:205:THR:O	2:B:207:HIS:N	2.41	0.50
2:B:350:SER:O	2:B:352:ASN:N	2.44	0.50
2:B:375:THR:HG23	2:B:379:LEU:HD12	1.94	0.50
3:C:32:CYS:O	3:C:35:ALA:HB3	2.11	0.50
1:D:482:ILE:O	1:D:483:ILE:C	2.53	0.50
2:B:302:LEU:HA	2:B:305:ILE:HB	1.93	0.50
1:D:373:LEU:HD22	1:D:384:ILE:HG21	1.94	0.50
1:A:343:SER:HA	1:A:380:VAL:HG22	1.94	0.50
1:A:456:TYR:O	1:A:457:ALA:C	2.54	0.50
1:A:487:LEU:HD22	1:A:524:THR:OG1	2.11	0.50
3:C:159:VAL:HG11	3:C:278:LEU:HD12	1.94	0.50
1:D:146:SER:O	1:D:147:ALA:C	2.55	0.50
1:D:456:TYR:O	1:D:457:ALA:C	2.54	0.50
1:D:463:THR:HG22	1:D:507:VAL:HG21	1.93	0.50
2:B:107:GLU:HG3	2:B:108:PHE:CD1	2.47	0.50
1:A:102:THR:O	1:A:105:ARG:HG2	2.11	0.50
2:B:120:ALA:C	2:B:122:PRO:HD2	2.36	0.50
2:B:315:GLU:O	2:B:319:ARG:HB2	2.11	0.50
3:C:172:PRO:HG3	3:C:209:TRP:CE3	2.47	0.50
2:E:138:PRO:C	2:E:140:PHE:H	2.20	0.50
3:F:128:GLY:O	3:F:129:PHE:C	2.54	0.50
1:A:303:SER:HB3	1:A:345:LEU:HB2	1.94	0.50
1:A:362:ILE:HG23	1:A:366:LEU:HD23	1.94	0.50
2:B:110:PRO:HA	2:B:113:ASP:OD2	2.12	0.50
2:B:255:PRO:HG2	2:B:256:GLN:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:ALA:CB	2:B:390:MET:HE3	2.41	0.50
2:E:350:SER:O	2:E:352:ASN:N	2.45	0.50
3:C:276:MET:HE3	3:C:278:LEU:CD2	2.26	0.50
2:E:180:TYR:CE1	2:E:187:ARG:HA	2.47	0.50
2:E:287:HIS:CE1	2:E:289:PRO:HB2	2.47	0.50
1:A:25:VAL:CG2	1:A:62:GLU:HG2	2.42	0.49
1:D:71:GLU:HG3	1:D:107:LYS:CE	2.42	0.49
1:D:522:LEU:O	1:D:526:LEU:HG	2.11	0.49
2:E:39:CYS:O	2:E:42:LEU:N	2.45	0.49
2:E:304:VAL:HG12	2:E:304:VAL:O	2.12	0.49
1:A:570:ASP:OD2	1:A:571:GLN:N	2.44	0.49
2:B:350:SER:C	2:B:352:ASN:N	2.70	0.49
3:C:44:ASN:ND2	3:C:185:ARG:HH11	2.11	0.49
3:C:117:ASN:CG	3:C:241:HIS:CE1	2.90	0.49
3:F:156:THR:HG22	3:F:166:LEU:HB3	1.93	0.49
3:F:166:LEU:HD23	3:F:239:ARG:HB3	1.94	0.49
1:A:141:PHE:C	1:A:141:PHE:CD1	2.90	0.49
1:A:162:VAL:O	1:A:163:LYS:C	2.54	0.49
3:C:128:GLY:O	3:C:129:PHE:C	2.54	0.49
3:C:194:PRO:HG2	3:C:195:MET:H	1.77	0.49
3:C:240:ALA:HB1	3:C:259:ILE:O	2.12	0.49
3:C:244:VAL:C	3:C:246:GLU:H	2.21	0.49
1:D:98:THR:HG22	1:D:98:THR:O	2.10	0.49
1:A:91:PRO:HB2	1:A:92:PRO:CD	2.42	0.49
2:B:134:PHE:C	2:B:134:PHE:HD2	2.18	0.49
1:D:521:MET:C	1:D:523:PRO:HD2	2.37	0.49
2:E:164:GLU:C	2:E:165:ASP:O	2.55	0.49
2:B:142:PRO:HG2	2:B:143:ASN:H	1.77	0.49
2:B:145:ALA:O	2:B:148:TYR:N	2.42	0.49
1:D:91:PRO:HB2	1:D:92:PRO:CD	2.43	0.49
1:D:436:VAL:HB	1:D:473:PHE:CD1	2.48	0.49
1:A:24:ASP:O	1:A:26:GLN:N	2.46	0.49
3:F:29:LYS:HB2	3:F:145:TYR:CE1	2.47	0.49
1:A:411:LEU:O	1:A:413:GLU:N	2.45	0.49
3:C:44:ASN:ND2	3:C:185:ARG:NH1	2.61	0.49
2:E:242:LEU:N	2:E:243:PRO:CD	2.75	0.49
2:B:138:PRO:C	2:B:140:PHE:H	2.20	0.49
2:B:350:SER:HA	2:B:390:MET:SD	2.53	0.49
1:D:330:ILE:HD13	1:D:352:LEU:HD11	1.94	0.49
1:D:509:SER:HA	1:D:521:MET:HE1	1.95	0.49
2:E:166:PRO:O	2:E:170:ASP:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:252:HIS:O	3:F:253:ASP:C	2.56	0.49
1:A:267:PHE:CE2	1:A:287:PHE:HB2	2.47	0.49
1:A:448:MET:HE1	1:A:466:LEU:HD21	1.95	0.49
3:C:277:GLU:HB2	3:C:285:SER:OG	2.13	0.49
1:D:489:MET:HB3	1:D:501:THR:HG1	1.77	0.49
2:E:103:PRO:HG3	2:E:108:PHE:CD2	2.48	0.49
2:E:273:GLU:N	2:E:274:PRO:HD2	2.28	0.49
2:E:346:MET:HE2	2:E:349:ILE:HD12	1.93	0.49
1:A:438:PHE:CD1	1:A:438:PHE:C	2.89	0.49
3:C:18:ASN:C	3:C:20:CYS:H	2.20	0.49
3:C:59:HIS:HE1	3:C:118:HIS:CD2	2.31	0.49
2:E:119:ALA:O	2:E:120:ALA:CB	2.61	0.49
2:E:250:LEU:C	2:E:252:VAL:N	2.70	0.49
1:A:11:TYR:O	1:A:14:ALA:N	2.45	0.48
1:A:25:VAL:O	1:A:26:GLN:C	2.55	0.48
2:B:59:LYS:O	2:B:63:LEU:HG	2.12	0.48
2:B:94:PHE:CE1	2:B:156:GLN:HB2	2.48	0.48
3:C:253:ASP:O	3:C:254:ARG:C	2.55	0.48
1:D:162:VAL:O	1:D:163:LYS:C	2.55	0.48
2:E:318:PHE:HB3	2:E:360:MET:HE3	1.94	0.48
3:F:137:TYR:CD2	3:F:142:VAL:HG21	2.48	0.48
3:F:248:TYR:CE2	3:F:286:PHE:CD2	3.01	0.48
1:A:330:ILE:HD13	1:A:352:LEU:HD11	1.95	0.48
1:A:420:ARG:HH21	1:A:453:ASP:CG	2.22	0.48
1:A:588:LEU:O	1:A:589:ALA:HB2	2.13	0.48
2:B:242:LEU:HD11	2:B:275:VAL:HG22	1.95	0.48
2:E:223:ASN:ND2	2:E:263:GLN:NE2	2.60	0.48
2:E:329:HIS:HA	3:F:125:GLN:OE1	2.13	0.48
2:B:70:ILE:O	2:B:70:ILE:HG22	2.14	0.48
2:B:170:ASP:O	2:B:173:LYS:HB3	2.13	0.48
3:C:73:GLY:HA3	3:C:78:THR:HG21	1.95	0.48
3:C:158:LEU:HD12	3:C:163:ILE:O	2.13	0.48
3:F:118:HIS:HA	3:F:123:ILE:HG21	1.96	0.48
1:A:155:TYR:CE1	1:A:163:LYS:HB3	2.48	0.48
1:A:492:ASP:O	1:A:498:ARG:HD3	2.13	0.48
3:C:94:VAL:HG23	3:C:132:GLU:OE2	2.14	0.48
1:D:29:LEU:HD12	1:D:65:VAL:HG22	1.95	0.48
2:E:238:LEU:O	2:E:243:PRO:HD3	2.13	0.48
2:E:407:LEU:HD23	2:E:411:LEU:HB2	1.94	0.48
3:F:253:ASP:O	3:F:254:ARG:C	2.56	0.48
1:A:118:GLU:OE2	1:A:118:GLU:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLN:HA	1:A:399:GLN:NE2	2.28	0.48
2:B:350:SER:C	2:B:352:ASN:H	2.21	0.48
1:D:101:GLU:HG2	2:E:246:LYS:HZ1	1.79	0.48
1:D:140:TRP:HH2	2:E:199:TYR:HH	1.60	0.48
2:E:77:ILE:HG22	2:E:77:ILE:O	2.14	0.48
2:E:78:THR:O	2:E:140:PHE:CE2	2.66	0.48
2:E:242:LEU:HD11	2:E:275:VAL:HA	1.96	0.48
2:E:299:GLU:O	2:E:302:LEU:N	2.46	0.48
3:F:79:ASN:OD1	3:F:110:ARG:HD3	2.13	0.48
3:F:264:ASN:ND2	3:F:267:TYR:HA	2.28	0.48
1:A:411:LEU:C	1:A:413:GLU:N	2.71	0.48
2:B:93:MET:SD	2:B:124:LEU:HD22	2.53	0.48
2:B:384:LEU:O	2:B:387:PHE:HB2	2.14	0.48
3:C:12:GLN:O	3:C:13:TRP:C	2.56	0.48
3:C:166:LEU:O	3:C:239:ARG:HA	2.14	0.48
3:C:203:PRO:HD2	3:C:242:GLN:OE1	2.13	0.48
1:D:35:LEU:HB3	1:D:72:GLN:HG2	1.96	0.48
1:D:350:MET:CE	1:D:353:SER:HB2	2.43	0.48
1:D:385:ILE:HD11	1:D:411:LEU:HG	1.96	0.48
1:D:476:GLU:CD	1:D:476:GLU:H	2.21	0.48
2:E:388:MET:C	2:E:390:MET:H	2.21	0.48
3:F:266:CYS:O	3:F:267:TYR:HB2	2.14	0.48
1:A:102:THR:CG2	2:B:203:TYR:HB3	2.44	0.48
2:B:257:LEU:O	2:B:258:ALA:C	2.56	0.48
1:D:415:ALA:O	1:D:420:ARG:NH1	2.46	0.48
1:D:446:LEU:H	1:D:446:LEU:CD1	2.26	0.48
2:E:136:GLU:CD	2:E:178:ARG:NH1	2.72	0.48
2:E:382:ASN:O	2:E:386:LEU:HD12	2.12	0.48
3:F:12:GLN:HE22	3:F:16:GLN:HB2	1.79	0.48
3:F:239:ARG:NH1	3:F:258:THR:HG23	2.28	0.48
2:B:164:GLU:C	2:B:165:ASP:O	2.56	0.48
2:B:304:VAL:HG12	2:B:304:VAL:O	2.13	0.48
3:C:56:GLY:HA3	3:C:259:ILE:O	2.14	0.48
1:D:23:GLU:O	1:D:23:GLU:HG2	2.13	0.48
1:D:25:VAL:HG22	1:D:62:GLU:HG2	1.95	0.48
1:D:356:LEU:HD12	1:D:365:LEU:HD11	1.94	0.48
2:E:407:LEU:HD23	2:E:407:LEU:C	2.39	0.48
1:A:11:TYR:N	1:A:12:PRO:HD2	2.28	0.48
1:A:204:GLU:C	1:A:207:PRO:HD2	2.39	0.48
1:A:320:ASN:O	1:A:323:MET:N	2.46	0.48
1:A:438:PHE:C	1:A:438:PHE:HD1	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:VAL:HG13	1:A:497:HIS:CD2	2.49	0.48
1:A:475:LYS:HG3	1:A:476:GLU:N	2.29	0.48
2:B:218:LEU:O	2:B:219:GLY:C	2.57	0.48
3:C:308:PHE:O	3:C:309:LEU:CG	2.60	0.48
1:D:119:HIS:O	1:D:157:ARG:NH2	2.38	0.48
2:E:384:LEU:HD22	2:E:395:PHE:CZ	2.49	0.48
2:B:142:PRO:C	2:B:144:ILE:H	2.22	0.48
3:C:190:PRO:HD3	3:C:195:MET:CE	2.32	0.48
1:D:52:LEU:HD11	1:D:89:LEU:HD12	1.95	0.48
1:D:129:VAL:HB	1:D:130:PRO:HD3	1.96	0.48
2:E:133:ARG:CA	2:E:136:GLU:HG2	2.38	0.48
3:F:160:ASP:C	3:F:162:GLN:H	2.22	0.48
1:D:40:LEU:C	1:D:42:LEU:N	2.69	0.47
1:D:570:ASP:OD2	1:D:571:GLN:N	2.46	0.47
1:A:120:SER:O	1:A:121:PRO:C	2.57	0.47
1:A:155:TYR:CE2	1:A:196:LEU:HD23	2.49	0.47
3:C:237:VAL:CB	3:C:256:VAL:HG22	2.36	0.47
2:E:313:ILE:O	2:E:316:PRO:HD2	2.14	0.47
2:E:381:TYR:HE2	2:E:385:LYS:CD	2.22	0.47
3:F:126:VAL:HG12	3:F:126:VAL:O	2.14	0.47
1:A:358:LYS:HA	1:A:394:VAL:HG12	1.95	0.47
1:A:399:GLN:HE21	1:A:399:GLN:CA	2.26	0.47
1:D:78:THR:O	1:D:80:VAL:N	2.47	0.47
1:D:479:HIS:O	1:D:479:HIS:CG	2.67	0.47
1:D:504:CYS:O	1:D:507:VAL:N	2.43	0.47
2:E:142:PRO:HG2	2:E:143:ASN:H	1.79	0.47
2:E:188:ALA:O	2:E:189:TYR:C	2.57	0.47
3:F:132:GLU:HG3	3:F:136:LYS:HE3	1.94	0.47
1:A:373:LEU:HD22	1:A:384:ILE:HG21	1.97	0.47
2:B:244:LEU:HD21	2:B:253:TYR:CE1	2.50	0.47
2:B:276:VAL:HG11	2:B:313:ILE:CG2	2.44	0.47
2:B:309:GLU:C	2:B:311:VAL:N	2.70	0.47
1:D:443:LEU:HA	1:D:446:LEU:HD13	1.97	0.47
1:D:483:ILE:O	1:D:487:LEU:HG	2.13	0.47
1:D:546:LYS:C	1:D:548:GLY:H	2.21	0.47
2:B:381:TYR:HE2	2:B:385:LYS:HD2	1.80	0.47
2:B:408:LYS:C	2:B:410:LYS:H	2.23	0.47
1:D:350:MET:HE2	1:D:350:MET:O	2.14	0.47
1:D:438:PHE:CD1	1:D:438:PHE:C	2.91	0.47
1:D:486:VAL:HG12	1:D:486:VAL:O	2.14	0.47
2:E:222:ILE:HA	2:E:225:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:159:VAL:HB	3:F:163:ILE:HB	1.96	0.47
2:B:72:HIS:O	2:B:74:ARG:N	2.47	0.47
2:B:90:ALA:O	2:B:94:PHE:HB2	2.14	0.47
3:C:104:LYS:CA	3:C:111:ILE:HD11	2.44	0.47
1:D:408:ILE:HD13	1:D:426:TYR:CE2	2.45	0.47
2:E:236:PHE:O	2:E:240:VAL:HB	2.15	0.47
2:E:357:LEU:N	2:E:358:PRO:HD2	2.30	0.47
1:A:155:TYR:CZ	1:A:163:LYS:HB3	2.49	0.47
1:A:264:ALA:O	1:A:267:PHE:HB2	2.15	0.47
1:A:349:ILE:HG23	1:A:350:MET:N	2.30	0.47
1:A:522:LEU:N	1:A:523:PRO:CD	2.78	0.47
2:B:262:VAL:O	2:B:265:LEU:N	2.47	0.47
2:B:313:ILE:O	2:B:314:MET:C	2.57	0.47
1:D:109:VAL:O	1:D:113:ARG:HG3	2.14	0.47
1:D:350:MET:HE2	1:D:353:SER:HB2	1.97	0.47
1:D:353:SER:HB3	1:D:354:PRO:CD	2.44	0.47
2:E:93:MET:SD	2:E:124:LEU:HD22	2.54	0.47
2:E:118:GLU:H	2:E:164:GLU:CG	2.22	0.47
2:E:223:ASN:HD22	2:E:263:GLN:NE2	2.13	0.47
3:F:12:GLN:NE2	3:F:16:GLN:HB2	2.30	0.47
3:F:237:VAL:CB	3:F:256:VAL:HG22	2.42	0.47
1:A:236:PRO:O	1:A:237:GLN:C	2.58	0.47
2:B:298:LEU:HD21	2:B:317:LEU:HD13	1.97	0.47
3:C:121:ARG:HG3	3:C:121:ARG:NH1	2.29	0.47
2:E:142:PRO:HG2	2:E:143:ASN:N	2.29	0.47
2:E:266:GLU:HG2	2:E:304:VAL:HG11	1.96	0.47
2:B:91:VAL:HG12	2:B:91:VAL:O	2.14	0.47
2:B:118:GLU:H	2:B:164:GLU:CG	2.25	0.47
2:B:239:LYS:O	2:B:243:PRO:HG3	2.14	0.47
3:C:2:ASP:O	3:C:5:VAL:HB	2.15	0.47
3:C:294:ARG:HH11	3:C:294:ARG:HG2	1.78	0.47
1:D:155:TYR:CZ	1:D:196:LEU:CD2	2.98	0.47
1:D:368:LEU:O	1:D:371:ALA:HB3	2.15	0.47
1:D:564:LEU:O	1:D:564:LEU:HD23	2.15	0.47
2:E:244:LEU:CD2	2:E:253:TYR:CE1	2.98	0.47
3:F:65:LEU:O	3:F:68:LEU:HB3	2.15	0.47
3:F:276:MET:HE3	3:F:278:LEU:CD2	2.37	0.47
1:A:105:ARG:NH1	1:A:142:THR:CG2	2.78	0.47
2:B:82:TYR:CG	2:B:82:TYR:O	2.68	0.47
1:D:427:MET:CE	1:D:430:LEU:HD12	2.43	0.47
1:D:503:PHE:O	1:D:506:ASN:HB2	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:107:GLU:HG3	2:E:108:PHE:CD1	2.50	0.47
2:E:371:HIS:HB2	2:E:376:ILE:HD11	1.97	0.47
1:A:25:VAL:HG22	1:A:62:GLU:HG2	1.98	0.46
1:A:377:CYS:SG	1:A:379:GLU:HG2	2.55	0.46
2:B:85:VAL:HG11	2:B:134:PHE:CD1	2.50	0.46
1:A:196:LEU:HD12	1:A:205:ILE:HD11	1.96	0.46
1:A:424:ILE:HG12	1:A:450:TRP:CE3	2.50	0.46
1:D:17:ILE:HG12	1:D:38:ILE:HG23	1.97	0.46
1:D:102:THR:O	1:D:103:VAL:C	2.58	0.46
1:D:111:SER:O	1:D:112:LEU:C	2.58	0.46
1:D:502:LEU:HD13	1:D:540:VAL:HA	1.96	0.46
2:E:70:ILE:HG22	2:E:70:ILE:O	2.14	0.46
2:E:244:LEU:HD23	2:E:244:LEU:C	2.40	0.46
3:F:71:ILE:N	3:F:71:ILE:HD12	2.31	0.46
3:F:169:GLY:O	3:F:198:LEU:HA	2.15	0.46
1:A:98:THR:HG23	1:A:143:SER:OG	2.15	0.46
1:A:405:LEU:HD13	1:A:405:LEU:O	2.15	0.46
1:A:427:MET:HB3	1:A:428:PRO:CD	2.45	0.46
1:A:498:ARG:NE	1:A:531:ASP:OD2	2.48	0.46
2:B:164:GLU:OE2	2:B:164:GLU:C	2.58	0.46
3:F:117:ASN:CG	3:F:241:HIS:CE1	2.92	0.46
3:F:276:MET:HG3	3:F:286:PHE:CE1	2.50	0.46
2:B:357:LEU:N	2:B:358:PRO:HD2	2.30	0.46
3:C:239:ARG:NH1	3:C:258:THR:HG23	2.29	0.46
1:D:291:MET:HB3	1:D:333:LEU:HD11	1.98	0.46
2:E:35:LYS:O	2:E:37:ARG:N	2.47	0.46
2:E:330:PHE:CD1	2:E:331:GLN:N	2.84	0.46
2:E:366:ARG:O	2:E:367:ASN:C	2.58	0.46
2:E:407:LEU:HD21	2:E:411:LEU:HD12	1.98	0.46
3:F:203:PRO:HA	3:F:220:PHE:CE1	2.51	0.46
1:A:101:GLU:C	1:A:101:GLU:OE1	2.59	0.46
1:A:206:ILE:HG21	1:A:243:LEU:HB3	1.97	0.46
2:B:247:VAL:CG1	2:B:248:LYS:N	2.78	0.46
2:B:305:ILE:HD13	2:B:306:GLU:N	2.30	0.46
2:B:384:LEU:HD22	2:B:395:PHE:CZ	2.50	0.46
3:C:308:PHE:O	3:C:309:LEU:CB	2.62	0.46
1:D:245:MET:O	1:D:249:ARG:HG3	2.16	0.46
2:E:242:LEU:HD11	2:E:275:VAL:HG22	1.97	0.46
2:E:250:LEU:O	2:E:252:VAL:N	2.48	0.46
2:E:288:SER:HB2	2:E:289:PRO:HD3	1.97	0.46
3:F:67:GLU:O	3:F:71:ILE:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:TRP:O	2:B:285:LYS:HE3	2.16	0.46
2:B:294:PHE:O	2:B:295:LEU:C	2.58	0.46
1:D:267:PHE:CZ	1:D:287:PHE:HB2	2.51	0.46
3:F:183:LEU:HD21	3:F:194:PRO:HG3	1.97	0.46
1:A:171:ARG:HG3	1:A:208:MET:HE2	1.97	0.46
1:A:214:SER:HA	1:A:221:ARG:CD	2.46	0.46
1:D:25:VAL:CG2	1:D:62:GLU:HG2	2.46	0.46
2:E:88:MET:HE1	2:E:127:VAL:HG22	1.98	0.46
2:E:309:GLU:C	2:E:311:VAL:N	2.72	0.46
3:F:12:GLN:O	3:F:13:TRP:C	2.58	0.46
3:F:13:TRP:HE1	3:F:27:GLN:HE21	1.64	0.46
1:A:552:ASP:OD1	1:A:554:SER:HB3	2.15	0.46
2:B:298:LEU:HB3	2:B:339:TYR:OH	2.16	0.46
2:B:357:LEU:HD12	2:B:357:LEU:O	2.16	0.46
2:B:412:LYS:O	2:B:414:LYS:N	2.42	0.46
3:C:81:LEU:C	3:C:81:LEU:HD23	2.41	0.46
1:D:470:VAL:HG21	1:D:508:LEU:HD12	1.98	0.46
2:E:72:HIS:O	2:E:73:ASN:C	2.59	0.46
2:E:78:THR:O	2:E:78:THR:HG22	2.15	0.46
2:E:136:GLU:O	2:E:136:GLU:HG3	2.15	0.46
2:E:288:SER:O	2:E:289:PRO:C	2.58	0.46
2:E:317:LEU:O	2:E:320:GLN:HB3	2.16	0.46
2:B:173:LYS:HA	2:B:217:ILE:HD11	1.98	0.46
2:B:381:TYR:O	2:B:382:ASN:C	2.59	0.46
1:D:35:LEU:HD21	1:D:55:LEU:CD1	2.37	0.46
1:D:94:GLU:HB2	1:D:131:LEU:HD12	1.97	0.46
1:D:489:MET:C	1:D:491:GLY:H	2.24	0.46
1:D:538:PHE:HB3	1:D:575:VAL:HA	1.98	0.46
2:E:39:CYS:C	2:E:41:VAL:N	2.74	0.46
3:F:117:ASN:ND2	3:F:241:HIS:HE1	2.12	0.46
3:F:190:PRO:CD	3:F:195:MET:HE2	2.39	0.46
2:B:151:GLN:HB3	2:B:189:TYR:CE2	2.51	0.46
1:D:98:THR:O	1:D:99:VAL:C	2.59	0.46
1:D:140:TRP:CZ2	2:E:239:LYS:HD2	2.51	0.46
1:A:327:LEU:HB3	1:A:328:PRO:HD3	1.98	0.45
2:B:86:VAL:HG12	2:B:87:HIS:N	2.31	0.45
2:B:93:MET:HE1	2:B:124:LEU:HD22	1.98	0.45
2:B:205:THR:C	2:B:207:HIS:N	2.74	0.45
2:B:373:ASN:O	2:B:375:THR:N	2.45	0.45
2:E:121:TRP:CD1	2:E:167:ARG:NH1	2.84	0.45
2:E:246:LYS:HE3	3:F:307:TYR:OH	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:407:LEU:CD2	2:E:411:LEU:HD12	2.45	0.45
1:A:327:LEU:HA	1:A:330:ILE:HD12	1.98	0.45
1:A:353:SER:HB3	1:A:354:PRO:HD3	1.97	0.45
2:B:83:PRO:CG	2:B:148:TYR:CD2	2.98	0.45
1:D:353:SER:HB3	1:D:354:PRO:HD3	1.98	0.45
1:D:450:TRP:C	1:D:452:VAL:H	2.24	0.45
1:D:522:LEU:HD22	1:D:551:LEU:HD22	1.99	0.45
2:E:373:ASN:O	2:E:375:THR:N	2.49	0.45
1:A:429:LEU:O	1:A:433:GLN:HG3	2.16	0.45
3:C:232:ASN:HB2	3:C:234:LEU:HG	1.99	0.45
3:C:244:VAL:C	3:C:246:GLU:N	2.74	0.45
1:D:24:ASP:O	1:D:26:GLN:N	2.49	0.45
1:D:385:ILE:HD12	1:D:423:ILE:CD1	2.46	0.45
2:E:54:LYS:C	2:E:56:LYS:H	2.23	0.45
3:F:137:TYR:CE2	3:F:142:VAL:HG21	2.52	0.45
1:A:404:LEU:H	1:A:406:PRO:HD2	1.82	0.45
1:A:429:LEU:C	1:A:431:ALA:N	2.75	0.45
2:E:54:LYS:O	2:E:56:LYS:N	2.48	0.45
2:E:278:ALA:O	2:E:281:LYS:HB3	2.15	0.45
4:Y:6:FGA:HG3	4:Y:7:DAM:HM1	1.76	0.45
1:A:499:MET:O	1:A:500:THR:C	2.59	0.45
1:A:561:LYS:N	1:A:562:PRO:CD	2.80	0.45
2:B:230:LYS:O	2:B:231:GLU:C	2.59	0.45
2:B:238:LEU:O	2:B:243:PRO:HD3	2.17	0.45
2:B:318:PHE:O	2:B:319:ARG:C	2.60	0.45
3:C:71:ILE:CG2	3:C:275:ILE:HD11	2.47	0.45
3:C:99:LEU:HD12	3:C:99:LEU:O	2.17	0.45
1:D:427:MET:HG2	1:D:447:CYS:SG	2.56	0.45
1:A:119:HIS:O	1:A:157:ARG:NH2	2.43	0.45
1:A:534:ALA:O	1:A:537:ARG:N	2.50	0.45
2:B:72:HIS:O	2:B:74:ARG:HG2	2.17	0.45
2:B:276:VAL:HG11	2:B:313:ILE:HG21	1.99	0.45
2:B:288:SER:O	2:B:291:GLU:HB3	2.17	0.45
1:D:16:LEU:HB3	1:D:38:ILE:HD11	1.98	0.45
1:D:28:ARG:HD3	1:D:60:TYR:HE2	1.81	0.45
1:D:29:LEU:CD1	1:D:65:VAL:HG22	2.47	0.45
1:D:71:GLU:HG3	1:D:107:LYS:HE3	1.97	0.45
1:D:131:LEU:C	1:D:131:LEU:HD23	2.41	0.45
1:D:182:ARG:O	1:D:183:ARG:C	2.59	0.45
3:F:239:ARG:O	3:F:258:THR:HA	2.17	0.45
1:A:245:MET:O	1:A:249:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:ILE:HG22	3:C:72:GLY:N	2.31	0.45
2:E:337:LEU:O	2:E:340:TRP:HE3	1.99	0.45
1:A:209:PHE:CZ	1:A:228:CYS:HB2	2.52	0.45
1:A:350:MET:HE1	1:A:391:VAL:HG13	1.97	0.45
1:A:372:GLN:C	1:A:374:LYS:N	2.70	0.45
2:B:93:MET:O	2:B:160:LEU:HD21	2.16	0.45
2:B:268:ASP:OD1	2:B:268:ASP:C	2.60	0.45
3:C:76:PRO:HB3	3:C:107:TYR:CG	2.52	0.45
1:D:398:ARG:O	1:D:402:GLN:N	2.50	0.45
2:E:287:HIS:HE1	2:E:289:PRO:HB2	1.81	0.45
3:F:97:VAL:HG13	3:F:98:THR:N	2.31	0.45
1:A:245:MET:O	1:A:246:PRO:C	2.59	0.45
1:A:538:PHE:HB2	1:A:578:PHE:CD2	2.51	0.45
3:C:118:HIS:ND1	3:C:123:ILE:HG21	2.32	0.45
1:D:296:ALA:O	1:D:297:GLU:C	2.58	0.45
2:E:76:VAL:O	2:E:76:VAL:CG1	2.64	0.45
2:E:361:PHE:N	2:E:362:PRO:HD2	2.32	0.45
3:F:32:CYS:O	3:F:35:ALA:HB3	2.17	0.45
3:F:134:LEU:HD12	3:F:139:ASN:O	2.17	0.45
1:A:322:ILE:CG2	1:A:356:LEU:HD21	2.47	0.45
2:B:329:HIS:HA	3:C:125:GLN:OE1	2.16	0.45
3:C:51:PRO:HA	3:C:278:LEU:O	2.17	0.45
1:D:538:PHE:HB2	1:D:578:PHE:CD2	2.50	0.45
2:E:227:LEU:HB2	2:E:228:PRO:CD	2.45	0.45
2:E:273:GLU:CA	2:E:313:ILE:HD11	2.32	0.45
2:B:145:ALA:O	2:B:147:LYS:N	2.49	0.44
2:B:158:LEU:O	2:B:159:GLU:C	2.59	0.44
2:E:145:ALA:O	2:E:147:LYS:N	2.50	0.44
3:F:132:GLU:CG	3:F:136:LYS:HE3	2.47	0.44
1:A:38:ILE:O	1:A:42:LEU:HB2	2.17	0.44
3:C:211:ILE:O	3:C:211:ILE:HG22	2.17	0.44
1:D:155:TYR:HB3	1:D:156:PRO:HD3	1.99	0.44
2:E:384:LEU:O	2:E:387:PHE:HB2	2.17	0.44
2:E:408:LYS:C	2:E:410:LYS:H	2.24	0.44
1:A:99:VAL:HG21	1:A:104:VAL:HG11	1.99	0.44
1:A:183:ARG:O	1:A:186:ALA:HB3	2.18	0.44
2:B:72:HIS:O	2:B:73:ASN:C	2.61	0.44
2:B:164:GLU:HB3	2:B:168:GLU:CB	2.39	0.44
2:B:382:ASN:O	2:B:386:LEU:HD12	2.17	0.44
1:D:28:ARG:NH1	1:D:62:GLU:OE1	2.50	0.44
1:D:196:LEU:HD12	1:D:205:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:453:ASP:OD1	1:D:454:HIS:N	2.49	0.44
1:D:456:TYR:CD1	1:D:456:TYR:C	2.95	0.44
1:D:475:LYS:HG2	1:D:476:GLU:OE2	2.18	0.44
1:D:522:LEU:N	1:D:523:PRO:CD	2.80	0.44
1:D:529:ALA:CB	1:D:563:ILE:HD11	2.47	0.44
2:E:345:ILE:O	2:E:349:ILE:HG13	2.18	0.44
1:A:28:ARG:HD3	1:A:60:TYR:CE2	2.53	0.44
1:A:248:LEU:HD11	1:A:270:LEU:HD13	1.99	0.44
1:A:503:PHE:O	1:A:506:ASN:HB2	2.18	0.44
2:B:186:LEU:C	2:B:190:ILE:HD13	2.43	0.44
2:B:242:LEU:HD11	2:B:275:VAL:HA	2.00	0.44
2:E:63:LEU:C	2:E:65:GLU:N	2.73	0.44
2:E:102:ASN:ND2	2:E:113:ASP:HB3	2.31	0.44
2:E:408:LYS:C	2:E:410:LYS:N	2.76	0.44
3:F:119:GLU:OE1	3:F:119:GLU:N	2.50	0.44
1:A:52:LEU:O	1:A:53:PRO:C	2.60	0.44
1:A:492:ASP:OD2	1:A:493:PRO:CD	2.65	0.44
1:D:408:ILE:CD1	1:D:426:TYR:HE2	2.29	0.44
1:D:450:TRP:C	1:D:452:VAL:N	2.75	0.44
2:E:72:HIS:C	2:E:74:ARG:N	2.75	0.44
2:E:315:GLU:HB2	2:E:316:PRO:CD	2.48	0.44
3:F:117:ASN:HB2	3:F:200:TRP:CE2	2.53	0.44
3:F:276:MET:CG	3:F:286:PHE:CE1	3.00	0.44
1:A:365:LEU:HB3	1:A:369:PHE:CZ	2.52	0.44
2:B:71:THR:O	2:B:73:ASN:N	2.50	0.44
3:C:160:ASP:C	3:C:162:GLN:H	2.25	0.44
1:D:215:ASP:H	1:D:221:ARG:HG2	1.81	0.44
2:E:79:GLU:O	2:E:80:PRO:C	2.59	0.44
2:E:120:ALA:C	2:E:122:PRO:HD2	2.39	0.44
2:E:277:MET:HE2	2:E:280:LEU:HD12	1.99	0.44
2:E:314:MET:HG3	2:E:356:ILE:HD11	1.99	0.44
1:A:296:ALA:O	1:A:297:GLU:C	2.61	0.44
1:A:499:MET:C	1:A:501:THR:N	2.72	0.44
2:B:76:VAL:O	2:B:76:VAL:CG1	2.65	0.44
2:B:242:LEU:HD23	2:B:242:LEU:HA	1.84	0.44
3:C:118:HIS:HA	3:C:123:ILE:HG21	2.00	0.44
1:D:322:ILE:CG2	1:D:356:LEU:HD21	2.48	0.44
1:D:429:LEU:O	1:D:433:GLN:HG3	2.17	0.44
2:E:134:PHE:C	2:E:134:PHE:HD2	2.26	0.44
3:F:308:PHE:O	3:F:309:LEU:CB	2.66	0.44
1:A:268:THR:HG23	1:A:305:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:MET:O	1:A:491:GLY:N	2.51	0.44
2:B:283:TRP:O	2:B:285:LYS:CE	2.66	0.44
1:D:70:ALA:CB	1:D:96:LEU:HD13	2.45	0.44
1:D:218:ASP:OD1	1:D:219:SER:N	2.51	0.44
1:D:492:ASP:OD2	1:D:493:PRO:CD	2.62	0.44
1:D:506:ASN:ND2	1:D:543:SER:HA	2.32	0.44
1:A:266:LYS:O	1:A:269:GLU:HB2	2.18	0.44
1:A:302:ALA:O	1:A:303:SER:C	2.61	0.44
1:A:388:LEU:C	1:A:390:CYS:N	2.73	0.44
1:A:427:MET:O	1:A:431:ALA:N	2.47	0.44
3:C:140:ALA:O	3:C:143:TRP:HB3	2.17	0.44
3:C:143:TRP:CZ2	3:C:147:THR:HG21	2.53	0.44
1:D:144:ARG:HH21	1:D:176:ASP:CG	2.26	0.44
1:D:223:LEU:O	1:D:224:ALA:C	2.58	0.44
1:D:427:MET:O	1:D:431:ALA:N	2.42	0.44
2:E:56:LYS:O	2:E:58:VAL:HG23	2.18	0.44
2:E:254:HIS:CE1	2:E:297:GLU:HB2	2.53	0.44
2:E:257:LEU:O	2:E:258:ALA:C	2.61	0.44
2:E:330:PHE:CG	2:E:331:GLN:N	2.86	0.44
1:A:229:VAL:HG22	1:A:270:LEU:HD23	2.00	0.43
1:A:502:LEU:CD2	1:A:540:VAL:HG23	2.48	0.43
1:A:538:PHE:O	1:A:542:LYS:HG3	2.17	0.43
2:B:79:GLU:N	2:B:80:PRO:HD2	2.24	0.43
2:B:330:PHE:CZ	3:C:122:GLN:HG3	2.53	0.43
3:C:301:THR:CG2	3:C:302:ARG:H	2.09	0.43
1:D:279:THR:O	1:D:284:VAL:HG23	2.18	0.43
2:E:109:ASP:OD1	2:E:111:GLU:HB2	2.18	0.43
2:E:376:ILE:O	2:E:377:HIS:C	2.61	0.43
3:F:6:PHE:O	3:F:9:GLU:N	2.50	0.43
3:F:46:GLN:O	3:F:158:LEU:N	2.41	0.43
3:F:200:TRP:HZ3	4:Y:5:1ZN:H20	1.83	0.43
1:A:86:VAL:C	1:A:88:CYS:H	2.26	0.43
1:A:209:PHE:HE1	1:A:224:ALA:O	2.01	0.43
1:A:314:SER:HB3	1:A:317:CYS:SG	2.58	0.43
2:B:230:LYS:HB2	2:B:233:HIS:HD2	1.83	0.43
2:E:164:GLU:OE1	2:E:167:ARG:NH1	2.51	0.43
3:F:163:ILE:HD13	3:F:236:LEU:HD23	2.01	0.43
1:A:102:THR:HA	1:A:105:ARG:NE	2.33	0.43
1:A:346:ALA:HB2	1:A:380:VAL:HG13	1.99	0.43
2:B:64:SER:O	2:B:68:GLU:HG3	2.18	0.43
2:B:288:SER:O	2:B:289:PRO:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:366:ARG:O	2:B:368:SER:N	2.52	0.43
2:B:393:LYS:O	2:B:394:LEU:C	2.60	0.43
3:C:208:GLY:C	3:C:224:ILE:HD11	2.43	0.43
3:C:243:LEU:HD21	3:C:269:CYS:HB3	2.00	0.43
1:D:378:PRO:O	1:D:379:GLU:C	2.62	0.43
1:D:556:LEU:O	1:D:558:SER:N	2.45	0.43
2:E:93:MET:HE3	2:E:93:MET:HA	1.99	0.43
1:A:398:ARG:HH11	1:A:398:ARG:CB	2.31	0.43
1:A:412:ALA:HB1	1:A:450:TRP:CZ2	2.50	0.43
1:A:502:LEU:HD13	1:A:540:VAL:CA	2.47	0.43
2:B:165:ASP:C	2:B:167:ARG:N	2.76	0.43
3:C:278:LEU:HB3	3:C:282:LEU:HD23	2.00	0.43
1:D:101:GLU:OE1	1:D:101:GLU:C	2.61	0.43
1:D:283:LEU:O	1:D:284:VAL:C	2.62	0.43
2:E:78:THR:C	2:E:80:PRO:CD	2.82	0.43
3:F:24:SER:OG	3:F:27:GLN:HG3	2.19	0.43
3:F:277:GLU:HB2	3:F:285:SER:OG	2.17	0.43
1:A:217:GLN:HE22	2:B:155:LEU:HD11	1.83	0.43
1:A:390:CYS:O	1:A:391:VAL:C	2.60	0.43
1:A:418:ARG:HH12	3:C:67:GLU:CD	2.26	0.43
1:A:479:HIS:O	1:A:479:HIS:CG	2.70	0.43
1:A:548:GLY:HA3	1:A:586:LEU:HD21	2.00	0.43
1:D:482:ILE:C	1:D:484:PRO:HD2	2.43	0.43
2:E:39:CYS:CB	2:E:66:MET:HE1	2.49	0.43
3:F:121:ARG:HG3	3:F:121:ARG:HH11	1.82	0.43
3:F:183:LEU:HD21	3:F:194:PRO:HG2	2.00	0.43
1:A:90:LEU:HD11	1:A:119:HIS:HE1	1.84	0.43
1:A:182:ARG:NE	1:A:215:ASP:OD2	2.46	0.43
1:D:392:ASN:HB3	1:D:400:LEU:HD22	2.01	0.43
2:E:110:PRO:HA	2:E:113:ASP:OD2	2.18	0.43
2:E:176:LEU:O	2:E:177:HIS:C	2.62	0.43
2:E:218:LEU:O	2:E:219:GLY:C	2.59	0.43
3:F:164:PHE:HB2	3:F:234:LEU:HD13	2.01	0.43
1:A:124:LEU:HD23	1:A:124:LEU:HA	1.89	0.43
2:B:278:ALA:O	2:B:281:LYS:HB3	2.19	0.43
2:B:329:HIS:HD2	2:B:332:VAL:H	1.67	0.43
2:B:362:PRO:O	2:B:366:ARG:HB2	2.18	0.43
1:D:398:ARG:CB	1:D:398:ARG:NH1	2.81	0.43
3:F:131:ASP:O	3:F:132:GLU:C	2.61	0.43
1:A:11:TYR:O	1:A:12:PRO:C	2.62	0.43
1:A:475:LYS:CG	1:A:476:GLU:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:GLU:HB2	2:B:316:PRO:CD	2.49	0.43
2:B:361:PHE:HB3	2:B:362:PRO:CD	2.49	0.43
2:B:407:LEU:O	2:B:408:LYS:C	2.59	0.43
3:C:118:HIS:ND1	3:C:123:ILE:CG2	2.82	0.43
3:C:292:ALA:HB1	3:C:293:PRO:HD2	2.01	0.43
1:D:349:ILE:CG2	1:D:350:MET:N	2.80	0.43
1:D:489:MET:C	1:D:491:GLY:N	2.76	0.43
2:E:217:ILE:HG22	2:E:221:ILE:CD1	2.48	0.43
3:F:211:ILE:O	3:F:211:ILE:HG22	2.18	0.43
1:A:77:THR:CG2	1:A:118:GLU:HG3	2.37	0.43
2:B:80:PRO:HG2	2:B:82:TYR:CE2	2.54	0.43
2:B:313:ILE:N	2:B:313:ILE:HD12	2.34	0.43
2:B:329:HIS:HE1	3:C:125:GLN:O	2.01	0.43
2:B:373:ASN:HD21	2:B:375:THR:CG2	2.32	0.43
3:C:174:ILE:HD13	3:C:180:ILE:CG1	2.36	0.43
3:C:264:ASN:O	3:C:265:TYR:C	2.62	0.43
1:D:29:LEU:HD12	1:D:65:VAL:HA	2.00	0.43
1:D:262:MET:O	1:D:263:VAL:C	2.62	0.43
1:D:313:LEU:HD13	1:D:321:VAL:CG2	2.49	0.43
1:D:403:SER:O	1:D:404:LEU:CB	2.67	0.43
3:F:244:VAL:C	3:F:246:GLU:N	2.74	0.43
2:B:142:PRO:C	2:B:144:ILE:N	2.76	0.43
2:B:241:LEU:HA	2:B:241:LEU:HD23	1.84	0.43
3:C:156:THR:HG22	3:C:166:LEU:HB2	2.00	0.43
1:D:517:THR:HA	1:D:521:MET:CE	2.44	0.43
2:E:194:ILE:HG23	2:E:214:LEU:HD22	1.99	0.43
2:E:205:THR:C	2:E:207:HIS:H	2.26	0.43
2:E:318:PHE:O	2:E:360:MET:HE1	2.19	0.43
3:F:301:THR:CG2	3:F:302:ARG:H	2.12	0.43
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.88	0.42
2:B:191:ARG:O	2:B:192:LYS:C	2.62	0.42
2:B:237:LEU:CA	2:B:241:LEU:HB2	2.42	0.42
2:B:388:MET:O	2:B:390:MET:N	2.46	0.42
3:C:183:LEU:HD21	3:C:194:PRO:CG	2.49	0.42
3:C:279:ASP:C	3:C:281:THR:N	2.76	0.42
1:D:40:LEU:O	1:D:42:LEU:N	2.52	0.42
2:E:78:THR:HG22	2:E:82:TYR:OH	2.19	0.42
3:F:44:ASN:N	3:F:44:ASN:ND2	2.58	0.42
3:F:240:ALA:HA	3:F:258:THR:HG23	2.01	0.42
1:A:336:ASP:OD1	1:A:337:ALA:N	2.51	0.42
2:B:376:ILE:HD12	2:B:380:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408:LYS:O	2:B:410:LYS:N	2.53	0.42
3:C:240:ALA:O	3:C:241:HIS:HB2	2.17	0.42
1:D:392:ASN:ND2	1:D:433:GLN:NE2	2.64	0.42
2:E:64:SER:O	2:E:68:GLU:HG3	2.19	0.42
2:E:226:ALA:O	2:E:227:LEU:C	2.62	0.42
2:E:268:ASP:OD1	2:E:270:THR:N	2.52	0.42
3:F:160:ASP:O	3:F:162:GLN:N	2.52	0.42
3:F:163:ILE:HG12	3:F:236:LEU:HB3	2.01	0.42
3:F:239:ARG:HH11	3:F:258:THR:HG23	1.83	0.42
1:A:78:THR:O	1:A:80:VAL:N	2.53	0.42
1:A:583:LEU:O	1:A:584:THR:C	2.62	0.42
2:B:86:VAL:O	2:B:87:HIS:C	2.63	0.42
3:C:208:GLY:CA	3:C:224:ILE:HD11	2.48	0.42
1:D:408:ILE:O	1:D:408:ILE:HG22	2.19	0.42
2:E:103:PRO:HB2	2:E:108:PHE:CE1	2.54	0.42
2:E:110:PRO:HA	2:E:113:ASP:CG	2.45	0.42
2:E:154:VAL:HG11	2:E:190:ILE:HG13	2.01	0.42
3:F:17:LEU:HD13	3:F:99:LEU:N	2.34	0.42
3:F:120:SER:OG	3:F:123:ILE:HB	2.19	0.42
1:A:55:LEU:HD13	1:A:69:LEU:HD11	2.00	0.42
1:A:274:VAL:CG1	1:A:278:ILE:HB	2.49	0.42
1:A:352:LEU:O	1:A:353:SER:C	2.62	0.42
1:A:399:GLN:NE2	1:A:399:GLN:CA	2.81	0.42
1:A:486:VAL:HG12	1:A:486:VAL:O	2.19	0.42
1:D:278:ILE:O	1:D:282:ASP:N	2.40	0.42
1:D:455:VAL:HG13	1:D:455:VAL:O	2.19	0.42
1:D:525:VAL:HG11	1:D:544:LEU:CD2	2.49	0.42
2:E:393:LYS:O	2:E:394:LEU:C	2.61	0.42
1:A:13:ILE:O	1:A:17:ILE:HG13	2.19	0.42
1:A:67:LEU:HD13	1:A:103:VAL:HG12	2.01	0.42
1:A:91:PRO:HB2	1:A:92:PRO:HD3	2.00	0.42
3:C:62:PHE:HB2	3:C:92:TYR:HB2	2.01	0.42
1:D:124:LEU:HA	1:D:124:LEU:HD23	1.74	0.42
1:D:412:ALA:HB1	1:D:450:TRP:CZ2	2.53	0.42
2:E:232:GLU:HG3	2:E:233:HIS:N	2.34	0.42
2:E:276:VAL:HG11	2:E:313:ILE:CG2	2.50	0.42
2:E:373:ASN:ND2	2:E:376:ILE:HG23	2.34	0.42
3:F:263:PRO:HD3	3:F:273:ALA:CB	2.50	0.42
1:A:12:PRO:O	1:A:15:VAL:HB	2.20	0.42
1:A:28:ARG:CD	1:A:60:TYR:CE2	3.02	0.42
1:A:443:LEU:HA	1:A:446:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:LEU:HD13	2:B:162:ASP:HB3	2.01	0.42
2:B:257:LEU:O	2:B:261:VAL:HG23	2.18	0.42
2:B:371:HIS:HB2	2:B:376:ILE:HD11	2.01	0.42
2:B:380:ILE:O	2:B:383:ALA:HB3	2.20	0.42
3:C:4:LYS:O	3:C:5:VAL:C	2.62	0.42
3:C:185:ARG:O	3:C:187:GLN:N	2.53	0.42
3:C:237:VAL:O	3:C:256:VAL:HG13	2.19	0.42
1:D:11:TYR:O	1:D:12:PRO:C	2.60	0.42
1:D:24:ASP:C	1:D:24:ASP:OD2	2.62	0.42
3:F:160:ASP:C	3:F:162:GLN:N	2.78	0.42
3:F:266:CYS:SG	4:Y:2:LEU:HD12	2.59	0.42
1:A:278:ILE:HA	1:A:281:THR:HB	2.02	0.42
1:A:515:ASP:O	1:A:516:ILE:C	2.63	0.42
2:B:96:THR:O	2:B:97:LEU:C	2.63	0.42
2:B:186:LEU:O	2:B:187:ARG:C	2.62	0.42
2:B:239:LYS:C	2:B:243:PRO:HG3	2.45	0.42
2:B:367:ASN:C	2:B:369:LYS:H	2.26	0.42
1:D:257:TRP:CE2	2:E:99:PRO:HD3	2.54	0.42
1:D:321:VAL:CG2	1:D:322:ILE:N	2.81	0.42
1:D:372:GLN:C	1:D:374:LYS:N	2.76	0.42
1:D:526:LEU:HA	1:D:563:ILE:HD13	2.02	0.42
2:E:158:LEU:HB3	2:E:197:ILE:HD11	2.02	0.42
2:E:412:LYS:O	2:E:414:LYS:N	2.45	0.42
1:A:269:GLU:OE2	1:A:305:LYS:NZ	2.53	0.42
1:A:391:VAL:C	1:A:393:GLU:N	2.76	0.42
1:A:392:ASN:ND2	1:A:433:GLN:OE1	2.53	0.42
2:B:78:THR:HG22	2:B:78:THR:O	2.20	0.42
2:B:79:GLU:O	2:B:80:PRO:C	2.58	0.42
2:B:402:PHE:O	2:B:406:LYS:HB2	2.19	0.42
1:D:22:ASN:O	1:D:22:ASN:CG	2.62	0.42
1:D:317:CYS:O	1:D:318:ARG:C	2.63	0.42
1:D:330:ILE:CD1	1:D:352:LEU:HD11	2.49	0.42
2:E:199:TYR:CZ	2:E:240:VAL:HG22	2.54	0.42
3:F:6:PHE:CE2	3:F:34:LYS:HE3	2.54	0.42
3:F:76:PRO:HB3	3:F:107:TYR:CG	2.55	0.42
1:A:102:THR:O	1:A:103:VAL:C	2.63	0.42
1:A:303:SER:O	1:A:306:VAL:HG23	2.19	0.42
1:A:535:ASN:ND2	3:C:77:ASP:O	2.49	0.42
3:C:278:LEU:HD13	3:C:282:LEU:CD2	2.49	0.42
1:D:398:ARG:O	1:D:399:GLN:C	2.62	0.42
2:E:86:VAL:O	2:E:87:HIS:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:318:PHE:O	2:E:319:ARG:C	2.62	0.42
3:F:31:LEU:HD11	3:F:102:ALA:HA	2.01	0.42
3:F:143:TRP:CZ2	3:F:147:THR:HG21	2.55	0.42
1:A:111:SER:O	1:A:114:ALA:N	2.53	0.42
2:B:130:PHE:O	2:B:131:PHE:C	2.62	0.42
2:B:309:GLU:C	2:B:311:VAL:H	2.28	0.42
2:B:381:TYR:HD2	2:B:381:TYR:O	2.02	0.42
3:C:10:LEU:HD23	3:C:13:TRP:HE3	1.85	0.42
1:D:52:LEU:CD1	1:D:88:CYS:HB3	2.50	0.42
2:E:162:ASP:O	2:E:163:SER:HB2	2.20	0.42
2:E:180:TYR:CE2	2:E:221:ILE:HG23	2.55	0.42
2:E:367:ASN:C	2:E:369:LYS:H	2.28	0.42
3:F:137:TYR:CG	3:F:142:VAL:HG21	2.55	0.42
3:F:187:GLN:HE21	3:F:187:GLN:HB2	1.69	0.42
1:A:68:ALA:O	1:A:69:LEU:C	2.62	0.41
1:A:323:MET:CE	1:A:356:LEU:HD22	2.50	0.41
1:A:437:GLU:CG	1:A:438:PHE:N	2.83	0.41
1:A:446:LEU:H	1:A:446:LEU:CD1	2.32	0.41
1:D:198:LEU:O	1:D:201:VAL:HB	2.20	0.41
1:D:537:ARG:HG3	1:D:537:ARG:HH11	1.85	0.41
2:E:186:LEU:O	2:E:187:ARG:C	2.62	0.41
2:E:313:ILE:O	2:E:314:MET:C	2.63	0.41
3:F:74:LYS:HE2	3:F:74:LYS:HB3	1.86	0.41
3:F:88:ASP:O	3:F:89:ARG:HB2	2.19	0.41
1:A:13:ILE:HG21	1:A:41:ALA:HB3	2.02	0.41
2:B:76:VAL:O	2:B:76:VAL:HG12	2.20	0.41
3:C:17:LEU:CD1	3:C:98:THR:HG22	2.50	0.41
3:C:103:LEU:HD23	3:C:103:LEU:HA	1.89	0.41
3:C:189:VAL:HA	3:C:195:MET:CE	2.50	0.41
1:D:20:LEU:CD2	1:D:31:SER:HB3	2.49	0.41
1:D:69:LEU:O	1:D:73:LEU:HG	2.19	0.41
1:D:534:ALA:O	1:D:535:ASN:C	2.63	0.41
2:E:169:ARG:O	2:E:172:LEU:HB2	2.20	0.41
2:E:169:ARG:HB3	2:E:213:GLU:HG2	2.03	0.41
2:E:322:ALA:H	2:E:360:MET:HE1	1.84	0.41
3:F:45:VAL:HG22	3:F:156:THR:OG1	2.20	0.41
3:F:81:LEU:C	3:F:81:LEU:HD23	2.45	0.41
3:F:264:ASN:O	3:F:265:TYR:C	2.62	0.41
1:A:77:THR:O	1:A:80:VAL:HG12	2.20	0.41
1:A:372:GLN:C	1:A:374:LYS:H	2.29	0.41
2:B:220:SER:O	2:B:221:ILE:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:SER:O	2:B:270:THR:C	2.64	0.41
2:B:408:LYS:C	2:B:410:LYS:N	2.77	0.41
3:C:76:PRO:HD3	3:C:107:TYR:CZ	2.53	0.41
3:C:203:PRO:HA	3:C:220:PHE:CE1	2.55	0.41
1:D:438:PHE:O	1:D:439:PHE:C	2.62	0.41
2:B:63:LEU:C	2:B:65:GLU:N	2.76	0.41
2:B:142:PRO:HG2	2:B:143:ASN:N	2.36	0.41
2:B:255:PRO:HG2	2:B:256:GLN:CD	2.45	0.41
1:D:288:GLN:HA	1:D:291:MET:HE3	2.02	0.41
2:E:169:ARG:O	2:E:170:ASP:C	2.64	0.41
1:A:536:VAL:O	1:A:540:VAL:HB	2.20	0.41
2:B:136:GLU:O	2:B:136:GLU:HG3	2.21	0.41
2:B:222:ILE:O	2:B:224:GLY:N	2.52	0.41
3:C:130:TYR:HA	3:C:143:TRP:CD1	2.56	0.41
3:C:252:HIS:O	3:C:253:ASP:C	2.63	0.41
1:D:214:SER:HA	1:D:221:ARG:CD	2.50	0.41
1:D:398:ARG:O	1:D:402:GLN:HB2	2.21	0.41
2:E:381:TYR:O	2:E:382:ASN:C	2.63	0.41
3:F:163:ILE:HD12	3:F:278:LEU:HD13	2.03	0.41
1:A:29:LEU:CD1	1:A:65:VAL:HA	2.50	0.41
1:A:29:LEU:CD1	1:A:65:VAL:HG22	2.50	0.41
1:A:284:VAL:N	1:A:285:PRO:CD	2.83	0.41
1:A:436:VAL:HG13	1:A:437:GLU:N	2.35	0.41
2:B:392:GLN:O	2:B:393:LYS:C	2.63	0.41
3:C:117:ASN:ND2	3:C:241:HIS:HE1	2.19	0.41
3:C:222:GLN:HA	3:C:252:HIS:CG	2.55	0.41
1:D:121:PRO:O	1:D:124:LEU:HB2	2.20	0.41
1:D:411:LEU:C	1:D:413:GLU:N	2.79	0.41
1:D:521:MET:O	1:D:522:LEU:C	2.62	0.41
2:E:141:GLN:HB3	2:E:142:PRO:CD	2.46	0.41
2:E:270:THR:C	2:E:272:THR:H	2.28	0.41
3:F:17:LEU:HD13	3:F:99:LEU:CA	2.50	0.41
1:A:105:ARG:HH11	1:A:142:THR:HB	1.86	0.41
1:A:221:ARG:O	1:A:224:ALA:HB3	2.20	0.41
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.78	0.41
2:B:310:PHE:CZ	2:B:318:PHE:HE1	2.39	0.41
2:B:368:SER:HB2	2:B:377:HIS:CD2	2.56	0.41
1:D:514:GLN:HG3	1:D:550:ILE:O	2.20	0.41
2:E:121:TRP:CG	2:E:167:ARG:HH12	2.39	0.41
2:E:329:HIS:CD2	2:E:331:GLN:HB2	2.56	0.41
3:F:44:ASN:ND2	3:F:185:ARG:HH11	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:115:ARG:HH12	3:F:151:ASP:HA	1.85	0.41
1:A:109:VAL:O	1:A:110:GLU:C	2.63	0.41
1:A:353:SER:HB3	1:A:354:PRO:CD	2.51	0.41
1:A:518:THR:OG1	1:A:551:LEU:HD23	2.21	0.41
2:B:154:VAL:HG11	2:B:190:ILE:HG13	2.02	0.41
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.86	0.41
2:B:356:ILE:O	2:B:359:ILE:HB	2.21	0.41
2:B:388:MET:C	2:B:390:MET:N	2.78	0.41
3:C:29:LYS:HB2	3:C:145:TYR:HE1	1.83	0.41
3:C:158:LEU:CD2	3:C:161:GLY:HA2	2.50	0.41
3:C:206:ARG:O	3:C:207:GLY:O	2.39	0.41
3:C:207:GLY:HA2	3:C:221:GLY:HA3	2.03	0.41
3:C:248:TYR:CE2	3:C:286:PHE:CD2	3.09	0.41
1:D:155:TYR:CE1	1:D:163:LYS:HB3	2.56	0.41
1:D:463:THR:HG23	1:D:504:CYS:HA	2.03	0.41
2:E:247:VAL:CG1	2:E:248:LYS:N	2.84	0.41
3:F:29:LYS:O	3:F:33:GLU:HG2	2.20	0.41
3:F:110:ARG:HD3	3:F:110:ARG:HA	1.93	0.41
3:F:206:ARG:O	3:F:207:GLY:O	2.39	0.41
1:A:24:ASP:C	1:A:24:ASP:OD2	2.63	0.41
1:A:405:LEU:HD23	1:A:430:LEU:HD11	2.03	0.41
1:A:424:ILE:CD1	1:A:458:ILE:HG23	2.51	0.41
1:A:502:LEU:HB3	1:A:543:SER:OG	2.20	0.41
2:B:39:CYS:C	2:B:41:VAL:N	2.78	0.41
2:B:227:LEU:HB2	2:B:228:PRO:CD	2.51	0.41
2:B:293:MET:O	2:B:294:PHE:C	2.62	0.41
2:B:313:ILE:O	2:B:316:PRO:HD2	2.21	0.41
3:C:103:LEU:CB	3:C:111:ILE:HD13	2.50	0.41
3:C:225:SER:HG	3:C:252:HIS:HD1	1.67	0.41
3:C:239:ARG:O	3:C:258:THR:HA	2.21	0.41
1:D:107:LYS:O	1:D:108:ALA:C	2.64	0.41
1:D:155:TYR:CZ	1:D:163:LYS:HB3	2.56	0.41
1:D:230:ASN:O	1:D:234:LEU:HG	2.21	0.41
1:D:253:GLU:O	1:D:254:ASP:C	2.63	0.41
1:D:327:LEU:HB3	1:D:328:PRO:HD3	2.01	0.41
1:D:368:LEU:O	1:D:369:PHE:C	2.64	0.41
1:D:398:ARG:H	1:D:398:ARG:HG2	1.67	0.41
2:E:31:LEU:C	2:E:33:ILE:N	2.78	0.41
2:E:221:ILE:H	2:E:221:ILE:HG13	1.66	0.41
2:E:366:ARG:O	2:E:368:SER:N	2.53	0.41
3:F:73:GLY:HA3	3:F:78:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:CYS:O	2:B:42:LEU:N	2.54	0.41
2:B:63:LEU:O	2:B:64:SER:C	2.63	0.41
3:C:94:VAL:O	3:C:95:GLU:C	2.64	0.41
1:D:86:VAL:HG13	1:D:87:HIS:N	2.36	0.41
1:D:248:LEU:HD11	1:D:270:LEU:HD13	2.03	0.41
1:D:424:ILE:CD1	1:D:458:ILE:HG23	2.51	0.41
1:D:483:ILE:N	1:D:484:PRO:CD	2.84	0.41
2:E:31:LEU:O	2:E:33:ILE:N	2.46	0.41
2:E:145:ALA:C	2:E:147:LYS:N	2.79	0.41
2:E:175:THR:HG22	2:E:179:ILE:HD11	2.03	0.41
2:E:200:ARG:HG3	2:E:204:GLU:OE1	2.20	0.41
2:E:390:MET:O	2:E:391:ASN:HB2	2.21	0.41
3:F:278:LEU:HB3	3:F:282:LEU:HD23	2.02	0.41
1:A:75:THR:C	1:A:77:THR:H	2.28	0.40
1:A:102:THR:HG22	1:A:105:ARG:CZ	2.48	0.40
1:A:384:ILE:HD13	1:A:384:ILE:O	2.21	0.40
1:A:535:ASN:O	1:A:539:ASN:HB2	2.20	0.40
2:B:54:LYS:C	2:B:56:LYS:H	2.29	0.40
2:B:124:LEU:O	2:B:125:GLN:C	2.63	0.40
2:B:244:LEU:HD21	2:B:253:TYR:CZ	2.56	0.40
2:B:254:HIS:HE1	2:B:297:GLU:OE1	2.04	0.40
3:C:6:PHE:O	3:C:9:GLU:N	2.54	0.40
3:C:244:VAL:O	3:C:244:VAL:CG2	2.66	0.40
1:D:78:THR:C	1:D:80:VAL:N	2.79	0.40
1:D:86:VAL:C	1:D:88:CYS:H	2.28	0.40
1:D:521:MET:C	1:D:523:PRO:CD	2.94	0.40
3:F:4:LYS:O	3:F:5:VAL:C	2.64	0.40
3:F:28:VAL:HG11	3:F:142:VAL:HG13	2.03	0.40
3:F:240:ALA:HB2	3:F:259:ILE:H	1.85	0.40
1:A:178:THR:HA	1:A:179:PRO:HD3	1.89	0.40
1:A:411:LEU:HB3	1:A:423:ILE:HG13	2.03	0.40
1:A:463:THR:O	1:A:466:LEU:HB2	2.22	0.40
2:B:329:HIS:CD2	2:B:331:GLN:HB2	2.56	0.40
3:C:263:PRO:CD	3:C:273:ALA:HB2	2.51	0.40
1:D:343:SER:HA	1:D:380:VAL:HG22	2.03	0.40
1:D:557:GLN:HG2	1:D:588:LEU:HD22	2.03	0.40
1:A:182:ARG:O	1:A:183:ARG:C	2.64	0.40
1:A:279:THR:O	1:A:284:VAL:HG23	2.22	0.40
1:A:392:ASN:HD21	1:A:433:GLN:HE22	1.70	0.40
1:A:456:TYR:HD1	1:A:457:ALA:N	2.19	0.40
1:A:509:SER:O	1:A:510:GLU:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:222:GLN:HA	3:F:252:HIS:CG	2.57	0.40
1:A:90:LEU:HB2	1:A:91:PRO:HD3	2.03	0.40
1:A:131:LEU:C	1:A:131:LEU:HD23	2.46	0.40
1:A:534:ALA:O	1:A:535:ASN:C	2.63	0.40
1:A:583:LEU:O	1:A:586:LEU:N	2.55	0.40
2:B:121:TRP:CD1	2:B:167:ARG:NH1	2.90	0.40
2:B:226:ALA:O	2:B:227:LEU:C	2.64	0.40
2:B:318:PHE:C	2:B:320:GLN:N	2.78	0.40
1:D:32:ILE:O	1:D:35:LEU:HB2	2.22	0.40
3:F:10:LEU:O	3:F:11:ASP:C	2.64	0.40
3:F:165:CYS:SG	3:F:238:SER:HB3	2.62	0.40
1:A:28:ARG:CD	1:A:60:TYR:HE2	2.35	0.40
2:B:39:CYS:CB	2:B:66:MET:HE1	2.51	0.40
2:B:150:ASP:CG	2:B:151:GLN:H	2.29	0.40
2:B:189:TYR:O	2:B:190:ILE:C	2.64	0.40
3:C:76:PRO:CB	3:C:110:ARG:HG3	2.46	0.40
3:C:212:SER:HA	3:C:219:THR:CG2	2.52	0.40
1:D:18:ASP:C	1:D:20:LEU:H	2.29	0.40
1:D:90:LEU:O	1:D:91:PRO:C	2.65	0.40
1:D:282:ASP:O	1:D:285:PRO:HD2	2.22	0.40
1:D:438:PHE:C	1:D:438:PHE:HD1	2.28	0.40
2:E:242:LEU:C	2:E:244:LEU:N	2.79	0.40
3:F:43:SER:OG	3:F:45:VAL:C	2.64	0.40
3:F:309:LEU:HD23	3:F:309:LEU:HA	1.85	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	580/589 (98%)	469 (81%)	94 (16%)	17 (3%)	3 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	580/589 (98%)	481 (83%)	85 (15%)	14 (2%)	4	24
2	B	386/449 (86%)	273 (71%)	78 (20%)	35 (9%)	0	3
2	E	386/449 (86%)	277 (72%)	72 (19%)	37 (10%)	0	3
3	C	306/309 (99%)	245 (80%)	44 (14%)	17 (6%)	1	9
3	F	306/309 (99%)	250 (82%)	42 (14%)	14 (5%)	2	13
4	X	1/7 (14%)	1 (100%)	0	0	100	100
4	Y	1/7 (14%)	1 (100%)	0	0	100	100
All	All	2546/2708 (94%)	1997 (78%)	415 (16%)	134 (5%)	1	10

All (134) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	391	VAL
2	B	43	PHE
2	B	45	PHE
2	B	55	TRP
2	B	57	GLU
2	B	73	ASN
2	B	76	VAL
2	B	134	PHE
2	B	165	ASP
2	B	314	MET
2	B	367	ASN
3	C	183	LEU
3	C	245	MET
1	D	25	VAL
1	D	391	VAL
1	D	404	LEU
2	E	43	PHE
2	E	45	PHE
2	E	55	TRP
2	E	57	GLU
2	E	73	ASN
2	E	76	VAL
2	E	165	ASP
2	E	314	MET
2	E	367	ASN
3	F	245	MET
1	A	318	ARG

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Mol	Chain	Res	Type
1	A	404	LEU
1	A	412	ALA
1	A	415	ALA
1	A	443	LEU
1	A	558	SER
2	B	33	ILE
2	B	72	HIS
2	B	146	LYS
2	B	161	PHE
2	B	223	ASN
2	B	393	LYS
3	C	106	ARG
3	C	207	GLY
3	C	241	HIS
3	C	254	ARG
3	C	265	TYR
3	C	269	CYS
3	C	301	THR
1	D	79	LEU
1	D	318	ARG
1	D	558	SER
2	E	33	ILE
2	E	36	LEU
2	E	72	HIS
2	E	134	PHE
2	E	146	LYS
2	E	161	PHE
2	E	251	SER
2	E	391	ASN
3	F	183	LEU
3	F	186	LEU
3	F	207	GLY
3	F	265	TYR
3	F	285	SER
3	F	301	THR
1	A	41	ALA
1	A	76	PHE
1	A	79	LEU
1	A	103	VAL
1	A	556	LEU
2	B	104	THR
2	B	142	PRO

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Mol	Chain	Res	Type
2	B	163	SER
2	B	166	PRO
2	B	351	ASP
2	B	374	LYS
2	B	391	ASN
2	B	409	GLU
3	C	285	SER
1	D	415	ALA
1	D	443	LEU
1	D	556	LEU
2	E	51	SER
2	E	104	THR
2	E	142	PRO
2	E	166	PRO
2	E	188	ALA
2	E	351	ASP
2	E	393	LYS
3	F	106	ARG
3	F	129	PHE
3	F	241	HIS
3	F	254	ARG
1	A	320	ASN
2	B	167	ARG
2	B	187	ARG
3	C	280	ASP
1	D	103	VAL
2	E	167	ARG
2	E	271	LEU
2	E	334	GLU
2	E	413	MET
2	B	413	MET
3	C	41	LYS
3	C	161	GLY
1	D	41	ALA
2	E	163	SER
2	E	223	ASN
2	E	224	GLY
2	E	374	LYS
3	F	161	GLY
1	A	584	THR
2	B	36	LEU
2	B	81	ILE

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Mol	Chain	Res	Type
2	B	143	ASN
2	B	188	ALA
2	B	224	GLY
2	B	389	GLU
1	D	412	ALA
2	E	32	PHE
2	E	409	GLU
1	D	484	PRO
3	F	300	VAL
1	A	306	VAL
2	B	79	GLU
2	B	103	PRO
2	E	79	GLU
2	E	228	PRO
1	A	548	GLY
3	C	5	VAL
3	C	300	VAL
2	E	81	ILE
3	F	194	PRO
3	C	168	GLY
3	C	297	GLU
1	D	104	VAL

5.3.2 Protein sidechains [i](#)

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	509/512 (99%)	474 (93%)	35 (7%)	14	41
1	D	509/512 (99%)	475 (93%)	34 (7%)	15	42
2	B	331/414 (80%)	304 (92%)	27 (8%)	10	35
2	E	331/414 (80%)	303 (92%)	28 (8%)	10	33
3	C	273/274 (100%)	259 (95%)	14 (5%)	21	50
3	F	273/274 (100%)	259 (95%)	14 (5%)	21	50
4	X	2/2 (100%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Y	2/2 (100%)	2 (100%)	0	100	100
All	All	2230/2404 (93%)	2078 (93%)	152 (7%)	14	42

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	40	LEU
1	A	44	VAL
1	A	88	CYS
1	A	89	LEU
1	A	91	PRO
1	A	101	GLU
1	A	122	SER
1	A	145	THR
1	A	160	SER
1	A	177	ASP
1	A	178	THR
1	A	180	MET
1	A	197	GLU
1	A	198	LEU
1	A	217	GLN
1	A	222	LEU
1	A	237	GLN
1	A	294	CYS
1	A	295	GLU
1	A	348	VAL
1	A	350	MET
1	A	370	LEU
1	A	382	LEU
1	A	384	ILE
1	A	389	ASP
1	A	391	VAL
1	A	398	ARG
1	A	399	GLN
1	A	404	LEU
1	A	409	VAL
1	A	411	LEU
1	A	456	TYR
1	A	476	GLU
1	A	540	VAL
2	B	76	VAL

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Mol	Chain	Res	Type
2	B	95	ARG
2	B	96	THR
2	B	101	SER
2	B	132	LEU
2	B	134	PHE
2	B	135	LEU
2	B	139	ASP
2	B	162	ASP
2	B	166	PRO
2	B	167	ARG
2	B	170	ASP
2	B	186	LEU
2	B	256	GLN
2	B	263	GLN
2	B	264	PHE
2	B	285	LYS
2	B	289	PRO
2	B	305	ILE
2	B	317	LEU
2	B	337	LEU
2	B	357	LEU
2	B	371	HIS
2	B	375	THR
2	B	381	TYR
2	B	413	MET
2	B	415	GLU
3	C	7	THR
3	C	10	LEU
3	C	34	LYS
3	C	44	ASN
3	C	75	SER
3	C	76	PRO
3	C	119	GLU
3	C	211	ILE
3	C	235	THR
3	C	239	ARG
3	C	242	GLN
3	C	280	ASP
3	C	284	TYR
3	C	304	THR
1	D	36	SER
1	D	37	THR

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Mol	Chain	Res	Type
1	D	40	LEU
1	D	44	VAL
1	D	91	PRO
1	D	101	GLU
1	D	122	SER
1	D	145	THR
1	D	177	ASP
1	D	178	THR
1	D	180	MET
1	D	197	GLU
1	D	198	LEU
1	D	204	GLU
1	D	210	SER
1	D	237	GLN
1	D	294	CYS
1	D	295	GLU
1	D	321	VAL
1	D	350	MET
1	D	370	LEU
1	D	373	LEU
1	D	382	LEU
1	D	384	ILE
1	D	391	VAL
1	D	398	ARG
1	D	399	GLN
1	D	403	SER
1	D	409	VAL
1	D	411	LEU
1	D	414	ASP
1	D	476	GLU
1	D	515	ASP
1	D	540	VAL
2	E	76	VAL
2	E	83	PRO
2	E	95	ARG
2	E	132	LEU
2	E	134	PHE
2	E	135	LEU
2	E	139	ASP
2	E	162	ASP
2	E	165	ASP
2	E	166	PRO

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Mol	Chain	Res	Type
2	E	167	ARG
2	E	170	ASP
2	E	214	LEU
2	E	232	GLU
2	E	256	GLN
2	E	263	GLN
2	E	264	PHE
2	E	285	LYS
2	E	305	ILE
2	E	317	LEU
2	E	337	LEU
2	E	357	LEU
2	E	371	HIS
2	E	375	THR
2	E	379	LEU
2	E	381	TYR
2	E	413	MET
2	E	415	GLU
3	F	7	THR
3	F	10	LEU
3	F	34	LYS
3	F	43	SER
3	F	44	ASN
3	F	76	PRO
3	F	119	GLU
3	F	134	LEU
3	F	187	GLN
3	F	211	ILE
3	F	239	ARG
3	F	242	GLN
3	F	280	ASP
3	F	284	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	72	GLN
1	A	119	HIS
1	A	127	HIS
1	A	200	ASN
1	A	217	GLN

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Mol	Chain	Res	Type
1	A	230	ASN
1	A	271	GLN
1	A	325	GLN
1	A	338	ASN
1	A	364	HIS
1	A	387	ASN
1	A	392	ASN
1	A	399	GLN
1	A	433	GLN
1	A	444	ASN
1	A	465	ASN
1	A	497	HIS
1	A	506	ASN
1	A	520	HIS
1	A	545	GLN
1	A	571	GLN
1	A	580	GLN
2	B	123	HIS
2	B	143	ASN
2	B	156	GLN
2	B	193	GLN
2	B	207	HIS
2	B	208	HIS
2	B	233	HIS
2	B	254	HIS
2	B	329	HIS
2	B	331	GLN
2	B	373	ASN
2	B	377	HIS
2	B	382	ASN
2	B	392	GLN
3	C	12	GLN
3	C	44	ASN
3	C	179	HIS
3	C	187	GLN
1	D	22	ASN
1	D	72	GLN
1	D	119	HIS
1	D	200	ASN
1	D	217	GLN
1	D	230	ASN
1	D	304	HIS

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Mol	Chain	Res	Type
1	D	338	ASN
1	D	383	ASN
1	D	392	ASN
1	D	399	GLN
1	D	433	GLN
1	D	444	ASN
1	D	465	ASN
1	D	479	HIS
1	D	506	ASN
1	D	545	GLN
1	D	553	ASN
1	D	571	GLN
1	D	580	GLN
2	E	92	ASN
2	E	156	GLN
2	E	207	HIS
2	E	208	HIS
2	E	223	ASN
2	E	254	HIS
2	E	263	GLN
2	E	329	HIS
2	E	331	GLN
2	E	373	ASN
2	E	377	HIS
2	E	382	ASN
2	E	392	GLN
3	F	12	GLN
3	F	44	ASN
3	F	179	HIS
3	F	187	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FGA	Y	6	4	5,6,9	1.33	1 (20%)	5,6,11	0.53	0
4	ACB	X	3	-	7,8,9	2.05	1 (14%)	8,10,12	0.96	0
4	DAM	Y	7	4,3	4,5,6	1.58	1 (25%)	3,5,7	4.13	2 (66%)
4	DAM	X	7	4,3	4,5,6	1.84	1 (25%)	3,5,7	4.21	3 (100%)
4	FGA	X	6	4	5,6,9	1.22	0	5,6,11	0.36	0
4	1ZN	Y	5	4	21,23,24	1.22	2 (9%)	25,29,31	0.80	0
4	ACB	Y	3	-	7,8,9	1.89	1 (14%)	8,10,12	1.00	0
4	1ZN	X	5	4	21,23,24	1.20	2 (9%)	25,29,31	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FGA	Y	6	4	-	0/4/4/9	-
4	ACB	X	3	-	-	2/10/10/12	-
4	DAM	Y	7	4,3	-	0/0/4/6	-
4	DAM	X	7	4,3	-	0/0/4/6	-
4	FGA	X	6	4	-	1/4/4/9	-
4	1ZN	Y	5	4	-	1/23/25/27	0/1/1/1
4	ACB	Y	3	-	-	2/10/10/12	-
4	1ZN	X	5	4	-	1/23/25/27	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	3	ACB	CA-N	4.59	1.60	1.47
4	Y	3	ACB	CA-N	4.33	1.59	1.47
4	X	7	DAM	C-CA	3.12	1.50	1.45
4	Y	7	DAM	C-CA	2.54	1.49	1.45
4	X	5	1ZN	C9-C4	2.37	1.43	1.38
4	Y	5	1ZN	C3-C2	2.30	1.55	1.52
4	X	5	1ZN	C3-C2	2.23	1.55	1.52
4	Y	5	1ZN	C9-C4	2.22	1.43	1.38
4	Y	6	FGA	CB-CA	-2.16	1.50	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	7	DAM	O-C-CA	-5.32	118.41	125.33
4	Y	7	DAM	O-C-CA	-4.89	118.97	125.33
4	Y	7	DAM	CM-N-CA	-4.81	116.68	123.98
4	X	7	DAM	CM-N-CA	-4.47	117.20	123.98
4	X	7	DAM	CB-CA-N	-2.23	120.35	125.84

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	3	ACB	C4-CB-CG-OD1
4	Y	3	ACB	C4-CB-CG-OD1
4	X	3	ACB	CA-CB-CG-OD1
4	Y	3	ACB	CA-CB-CG-OD1
4	X	5	1ZN	C10-C2-C3-C4
4	Y	5	1ZN	C10-C2-C3-C4
4	X	6	FGA	CA-CB-CG-CD

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	6	FGA	1	0
4	Y	7	DAM	3	0
4	X	7	DAM	2	0
4	Y	5	1ZN	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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

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	582/589 (98%)	-0.30	4 (0%) 84 70	25, 65, 112, 147	0
1	D	582/589 (98%)	-0.38	3 (0%) 87 76	22, 53, 109, 145	0
2	B	388/449 (86%)	0.13	13 (3%) 48 32	31, 81, 140, 155	0
2	E	388/449 (86%)	0.04	21 (5%) 31 21	28, 75, 136, 155	0
3	C	308/309 (99%)	-0.26	3 (0%) 79 63	26, 68, 110, 168	0
3	F	308/309 (99%)	-0.03	5 (1%) 70 52	27, 64, 109, 169	0
4	X	2/7 (28%)	0.69	0 100 100	91, 91, 91, 103	0
4	Y	2/7 (28%)	-0.17	0 100 100	76, 76, 76, 96	0
All	All	2560/2708 (94%)	-0.16	49 (1%) 66 48	22, 65, 127, 169	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	130	PHE	4.1
2	E	79	GLU	3.8
2	E	104	THR	3.5
2	E	52	ASP	3.5
2	B	83	PRO	3.4
2	E	75	ASN	3.2
2	E	415	GLU	3.1
3	F	284	TYR	3.1
2	B	28	GLN	3.1
2	B	39	CYS	3.0
2	E	28	GLN	2.9
2	E	83	PRO	2.9
2	E	134	PHE	2.8
1	D	390	CYS	2.8
2	B	51	SER	2.6
2	E	58	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	51	SER	2.6
2	B	415	GLU	2.6
3	F	80	TYR	2.5
3	F	300	VAL	2.5
1	A	389	ASP	2.4
2	B	73	ASN	2.4
1	A	391	VAL	2.4
1	A	588	LEU	2.4
3	F	214	ARG	2.3
3	C	298	PRO	2.3
3	F	82	PHE	2.3
2	E	369	LYS	2.3
3	C	309	LEU	2.2
2	E	367	ASN	2.2
2	E	131	PHE	2.2
2	E	49	PRO	2.2
2	B	134	PHE	2.2
2	E	139	ASP	2.2
2	E	82	TYR	2.2
2	E	53	LEU	2.2
1	D	447	CYS	2.2
2	E	140	PHE	2.1
2	B	48	ASP	2.1
2	B	30	LYS	2.1
2	B	227	LEU	2.1
2	E	137	SER	2.1
3	C	159	VAL	2.1
2	E	30	LYS	2.1
2	E	56	LYS	2.1
2	B	70	ILE	2.1
1	A	426	TYR	2.0
1	D	439	PHE	2.0
2	B	32	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
4	FGA	X	6	7/10	0.52	0.27	81,88,93,97	0
4	FGA	Y	6	7/10	0.68	0.26	77,81,87,93	0
4	ACB	X	3	9/10	0.92	0.12	93,97,99,101	0
4	DAL	Y	1	5/6	0.93	0.09	72,72,73,74	0
4	1ZN	Y	5	23/24	0.93	0.14	64,74,82,84	0
4	DAM	Y	7	6/7	0.93	0.09	72,77,79,81	0
4	DAM	X	7	6/7	0.94	0.08	76,80,81,82	0
4	1ZN	X	5	23/24	0.94	0.17	64,70,89,93	0
4	DAL	X	1	5/6	0.95	0.09	77,77,80,80	0
4	ACB	Y	3	9/10	0.96	0.11	80,85,92,93	0

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(\AA^2)	Q<0.9
5	MN	C	502	1/1	0.93	0.08	65,65,65,65	0
5	MN	F	502	1/1	0.94	0.06	56,56,56,56	0
5	MN	F	501	1/1	0.99	0.03	35,35,35,35	0
5	MN	C	501	1/1	0.99	0.04	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.