



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 09:23 AM EDT

PDB ID : 8BAL / pdb_00008bal
Title : Niako3494, a bacterial protein structure in glycoside hydrolase family 20
Authors : Dong, M.D.; Roth, C.R.; Jin, Y.J.
Deposited on : 2022-10-11
Resolution : 2.27 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

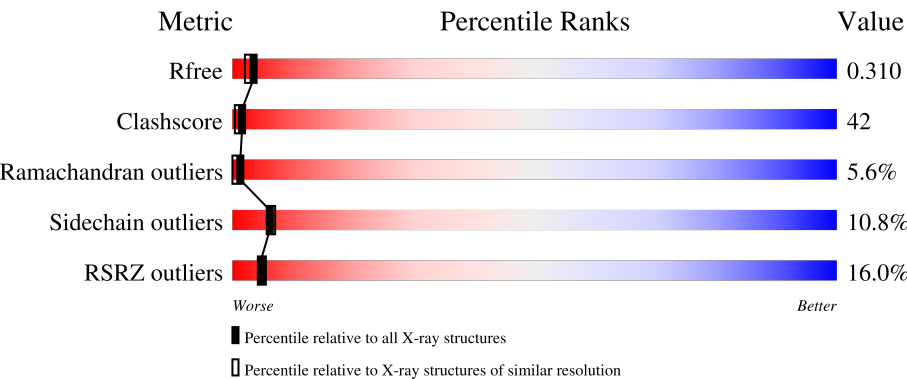
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	380	5% 32%49%9%•9%
1	C	380	20% 26%47%13%•13%
1	D	380	10% 36%46%6%•10%
1	E	380	18% 28%46%12%•12%
1	F	380	18% 32%51%8%8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13749 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 Beta-N-acetylhexosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	1	0
			2795	1802	472	500	21			
1	C	330	Total	C	N	O	S	0	0	0
			2657	1715	447	475	20			
1	D	343	Total	C	N	O	S	0	0	0
			2763	1783	467	494	19			
1	E	335	Total	C	N	O	S	0	0	0
			2697	1733	459	486	19			
1	F	348	Total	C	N	O	S	0	0	0
			2804	1808	473	503	20			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	C	3	Total	O	0	0
			3	3		

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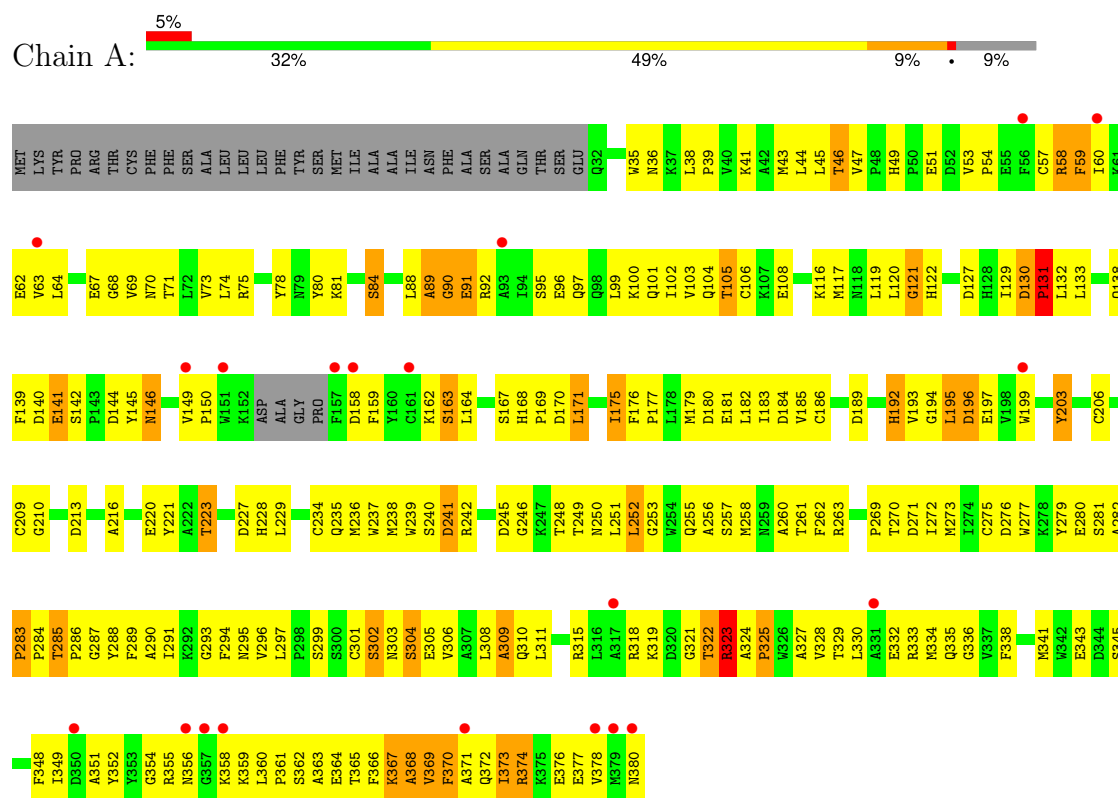
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	9	Total 9	O 9	0	0
3	E	3	Total 3	O 3	0	0
3	F	8	Total 8	O 8	0	0

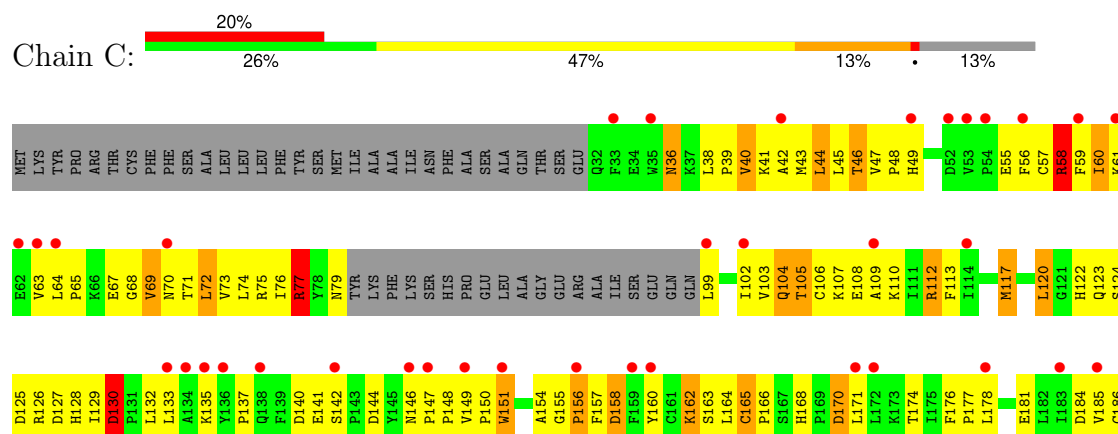
3 Residue-property plots

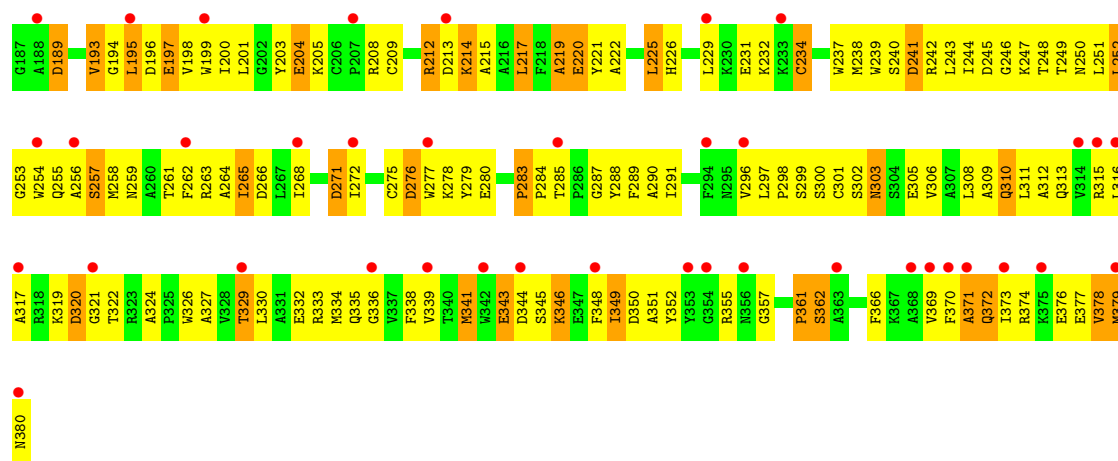
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

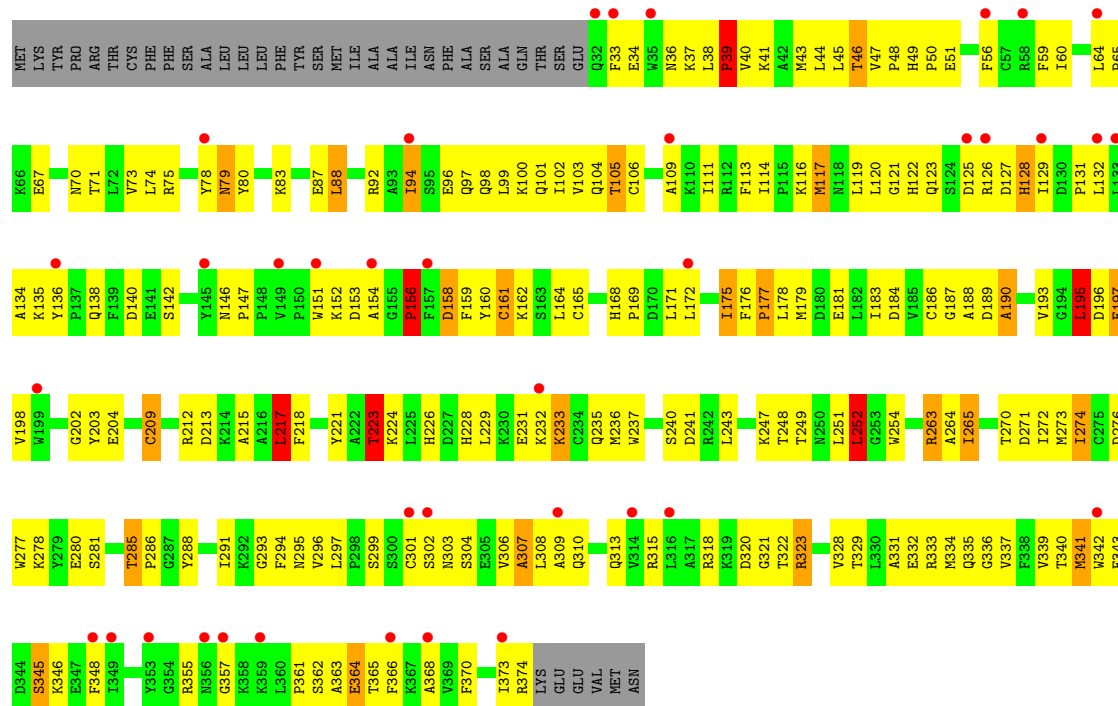


• Molecule 1: Beta-N-acetylhexosaminidase

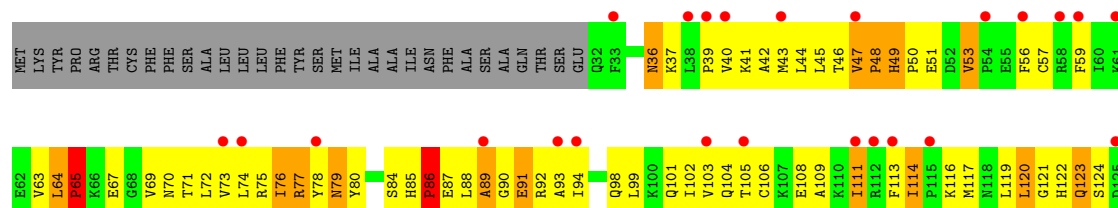


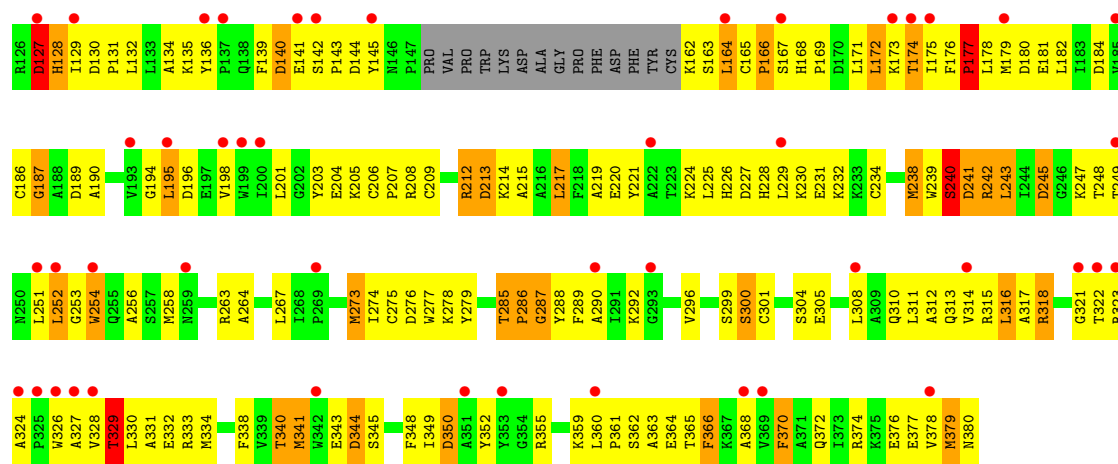


• Molecule 1: Beta-N-acetylhexosaminidase

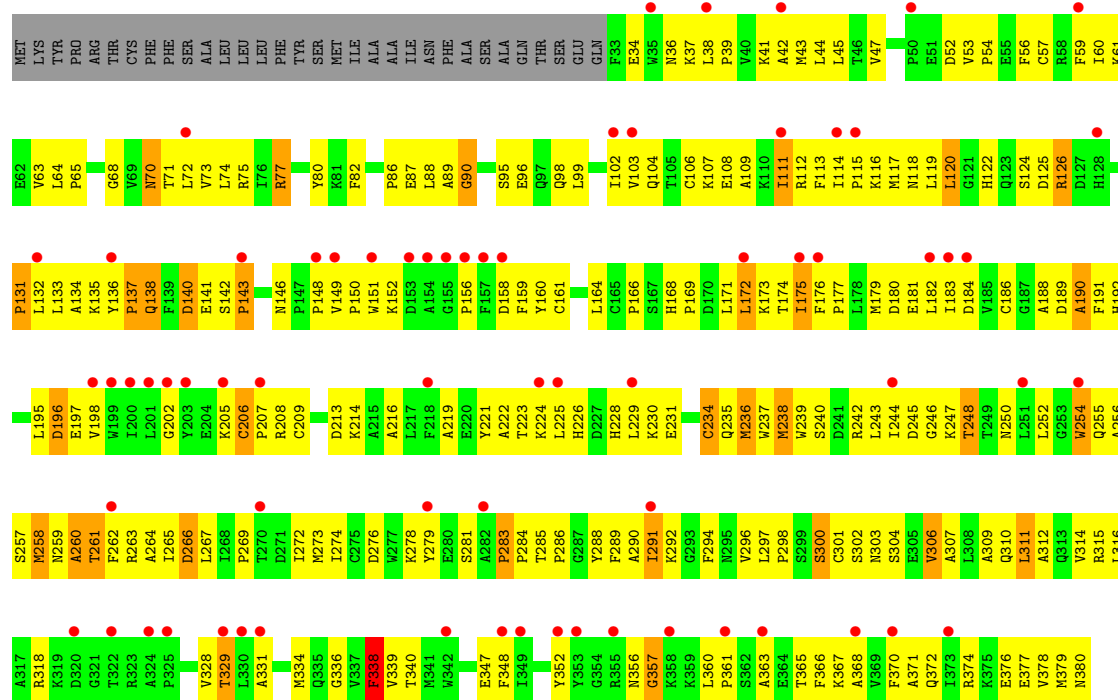


• Molecule 1: Beta-N-acetylhexosaminidase





● Molecule 1: Beta-N-acetylhexosaminidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	146.99Å 254.59Å 139.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.49 – 2.27 73.49 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.9 (73.49-2.27) 99.7 (73.49-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.283 , 0.356 0.248 , 0.310	Depositor DCC
R_{free} test set	6126 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.064 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.069 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
Reported twinning fraction	0.332 for H, K, L 0.334 for 1/2H+1/2K, 3/2H-1/2K, -L 0.334 for 1/2H-1/2K, -3/2H-1/2K, -L	Depositor
Outliers	0 of 120467 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13749	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.62	0/2872	1.28	11/3890 (0.3%)
1	C	0.54	0/2731	1.14	6/3703 (0.2%)
1	D	0.58	0/2842	1.24	11/3854 (0.3%)
1	E	0.54	0/2767	1.15	8/3745 (0.2%)
1	F	0.53	0/2883	1.13	6/3908 (0.2%)
All	All	0.56	0/14095	1.19	42/19100 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	C	0	6
1	D	0	3
1	E	0	6
1	F	0	1
All	All	0	21

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	PRO	N-CA-C	11.94	125.27	110.70
1	C	320	ASP	CA-CB-CG	9.57	122.17	112.60
1	A	196	ASP	CA-CB-CG	8.72	121.32	112.60
1	D	156	PRO	N-CA-CB	-8.64	94.18	103.25
1	D	223	THR	CA-CB-OG1	-7.89	97.77	109.60
1	E	65	PRO	N-CA-CB	-7.30	95.59	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	THR	CB-CA-C	6.79	122.40	110.85
1	D	271	ASP	CA-CB-CG	6.78	119.38	112.60
1	E	338	PHE	CA-CB-CG	6.71	120.51	113.80
1	E	36	ASN	CA-CB-CG	6.50	119.10	112.60
1	A	203	TYR	CB-CA-C	6.34	120.49	109.65
1	A	223	THR	CA-CB-OG1	-6.33	100.11	109.60
1	D	46	THR	CA-CB-OG1	-6.29	100.16	109.60
1	E	127	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	269	PRO	CB-CA-C	-6.10	102.99	110.98
1	F	137	PRO	N-CA-CB	-6.03	96.92	103.25
1	C	350	ASP	CB-CA-C	5.92	120.62	110.79
1	F	283	PRO	N-CA-C	5.89	117.89	110.70
1	A	127	ASP	CA-CB-CG	5.72	118.32	112.60
1	D	103	VAL	N-CA-C	-5.72	107.24	112.96
1	D	223	THR	CB-CA-C	5.69	121.74	110.42
1	D	156	PRO	N-CA-C	5.66	124.13	112.47
1	E	329	THR	CA-CB-OG1	-5.61	101.19	109.60
1	A	131	PRO	N-CA-C	5.57	122.05	113.75
1	A	141	GLU	N-CA-C	-5.57	106.84	113.97
1	F	70	ASN	CB-CA-C	5.55	118.02	109.03
1	C	271	ASP	CA-CB-CG	5.51	118.11	112.60
1	C	283	PRO	N-CA-C	5.47	117.38	110.70
1	F	283	PRO	CB-CA-C	-5.47	104.25	110.92
1	C	263	ARG	N-CA-C	-5.45	106.59	113.18
1	E	140	ASP	CA-CB-CG	5.39	117.99	112.60
1	C	125	ASP	CA-CB-CG	5.38	117.98	112.60
1	D	218	PHE	N-CA-C	-5.36	105.44	111.28
1	E	177	PRO	N-CA-CB	-5.31	97.67	103.25
1	A	146	ASN	CB-CA-C	5.31	117.03	108.91
1	D	217	LEU	CA-C-N	5.28	127.35	120.28
1	D	217	LEU	C-N-CA	5.28	127.35	120.28
1	F	254	TRP	N-CA-C	-5.25	106.93	113.55
1	A	297	LEU	CB-CA-C	-5.17	104.43	110.17
1	D	323	ARG	N-CA-C	-5.15	107.54	113.88
1	E	350	ASP	CA-CB-CG	5.13	117.73	112.60
1	F	138	GLN	N-CA-C	-5.04	106.98	112.72

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	203	TYR	Peptide
1	A	242	ARG	Sidechain
1	A	323	ARG	Sidechain
1	A	374	ARG	Sidechain
1	C	112	ARG	Sidechain
1	C	130	ASP	Peptide
1	C	154	ALA	Peptide
1	C	208	ARG	Sidechain
1	C	212	ARG	Sidechain
1	C	77	ARG	Sidechain
1	D	154	ALA	Peptide
1	D	263	ARG	Sidechain
1	D	297	LEU	Peptide
1	E	173	LYS	Peptide
1	E	212	ARG	Sidechain
1	E	240	SER	Peptide
1	E	242	ARG	Sidechain
1	E	318	ARG	Sidechain
1	E	76	ILE	Peptide
1	F	318	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2795	0	2771	226	0
1	C	2657	0	2638	279	0
1	D	2763	0	2741	212	0
1	E	2697	0	2686	251	0
1	F	2804	0	2780	240	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	5	0	0	3	0
3	C	3	0	0	0	0
3	D	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	3	0	0	4	0
3	F	8	0	0	6	0
All	All	13749	0	13616	1151	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 42.

All (1151) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:SER:O	1:A:365:THR:OG1	1.56	1.22
1:A:245:ASP:O	1:A:249:THR:OG1	1.69	1.09
1:E:165:CYS:SG	1:E:208:ARG:NH1	2.27	1.05
1:C:158:ASP:O	1:F:247:LYS:HE3	1.58	1.03
1:A:39:PRO:HD2	1:A:335:GLN:O	1.59	1.03
1:F:190:ALA:N	1:F:234:CYS:SG	2.32	1.03
1:C:158:ASP:O	1:F:247:LYS:CE	2.07	1.01
1:E:240:SER:OG	1:E:276:ASP:HA	1.61	1.00
1:D:87:GLU:OE1	1:D:136:TYR:OH	1.79	0.99
1:A:193:VAL:HG21	1:A:236:MET:HE3	1.43	0.98
1:F:133:LEU:HD13	1:F:140:ASP:HB2	1.45	0.96
1:A:51:GLU:HG3	1:E:98:GLN:NE2	1.82	0.94
1:A:84:SER:OG	1:A:181:GLU:OE2	1.86	0.92
1:A:318:ARG:HG2	1:A:318:ARG:HH11	1.32	0.92
1:F:296:VAL:O	1:F:297:LEU:HD23	1.69	0.91
1:E:120:LEU:HD12	1:E:164:LEU:HB2	1.52	0.90
1:E:374:ARG:O	1:E:378:VAL:HG23	1.72	0.90
1:C:164:LEU:O	1:C:166:PRO:HD3	1.72	0.89
1:D:160:TYR:OH	1:D:197:GLU:OE2	1.89	0.89
1:D:135:LYS:O	1:D:136:TYR:HD1	1.56	0.89
1:E:77:ARG:NH2	1:E:130:ASP:OD2	2.04	0.88
1:A:367:LYS:O	1:A:369:VAL:N	2.06	0.88
1:A:199:TRP:CH2	1:A:253:GLY:O	2.28	0.87
1:F:57:CYS:SG	1:F:102:ILE:HG12	2.14	0.87
1:C:200:ILE:HA	1:F:248:THR:HA	1.57	0.87
1:E:47:VAL:HG12	1:E:75:ARG:O	1.73	0.87
1:C:253:GLY:N	1:C:258:MET:HE2	1.91	0.86
1:D:135:LYS:O	1:D:136:TYR:CD1	2.29	0.85
1:A:324:ALA:HB1	1:A:325:PRO:HD2	1.58	0.85
1:C:156:PRO:O	1:C:254:TRP:CZ2	2.30	0.84
1:E:47:VAL:CG1	1:E:75:ARG:O	2.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:THR:N	1:F:266:ASP:OD2	2.11	0.84
1:A:370:PHE:HA	1:A:373:ILE:HD12	1.58	0.84
1:E:370:PHE:O	1:E:374:ARG:NH1	2.11	0.84
1:F:133:LEU:HD21	1:F:164:LEU:HD23	1.60	0.83
1:E:41:LYS:HE3	1:E:70:ASN:HD22	1.43	0.83
1:A:47:VAL:HG23	1:A:74:LEU:HD21	1.60	0.83
1:E:240:SER:OG	1:E:275:CYS:O	1.97	0.83
1:C:229:LEU:HB3	1:C:234:CYS:HB3	1.59	0.83
1:A:51:GLU:HG3	1:E:98:GLN:HE21	1.41	0.82
1:E:164:LEU:HD13	1:E:171:LEU:HD21	1.59	0.82
1:E:372:GLN:HG3	1:E:376:GLU:OE2	1.80	0.82
1:C:308:LEU:HD23	1:C:311:LEU:HD23	1.60	0.81
1:A:253:GLY:HA2	3:A:501:HOH:O	1.80	0.81
1:A:258:MET:N	3:A:501:HOH:O	2.14	0.81
1:D:36:ASN:O	1:D:315:ARG:NH1	2.12	0.81
1:C:76:ILE:O	1:C:79:ASN:ND2	2.13	0.81
1:A:64:LEU:HD13	1:A:69:VAL:HG11	1.60	0.81
1:A:302:SER:HA	1:A:362:SER:HA	1.63	0.81
1:C:122:HIS:NE2	1:C:197:GLU:OE2	2.14	0.81
1:D:229:LEU:HD12	1:D:236:MET:HB2	1.63	0.80
1:C:303:ASN:OD1	1:C:303:ASN:C	2.24	0.80
1:E:42:ALA:HA	1:E:71:THR:HB	1.64	0.79
1:A:245:ASP:C	1:A:249:THR:HG1	1.87	0.79
1:A:70:ASN:OD1	1:A:71:THR:OG1	1.99	0.79
1:A:246:GLY:O	1:A:250:ASN:HA	1.81	0.79
1:A:324:ALA:HB1	1:A:325:PRO:CD	2.12	0.79
1:D:215:ALA:HB3	1:D:263:ARG:NH1	1.97	0.79
1:E:290:ALA:HB2	1:E:334:MET:HE2	1.64	0.79
1:F:370:PHE:O	1:F:374:ARG:NH1	2.15	0.79
1:E:254:TRP:HA	3:E:502:HOH:O	1.84	0.78
1:A:323:ARG:HH11	1:A:323:ARG:CG	1.96	0.78
1:A:370:PHE:O	1:A:374:ARG:NH1	2.17	0.78
1:C:247:LYS:HB3	1:F:265:ILE:HG22	1.64	0.78
1:C:324:ALA:HB1	1:C:326:TRP:CE2	2.18	0.78
1:A:51:GLU:O	1:A:51:GLU:HG2	1.82	0.77
1:C:155:GLY:C	1:C:157:PHE:H	1.92	0.77
1:C:103:VAL:HG21	1:C:186:CYS:SG	2.23	0.77
1:E:53:VAL:HG11	1:E:98:GLN:HB3	1.65	0.77
1:C:156:PRO:O	1:C:157:PHE:HD1	1.66	0.77
1:E:245:ASP:OD1	1:E:248:THR:N	2.18	0.77
1:D:79:ASN:N	1:D:79:ASN:HD22	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:GLY:O	1:C:291:ILE:HD12	1.86	0.76
1:E:213:ASP:OD1	1:E:213:ASP:C	2.28	0.76
1:A:179:MET:HE2	1:A:229:LEU:HD21	1.68	0.75
1:E:87:GLU:OE1	1:E:136:TYR:OH	2.04	0.75
1:E:254:TRP:CG	3:E:502:HOH:O	2.38	0.75
1:E:349:ILE:O	1:E:352:TYR:HB3	1.86	0.75
1:E:47:VAL:O	1:E:47:VAL:HG13	1.87	0.74
1:F:213:ASP:CG	1:F:263:ARG:HH22	1.94	0.74
1:C:158:ASP:O	1:F:247:LYS:HE2	1.87	0.74
1:A:36:ASN:O	1:A:315:ARG:NH1	2.18	0.74
1:D:179:MET:O	1:D:183:ILE:HG13	1.88	0.74
1:C:129:ILE:O	1:C:130:ASP:C	2.31	0.74
1:E:254:TRP:CA	3:E:502:HOH:O	2.33	0.74
1:C:199:TRP:CE3	1:F:247:LYS:HD3	2.24	0.73
1:E:196:ASP:HA	1:E:241:ASP:OD2	1.88	0.73
1:F:328:VAL:O	1:F:329:THR:C	2.31	0.73
1:A:305:GLU:HB3	1:D:323:ARG:HH12	1.53	0.73
1:F:283:PRO:O	1:F:285:THR:N	2.19	0.73
1:C:253:GLY:CA	1:C:258:MET:HE2	2.18	0.73
1:F:228:HIS:O	1:F:231:GLU:N	2.20	0.73
1:C:140:ASP:OD2	1:C:162:LYS:NZ	2.17	0.72
1:A:374:ARG:O	1:A:378:VAL:HG23	1.88	0.72
1:E:129:ILE:HG22	1:E:134:ALA:HB2	1.71	0.72
1:A:70:ASN:O	1:A:71:THR:OG1	2.06	0.72
1:F:182:LEU:HD12	1:F:191:PHE:CE2	2.24	0.72
1:F:132:LEU:HD23	1:F:164:LEU:HD21	1.71	0.72
1:D:160:TYR:CZ	1:D:197:GLU:OE2	2.42	0.71
1:F:37:LYS:NZ	1:F:377:GLU:O	2.23	0.71
1:C:165:CYS:SG	1:C:165:CYS:O	2.47	0.71
1:D:46:THR:OG1	1:D:341:MET:SD	2.48	0.71
1:C:67:GLU:HA	1:C:374:ARG:HH11	1.54	0.71
1:C:277:TRP:HB3	1:C:299:SER:HB2	1.72	0.71
1:E:286:PRO:O	1:E:287:GLY:C	2.32	0.71
1:F:45:LEU:HD11	1:F:59:PHE:HE2	1.53	0.71
1:C:166:PRO:HA	1:C:171:LEU:HD22	1.71	0.71
1:D:59:PHE:CE2	1:D:64:LEU:HD21	2.25	0.71
1:D:87:GLU:OE2	1:D:87:GLU:N	2.21	0.71
1:C:156:PRO:O	1:C:254:TRP:HZ2	1.74	0.71
1:F:189:ASP:O	1:F:190:ALA:HB2	1.90	0.71
1:A:311:LEU:HD23	1:A:376:GLU:OE1	1.91	0.71
1:D:168:HIS:ND1	1:D:169:PRO:CD	2.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:LEU:HD12	1:F:72:LEU:HD11	1.71	0.71
1:E:174:THR:O	1:E:178:LEU:HG	1.90	0.70
1:C:57:CYS:O	1:C:60:ILE:N	2.24	0.70
1:A:39:PRO:CD	1:A:335:GLN:O	2.39	0.70
1:C:250:ASN:ND2	1:F:216:ALA:HB2	2.06	0.70
1:C:219:ALA:O	1:C:222:ALA:N	2.23	0.70
1:F:57:CYS:SG	1:F:102:ILE:CG1	2.79	0.70
1:D:168:HIS:ND1	1:D:169:PRO:HD2	2.06	0.70
1:C:371:ALA:O	1:C:372:GLN:C	2.33	0.70
1:D:189:ASP:O	1:D:190:ALA:HB2	1.90	0.69
1:F:370:PHE:O	1:F:374:ARG:CZ	2.39	0.69
1:D:44:LEU:HD13	1:D:340:THR:HB	1.73	0.69
1:D:203:TYR:O	1:D:204:GLU:C	2.36	0.69
1:E:182:LEU:O	1:E:186:CYS:SG	2.50	0.69
1:E:287:GLY:N	1:E:334:MET:HE1	2.07	0.69
1:D:102:ILE:HG22	1:D:102:ILE:O	1.93	0.69
1:A:318:ARG:HG2	1:A:318:ARG:NH1	2.06	0.68
1:A:323:ARG:HH11	1:A:323:ARG:HG3	1.57	0.68
1:E:186:CYS:O	1:E:187:GLY:C	2.36	0.68
1:F:252:LEU:O	1:F:256:ALA:HB3	1.94	0.68
1:A:141:GLU:OE1	1:A:206:CYS:CB	2.35	0.68
1:E:345:SER:O	1:E:349:ILE:HG13	1.93	0.68
1:A:196:ASP:HB3	1:A:239:TRP:CD1	2.29	0.68
1:A:311:LEU:CD2	1:A:376:GLU:OE1	2.42	0.68
1:E:242:ARG:NH2	1:E:253:GLY:O	2.24	0.68
1:D:39:PRO:O	1:D:70:ASN:ND2	2.19	0.67
1:E:78:TYR:OH	1:E:123:GLN:NE2	2.26	0.67
1:E:361:PRO:O	1:E:364:GLU:N	2.26	0.67
1:A:70:ASN:C	1:A:71:THR:OG1	2.34	0.67
1:C:126:ARG:HG2	1:C:151:TRP:CE3	2.28	0.67
1:D:243:LEU:HD22	1:D:265:ILE:HA	1.76	0.67
1:E:117:MET:SD	1:E:182:LEU:HD11	2.34	0.67
1:F:279:TYR:CG	1:F:301:CYS:HB3	2.29	0.67
1:A:237:TRP:CD2	1:A:273:MET:HG2	2.28	0.67
1:C:124:SER:OG	1:C:162:LYS:HB2	1.93	0.67
1:A:308:LEU:O	1:A:309:ALA:C	2.37	0.67
1:C:69:VAL:HG22	1:C:370:PHE:CZ	2.30	0.67
1:E:171:LEU:O	1:E:172:LEU:HD23	1.95	0.67
1:C:41:LYS:N	1:C:70:ASN:OD1	2.27	0.67
1:C:126:ARG:HA	1:C:151:TRP:CE2	2.30	0.67
1:C:203:TYR:C	1:C:205:LYS:H	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:VAL:O	1:D:307:ALA:C	2.38	0.67
1:D:213:ASP:CG	1:D:263:ARG:HH12	2.03	0.67
1:D:248:THR:O	1:D:248:THR:HG22	1.94	0.67
1:E:120:LEU:HA	1:E:164:LEU:HD12	1.77	0.67
1:C:245:ASP:O	1:C:249:THR:OG1	2.11	0.66
1:C:255:GLN:HB3	1:C:278:LYS:HD3	1.78	0.66
1:E:127:ASP:OD1	1:E:127:ASP:O	2.13	0.66
1:E:57:CYS:SG	1:E:102:ILE:HG12	2.35	0.66
1:D:190:ALA:HA	1:D:235:GLN:O	1.95	0.66
1:E:213:ASP:OD1	1:E:215:ALA:N	2.28	0.66
1:A:100:LYS:HG3	1:A:185:VAL:HG13	1.78	0.66
1:C:343:GLU:OE1	1:C:362:SER:OG	2.12	0.66
1:F:339:VAL:HG11	1:F:366:PHE:HA	1.77	0.66
1:E:286:PRO:O	1:E:288:TYR:N	2.29	0.66
1:A:141:GLU:OE1	1:A:209:CYS:HB2	1.94	0.66
1:C:157:PHE:O	1:F:258:MET:SD	2.53	0.66
1:A:335:GLN:HE21	1:A:335:GLN:HA	1.60	0.66
1:C:255:GLN:HB3	1:C:278:LYS:CD	2.25	0.66
1:D:153:ASP:OD1	1:D:158:ASP:HB2	1.96	0.66
1:C:156:PRO:O	1:C:157:PHE:CD1	2.47	0.66
1:C:275:CYS:HG	1:C:338:PHE:HD2	1.39	0.66
1:D:38:LEU:HD22	1:D:336:GLY:HA2	1.77	0.66
1:D:341:MET:HE1	1:D:345:SER:HA	1.76	0.66
1:E:41:LYS:HB2	1:E:70:ASN:ND2	2.10	0.66
1:F:103:VAL:O	1:F:106:CYS:N	2.28	0.66
1:C:147:PRO:O	1:C:149:VAL:HG23	1.96	0.66
1:A:361:PRO:O	1:A:365:THR:N	2.27	0.66
1:F:172:LEU:HD13	1:F:176:PHE:CZ	2.31	0.66
1:C:371:ALA:O	1:C:373:ILE:N	2.29	0.65
1:A:180:ASP:CG	1:A:228:HIS:HE2	2.05	0.65
1:C:247:LYS:HE2	1:C:258:MET:HA	1.78	0.65
1:E:171:LEU:C	1:E:172:LEU:HD23	2.22	0.65
1:A:41:LYS:NZ	1:A:68:GLY:O	2.30	0.65
1:A:73:VAL:HG21	1:A:338:PHE:CZ	2.32	0.65
1:A:306:VAL:O	1:A:309:ALA:HB3	1.96	0.65
1:D:65:PRO:HG3	1:D:109:ALA:HB1	1.78	0.65
1:A:246:GLY:O	1:A:250:ASN:CA	2.43	0.65
1:C:132:LEU:O	1:C:135:LYS:N	2.29	0.65
1:A:182:LEU:O	1:A:186:CYS:SG	2.55	0.65
1:E:106:CYS:HB3	1:E:111:ILE:HG22	1.77	0.65
1:C:39:PRO:C	1:C:70:ASN:HD21	2.05	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:VAL:HA	1:D:74:LEU:HD11	1.77	0.65
1:F:125:ASP:O	1:F:126:ARG:CB	2.45	0.65
1:F:176:PHE:O	1:F:177:PRO:C	2.40	0.64
1:E:120:LEU:HD12	1:E:164:LEU:CB	2.25	0.64
1:C:55:GLU:OE2	1:C:346:LYS:HE3	1.97	0.64
1:C:219:ALA:O	1:C:221:TYR:N	2.31	0.64
1:E:141:GLU:OE2	1:E:206:CYS:SG	2.55	0.64
1:E:245:ASP:OD2	3:E:501:HOH:O	2.14	0.64
1:F:141:GLU:OE1	1:F:209:CYS:HB2	1.97	0.64
1:E:41:LYS:H	1:E:70:ASN:HD21	1.45	0.64
1:E:372:GLN:HE21	1:E:376:GLU:HG3	1.61	0.64
1:F:42:ALA:HB3	1:F:338:PHE:HB2	1.79	0.64
1:C:250:ASN:HD21	1:F:216:ALA:HB2	1.60	0.64
1:F:125:ASP:O	1:F:126:ARG:HB2	1.97	0.64
1:A:199:TRP:CZ2	1:A:253:GLY:O	2.50	0.64
1:D:277:TRP:O	1:D:278:LYS:HD3	1.98	0.64
1:A:367:LYS:O	1:A:368:ALA:C	2.40	0.64
1:C:258:MET:O	1:F:245:ASP:HB2	1.98	0.64
1:D:45:LEU:HD13	1:D:56:PHE:CE1	2.33	0.64
1:D:80:TYR:CE1	1:D:99:LEU:HD23	2.33	0.63
1:D:50:PRO:HD3	1:D:94:ILE:HG22	1.80	0.63
1:A:193:VAL:CG2	1:A:236:MET:HE3	2.22	0.63
1:F:160:TYR:OH	1:F:197:GLU:OE2	2.10	0.63
1:E:376:GLU:HA	1:E:379:MET:SD	2.39	0.63
1:D:343:GLU:OE2	1:D:362:SER:OG	2.11	0.63
1:A:58:ARG:NH1	1:A:62:GLU:OE2	2.32	0.63
1:A:146:ASN:OD1	1:A:162:LYS:NZ	2.23	0.63
1:C:203:TYR:O	1:C:205:LYS:N	2.31	0.62
1:C:251:LEU:O	1:C:252:LEU:HB2	1.97	0.62
1:C:277:TRP:CE3	1:C:279:TYR:CE2	2.87	0.62
1:E:101:GLN:O	1:E:105:THR:OG1	2.14	0.62
1:E:206:CYS:SG	1:E:207:PRO:HD2	2.39	0.62
1:C:195:LEU:HD23	1:C:195:LEU:N	2.15	0.62
1:D:99:LEU:O	1:D:102:ILE:N	2.29	0.62
1:D:45:LEU:HD23	1:D:341:MET:HE3	1.80	0.62
1:E:85:HIS:CB	1:E:88:LEU:HD12	2.29	0.62
1:F:243:LEU:HA	1:F:262:PHE:HA	1.81	0.62
1:C:247:LYS:HG2	1:F:263:ARG:HA	1.81	0.62
1:C:329:THR:O	1:C:332:GLU:HB2	1.99	0.62
1:F:115:PRO:HD2	1:F:190:ALA:O	1.99	0.62
1:E:310:GLN:O	1:E:314:VAL:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:MET:HE1	1:F:263:ARG:HE	1.64	0.62
1:F:73:VAL:HG13	1:F:114:ILE:HG22	1.82	0.62
1:F:73:VAL:HG22	1:F:114:ILE:HB	1.81	0.62
1:C:140:ASP:C	1:C:140:ASP:OD1	2.38	0.62
1:F:205:LYS:O	1:F:206:CYS:C	2.42	0.62
1:D:45:LEU:CD2	1:D:341:MET:HE3	2.30	0.61
1:D:140:ASP:O	3:D:501:HOH:O	2.15	0.61
1:F:45:LEU:HD13	1:F:56:PHE:CE1	2.35	0.61
1:D:36:ASN:C	1:D:315:ARG:HH12	2.07	0.61
1:F:132:LEU:HD23	1:F:164:LEU:HD11	1.81	0.61
1:E:290:ALA:O	1:E:333:ARG:NH1	2.29	0.61
1:C:345:SER:O	1:C:349:ILE:HG13	2.00	0.61
1:E:165:CYS:O	1:E:171:LEU:HD22	2.00	0.61
1:D:193:VAL:O	1:D:195:LEU:HD23	2.01	0.61
1:F:314:VAL:HG11	1:F:336:GLY:HA2	1.82	0.61
1:D:306:VAL:O	1:D:309:ALA:HB3	2.00	0.61
1:A:121:GLY:HA2	1:A:163:SER:HA	1.83	0.61
1:A:180:ASP:OD2	1:A:228:HIS:NE2	2.29	0.61
1:A:359:LYS:O	1:A:360:LEU:HD23	2.01	0.61
1:C:47:VAL:HA	1:C:74:LEU:HD11	1.82	0.61
1:C:259:ASN:ND2	1:F:248:THR:HG21	2.15	0.61
1:A:301:CYS:O	1:A:365:THR:HG21	2.01	0.61
1:C:40:VAL:HG11	1:C:297:LEU:HD11	1.83	0.61
1:C:57:CYS:O	1:C:59:PHE:N	2.34	0.61
1:F:222:ALA:O	1:F:223:THR:C	2.43	0.61
1:A:36:ASN:O	1:A:377:GLU:OE1	2.19	0.60
1:C:141:GLU:OE2	1:C:141:GLU:HA	1.99	0.60
1:E:59:PHE:CE2	1:E:64:LEU:HD21	2.36	0.60
1:E:328:VAL:O	1:E:329:THR:C	2.44	0.60
1:A:302:SER:HA	1:A:362:SER:CA	2.30	0.60
1:A:237:TRP:CE2	1:A:273:MET:HG2	2.36	0.60
1:C:133:LEU:O	1:C:137:PRO:HA	2.01	0.60
1:E:372:GLN:NE2	1:E:376:GLU:HG3	2.16	0.60
1:C:324:ALA:HB1	1:C:326:TRP:CZ2	2.36	0.60
1:D:328:VAL:O	1:D:329:THR:C	2.43	0.60
1:F:63:VAL:HG13	1:F:352:TYR:CZ	2.36	0.60
1:F:89:ALA:O	1:F:90:GLY:O	2.20	0.60
1:A:245:ASP:O	1:A:249:THR:CB	2.50	0.60
1:C:258:MET:HB3	1:F:245:ASP:HB2	1.84	0.60
1:C:376:GLU:O	1:C:380:ASN:OD1	2.20	0.60
1:C:348:PHE:O	1:C:351:ALA:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:PRO:O	1:F:151:TRP:HA	2.02	0.60
1:A:36:ASN:O	1:A:377:GLU:CD	2.45	0.60
1:D:160:TYR:CD2	1:D:161:CYS:SG	2.96	0.59
1:D:304:SER:O	1:D:308:LEU:HG	2.02	0.59
1:E:139:PHE:O	1:E:165:CYS:N	2.34	0.59
1:D:50:PRO:HG3	1:D:94:ILE:HA	1.82	0.59
1:D:294:PHE:O	1:D:333:ARG:HB3	2.02	0.59
1:F:99:LEU:O	1:F:103:VAL:HG23	2.03	0.59
1:F:328:VAL:O	1:F:329:THR:O	2.20	0.59
1:E:296:VAL:HG13	1:E:334:MET:SD	2.42	0.59
1:F:80:TYR:OH	1:F:96:GLU:OE2	2.19	0.59
1:C:197:GLU:HB3	1:C:199:TRP:CD1	2.37	0.59
1:E:315:ARG:O	1:E:318:ARG:N	2.34	0.59
1:E:341:MET:HG2	1:E:348:PHE:CD2	2.36	0.59
1:F:45:LEU:HD11	1:F:59:PHE:CE2	2.36	0.59
1:E:56:PHE:O	1:E:56:PHE:CD1	2.56	0.59
1:F:41:LYS:HE2	1:F:70:ASN:ND2	2.18	0.59
1:D:50:PRO:CD	1:D:94:ILE:HG22	2.33	0.58
1:D:295:ASN:HB3	1:D:335:GLN:HG3	1.84	0.58
1:C:309:ALA:O	1:C:310:GLN:C	2.45	0.58
1:E:79:ASN:HD22	1:E:79:ASN:N	2.00	0.58
1:E:85:HIS:HB3	1:E:88:LEU:HD12	1.84	0.58
1:E:290:ALA:CB	1:E:334:MET:HE2	2.33	0.58
1:C:242:ARG:O	1:C:261:THR:O	2.21	0.58
1:A:319:LYS:O	1:A:322:THR:OG1	2.19	0.58
1:E:285:THR:O	1:E:288:TYR:HB3	2.04	0.58
1:E:41:LYS:CE	1:E:70:ASN:HD22	2.13	0.58
1:A:38:LEU:HD22	1:A:336:GLY:HA2	1.86	0.58
1:A:335:GLN:HA	1:A:335:GLN:NE2	2.19	0.58
1:D:44:LEU:HB3	1:D:340:THR:HA	1.83	0.58
1:D:73:VAL:HA	1:D:114:ILE:O	2.04	0.58
1:A:213:ASP:OD2	1:A:263:ARG:NH1	2.32	0.58
1:C:124:SER:HB2	1:C:128:HIS:O	2.04	0.58
1:D:270:THR:HB	1:D:293:GLY:O	2.03	0.58
1:F:189:ASP:C	1:F:234:CYS:SG	2.86	0.58
1:D:156:PRO:O	1:D:254:TRP:CZ2	2.57	0.57
1:E:63:VAL:HG13	1:E:352:TYR:CZ	2.39	0.57
1:F:103:VAL:HG22	3:F:505:HOH:O	2.02	0.57
1:A:142:SER:O	1:A:142:SER:OG	2.21	0.57
1:E:48:PRO:HD3	1:E:56:PHE:CE2	2.40	0.57
1:F:64:LEU:CD1	1:F:72:LEU:HD13	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:LEU:HD13	1:F:140:ASP:CB	2.30	0.57
1:A:41:LYS:HE3	1:A:70:ASN:ND2	2.19	0.57
1:C:129:ILE:O	1:C:130:ASP:O	2.21	0.57
1:E:331:ALA:O	1:E:332:GLU:C	2.46	0.57
1:C:60:ILE:HG21	1:C:105:THR:HB	1.85	0.57
1:D:340:THR:O	1:D:340:THR:OG1	2.23	0.57
1:E:203:TYR:CE2	1:E:205:LYS:HB2	2.40	0.57
1:A:41:LYS:CE	1:A:70:ASN:HD22	2.18	0.57
1:C:279:TYR:CD1	1:C:301:CYS:HB2	2.40	0.57
1:C:44:LEU:HD23	1:C:341:MET:O	2.05	0.57
1:C:244:ILE:HG22	1:C:256:ALA:HB1	1.86	0.57
1:C:329:THR:HG22	1:C:333:ARG:NE	2.19	0.57
1:F:221:TYR:CZ	1:F:225:LEU:HD11	2.39	0.57
1:F:240:SER:O	1:F:243:LEU:HB2	2.05	0.57
1:F:304:SER:O	1:F:307:ALA:N	2.38	0.57
1:C:199:TRP:O	1:F:248:THR:CA	2.53	0.56
1:C:311:LEU:HD22	1:C:369:VAL:HG13	1.87	0.56
1:C:376:GLU:HA	1:C:379:MET:HE2	1.87	0.56
1:D:117:MET:HG2	1:D:119:LEU:HD21	1.86	0.56
1:F:213:ASP:C	1:F:213:ASP:OD1	2.47	0.56
1:A:193:VAL:HG22	1:A:237:TRP:O	2.05	0.56
1:C:155:GLY:O	1:C:157:PHE:N	2.38	0.56
1:C:253:GLY:CA	1:C:258:MET:CE	2.83	0.56
1:D:189:ASP:O	1:D:190:ALA:CB	2.53	0.56
1:F:39:PRO:O	1:F:70:ASN:ND2	2.36	0.56
1:F:104:GLN:NE2	1:F:108:GLU:HG3	2.20	0.56
1:A:189:ASP:O	1:A:234:CYS:HA	2.04	0.56
1:C:198:VAL:HG12	1:C:198:VAL:O	2.05	0.56
1:C:258:MET:HB2	1:F:245:ASP:OD2	2.06	0.56
1:F:41:LYS:HE3	1:F:68:GLY:O	2.06	0.56
1:F:124:SER:OG	1:F:161:CYS:CB	2.53	0.56
1:F:189:ASP:O	1:F:190:ALA:CB	2.54	0.56
1:F:285:THR:N	1:F:286:PRO:CD	2.68	0.56
1:F:303:ASN:HB3	1:F:306:VAL:HB	1.87	0.56
1:A:216:ALA:O	1:A:220:GLU:HB2	2.06	0.56
1:A:315:ARG:NH2	1:A:377:GLU:OE1	2.38	0.56
1:A:351:ALA:HA	1:A:358:LYS:HB3	1.88	0.56
1:D:117:MET:CG	1:D:119:LEU:HD21	2.35	0.56
1:D:119:LEU:HD12	1:D:179:MET:HE3	1.87	0.56
1:A:103:VAL:O	1:A:104:GLN:C	2.49	0.56
1:C:140:ASP:OD1	1:C:142:SER:N	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:VAL:O	1:D:336:GLY:HA3	2.06	0.56
1:A:255:GLN:O	1:A:256:ALA:HB2	2.06	0.56
1:C:209:CYS:O	1:C:212:ARG:HG3	2.05	0.56
1:D:243:LEU:HD22	1:D:265:ILE:CA	2.35	0.56
1:D:348:PHE:C	1:D:348:PHE:CD1	2.84	0.56
1:C:68:GLY:O	1:C:69:VAL:C	2.48	0.56
1:F:131:PRO:HA	1:F:134:ALA:HB3	1.89	0.56
1:A:368:ALA:O	1:A:372:GLN:N	2.36	0.55
1:D:355:ARG:C	1:D:357:GLY:H	2.14	0.55
1:C:241:ASP:O	1:C:243:LEU:N	2.39	0.55
1:E:318:ARG:HA	1:E:331:ALA:HB1	1.88	0.55
1:A:281:SER:C	1:A:283:PRO:HD3	2.31	0.55
1:E:239:TRP:CE3	1:E:275:CYS:HB3	2.41	0.55
1:F:87:GLU:OE1	1:F:88:LEU:HG	2.06	0.55
1:F:61:LYS:O	1:F:61:LYS:HG2	2.06	0.55
1:C:130:ASP:O	1:C:132:LEU:N	2.40	0.55
1:D:60:ILE:CD1	1:D:102:ILE:HG23	2.37	0.55
1:D:104:GLN:O	1:D:105:THR:C	2.49	0.55
1:A:168:HIS:ND1	1:A:169:PRO:HD2	2.22	0.55
1:E:240:SER:OG	1:E:276:ASP:CA	2.47	0.55
1:E:365:THR:O	1:E:366:PHE:C	2.50	0.55
1:F:214:LYS:HD2	1:F:260:ALA:HB3	1.88	0.55
1:C:255:GLN:HB3	1:C:278:LYS:CE	2.37	0.55
1:D:117:MET:HE1	1:D:178:LEU:HD13	1.89	0.55
1:E:276:ASP:OD2	1:E:285:THR:HB	2.07	0.55
1:C:219:ALA:O	1:C:220:GLU:C	2.50	0.55
1:E:80:TYR:C	1:E:93:ALA:HB1	2.31	0.55
1:E:164:LEU:HD22	1:E:171:LEU:HD11	1.89	0.55
1:F:372:GLN:HE21	1:F:376:GLU:CD	2.15	0.55
1:D:120:LEU:HD13	1:D:221:TYR:CD2	2.42	0.55
1:E:140:ASP:OD1	1:E:141:GLU:N	2.39	0.55
1:C:140:ASP:OD1	1:C:141:GLU:N	2.40	0.54
1:E:239:TRP:HA	1:E:275:CYS:HB2	1.88	0.54
1:F:190:ALA:HA	1:F:235:GLN:O	2.07	0.54
1:C:155:GLY:C	1:C:157:PHE:N	2.58	0.54
1:C:245:ASP:OD1	1:C:247:LYS:HB2	2.08	0.54
1:F:272:ILE:HG22	1:F:273:MET:O	2.06	0.54
1:C:123:GLN:NE2	1:C:164:LEU:HD11	2.22	0.54
1:C:247:LYS:HE3	1:C:258:MET:C	2.33	0.54
1:E:116:LYS:O	1:E:117:MET:HG3	2.06	0.54
1:C:55:GLU:OE2	1:C:346:LYS:CE	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:GLU:HA	1:C:380:ASN:HB2	1.90	0.54
1:D:302:SER:OG	1:D:303:ASN:N	2.41	0.54
1:E:194:GLY:O	1:E:195:LEU:HB2	2.08	0.54
1:F:196:ASP:HB3	1:F:239:TRP:CD1	2.42	0.54
1:D:121:GLY:O	1:D:122:HIS:C	2.50	0.54
1:E:64:LEU:N	1:E:64:LEU:HD23	2.23	0.54
1:E:90:GLY:O	1:E:92:ARG:N	2.40	0.54
1:E:286:PRO:O	1:E:289:PHE:N	2.40	0.54
1:F:119:LEU:O	1:F:221:TYR:OH	2.20	0.54
1:F:124:SER:OG	1:F:161:CYS:HB2	2.07	0.54
1:D:122:HIS:NE2	1:D:197:GLU:HB2	2.23	0.54
1:D:361:PRO:O	1:D:365:THR:OG1	2.25	0.54
1:E:213:ASP:OD1	1:E:214:LYS:N	2.40	0.54
1:F:132:LEU:HD23	1:F:164:LEU:CD2	2.37	0.54
1:C:343:GLU:OE2	1:C:343:GLU:O	2.26	0.54
1:E:168:HIS:ND1	1:E:169:PRO:HD2	2.22	0.54
1:F:274:ILE:O	1:F:296:VAL:HG23	2.08	0.54
1:C:176:PHE:HB2	1:C:177:PRO:HD3	1.89	0.54
1:F:206:CYS:O	1:F:206:CYS:SG	2.65	0.54
1:A:328:VAL:O	1:A:329:THR:C	2.49	0.54
1:C:250:ASN:HA	1:F:263:ARG:HH11	1.73	0.54
1:E:344:ASP:CG	1:E:345:SER:H	2.16	0.54
1:A:80:TYR:CE1	1:A:99:LEU:HD23	2.43	0.54
1:C:226:HIS:HE2	1:C:271:ASP:CG	2.16	0.54
1:C:258:MET:O	1:F:245:ASP:CB	2.55	0.54
1:D:120:LEU:HD13	1:D:221:TYR:CE2	2.42	0.54
1:E:85:HIS:O	1:E:88:LEU:N	2.28	0.54
1:F:116:LYS:NZ	1:F:118:ASN:ND2	2.56	0.54
1:A:287:GLY:O	1:A:288:TYR:C	2.51	0.53
1:C:308:LEU:HD23	1:C:311:LEU:CD2	2.34	0.53
1:D:196:ASP:O	1:D:197:GLU:C	2.51	0.53
1:E:221:TYR:O	1:E:224:LYS:HB2	2.08	0.53
1:E:278:LYS:HB2	1:E:310:GLN:HE22	1.73	0.53
1:A:122:HIS:NE2	1:A:197:GLU:OE2	2.42	0.53
1:E:127:ASP:O	1:E:128:HIS:HB2	2.08	0.53
1:F:279:TYR:CD2	1:F:301:CYS:HB3	2.43	0.53
1:D:67:GLU:OE2	1:D:374:ARG:NH1	2.40	0.53
1:F:365:THR:O	1:F:366:PHE:C	2.51	0.53
1:D:135:LYS:C	1:D:136:TYR:CD1	2.86	0.53
1:A:293:GLY:HA2	1:D:248:THR:CG2	2.39	0.53
1:C:48:PRO:HD3	1:C:56:PHE:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:PHE:O	1:D:60:ILE:HG13	2.09	0.53
1:E:59:PHE:CE1	1:E:349:ILE:HG12	2.43	0.53
1:F:261:THR:OG1	1:F:262:PHE:N	2.41	0.53
1:F:309:ALA:O	1:F:312:ALA:HB3	2.08	0.53
1:E:47:VAL:CG1	1:E:47:VAL:O	2.57	0.53
1:A:164:LEU:HD13	1:A:171:LEU:HD11	1.90	0.53
1:A:303:ASN:OD1	1:A:306:VAL:HG23	2.08	0.53
1:E:328:VAL:O	1:E:331:ALA:N	2.41	0.53
1:E:366:PHE:O	1:E:370:PHE:HB2	2.08	0.53
1:F:246:GLY:O	1:F:250:ASN:HA	2.09	0.53
1:C:76:ILE:O	1:C:77:ARG:HB2	2.09	0.53
1:E:36:ASN:HD22	1:E:380:ASN:HB3	1.74	0.53
1:E:245:ASP:O	1:E:249:THR:OG1	2.22	0.53
1:F:36:ASN:HD21	1:F:37:LYS:HE2	1.73	0.53
1:F:289:PHE:C	1:F:291:ILE:N	2.66	0.53
1:A:195:LEU:HD12	1:A:238:MET:HE3	1.91	0.52
1:A:306:VAL:O	1:A:310:GLN:HG3	2.09	0.52
1:C:104:GLN:HE22	1:C:107:LYS:HD3	1.72	0.52
1:D:243:LEU:HB3	1:D:265:ILE:HD12	1.91	0.52
1:A:70:ASN:OD1	1:A:70:ASN:C	2.53	0.52
1:C:123:GLN:CD	1:C:164:LEU:HD21	2.35	0.52
1:C:246:GLY:HA2	1:C:256:ALA:HB3	1.89	0.52
1:C:275:CYS:SG	1:C:338:PHE:HD2	2.32	0.52
1:D:50:PRO:HB3	1:D:98:GLN:NE2	2.24	0.52
1:E:300:SER:O	1:E:340:THR:HG23	2.10	0.52
1:F:198:VAL:HG12	1:F:198:VAL:O	2.08	0.52
1:A:238:MET:O	1:A:275:CYS:HB2	2.09	0.52
1:D:285:THR:N	1:D:286:PRO:CD	2.72	0.52
1:F:171:LEU:O	1:F:175:ILE:N	2.41	0.52
1:A:192:HIS:CE1	1:A:194:GLY:H	2.28	0.52
1:A:235:GLN:HE22	1:A:273:MET:HE2	1.74	0.52
1:C:128:HIS:HD2	1:C:130:ASP:OD1	1.93	0.52
1:C:203:TYR:C	1:C:205:LYS:N	2.67	0.52
1:E:348:PHE:HA	1:E:360:LEU:HD12	1.90	0.52
1:E:365:THR:O	1:E:368:ALA:N	2.42	0.52
1:F:266:ASP:OD1	1:F:292:LYS:HD2	2.08	0.52
1:F:279:TYR:CD1	1:F:301:CYS:HB3	2.43	0.52
1:A:301:CYS:SG	1:A:302:SER:N	2.83	0.52
1:D:223:THR:O	1:D:226:HIS:N	2.42	0.52
1:E:229:LEU:O	1:E:234:CYS:HB2	2.09	0.52
1:F:213:ASP:OD1	1:F:263:ARG:NH2	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:MET:HE3	1:A:366:PHE:CZ	2.45	0.52
1:C:43:MET:CE	1:C:366:PHE:CD1	2.93	0.52
1:C:225:LEU:N	1:C:225:LEU:HD23	2.24	0.52
1:C:250:ASN:OD1	1:F:263:ARG:NH1	2.43	0.52
1:D:44:LEU:HD22	1:D:341:MET:O	2.10	0.52
1:D:116:LYS:HG2	1:D:117:MET:N	2.23	0.52
1:E:175:ILE:HG22	1:E:179:MET:SD	2.49	0.52
1:D:213:ASP:OD2	1:D:263:ARG:NH1	2.43	0.52
1:E:43:MET:HE2	1:E:45:LEU:HD21	1.92	0.52
1:E:286:PRO:C	1:E:334:MET:HE1	2.35	0.52
1:A:51:GLU:O	1:A:51:GLU:CG	2.51	0.52
1:F:206:CYS:SG	1:F:209:CYS:HB2	2.49	0.52
1:D:226:HIS:C	1:D:226:HIS:ND1	2.67	0.52
1:E:104:GLN:O	1:E:108:GLU:N	2.32	0.52
1:F:348:PHE:HA	1:F:360:LEU:HD13	1.92	0.52
1:C:254:TRP:HB2	1:C:255:GLN:HE21	1.75	0.51
1:C:257:SER:OG	1:C:258:MET:N	2.43	0.51
1:F:138:GLN:HG3	3:F:507:HOH:O	2.10	0.51
1:F:278:LYS:HE2	1:F:285:THR:HG21	1.93	0.51
1:C:74:LEU:HD22	1:C:102:ILE:HG21	1.92	0.51
1:C:156:PRO:O	1:C:254:TRP:CH2	2.63	0.51
1:C:280:GLU:C	1:C:306:VAL:HG21	2.35	0.51
1:E:317:ALA:HB1	1:E:334:MET:HG3	1.91	0.51
1:C:242:ARG:HA	1:C:257:SER:HB2	1.91	0.51
1:D:119:LEU:CD1	1:D:179:MET:HE3	2.40	0.51
1:E:39:PRO:O	1:E:70:ASN:CG	2.53	0.51
1:E:166:PRO:HD2	1:E:209:CYS:SG	2.50	0.51
1:E:312:ALA:O	1:E:313:GLN:C	2.53	0.51
1:A:223:THR:O	1:A:227:ASP:N	2.37	0.51
1:C:245:ASP:HA	1:C:262:PHE:CD2	2.45	0.51
1:E:287:GLY:O	1:E:290:ALA:HB3	2.10	0.51
1:C:109:ALA:O	1:C:110:LYS:HB2	2.10	0.51
1:D:48:PRO:O	1:D:94:ILE:HG21	2.11	0.51
1:D:196:ASP:HA	1:D:241:ASP:OD1	2.11	0.51
1:D:328:VAL:O	1:D:332:GLU:N	2.36	0.51
1:A:271:ASP:OD1	1:A:271:ASP:C	2.53	0.51
1:A:348:PHE:CZ	1:A:363:ALA:HA	2.46	0.51
1:D:237:TRP:CD2	1:D:273:MET:HG2	2.45	0.51
1:A:57:CYS:SG	1:A:102:ILE:HA	2.51	0.51
1:A:120:LEU:O	1:A:164:LEU:N	2.34	0.51
1:E:176:PHE:HD1	1:E:179:MET:SD	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:ARG:NH2	1:F:122:HIS:O	2.44	0.51
1:F:103:VAL:CG2	3:F:505:HOH:O	2.57	0.51
1:C:193:VAL:HG22	1:C:237:TRP:O	2.11	0.51
1:C:226:HIS:NE2	1:C:271:ASP:OD1	2.38	0.51
1:C:324:ALA:CB	1:C:326:TRP:CE2	2.91	0.51
1:D:105:THR:O	1:D:106:CYS:C	2.53	0.51
1:D:363:ALA:O	1:D:366:PHE:N	2.44	0.51
1:C:120:LEU:HD13	1:C:166:PRO:HG3	1.93	0.51
1:C:248:THR:HA	1:F:266:ASP:HB2	1.92	0.51
1:D:264:ALA:O	1:D:265:ILE:C	2.54	0.51
1:E:168:HIS:CD2	1:E:208:ARG:CZ	2.94	0.51
1:C:133:LEU:O	1:C:137:PRO:CA	2.59	0.50
1:C:268:ILE:HD12	1:C:272:ILE:HD12	1.93	0.50
1:D:73:VAL:HG13	1:D:116:LYS:HB2	1.93	0.50
1:E:243:LEU:CD1	1:E:274:ILE:HD12	2.40	0.50
1:C:194:GLY:HA2	1:C:239:TRP:CD1	2.46	0.50
1:C:247:LYS:CB	1:F:263:ARG:HA	2.41	0.50
1:D:50:PRO:HG3	1:D:94:ILE:HG22	1.92	0.50
1:A:171:LEU:O	1:A:175:ILE:HB	2.12	0.50
1:A:270:THR:HA	1:A:294:PHE:CE1	2.46	0.50
1:C:123:GLN:HB2	1:C:162:LYS:O	2.10	0.50
1:E:64:LEU:HB2	1:E:65:PRO:HD2	1.93	0.50
1:E:242:ARG:CZ	1:E:256:ALA:O	2.59	0.50
1:E:328:VAL:O	1:E:331:ALA:HB3	2.10	0.50
1:F:120:LEU:HD12	1:F:164:LEU:O	2.11	0.50
1:A:240:SER:HB3	1:A:276:ASP:HA	1.92	0.50
1:C:59:PHE:O	1:C:61:LYS:N	2.45	0.50
1:F:328:VAL:HA	1:F:331:ALA:HB3	1.93	0.50
1:A:41:LYS:CE	1:A:70:ASN:ND2	2.75	0.50
1:A:240:SER:CB	1:A:276:ASP:HA	2.42	0.50
1:F:221:TYR:CE2	1:F:225:LEU:HD11	2.47	0.50
1:A:295:ASN:HB3	1:A:335:GLN:CG	2.41	0.50
1:A:323:ARG:HG3	1:A:323:ARG:NH1	2.26	0.50
1:E:39:PRO:HG2	1:E:40:VAL:HG23	1.93	0.50
1:E:345:SER:O	1:E:349:ILE:CG1	2.60	0.50
1:A:246:GLY:O	1:A:250:ASN:N	2.45	0.50
1:A:348:PHE:CE2	1:A:363:ALA:HA	2.47	0.50
1:D:131:PRO:HA	1:D:134:ALA:HB3	1.94	0.50
1:F:278:LYS:HB2	1:F:310:GLN:HE22	1.77	0.50
1:E:79:ASN:N	1:E:79:ASN:ND2	2.60	0.50
1:E:85:HIS:O	1:E:86:PRO:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:343:GLU:OE2	1:E:343:GLU:N	2.45	0.50
1:F:117:MET:HB3	1:F:191:PHE:CZ	2.47	0.50
1:C:59:PHE:O	1:C:60:ILE:C	2.54	0.50
1:C:181:GLU:O	1:C:185:VAL:HG23	2.12	0.50
1:C:214:LYS:NZ	1:F:248:THR:O	2.45	0.50
1:F:192:HIS:CE1	1:F:238:MET:HA	2.47	0.50
1:A:96:GLU:O	1:A:97:GLN:C	2.55	0.49
1:C:229:LEU:CB	1:C:234:CYS:HB3	2.38	0.49
1:D:320:ASP:C	1:D:322:THR:H	2.20	0.49
1:E:39:PRO:O	1:E:70:ASN:ND2	2.45	0.49
1:F:70:ASN:O	1:F:111:ILE:HA	2.11	0.49
1:A:63:VAL:HG13	1:A:352:TYR:CZ	2.46	0.49
1:C:287:GLY:O	1:C:291:ILE:CD1	2.60	0.49
1:E:376:GLU:O	1:E:379:MET:N	2.35	0.49
1:F:45:LEU:O	1:F:74:LEU:HD12	2.12	0.49
1:A:364:GLU:O	1:A:367:LYS:HB2	2.12	0.49
1:C:55:GLU:OE2	1:C:346:LYS:NZ	2.45	0.49
1:C:275:CYS:SG	1:C:338:PHE:CD2	2.98	0.49
1:D:240:SER:OG	1:D:276:ASP:HA	2.13	0.49
1:E:84:SER:C	1:E:86:PRO:HD2	2.38	0.49
1:A:281:SER:C	1:A:283:PRO:CD	2.85	0.49
1:C:72:LEU:HD22	1:C:106:CYS:SG	2.53	0.49
1:C:112:ARG:HH21	1:C:189:ASP:HB2	1.77	0.49
1:C:315:ARG:O	1:C:319:LYS:N	2.39	0.49
1:D:43:MET:CG	1:D:44:LEU:N	2.75	0.49
1:D:160:TYR:CE2	1:D:161:CYS:SG	3.06	0.49
1:E:131:PRO:O	1:E:135:LYS:HB2	2.12	0.49
1:E:220:GLU:O	1:E:224:LYS:HG3	2.11	0.49
1:F:173:LYS:O	1:F:177:PRO:HG2	2.13	0.49
1:F:356:ASN:O	1:F:357:GLY:C	2.54	0.49
1:A:192:HIS:ND1	1:A:192:HIS:C	2.70	0.49
1:C:170:ASP:OD1	1:C:170:ASP:N	2.46	0.49
1:E:240:SER:N	1:E:275:CYS:O	2.42	0.49
1:F:103:VAL:HG13	3:F:505:HOH:O	2.12	0.49
1:A:289:PHE:O	1:A:290:ALA:C	2.56	0.49
1:D:228:HIS:O	1:D:231:GLU:HB2	2.12	0.49
1:C:324:ALA:O	1:C:327:ALA:HB3	2.12	0.49
1:D:37:LYS:O	1:D:39:PRO:HD3	2.13	0.49
1:D:209:CYS:HB3	1:D:217:LEU:HD11	1.94	0.49
1:E:279:TYR:CZ	1:E:301:CYS:HB2	2.47	0.49
1:E:296:VAL:CG1	1:E:334:MET:SD	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:SER:OG	1:A:261:THR:OG1	2.18	0.49
1:D:146:ASN:OD1	1:D:162:LYS:NZ	2.43	0.49
1:E:48:PRO:HD3	1:E:56:PHE:CZ	2.48	0.49
1:E:144:ASP:OD1	1:E:203:TYR:OH	2.23	0.49
1:F:206:CYS:O	1:F:208:ARG:N	2.46	0.49
1:A:315:ARG:NE	1:A:376:GLU:OE2	2.43	0.49
1:C:68:GLY:O	1:C:69:VAL:O	2.30	0.49
1:D:172:LEU:HD21	1:D:221:TYR:HE1	1.77	0.49
1:A:237:TRP:CD1	1:A:273:MET:HB3	2.48	0.48
1:A:369:VAL:O	1:A:372:GLN:N	2.46	0.48
1:F:379:MET:O	1:F:380:ASN:C	2.56	0.48
1:A:282:ALA:HB2	1:A:309:ALA:HB1	1.95	0.48
1:C:184:ASP:CG	1:C:232:LYS:HZ2	2.21	0.48
1:C:321:GLY:HA2	1:C:327:ALA:O	2.13	0.48
1:D:138:GLN:OE1	1:D:138:GLN:N	2.39	0.48
1:C:165:CYS:O	1:C:168:HIS:HB2	2.13	0.48
1:C:290:ALA:O	1:C:333:ARG:NH1	2.46	0.48
1:E:144:ASP:CG	1:E:145:TYR:N	2.71	0.48
1:A:59:PHE:CD2	1:A:349:ILE:HG12	2.48	0.48
1:A:167:SER:O	1:A:168:HIS:C	2.57	0.48
1:D:302:SER:O	1:D:303:ASN:C	2.55	0.48
1:E:59:PHE:O	1:E:63:VAL:HB	2.13	0.48
1:E:90:GLY:C	1:E:92:ARG:N	2.70	0.48
1:E:194:GLY:O	1:E:195:LEU:CB	2.61	0.48
1:F:36:ASN:HD21	1:F:37:LYS:CE	2.27	0.48
1:A:63:VAL:CG1	1:A:352:TYR:CZ	2.96	0.48
1:A:322:THR:O	1:A:323:ARG:C	2.55	0.48
1:C:57:CYS:O	1:C:58:ARG:C	2.55	0.48
1:C:129:ILE:O	1:C:129:ILE:HG22	2.14	0.48
1:D:301:CYS:HA	1:D:340:THR:O	2.14	0.48
1:F:89:ALA:C	1:F:90:GLY:O	2.57	0.48
1:F:189:ASP:CA	1:F:234:CYS:SG	3.01	0.48
1:A:367:LYS:C	1:A:369:VAL:N	2.71	0.48
1:C:42:ALA:HB2	1:C:71:THR:HB	1.95	0.48
1:C:324:ALA:CB	1:C:326:TRP:CZ2	2.97	0.48
1:E:227:ASP:O	1:E:230:LYS:HB3	2.14	0.48
1:E:276:ASP:OD2	1:E:285:THR:CB	2.62	0.48
1:E:350:ASP:HB3	1:E:355:ARG:HB2	1.95	0.48
1:A:323:ARG:CG	1:A:323:ARG:NH1	2.65	0.48
1:C:317:ALA:O	1:C:320:ASP:HB3	2.13	0.48
1:D:60:ILE:HD13	1:D:102:ILE:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ASP:O	1:D:198:VAL:N	2.47	0.48
1:E:184:ASP:CG	1:E:232:LYS:HZ3	2.21	0.48
1:A:368:ALA:O	1:A:371:ALA:HB3	2.14	0.48
1:D:88:LEU:HD13	1:D:132:LEU:HB2	1.95	0.48
1:F:298:PRO:HB3	1:F:310:GLN:OE1	2.14	0.48
1:D:34:GLU:O	1:D:318:ARG:NH2	2.47	0.48
1:D:74:LEU:HB2	1:D:113:PHE:CZ	2.48	0.48
1:E:43:MET:HG2	1:E:44:LEU:N	2.29	0.48
1:F:348:PHE:HA	1:F:360:LEU:CD1	2.44	0.48
1:C:248:THR:O	1:F:267:LEU:HD21	2.14	0.48
1:C:258:MET:SD	1:F:263:ARG:HG3	2.54	0.48
1:D:88:LEU:HD22	1:D:131:PRO:O	2.14	0.48
1:D:251:LEU:C	1:D:252:LEU:HG	2.39	0.48
1:A:121:GLY:CA	1:A:163:SER:HB3	2.44	0.47
1:C:38:LEU:C	1:C:40:VAL:H	2.22	0.47
1:D:320:ASP:C	1:D:322:THR:N	2.72	0.47
1:E:46:THR:O	1:E:47:VAL:C	2.56	0.47
1:F:276:ASP:OD1	1:F:285:THR:HG22	2.14	0.47
1:C:258:MET:HE1	1:F:263:ARG:NE	2.28	0.47
1:E:69:VAL:HG12	1:E:111:ILE:HD11	1.96	0.47
1:F:82:PHE:O	1:F:86:PRO:HA	2.13	0.47
1:F:259:ASN:O	1:F:260:ALA:CB	2.62	0.47
1:A:324:ALA:CB	1:A:325:PRO:CD	2.86	0.47
1:D:123:GLN:OE1	1:D:164:LEU:HD21	2.15	0.47
1:D:363:ALA:O	1:D:364:GLU:C	2.56	0.47
1:E:56:PHE:CZ	1:E:74:LEU:HD11	2.49	0.47
1:F:166:PRO:HD2	1:F:209:CYS:SG	2.54	0.47
1:F:182:LEU:HD12	1:F:191:PHE:CZ	2.50	0.47
1:A:116:LYS:HA	1:A:192:HIS:O	2.13	0.47
1:D:165:CYS:O	1:D:171:LEU:HD22	2.14	0.47
1:E:117:MET:SD	1:E:182:LEU:CD1	3.03	0.47
1:E:174:THR:O	1:E:178:LEU:CG	2.58	0.47
1:F:176:PHE:C	1:F:180:ASP:OD2	2.57	0.47
1:A:150:PRO:HB2	1:C:146:ASN:HB2	1.97	0.47
1:C:43:MET:HE3	1:C:339:VAL:HG12	1.95	0.47
1:C:199:TRP:C	1:F:248:THR:HG23	2.39	0.47
1:D:156:PRO:O	1:D:254:TRP:HZ2	1.98	0.47
1:D:223:THR:O	1:D:224:LYS:C	2.56	0.47
1:F:106:CYS:O	1:F:109:ALA:N	2.48	0.47
1:F:279:TYR:CZ	1:F:301:CYS:HB2	2.49	0.47
1:C:99:LEU:O	1:C:103:VAL:N	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:LEU:O	1:C:163:SER:HA	2.14	0.47
1:C:120:LEU:CD1	1:C:166:PRO:HG3	2.45	0.47
1:C:341:MET:SD	1:C:343:GLU:OE2	2.73	0.47
1:E:39:PRO:O	1:E:70:ASN:OD1	2.33	0.47
1:E:360:LEU:O	1:E:363:ALA:N	2.47	0.47
1:A:49:HIS:CD2	1:A:92:ARG:NH2	2.83	0.47
1:A:73:VAL:HG21	1:A:338:PHE:HZ	1.76	0.47
1:A:213:ASP:OD1	1:A:263:ARG:NH2	2.46	0.47
1:A:368:ALA:HA	1:A:371:ALA:HB3	1.96	0.47
1:C:148:PRO:O	1:C:150:PRO:O	2.33	0.47
1:C:302:SER:HA	1:C:361:PRO:O	2.15	0.47
1:D:79:ASN:HD22	1:D:79:ASN:H	1.60	0.47
1:D:147:PRO:HD3	1:D:162:LYS:HE2	1.97	0.47
1:D:186:CYS:O	1:D:187:GLY:C	2.58	0.47
1:D:310:GLN:O	1:D:313:GLN:HB2	2.15	0.47
1:D:328:VAL:O	1:D:331:ALA:N	2.48	0.47
1:E:88:LEU:O	1:E:89:ALA:C	2.58	0.47
1:E:119:LEU:O	1:E:221:TYR:OH	2.23	0.47
1:E:273:MET:SD	1:E:273:MET:C	2.97	0.47
1:E:329:THR:CG2	1:E:333:ARG:NH2	2.78	0.47
1:F:240:SER:HB2	1:F:244:ILE:HD11	1.97	0.47
1:D:79:ASN:N	1:D:79:ASN:ND2	2.54	0.47
1:D:168:HIS:CE1	1:D:169:PRO:HD2	2.50	0.47
1:F:338:PHE:CD1	1:F:338:PHE:C	2.93	0.47
1:D:64:LEU:N	1:D:65:PRO:CD	2.78	0.47
1:D:228:HIS:O	1:D:231:GLU:N	2.32	0.47
1:D:320:ASP:O	1:D:322:THR:N	2.47	0.47
1:E:49:HIS:O	1:E:50:PRO:C	2.57	0.47
1:E:212:ARG:HB2	1:E:217:LEU:CD1	2.45	0.47
1:E:227:ASP:O	1:E:228:HIS:C	2.58	0.47
1:F:60:ILE:HA	1:F:64:LEU:HG	1.97	0.47
1:A:352:TYR:CD1	1:A:352:TYR:C	2.93	0.47
1:C:247:LYS:CB	1:F:265:ILE:HG22	2.39	0.47
1:D:99:LEU:C	1:D:101:GLN:N	2.70	0.47
1:F:112:ARG:NH2	1:F:189:ASP:O	2.48	0.47
1:F:182:LEU:O	1:F:186:CYS:HB2	2.15	0.47
1:A:64:LEU:HD22	1:A:69:VAL:HG21	1.97	0.46
1:A:304:SER:HB3	1:A:365:THR:HG23	1.96	0.46
1:A:341:MET:C	1:A:341:MET:SD	2.98	0.46
1:C:249:THR:HB	1:C:251:LEU:HG	1.97	0.46
1:D:184:ASP:OD1	1:D:232:LYS:NZ	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:VAL:HA	1:D:331:ALA:HB3	1.96	0.46
1:F:159:PHE:CD1	1:F:159:PHE:C	2.93	0.46
1:F:289:PHE:C	1:F:291:ILE:H	2.22	0.46
1:A:369:VAL:C	1:A:371:ALA:N	2.71	0.46
1:C:117:MET:HE1	1:C:178:LEU:CB	2.46	0.46
1:D:175:ILE:C	1:D:177:PRO:HD2	2.40	0.46
1:E:67:GLU:O	1:E:374:ARG:NH1	2.43	0.46
1:E:85:HIS:N	1:E:86:PRO:CD	2.78	0.46
1:E:119:LEU:O	1:E:164:LEU:HD12	2.14	0.46
1:E:341:MET:HG2	1:E:348:PHE:CE2	2.50	0.46
1:F:265:ILE:HG23	1:F:266:ASP:OD1	2.14	0.46
1:F:274:ILE:HD11	1:F:294:PHE:CE1	2.51	0.46
1:A:60:ILE:HA	1:A:64:LEU:HD12	1.96	0.46
1:A:378:VAL:O	1:A:380:ASN:N	2.45	0.46
1:D:88:LEU:HD22	1:D:131:PRO:C	2.41	0.46
1:F:168:HIS:ND1	1:F:169:PRO:HD2	2.29	0.46
1:A:119:LEU:O	1:A:221:TYR:HE2	1.98	0.46
1:A:245:ASP:O	1:A:249:THR:CG2	2.63	0.46
1:E:285:THR:N	1:E:286:PRO:HD2	2.31	0.46
1:C:241:ASP:O	1:C:242:ARG:C	2.57	0.46
1:D:97:GLN:C	1:D:99:LEU:H	2.23	0.46
1:D:195:LEU:HD23	1:D:195:LEU:N	2.31	0.46
1:D:272:ILE:HG22	1:D:274:ILE:HD13	1.97	0.46
1:E:76:ILE:HG22	1:E:77:ARG:O	2.16	0.46
1:E:120:LEU:O	1:E:163:SER:HA	2.16	0.46
1:E:252:LEU:HD23	1:E:252:LEU:N	2.30	0.46
1:E:288:TYR:O	1:E:292:LYS:HG2	2.16	0.46
1:A:240:SER:OG	1:A:276:ASP:HA	2.15	0.46
1:C:42:ALA:CB	1:C:71:THR:HB	2.45	0.46
1:C:244:ILE:HD11	1:C:289:PHE:CE2	2.50	0.46
1:C:248:THR:O	1:F:267:LEU:CD2	2.63	0.46
1:D:33:PHE:CE1	1:D:328:VAL:HG13	2.50	0.46
1:D:73:VAL:HG22	1:D:114:ILE:CG2	2.45	0.46
1:A:101:GLN:O	1:A:105:THR:OG1	2.33	0.46
1:A:251:LEU:O	1:A:252:LEU:HG	2.15	0.46
1:C:104:GLN:O	1:C:104:GLN:NE2	2.48	0.46
1:D:248:THR:O	1:D:248:THR:CG2	2.64	0.46
1:F:70:ASN:OD1	1:F:71:THR:OG1	2.33	0.46
1:F:226:HIS:ND1	1:F:269:PRO:HG2	2.31	0.46
1:A:241:ASP:O	1:A:256:ALA:HA	2.15	0.46
1:C:41:LYS:O	1:C:69:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:PHE:C	1:F:247:LYS:HE3	2.41	0.46
1:C:265:ILE:HG23	1:C:266:ASP:OD1	2.16	0.46
1:C:349:ILE:O	1:C:352:TYR:HB3	2.16	0.46
1:D:147:PRO:HB3	1:D:159:PHE:CD1	2.50	0.46
1:E:175:ILE:O	1:E:178:LEU:HB2	2.15	0.46
1:E:376:GLU:O	1:E:379:MET:HE2	2.16	0.46
1:A:70:ASN:OD1	1:A:70:ASN:O	2.34	0.46
1:C:240:SER:O	1:C:241:ASP:C	2.58	0.46
1:C:246:GLY:CA	1:C:256:ALA:HB3	2.46	0.46
1:D:78:TYR:CE1	1:D:117:MET:CE	2.99	0.46
1:D:183:ILE:HG23	1:D:188:ALA:HB3	1.96	0.46
1:D:240:SER:CB	1:D:276:ASP:HA	2.46	0.46
1:A:237:TRP:CZ2	1:A:273:MET:HE3	2.51	0.46
1:A:361:PRO:O	1:A:365:THR:OG1	2.34	0.46
1:C:324:ALA:HB1	1:C:326:TRP:CD2	2.50	0.46
1:E:179:MET:HE1	1:E:225:LEU:HD22	1.97	0.46
1:F:214:LYS:HB2	1:F:260:ALA:O	2.15	0.46
1:F:238:MET:HE3	1:F:238:MET:HB2	1.76	0.46
1:A:246:GLY:HA2	1:A:249:THR:OG1	2.16	0.45
1:C:247:LYS:CG	1:F:263:ARG:HA	2.44	0.45
1:E:64:LEU:HB2	1:E:65:PRO:CD	2.46	0.45
1:E:79:ASN:O	1:E:94:ILE:N	2.48	0.45
1:F:103:VAL:CG1	3:F:505:HOH:O	2.64	0.45
1:A:41:LYS:HE3	1:A:70:ASN:HD22	1.77	0.45
1:A:323:ARG:HH11	1:A:323:ARG:HG2	1.76	0.45
1:C:355:ARG:C	1:C:357:GLY:N	2.72	0.45
1:D:121:GLY:O	1:D:123:GLN:HG2	2.15	0.45
1:D:212:ARG:NH1	1:D:217:LEU:HD21	2.31	0.45
1:E:43:MET:CE	1:E:45:LEU:HD21	2.46	0.45
1:F:151:TRP:CZ3	1:F:152:LYS:O	2.69	0.45
1:A:355:ARG:O	1:A:358:LYS:HB2	2.16	0.45
1:C:43:MET:SD	1:C:366:PHE:CE1	3.09	0.45
1:C:74:LEU:CD2	1:C:102:ILE:HG21	2.46	0.45
1:C:303:ASN:OD1	1:C:305:GLU:N	2.45	0.45
1:C:345:SER:O	1:C:349:ILE:CG1	2.63	0.45
1:E:245:ASP:OD1	1:E:245:ASP:C	2.60	0.45
1:E:245:ASP:O	1:E:249:THR:HG23	2.15	0.45
1:E:278:LYS:HB2	1:E:310:GLN:NE2	2.30	0.45
1:F:132:LEU:HD23	1:F:164:LEU:CD1	2.45	0.45
1:F:141:GLU:OE1	1:F:209:CYS:CB	2.64	0.45
1:C:40:VAL:HG21	1:C:335:GLN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:LEU:HB2	1:D:41:LYS:HD3	1.98	0.45
1:E:238:MET:HE3	1:E:238:MET:HB2	1.86	0.45
1:E:239:TRP:CZ3	1:E:275:CYS:HB3	2.52	0.45
1:A:132:LEU:CD2	1:A:164:LEU:HD21	2.47	0.45
1:C:253:GLY:HA3	1:C:258:MET:CE	2.47	0.45
1:C:283:PRO:HB2	1:C:284:PRO:HD2	1.97	0.45
1:D:363:ALA:O	1:D:365:THR:N	2.50	0.45
1:E:240:SER:HB3	1:E:274:ILE:CG2	2.46	0.45
1:E:308:LEU:HD23	1:E:308:LEU:HA	1.87	0.45
1:F:366:PHE:O	1:F:370:PHE:HD1	1.99	0.45
1:A:329:THR:HG22	1:A:333:ARG:CZ	2.47	0.45
1:E:219:ALA:HB2	1:E:264:ALA:HB1	1.98	0.45
1:F:36:ASN:ND2	1:F:37:LYS:CE	2.79	0.45
1:F:360:LEU:O	1:F:363:ALA:N	2.47	0.45
1:A:47:VAL:HA	1:A:74:LEU:HD11	1.98	0.45
1:C:244:ILE:HD13	1:C:285:THR:CG2	2.47	0.45
1:D:43:MET:HE2	1:D:45:LEU:CD2	2.47	0.45
1:D:67:GLU:HG3	1:D:366:PHE:HE2	1.81	0.45
1:E:226:HIS:O	1:E:230:LYS:HB2	2.16	0.45
1:E:343:GLU:N	1:E:343:GLU:CD	2.75	0.45
1:F:125:ASP:O	1:F:126:ARG:CG	2.65	0.45
1:F:151:TRP:CE3	1:F:152:LYS:O	2.70	0.45
1:F:289:PHE:O	1:F:290:ALA:C	2.59	0.45
1:A:295:ASN:HB3	1:A:335:GLN:HG2	1.98	0.45
1:C:212:ARG:HD3	1:C:217:LEU:HD12	1.98	0.45
1:C:258:MET:HE1	1:F:263:ARG:HG3	1.98	0.45
1:C:312:ALA:O	1:C:313:GLN:C	2.60	0.45
1:D:59:PHE:CZ	1:D:64:LEU:HD21	2.52	0.45
1:F:133:LEU:HD22	1:F:140:ASP:N	2.31	0.45
1:F:219:ALA:HB2	1:F:264:ALA:HB1	1.99	0.45
1:A:285:THR:O	1:A:288:TYR:HB3	2.16	0.45
1:E:308:LEU:O	1:E:311:LEU:N	2.50	0.45
1:F:73:VAL:HA	1:F:114:ILE:O	2.17	0.45
1:A:78:TYR:CD2	1:A:131:PRO:HD2	2.52	0.44
1:C:298:PRO:O	1:C:338:PHE:N	2.44	0.44
1:C:43:MET:HE1	1:C:366:PHE:CG	2.53	0.44
1:E:85:HIS:O	1:E:88:LEU:HB2	2.17	0.44
1:E:121:GLY:O	1:E:122:HIS:HB2	2.18	0.44
1:E:239:TRP:HZ3	1:E:299:SER:CB	2.29	0.44
1:F:42:ALA:HB3	1:F:338:PHE:CB	2.46	0.44
1:A:167:SER:O	1:A:168:HIS:O	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:TRP:HA	1:A:299:SER:O	2.17	0.44
1:C:203:TYR:HE1	1:F:250:ASN:CG	2.25	0.44
1:C:240:SER:OG	1:C:276:ASP:HA	2.16	0.44
1:C:250:ASN:HB2	1:F:267:LEU:HD11	2.00	0.44
1:A:104:GLN:HE21	1:A:108:GLU:HG3	1.83	0.44
1:A:255:GLN:CD	1:A:280:GLU:OE2	2.61	0.44
1:C:156:PRO:C	1:C:157:PHE:CD1	2.95	0.44
1:C:330:LEU:HD23	1:C:333:ARG:HH11	1.83	0.44
1:D:65:PRO:HG3	1:D:109:ALA:CB	2.47	0.44
1:D:88:LEU:HD11	1:D:132:LEU:HD13	1.99	0.44
1:A:284:PRO:HB2	1:D:291:ILE:HD11	1.98	0.44
1:C:45:LEU:N	1:C:73:VAL:O	2.38	0.44
1:C:99:LEU:HD11	1:C:186:CYS:SG	2.58	0.44
1:C:199:TRP:O	1:F:248:THR:N	2.50	0.44
1:D:46:THR:HG21	1:D:343:GLU:O	2.17	0.44
1:E:359:LYS:O	1:E:360:LEU:HD23	2.17	0.44
1:F:301:CYS:O	1:F:302:SER:C	2.61	0.44
1:E:37:LYS:HA	1:E:377:GLU:OE1	2.17	0.44
1:E:123:GLN:O	1:E:130:ASP:HB2	2.18	0.44
1:A:366:PHE:O	1:A:367:LYS:O	2.36	0.44
1:D:138:GLN:H	1:D:138:GLN:CD	2.25	0.44
1:D:177:PRO:O	1:D:178:LEU:C	2.60	0.44
1:D:196:ASP:OD1	1:D:196:ASP:N	2.50	0.44
1:D:226:HIS:HD2	1:D:272:ILE:CG1	2.30	0.44
1:D:339:VAL:HG21	1:D:370:PHE:CE2	2.53	0.44
1:D:373:ILE:O	1:D:374:ARG:C	2.61	0.44
1:E:114:ILE:HG23	1:E:190:ALA:HB3	1.99	0.44
1:E:340:THR:OG1	1:E:341:MET:N	2.49	0.44
1:F:37:LYS:HB2	3:F:502:HOH:O	2.16	0.44
1:F:189:ASP:HA	1:F:234:CYS:SG	2.58	0.44
1:C:165:CYS:SG	1:C:168:HIS:HB2	2.58	0.44
1:D:83:LYS:HG3	1:D:181:GLU:OE1	2.17	0.44
1:D:176:PHE:N	1:D:177:PRO:CD	2.80	0.44
1:D:226:HIS:HD2	1:D:272:ILE:HG12	1.83	0.44
1:E:228:HIS:C	1:E:228:HIS:CD2	2.96	0.44
1:F:183:ILE:HD11	1:F:229:LEU:HD21	2.00	0.44
1:F:372:GLN:O	1:F:376:GLU:HG3	2.17	0.44
1:C:247:LYS:HA	1:F:263:ARG:CB	2.48	0.44
1:C:279:TYR:CE1	1:C:301:CYS:HB2	2.53	0.44
1:C:297:LEU:CD2	1:C:336:GLY:N	2.81	0.44
1:C:122:HIS:CE1	1:C:197:GLU:OE2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:MET:SD	1:C:272:ILE:HG21	2.58	0.43
1:D:50:PRO:CG	1:D:94:ILE:HG22	2.47	0.43
1:E:242:ARG:NH2	1:E:256:ALA:O	2.51	0.43
1:F:37:LYS:O	1:F:38:LEU:C	2.61	0.43
1:F:149:VAL:HA	1:F:150:PRO:C	2.43	0.43
1:C:38:LEU:O	1:C:40:VAL:N	2.51	0.43
1:C:316:LEU:HA	1:C:319:LYS:HB3	1.99	0.43
1:C:371:ALA:O	1:C:374:ARG:N	2.52	0.43
1:E:84:SER:C	1:E:86:PRO:CD	2.91	0.43
1:F:175:ILE:HG23	1:F:179:MET:SD	2.58	0.43
1:D:346:LYS:C	1:D:348:PHE:N	2.75	0.43
1:F:188:ALA:O	1:F:234:CYS:SG	2.71	0.43
1:F:378:VAL:HG12	1:F:378:VAL:O	2.17	0.43
1:A:51:GLU:HG3	1:E:98:GLN:HE22	1.77	0.43
1:A:64:LEU:HD23	1:A:64:LEU:HA	1.80	0.43
1:A:237:TRP:CE3	1:A:273:MET:HG2	2.53	0.43
1:A:291:ILE:HA	1:D:249:THR:HG22	1.99	0.43
1:A:330:LEU:HD21	1:D:249:THR:HA	2.00	0.43
1:A:369:VAL:O	1:A:371:ALA:N	2.51	0.43
1:A:370:PHE:CD1	1:A:373:ILE:HD12	2.53	0.43
1:C:203:TYR:CE1	1:F:250:ASN:CB	3.01	0.43
1:D:80:TYR:HE1	1:D:99:LEU:HD23	1.83	0.43
1:D:265:ILE:HD13	1:D:288:TYR:CE2	2.53	0.43
1:F:311:LEU:HD11	1:F:315:ARG:HH21	1.83	0.43
1:A:63:VAL:HG12	1:A:67:GLU:CG	2.47	0.43
1:A:293:GLY:CA	1:D:248:THR:CG2	2.96	0.43
1:A:366:PHE:CE1	1:A:370:PHE:CD2	3.06	0.43
1:D:71:THR:N	1:D:111:ILE:HG23	2.32	0.43
1:D:277:TRP:O	1:D:278:LYS:CD	2.67	0.43
1:E:198:VAL:CG2	1:E:242:ARG:HG3	2.49	0.43
1:F:57:CYS:SG	1:F:102:ILE:HG13	2.59	0.43
1:C:69:VAL:CG1	1:C:71:THR:O	2.67	0.43
1:D:49:HIS:CG	1:D:92:ARG:NH2	2.86	0.43
1:E:328:VAL:O	1:E:329:THR:O	2.37	0.43
1:A:41:LYS:CE	1:A:68:GLY:O	2.66	0.43
1:C:64:LEU:HB2	1:C:65:PRO:HD3	2.00	0.43
1:C:103:VAL:CG2	1:C:186:CYS:SG	3.02	0.43
1:C:177:PRO:HB3	1:E:184:ASP:HB3	2.00	0.43
1:C:215:ALA:O	1:C:264:ALA:HB2	2.19	0.43
1:C:348:PHE:O	1:C:349:ILE:C	2.61	0.43
1:D:117:MET:HG2	1:D:119:LEU:CD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ILE:C	1:D:177:PRO:CD	2.92	0.43
1:D:365:THR:O	1:D:368:ALA:HB3	2.19	0.43
1:E:90:GLY:O	1:E:91:GLU:C	2.62	0.43
1:A:132:LEU:CD2	1:A:164:LEU:CD2	2.96	0.43
1:A:329:THR:O	1:A:332:GLU:N	2.52	0.43
1:E:47:VAL:HA	1:E:74:LEU:HD21	2.01	0.43
1:E:114:ILE:HG23	1:E:190:ALA:O	2.19	0.43
1:F:64:LEU:N	1:F:64:LEU:HD23	2.34	0.43
1:F:367:LYS:O	1:F:368:ALA:C	2.61	0.43
1:A:89:ALA:C	1:A:90:GLY:O	2.62	0.43
1:C:259:ASN:CB	1:F:248:THR:HB	2.49	0.43
1:D:125:ASP:O	1:D:126:ARG:C	2.60	0.43
1:F:64:LEU:N	1:F:65:PRO:HD2	2.34	0.43
1:A:35:TRP:HB2	1:A:318:ARG:HB3	2.01	0.43
1:A:44:LEU:HD23	1:A:44:LEU:C	2.44	0.43
1:D:83:LYS:CB	1:D:181:GLU:OE1	2.67	0.43
1:A:119:LEU:O	1:A:221:TYR:CE2	2.71	0.42
1:C:103:VAL:HG22	1:C:113:PHE:CE2	2.54	0.42
1:C:251:LEU:O	1:C:252:LEU:CB	2.65	0.42
1:C:378:VAL:HG12	1:C:379:MET:N	2.33	0.42
1:D:96:GLU:HG2	1:D:100:LYS:HE3	2.01	0.42
1:D:128:HIS:C	1:D:129:ILE:HD13	2.44	0.42
1:D:151:TRP:CD2	1:D:151:TRP:C	2.97	0.42
1:D:361:PRO:HA	1:D:364:GLU:HB2	2.00	0.42
1:E:48:PRO:HD3	1:E:56:PHE:CD2	2.53	0.42
1:E:360:LEU:HB3	1:E:362:SER:OG	2.19	0.42
1:F:47:VAL:O	1:F:47:VAL:HG13	2.18	0.42
1:F:283:PRO:C	1:F:285:THR:N	2.76	0.42
1:F:300:SER:CB	1:F:307:ALA:HB1	2.49	0.42
1:A:321:GLY:HA2	1:A:327:ALA:O	2.19	0.42
1:E:44:LEU:HD12	1:E:239:TRP:HZ2	1.83	0.42
1:E:321:GLY:O	1:E:328:VAL:HG22	2.18	0.42
1:F:367:LYS:O	1:F:371:ALA:N	2.51	0.42
1:A:84:SER:CB	1:A:181:GLU:OE2	2.66	0.42
1:A:373:ILE:O	1:A:376:GLU:HB2	2.19	0.42
1:C:129:ILE:C	1:C:130:ASP:O	2.62	0.42
1:C:196:ASP:O	1:C:197:GLU:C	2.63	0.42
1:C:246:GLY:HA2	1:C:256:ALA:CB	2.49	0.42
1:D:240:SER:HB3	1:D:276:ASP:HA	2.00	0.42
1:E:120:LEU:HD11	1:E:166:PRO:HG3	2.01	0.42
1:E:321:GLY:HA3	1:E:331:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:TYR:HB3	1:A:88:LEU:O	2.19	0.42
1:C:59:PHE:CZ	1:C:63:VAL:HG11	2.54	0.42
1:C:371:ALA:C	1:C:373:ILE:N	2.77	0.42
1:E:198:VAL:HB	1:E:242:ARG:HG3	2.00	0.42
1:E:328:VAL:HG12	1:E:329:THR:N	2.33	0.42
1:C:40:VAL:HG11	1:C:297:LEU:CD1	2.49	0.42
1:C:204:GLU:HG3	1:C:204:GLU:O	2.18	0.42
1:D:151:TRP:CG	1:D:152:LYS:N	2.87	0.42
1:D:295:ASN:OD1	1:D:333:ARG:HA	2.20	0.42
1:D:301:CYS:SG	1:D:342:TRP:HD1	2.43	0.42
1:F:142:SER:HA	1:F:143:PRO:HD3	1.90	0.42
1:F:274:ILE:HG21	1:F:289:PHE:CZ	2.55	0.42
1:F:304:SER:O	1:F:306:VAL:N	2.52	0.42
1:A:258:MET:HB2	3:A:501:HOH:O	2.20	0.42
1:C:203:TYR:CE1	1:F:250:ASN:CG	2.98	0.42
1:C:259:ASN:CG	1:F:248:THR:HG21	2.44	0.42
1:D:120:LEU:HG	1:D:198:VAL:HG11	2.01	0.42
1:E:59:PHE:CZ	1:E:349:ILE:HG12	2.55	0.42
1:E:329:THR:O	1:E:331:ALA:N	2.53	0.42
1:F:116:LYS:NZ	1:F:118:ASN:HD21	2.17	0.42
1:F:315:ARG:HH12	1:F:377:GLU:CG	2.32	0.42
1:A:139:PHE:CZ	1:A:170:ASP:O	2.72	0.42
1:A:182:LEU:O	1:A:183:ILE:C	2.62	0.42
1:A:277:TRP:HB3	1:A:299:SER:HB2	2.01	0.42
1:C:36:ASN:C	1:C:36:ASN:HD22	2.27	0.42
1:C:57:CYS:C	1:C:59:PHE:N	2.77	0.42
1:C:103:VAL:HG22	1:C:113:PHE:CZ	2.55	0.42
1:E:76:ILE:HD12	1:E:182:LEU:HD13	2.02	0.42
1:F:64:LEU:HD11	1:F:72:LEU:HD13	2.00	0.42
1:C:117:MET:HE1	1:C:178:LEU:HB3	2.02	0.42
1:C:160:TYR:CD2	1:C:199:TRP:CD1	3.08	0.42
1:C:255:GLN:HB3	1:C:278:LYS:HE3	2.01	0.42
1:D:232:LYS:O	1:D:233:LYS:C	2.62	0.42
1:E:131:PRO:HA	1:E:134:ALA:HB3	2.01	0.42
1:E:212:ARG:HB2	1:E:217:LEU:HD12	2.02	0.42
1:F:44:LEU:HB2	1:F:338:PHE:HE1	1.84	0.42
1:F:213:ASP:OD2	1:F:263:ARG:NH1	2.51	0.42
1:F:304:SER:C	1:F:306:VAL:N	2.77	0.42
1:A:293:GLY:CA	1:D:248:THR:HG21	2.49	0.42
1:C:46:THR:HG23	1:C:75:ARG:NH2	2.35	0.42
1:C:127:ASP:OD1	1:C:127:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:TRP:CE3	1:D:273:MET:HG2	2.54	0.42
1:D:366:PHE:CE1	1:D:370:PHE:CE2	3.07	0.42
1:F:338:PHE:CE1	1:F:340:THR:HG22	2.54	0.42
1:C:199:TRP:O	1:F:248:THR:OG1	2.32	0.42
1:C:239:TRP:CE3	1:C:275:CYS:HB3	2.54	0.42
1:E:90:GLY:O	1:E:93:ALA:N	2.53	0.42
1:E:130:ASP:O	1:E:132:LEU:N	2.49	0.42
1:E:179:MET:C	1:E:181:GLU:H	2.27	0.42
1:E:290:ALA:O	1:E:330:LEU:HD22	2.19	0.42
1:F:43:MET:CE	1:F:45:LEU:HG	2.49	0.42
1:F:259:ASN:O	1:F:260:ALA:HB2	2.20	0.42
1:C:99:LEU:CD1	1:C:186:CYS:SG	3.07	0.41
1:D:50:PRO:HB3	1:D:98:GLN:CD	2.45	0.41
1:D:147:PRO:HB3	1:D:159:PHE:CE1	2.55	0.41
1:E:41:LYS:CB	1:E:70:ASN:ND2	2.79	0.41
1:E:201:LEU:HD23	1:E:214:LYS:HG2	2.01	0.41
1:E:263:ARG:O	1:E:267:LEU:CD1	2.68	0.41
1:F:47:VAL:HG12	1:F:75:ARG:O	2.19	0.41
1:A:58:ARG:O	1:A:62:GLU:CG	2.69	0.41
1:A:103:VAL:HG21	1:A:186:CYS:HA	2.01	0.41
1:A:279:TYR:CE2	1:A:301:CYS:HB2	2.55	0.41
1:A:322:THR:O	1:A:324:ALA:N	2.53	0.41
1:C:59:PHE:CE2	1:C:64:LEU:HD21	2.55	0.41
1:D:83:LYS:HB2	1:D:181:GLU:OE1	2.20	0.41
1:D:237:TRP:CG	1:D:273:MET:HB3	2.54	0.41
1:A:248:THR:O	1:D:333:ARG:NH1	2.39	0.41
1:A:308:LEU:O	1:A:311:LEU:N	2.53	0.41
1:C:99:LEU:O	1:C:103:VAL:HG23	2.20	0.41
1:C:253:GLY:HA2	1:C:258:MET:CG	2.49	0.41
1:C:285:THR:O	1:C:288:TYR:HB3	2.21	0.41
1:C:300:SER:HB3	1:C:339:VAL:HG22	2.01	0.41
1:E:77:ARG:CZ	1:E:122:HIS:O	2.68	0.41
1:E:99:LEU:C	1:E:101:GLN:H	2.29	0.41
1:E:225:LEU:O	1:E:226:HIS:C	2.63	0.41
1:F:95:SER:H	1:F:98:GLN:HB2	1.86	0.41
1:F:260:ALA:C	1:F:261:THR:HG23	2.46	0.41
1:A:53:VAL:HB	1:A:54:PRO:HD3	2.02	0.41
1:A:193:VAL:HG23	1:A:195:LEU:HG	2.01	0.41
1:C:59:PHE:CD1	1:C:349:ILE:HG12	2.56	0.41
1:C:241:ASP:C	1:C:243:LEU:N	2.77	0.41
1:D:160:TYR:CE2	1:D:197:GLU:OE2	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:SER:O	1:E:162:LYS:NZ	2.54	0.41
1:A:46:THR:HA	1:A:75:ARG:HB3	2.02	0.41
1:A:81:LYS:HD2	1:A:95:SER:HB3	2.02	0.41
1:C:69:VAL:CG2	1:C:370:PHE:CZ	3.03	0.41
1:D:45:LEU:HD13	1:D:56:PHE:CZ	2.56	0.41
1:D:50:PRO:HB3	1:D:98:GLN:HE22	1.85	0.41
1:D:102:ILE:O	1:D:102:ILE:CG2	2.64	0.41
1:F:135:LYS:C	1:F:136:TYR:HD1	2.27	0.41
1:A:63:VAL:HG11	1:A:352:TYR:CE2	2.56	0.41
1:A:64:LEU:HD13	1:A:69:VAL:CG1	2.41	0.41
1:A:138:GLN:C	1:A:140:ASP:H	2.28	0.41
1:C:166:PRO:HB2	1:C:221:TYR:CD1	2.56	0.41
1:C:255:GLN:O	1:C:278:LYS:NZ	2.31	0.41
1:D:36:ASN:OD1	1:D:36:ASN:N	2.51	0.41
1:E:263:ARG:O	1:E:267:LEU:HG	2.21	0.41
1:E:321:GLY:HA2	1:E:327:ALA:C	2.45	0.41
1:F:106:CYS:SG	1:F:113:PHE:HD2	2.44	0.41
1:F:236:MET:C	1:F:237:TRP:CD1	2.99	0.41
1:F:265:ILE:CD1	1:F:288:TYR:CZ	3.04	0.41
1:A:51:GLU:HA	1:E:51:GLU:HA	2.03	0.41
1:C:166:PRO:HA	1:C:171:LEU:CD2	2.45	0.41
1:C:247:LYS:O	1:F:263:ARG:O	2.38	0.41
1:C:247:LYS:CE	1:C:258:MET:C	2.93	0.41
1:E:45:LEU:HB2	1:E:72:LEU:HD11	2.02	0.41
1:E:69:VAL:HG12	1:E:111:ILE:CD1	2.51	0.41
1:E:189:ASP:O	1:E:234:CYS:HA	2.21	0.41
1:E:277:TRP:HB2	1:E:279:TYR:CE1	2.55	0.41
1:F:43:MET:HG2	1:F:44:LEU:N	2.35	0.41
1:F:226:HIS:CE1	1:F:230:LYS:HD2	2.55	0.41
1:A:295:ASN:HB3	1:A:335:GLN:HG3	2.01	0.41
1:D:47:VAL:HB	1:D:75:ARG:O	2.21	0.41
1:E:65:PRO:HG3	1:E:109:ALA:HB1	2.03	0.41
1:E:106:CYS:CB	1:E:111:ILE:HG22	2.49	0.41
1:F:224:LYS:O	1:F:225:LEU:C	2.64	0.41
1:A:41:LYS:HB3	1:A:370:PHE:CE1	2.55	0.41
1:A:41:LYS:HE2	1:A:70:ASN:HD22	1.85	0.41
1:A:129:ILE:O	1:A:130:ASP:C	2.63	0.41
1:A:176:PHE:CZ	1:A:228:HIS:HB2	2.56	0.41
1:A:182:LEU:C	1:A:184:ASP:N	2.77	0.41
1:A:251:LEU:O	1:A:252:LEU:CB	2.69	0.41
1:A:358:LYS:C	1:A:359:LYS:HG3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:GLN:NE2	1:C:108:GLU:HG3	2.36	0.41
1:C:129:ILE:HG23	1:C:133:LEU:HB2	2.03	0.41
1:E:59:PHE:CD1	1:E:349:ILE:HG23	2.56	0.41
1:F:146:ASN:O	1:F:159:PHE:CD2	2.74	0.41
1:F:274:ILE:CG1	1:F:294:PHE:CD1	3.03	0.41
1:C:38:LEU:C	1:C:40:VAL:N	2.78	0.41
1:D:228:HIS:O	1:D:229:LEU:C	2.64	0.41
1:D:280:GLU:O	1:D:281:SER:HB3	2.20	0.41
1:E:251:LEU:O	1:E:252:LEU:HB2	2.21	0.41
1:E:343:GLU:C	1:E:344:ASP:O	2.64	0.41
1:F:292:LYS:HA	1:F:292:LYS:HD3	1.90	0.41
1:A:45:LEU:O	1:A:74:LEU:HA	2.21	0.40
1:A:260:ALA:HA	1:A:262:PHE:CE2	2.56	0.40
1:C:41:LYS:H	1:C:70:ASN:CG	2.26	0.40
1:C:56:PHE:O	1:C:59:PHE:HB3	2.21	0.40
1:C:243:LEU:O	1:C:244:ILE:HG13	2.20	0.40
1:C:251:LEU:HD23	1:C:251:LEU:HA	1.94	0.40
1:E:36:ASN:ND2	1:E:37:LYS:HE2	2.37	0.40
1:E:324:ALA:HB1	1:E:326:TRP:CD2	2.56	0.40
1:F:367:LYS:O	1:F:370:PHE:N	2.54	0.40
1:A:122:HIS:NE2	1:A:196:ASP:OD2	2.54	0.40
1:A:145:TYR:CE2	1:A:159:PHE:HD2	2.38	0.40
1:C:60:ILE:CG2	1:C:105:THR:HB	2.51	0.40
1:C:160:TYR:CD2	1:C:199:TRP:HD1	2.39	0.40
1:C:258:MET:CB	1:F:245:ASP:OD2	2.68	0.40
1:D:83:LYS:N	1:D:181:GLU:OE1	2.45	0.40
1:D:106:CYS:O	1:D:109:ALA:N	2.54	0.40
1:D:196:ASP:O	1:D:198:VAL:HG23	2.21	0.40
1:E:63:VAL:HG13	1:E:352:TYR:OH	2.21	0.40
1:E:228:HIS:O	1:E:231:GLU:HB2	2.21	0.40
1:E:245:ASP:OD1	1:E:247:LYS:N	2.55	0.40
1:E:321:GLY:HA3	1:E:331:ALA:CB	2.51	0.40
1:E:322:THR:O	1:E:323:ARG:C	2.64	0.40
1:F:202:GLY:HA3	1:F:214:LYS:HG2	2.02	0.40
1:A:132:LEU:HD23	1:A:164:LEU:HD21	2.02	0.40
1:C:253:GLY:HA2	1:C:258:MET:HG2	2.03	0.40
1:E:103:VAL:HG22	1:E:113:PHE:CD1	2.56	0.40
1:E:341:MET:SD	1:E:341:MET:C	3.05	0.40
1:F:53:VAL:O	1:F:57:CYS:SG	2.73	0.40
1:F:286:PRO:O	1:F:334:MET:SD	2.79	0.40
1:A:58:ARG:O	1:A:62:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:SER:C	1:A:168:HIS:O	2.65	0.40
1:C:157:PHE:CE1	1:C:199:TRP:CH2	3.10	0.40
1:E:128:HIS:C	1:E:128:HIS:ND1	2.79	0.40
1:E:359:LYS:HB3	1:E:364:GLU:OE1	2.20	0.40
1:A:99:LEU:O	1:A:102:ILE:N	2.47	0.40
1:A:236:MET:HG2	1:A:272:ILE:HG23	2.03	0.40
1:A:324:ALA:CB	1:A:325:PRO:HD2	2.42	0.40
1:C:197:GLU:HG2	1:C:254:TRP:HE3	1.86	0.40
1:D:132:LEU:O	1:D:136:TYR:HB2	2.20	0.40
1:D:281:SER:HA	1:D:306:VAL:HG21	2.03	0.40
1:E:41:LYS:O	1:E:71:THR:HB	2.21	0.40
1:F:222:ALA:O	1:F:224:LYS:N	2.53	0.40
1:F:242:ARG:O	1:F:243:LEU:HD23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	342/380 (90%)	283 (83%)	44 (13%)	15 (4%)	2	1
1	C	326/380 (86%)	239 (73%)	67 (21%)	20 (6%)	1	0
1	D	341/380 (90%)	268 (79%)	59 (17%)	14 (4%)	2	1
1	E	331/380 (87%)	250 (76%)	54 (16%)	27 (8%)	0	0
1	F	346/380 (91%)	264 (76%)	64 (18%)	18 (5%)	1	0
All	All	1686/1900 (89%)	1304 (77%)	288 (17%)	94 (6%)	1	0

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	LEU

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Mol	Chain	Res	Type
1	A	367	LYS
1	A	368	ALA
1	A	369	VAL
1	C	58	ARG
1	C	204	GLU
1	C	219	ALA
1	C	220	GLU
1	C	252	LEU
1	D	156	PRO
1	E	164	LEU
1	E	195	LEU
1	E	286	PRO
1	E	329	THR
1	F	126	ARG
1	F	260	ALA
1	F	329	THR
1	A	90	GLY
1	C	69	VAL
1	C	77	ARG
1	C	197	GLU
1	C	213	ASP
1	D	128	HIS
1	D	190	ALA
1	D	197	GLU
1	D	202	GLY
1	D	252	LEU
1	D	321	GLY
1	E	65	PRO
1	E	77	ARG
1	E	91	GLU
1	E	128	HIS
1	E	187	GLY
1	E	287	GLY
1	F	77	ARG
1	F	90	GLY
1	F	107	LYS
1	F	190	ALA
1	F	261	THR
1	F	284	PRO
1	F	357	GLY
1	A	89	ALA
1	A	91	GLU

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Mol	Chain	Res	Type
1	A	309	ALA
1	A	343	GLU
1	A	354	GLY
1	C	120	LEU
1	C	156	PRO
1	C	344	ASP
1	C	371	ALA
1	D	195	LEU
1	D	364	GLU
1	E	127	ASP
1	E	174	THR
1	E	252	LEU
1	E	304	SER
1	E	305	GLU
1	F	338	PHE
1	A	356	ASN
1	C	310	GLN
1	C	372	GLN
1	D	307	ALA
1	E	120	LEU
1	E	143	PRO
1	E	316	LEU
1	F	206	CYS
1	A	370	PHE
1	C	60	ILE
1	C	130	ASP
1	D	105	THR
1	D	177	PRO
1	D	223	THR
1	E	47	VAL
1	E	86	PRO
1	E	166	PRO
1	E	177	PRO
1	E	344	ASP
1	E	366	PHE
1	E	370	PHE
1	F	54	PRO
1	F	120	LEU
1	F	207	PRO
1	F	361	PRO
1	C	241	ASP
1	E	89	ALA

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Mol	Chain	Res	Type
1	F	156	PRO
1	D	39	PRO
1	A	325	PRO
1	E	48	PRO
1	A	210	GLY
1	A	373	ILE
1	C	349	ILE
1	F	143	PRO
1	C	361	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/330 (92%)	273 (90%)	30 (10%)	7	8
1	C	288/330 (87%)	248 (86%)	40 (14%)	3	3
1	D	298/330 (90%)	271 (91%)	27 (9%)	9	10
1	E	292/330 (88%)	260 (89%)	32 (11%)	6	6
1	F	303/330 (92%)	272 (90%)	31 (10%)	7	7
All	All	1484/1650 (90%)	1324 (89%)	160 (11%)	6	6

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	THR
1	A	58	ARG
1	A	59	PHE
1	A	84	SER
1	A	91	GLU
1	A	105	THR
1	A	106	CYS
1	A	117	MET
1	A	130	ASP
1	A	131	PRO

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Mol	Chain	Res	Type
1	A	133	LEU
1	A	144	ASP
1	A	149	VAL
1	A	158	ASP
1	A	163	SER
1	A	171	LEU
1	A	175	ILE
1	A	177	PRO
1	A	192	HIS
1	A	195	LEU
1	A	241	ASP
1	A	285	THR
1	A	286	PRO
1	A	296	VAL
1	A	302	SER
1	A	304	SER
1	A	322	THR
1	A	323	ARG
1	A	334	MET
1	A	345	SER
1	C	36	ASN
1	C	40	VAL
1	C	44	LEU
1	C	46	THR
1	C	49	HIS
1	C	58	ARG
1	C	72	LEU
1	C	104	GLN
1	C	105	THR
1	C	117	MET
1	C	144	ASP
1	C	151	TRP
1	C	158	ASP
1	C	162	LYS
1	C	165	CYS
1	C	170	ASP
1	C	174	THR
1	C	189	ASP
1	C	193	VAL
1	C	195	LEU
1	C	201	LEU
1	C	214	LYS

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Mol	Chain	Res	Type
1	C	217	LEU
1	C	225	LEU
1	C	231	GLU
1	C	234	CYS
1	C	257	SER
1	C	265	ILE
1	C	276	ASP
1	C	296	VAL
1	C	303	ASN
1	C	322	THR
1	C	329	THR
1	C	334	MET
1	C	341	MET
1	C	343	GLU
1	C	346	LYS
1	C	362	SER
1	C	378	VAL
1	C	379	MET
1	D	39	PRO
1	D	51	GLU
1	D	79	ASN
1	D	88	LEU
1	D	94	ILE
1	D	117	MET
1	D	127	ASP
1	D	142	SER
1	D	156	PRO
1	D	158	ASP
1	D	161	CYS
1	D	175	ILE
1	D	195	LEU
1	D	209	CYS
1	D	217	LEU
1	D	233	LYS
1	D	247	LYS
1	D	252	LEU
1	D	265	ILE
1	D	274	ILE
1	D	285	THR
1	D	296	VAL
1	D	299	SER
1	D	334	MET

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Mol	Chain	Res	Type
1	D	337	VAL
1	D	341	MET
1	D	345	SER
1	E	49	HIS
1	E	53	VAL
1	E	64	LEU
1	E	65	PRO
1	E	73	VAL
1	E	79	ASN
1	E	86	PRO
1	E	111	ILE
1	E	114	ILE
1	E	123	GLN
1	E	124	SER
1	E	167	SER
1	E	172	LEU
1	E	177	PRO
1	E	180	ASP
1	E	204	GLU
1	E	213	ASP
1	E	217	LEU
1	E	238	MET
1	E	240	SER
1	E	241	ASP
1	E	243	LEU
1	E	245	ASP
1	E	254	TRP
1	E	258	MET
1	E	273	MET
1	E	285	THR
1	E	300	SER
1	E	316	LEU
1	E	340	THR
1	E	341	MET
1	E	379	MET
1	F	34	GLU
1	F	52	ASP
1	F	111	ILE
1	F	131	PRO
1	F	137	PRO
1	F	140	ASP
1	F	158	ASP

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Mol	Chain	Res	Type
1	F	172	LEU
1	F	174	THR
1	F	175	ILE
1	F	181	GLU
1	F	184	ASP
1	F	195	LEU
1	F	196	ASP
1	F	234	CYS
1	F	236	MET
1	F	238	MET
1	F	248	THR
1	F	254	TRP
1	F	255	GLN
1	F	257	SER
1	F	258	MET
1	F	266	ASP
1	F	281	SER
1	F	291	ILE
1	F	300	SER
1	F	306	VAL
1	F	311	LEU
1	F	316	LEU
1	F	338	PHE
1	F	347	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	104	GLN
1	A	118	ASN
1	A	128	HIS
1	A	335	GLN
1	C	36	ASN
1	C	104	GLN
1	C	118	ASN
1	C	123	GLN
1	C	128	HIS
1	C	235	GLN
1	C	255	GLN
1	C	372	GLN
1	D	79	ASN

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Mol	Chain	Res	Type
1	E	36	ASN
1	E	49	HIS
1	E	70	ASN
1	E	79	ASN
1	E	98	GLN
1	E	123	GLN
1	E	146	ASN
1	E	295	ASN
1	E	310	GLN
1	E	372	GLN
1	F	36	ASN
1	F	104	GLN
1	F	118	ASN
1	F	122	HIS
1	F	372	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 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	345/380 (90%)	0.60	20 (5%) 29 30	9, 24, 39, 51	1 (0%)
1	C	330/380 (86%)	1.36	75 (22%) 2 2	22, 36, 49, 61	0
1	D	343/380 (90%)	0.84	38 (11%) 10 11	12, 28, 43, 54	0
1	E	335/380 (88%)	1.31	70 (20%) 2 2	23, 35, 47, 58	0
1	F	348/380 (91%)	1.36	69 (19%) 3 3	20, 35, 48, 72	0
All	All	1701/1900 (89%)	1.09	272 (15%) 5 5	9, 33, 46, 72	1 (0%)

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	154	ALA	6.4
1	E	142	SER	5.7
1	C	353	TYR	5.4
1	F	262	PHE	4.9
1	F	157	PHE	4.6
1	F	148	PRO	4.4
1	A	157	PHE	4.4
1	E	322	THR	4.3
1	E	73	VAL	4.3
1	E	78	TYR	4.2
1	D	151	TRP	4.1
1	F	183	ILE	4.1
1	F	154	ALA	4.0
1	C	63	VAL	4.0
1	E	324	ALA	4.0
1	F	205	LYS	3.9
1	E	251	LEU	3.9
1	C	369	VAL	3.9
1	C	53	VAL	3.8
1	F	114	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	147	PRO	3.7
1	C	102	ILE	3.7
1	E	145	TYR	3.7
1	E	290	ALA	3.7
1	F	348	PHE	3.6
1	A	357	GLY	3.6
1	C	344	ASP	3.6
1	C	356	ASN	3.5
1	F	322	THR	3.5
1	E	33	PHE	3.5
1	F	155	GLY	3.5
1	D	126	ARG	3.5
1	F	324	ALA	3.4
1	D	56	PHE	3.4
1	C	342	TRP	3.3
1	D	78	TYR	3.3
1	F	218	PHE	3.3
1	D	125	ASP	3.3
1	C	348	PHE	3.3
1	E	167	SER	3.3
1	E	321	GLY	3.3
1	A	56	PHE	3.3
1	C	256	ALA	3.3
1	C	363	ALA	3.3
1	C	136	TYR	3.3
1	A	158	ASP	3.2
1	C	268	ILE	3.2
1	E	129	ILE	3.2
1	F	331	ALA	3.2
1	E	43	MET	3.2
1	F	342	TRP	3.2
1	E	195	LEU	3.2
1	F	207	PRO	3.2
1	C	134	ALA	3.1
1	C	178	LEU	3.1
1	C	229	LEU	3.1
1	E	164	LEU	3.1
1	F	172	LEU	3.1
1	C	339	VAL	3.1
1	C	54	PRO	3.1
1	C	146	ASN	3.1
1	F	282	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	185	VAL	3.1
1	E	193	VAL	3.1
1	F	156	PRO	3.1
1	F	355	ARG	3.1
1	F	151	TRP	3.1
1	E	136	TYR	3.0
1	E	173	LYS	3.0
1	D	33	PHE	3.0
1	A	379	MET	3.0
1	C	188	ALA	3.0
1	A	149	VAL	3.0
1	D	172	LEU	3.0
1	F	368	ALA	3.0
1	F	182	LEU	3.0
1	F	370	PHE	2.9
1	A	199	TRP	2.9
1	D	348	PHE	2.9
1	C	149	VAL	2.9
1	D	149	VAL	2.9
1	E	111	ILE	2.9
1	C	336	GLY	2.9
1	A	151	TRP	2.9
1	F	143	PRO	2.9
1	E	323	ARG	2.9
1	D	157	PHE	2.9
1	C	354	GLY	2.8
1	C	56	PHE	2.8
1	F	103	VAL	2.8
1	F	251	LEU	2.8
1	F	115	PRO	2.8
1	C	172	LEU	2.8
1	A	358	LYS	2.8
1	A	371	ALA	2.8
1	E	59	PHE	2.8
1	E	200	ILE	2.7
1	C	133	LEU	2.7
1	E	229	LEU	2.7
1	C	315	ARG	2.7
1	E	327	ALA	2.7
1	A	63	VAL	2.7
1	F	128	HIS	2.7
1	F	149	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	356	ASN	2.7
1	F	200	ILE	2.7
1	E	351	ALA	2.7
1	E	314	VAL	2.7
1	E	328	VAL	2.7
1	D	309	ALA	2.7
1	F	279	TYR	2.7
1	F	270	THR	2.7
1	F	102	ILE	2.7
1	D	302	SER	2.7
1	E	325	PRO	2.7
1	D	58	ARG	2.7
1	E	326	TRP	2.7
1	E	222	ALA	2.6
1	C	262	PHE	2.6
1	F	352	TYR	2.6
1	C	207	PRO	2.6
1	E	39	PRO	2.6
1	C	151	TRP	2.6
1	E	61	LYS	2.6
1	C	42	ALA	2.6
1	F	363	ALA	2.6
1	E	127	ASP	2.6
1	E	353	TYR	2.6
1	A	378	VAL	2.6
1	C	272	ILE	2.6
1	E	141	GLU	2.6
1	C	379	MET	2.6
1	D	314	VAL	2.6
1	F	175	ILE	2.6
1	F	349	ILE	2.6
1	A	161[A]	CYS	2.6
1	C	294	PHE	2.6
1	D	357	GLY	2.6
1	C	296	VAL	2.6
1	C	371	ALA	2.5
1	F	59	PHE	2.5
1	E	47	VAL	2.5
1	E	369	VAL	2.5
1	E	360	LEU	2.5
1	F	229	LEU	2.5
1	E	125	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	329	THR	2.5
1	E	113	PHE	2.5
1	F	136	TYR	2.5
1	E	368	ALA	2.5
1	F	153	ASP	2.5
1	C	33	PHE	2.5
1	C	183	ILE	2.5
1	C	185	VAL	2.5
1	D	35	TRP	2.5
1	E	112	ARG	2.5
1	F	35	TRP	2.5
1	D	359	LYS	2.5
1	F	358	LYS	2.5
1	D	199	TRP	2.4
1	C	99	LEU	2.4
1	F	72	LEU	2.4
1	F	320	ASP	2.4
1	F	42	ALA	2.4
1	A	60	ILE	2.4
1	C	373	ILE	2.4
1	D	129	ILE	2.4
1	E	94	ILE	2.4
1	F	291	ILE	2.4
1	E	38	LEU	2.4
1	E	252	LEU	2.4
1	C	70	ASN	2.4
1	C	138	GLN	2.4
1	C	109	ALA	2.4
1	F	199	TRP	2.4
1	A	356	ASN	2.4
1	E	105	THR	2.4
1	E	378	VAL	2.4
1	E	175	ILE	2.3
1	E	58	ARG	2.3
1	D	136	TYR	2.3
1	A	93	ALA	2.3
1	D	368	ALA	2.3
1	F	325	PRO	2.3
1	D	353	TYR	2.3
1	E	174	THR	2.3
1	F	329	THR	2.3
1	C	49	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	111	ILE	2.3
1	E	56	PHE	2.3
1	C	375	LYS	2.3
1	F	225	LEU	2.3
1	E	259	ASN	2.3
1	E	137	PRO	2.3
1	F	203	TYR	2.3
1	C	199	TRP	2.3
1	C	62	GLU	2.3
1	C	135	LYS	2.3
1	D	94	ILE	2.3
1	F	244	ILE	2.3
1	A	350	ASP	2.2
1	F	184	ASP	2.2
1	E	269	PRO	2.2
1	E	199	TRP	2.2
1	E	342	TRP	2.2
1	F	254	TRP	2.2
1	D	64	LEU	2.2
1	D	132	LEU	2.2
1	E	40	VAL	2.2
1	C	277	TRP	2.2
1	D	349	ILE	2.2
1	E	74	LEU	2.2
1	F	38	LEU	2.2
1	F	201	LEU	2.2
1	C	254	TRP	2.2
1	E	254	TRP	2.2
1	C	195	LEU	2.2
1	A	380	ASN	2.2
1	C	159	PHE	2.2
1	C	370	PHE	2.2
1	F	202	GLY	2.2
1	E	249	THR	2.2
1	D	145	TYR	2.1
1	F	373	ILE	2.1
1	C	35	TRP	2.1
1	F	198	VAL	2.1
1	F	50	PRO	2.1
1	C	142	SER	2.1
1	C	285	THR	2.1
1	E	89	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	160	TYR	2.1
1	C	64	LEU	2.1
1	C	316	LEU	2.1
1	C	380	ASN	2.1
1	F	158	ASP	2.1
1	D	32	GLN	2.1
1	E	115	PRO	2.1
1	C	321	GLY	2.1
1	D	301	CYS	2.1
1	C	317	ALA	2.1
1	E	93	ALA	2.1
1	F	224	LYS	2.1
1	D	133	LEU	2.1
1	D	316	LEU	2.1
1	F	353	TYR	2.1
1	E	103	VAL	2.1
1	D	366	PHE	2.1
1	C	61	LYS	2.1
1	C	233	LYS	2.1
1	D	109	ALA	2.1
1	F	330	LEU	2.1
1	E	198	VAL	2.1
1	C	59	PHE	2.1
1	E	293	GLY	2.1
1	D	232	LYS	2.0
1	C	368	ALA	2.0
1	E	179	MET	2.0
1	C	171	LEU	2.0
1	E	308	LEU	2.0
1	F	132	LEU	2.0
1	C	114	ILE	2.0
1	C	156	PRO	2.0
1	E	54	PRO	2.0
1	C	314	VAL	2.0
1	F	176	PHE	2.0
1	D	342	TRP	2.0
1	A	317	ALA	2.0
1	A	331	ALA	2.0
1	C	52	ASP	2.0
1	C	213	ASP	2.0
1	D	373	ILE	2.0
1	F	361	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

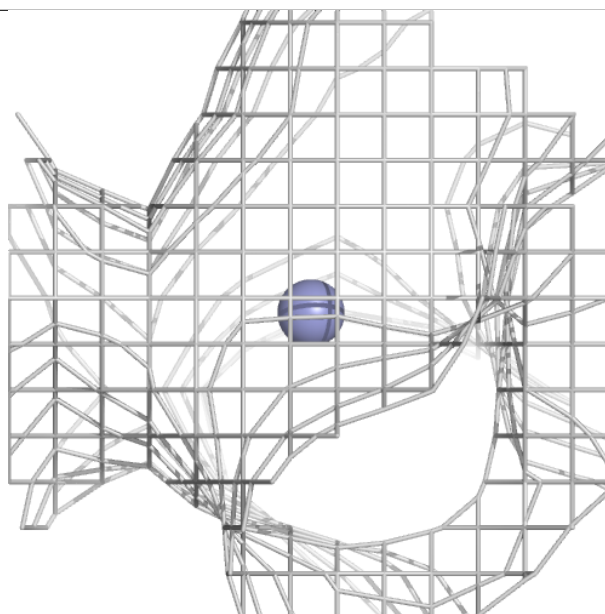
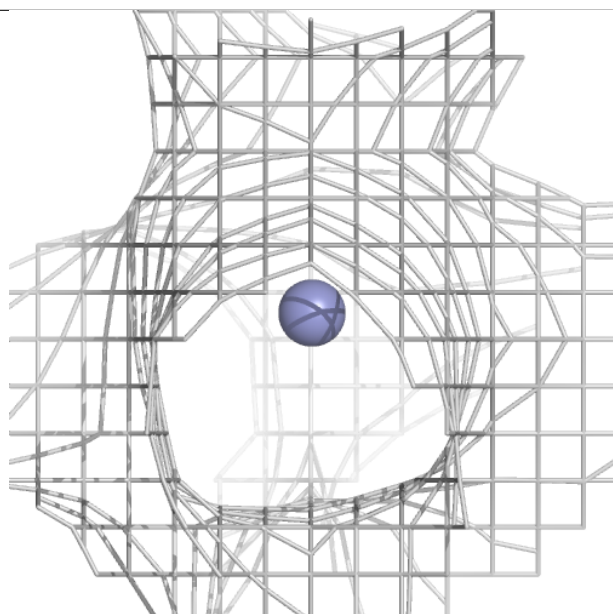
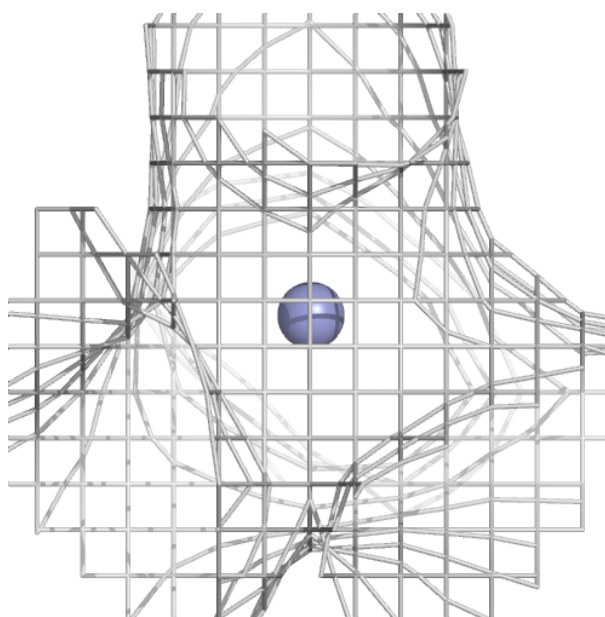
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	C	401	1/1	0.97	0.06	42,42,42,42	0
2	ZN	D	401	1/1	0.99	0.04	39,39,39,39	1
2	ZN	E	401	1/1	0.99	0.03	52,52,52,52	0
2	ZN	F	401	1/1	0.99	0.03	44,44,44,44	0
2	ZN	A	401	1/1	1.00	0.01	31,31,31,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

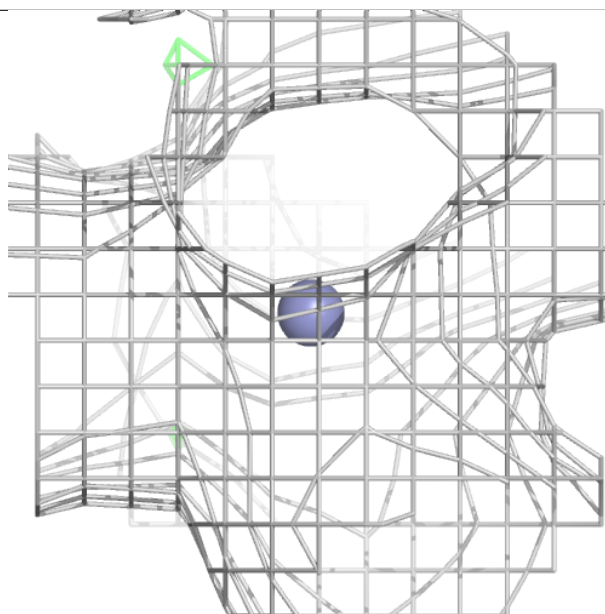
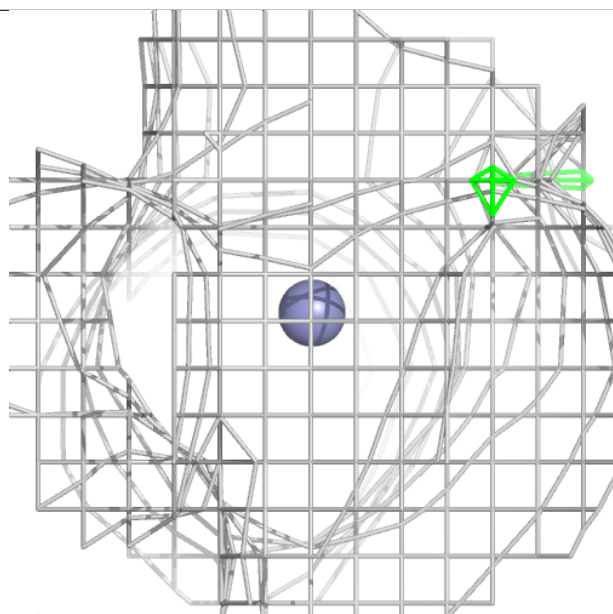
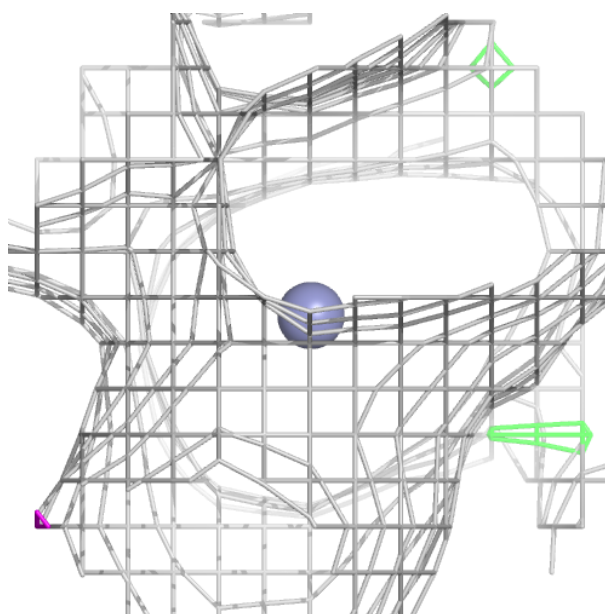
Electron density around ZN C 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



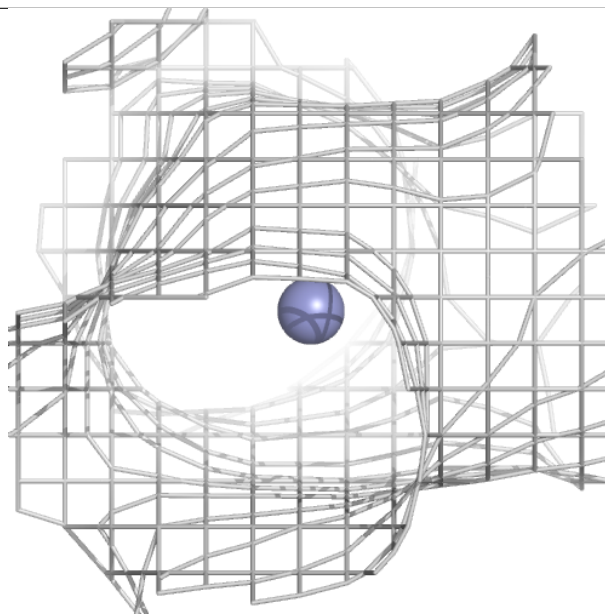
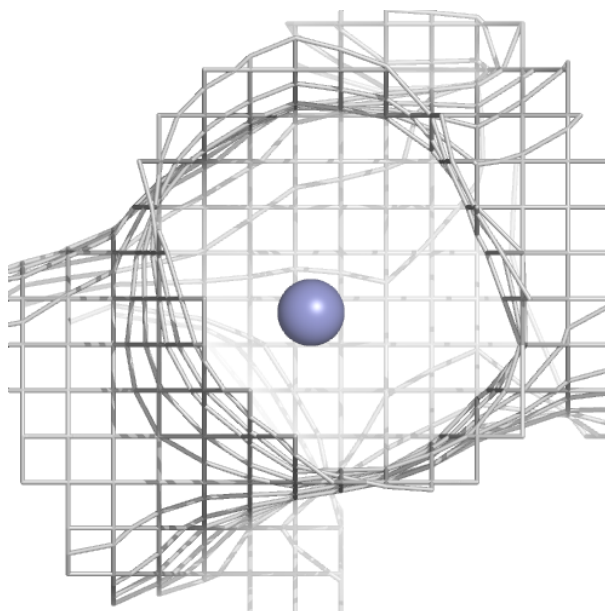
Electron density around ZN D 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



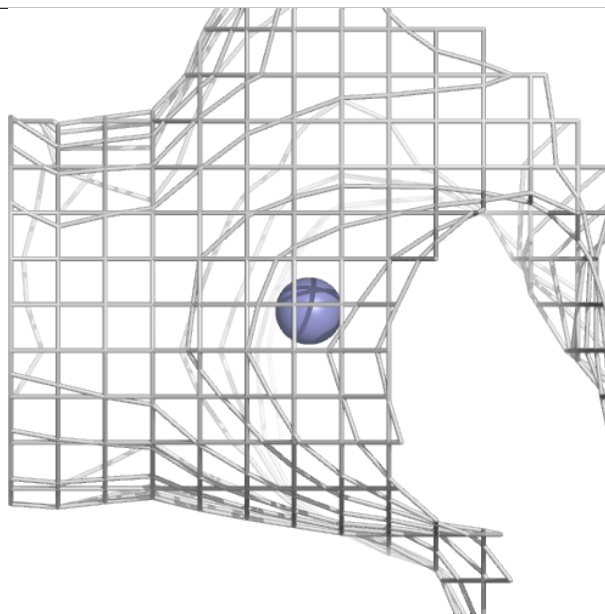
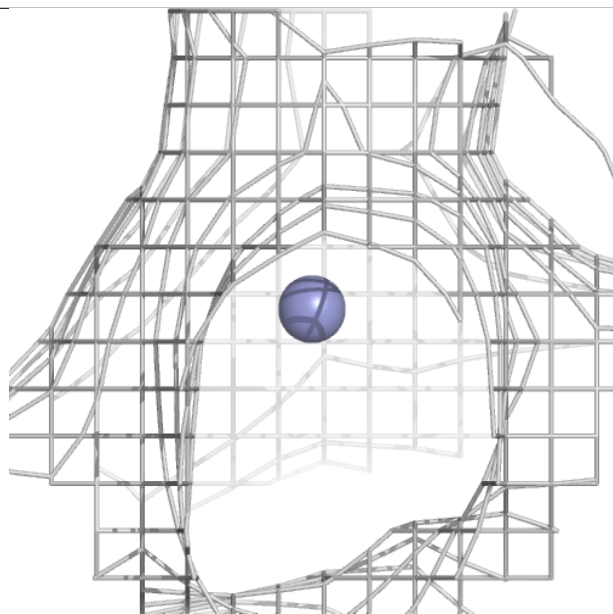
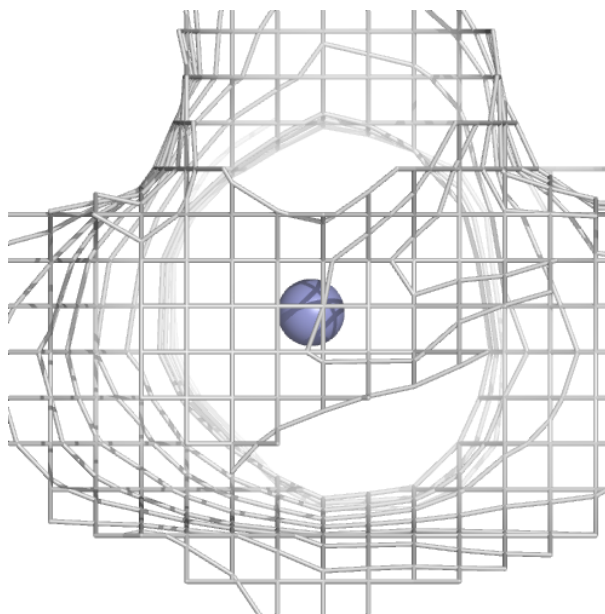
Electron density around ZN E 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



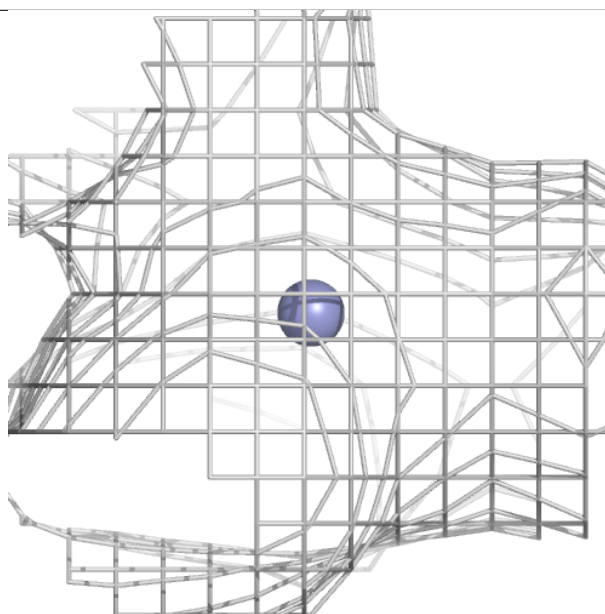
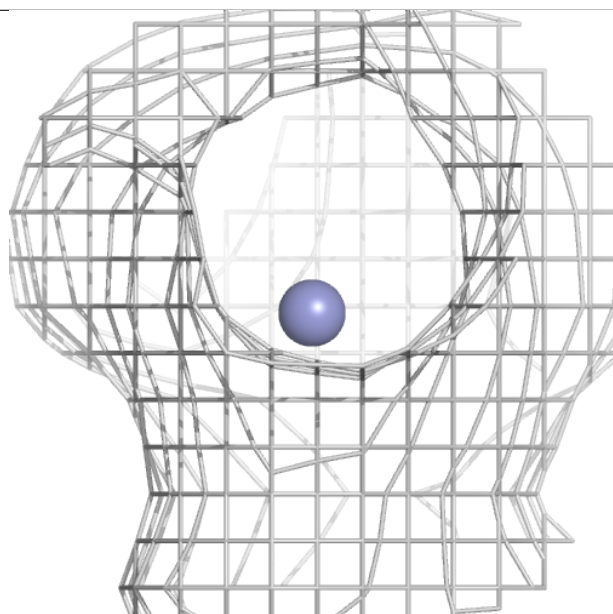
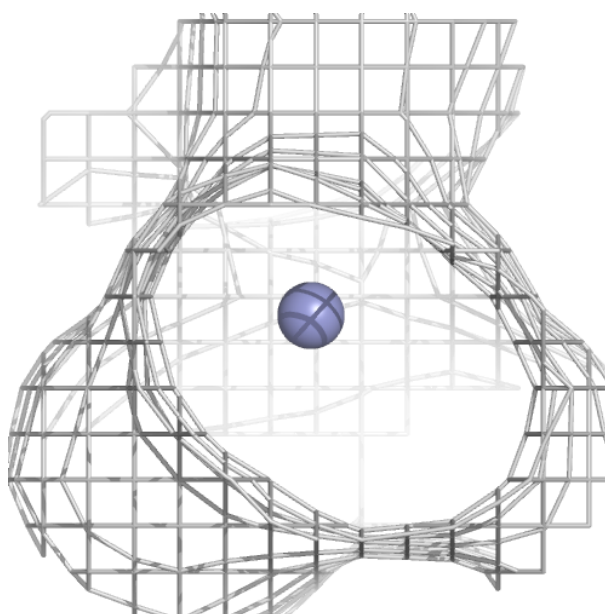
Electron density around ZN F 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.