



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 10:16 PM UTC

PDB ID : 1N8B / pdb_00001n8b
Title : Bacteriophage T4 baseplate structural protein gp8
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Deposited on : 2002-11-20
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

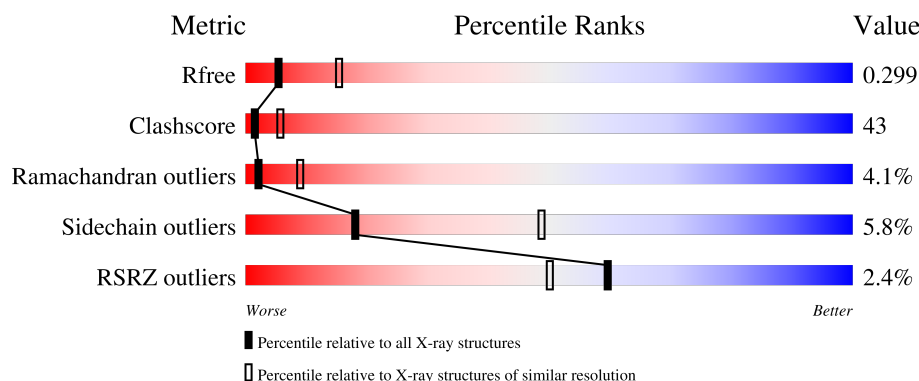
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	334	3% 34% 53% 10% ..
1	B	334	3% 40% 51% 7% ..
1	C	334	2% 37% 52% 9% .
1	D	334	3% 39% 54% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	A	342	-	-	X	-
2	BR	B	337	-	-	X	-
2	BR	B	343	-	-	X	-
2	BR	C	335	-	-	X	-
2	BR	C	339	-	-	X	-
2	BR	D	336	-	-	X	-
2	BR	D	337	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10842 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 baseplate structural protein gp8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2631	1677	430	507	17			
1	B	328	Total	C	N	O	S	0	0	0
			2631	1677	430	507	17			
1	C	328	Total	C	N	O	S	0	0	0
			2631	1677	430	507	17			
1	D	328	Total	C	N	O	S	0	0	0
			2631	1677	430	507	17			

- Molecule 2 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	Br	0	0
			9	9		
2	B	12	Total	Br	0	0
			12	12		
2	C	9	Total	Br	0	0
			9	9		
2	D	10	Total	Br	0	0
			10	10		

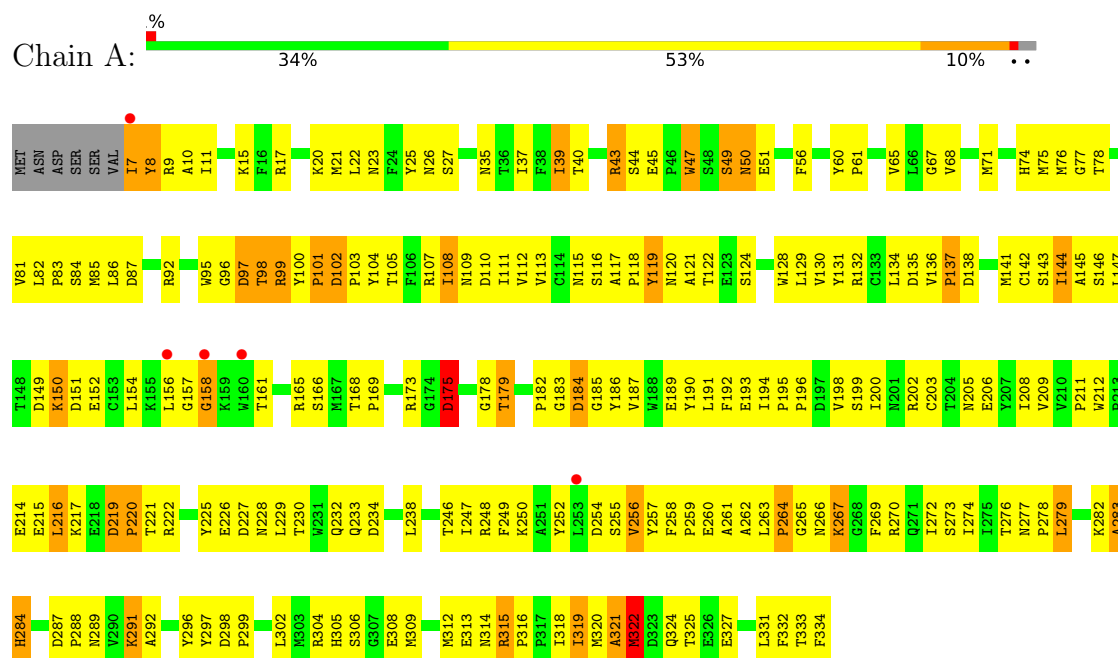
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	77	Total	O	0	0
			77	77		
3	B	59	Total	O	0	0
			59	59		
3	C	76	Total	O	0	0
			76	76		
3	D	66	Total	O	0	0
			66	66		

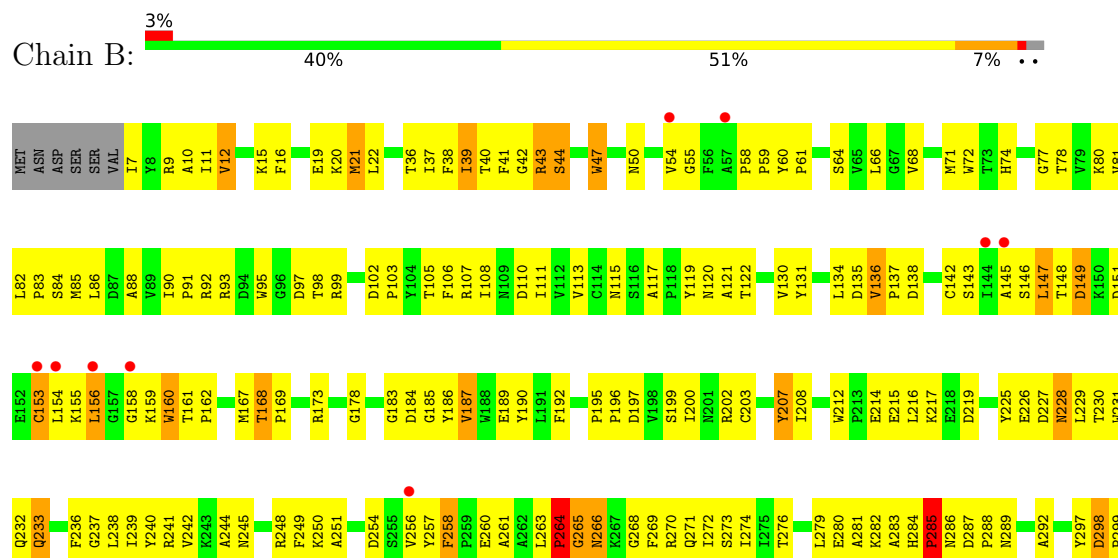
3 Residue-property plots

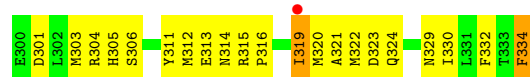
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: baseplate structural protein gp8

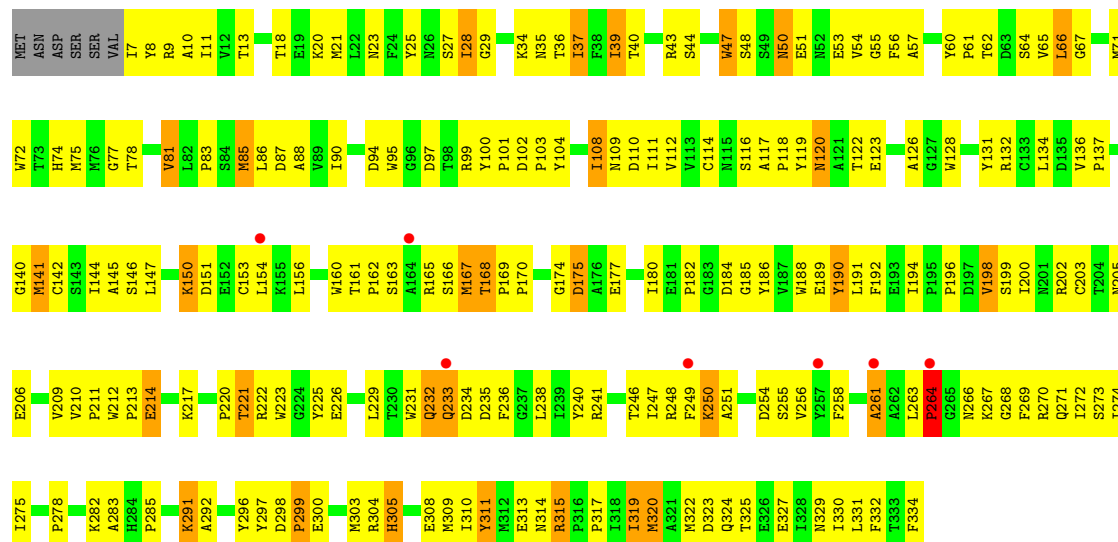


• Molecule 1: baseplate structural protein gp8

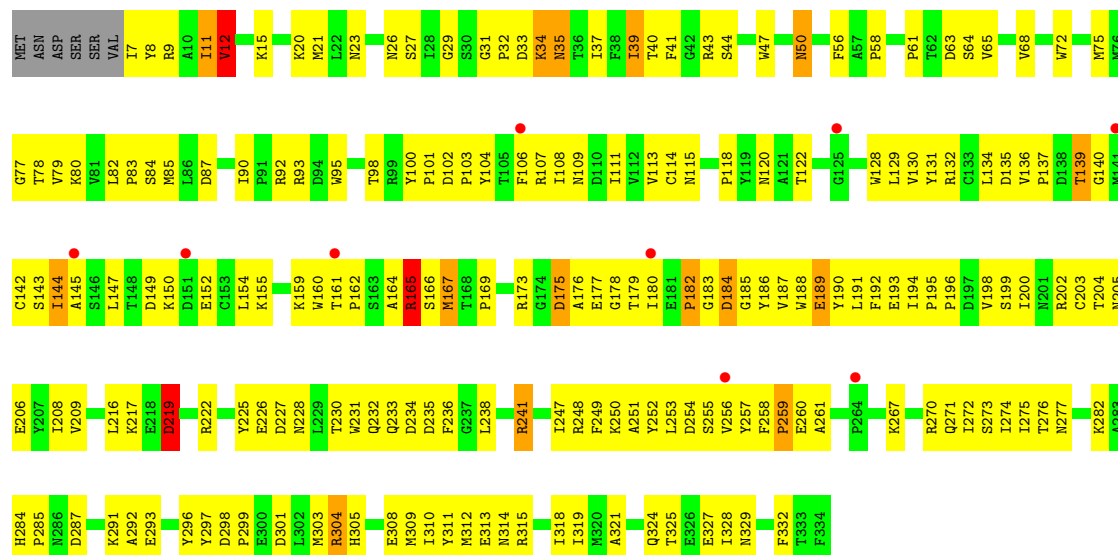




• Molecule 1: baseplate structural protein gp8



• Molecule 1: baseplate structural protein gp8



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.20Å 65.77Å 79.65Å 93.04° 100.32° 91.93°	Depositor
Resolution (Å)	30.98 – 2.90 30.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.98-2.90) 99.0 (30.98-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.53 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.300 0.222 , 0.299	Depositor DCC
R_{free} test set	1021 reflections (3.58%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10842	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: BR

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	0/2709	1.02	15/3694 (0.4%)
1	B	0.48	0/2709	0.98	16/3694 (0.4%)
1	C	0.52	0/2709	1.01	8/3694 (0.2%)
1	D	0.49	0/2709	0.95	8/3694 (0.2%)
All	All	0.50	0/10836	0.99	47/14776 (0.3%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	ASP	N-CA-C	-10.68	94.13	109.62
1	A	47	TRP	N-CA-C	-8.97	100.66	111.69
1	A	219	ASP	CA-C-N	7.89	129.71	119.84
1	A	219	ASP	C-N-CA	7.89	129.71	119.84
1	D	219	ASP	CA-C-N	7.41	127.27	119.05
1	D	219	ASP	C-N-CA	7.41	127.27	119.05
1	B	155	LYS	N-CA-C	-7.32	104.15	113.23
1	B	168	THR	CA-C-N	7.31	124.93	119.66
1	B	168	THR	C-N-CA	7.31	124.93	119.66
1	B	219	ASP	CA-C-N	6.71	126.22	119.24
1	B	219	ASP	C-N-CA	6.71	126.22	119.24
1	D	284	HIS	CA-C-N	6.50	127.97	119.84
1	D	284	HIS	C-N-CA	6.50	127.97	119.84
1	D	44	SER	N-CA-C	-6.36	105.34	113.23
1	C	88	ALA	N-CA-C	-6.19	99.91	109.76
1	B	161	THR	CA-C-N	6.09	126.06	120.21
1	B	161	THR	C-N-CA	6.09	126.06	120.21
1	C	315	ARG	N-CA-C	5.94	113.36	108.07
1	D	241	ARG	N-CA-C	5.93	119.77	112.54
1	B	160	TRP	N-CA-C	5.87	118.09	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	TYR	N-CA-C	-5.84	102.64	110.24
1	B	298	ASP	N-CA-C	-5.76	101.23	109.24
1	B	207	TYR	N-CA-C	5.74	117.91	109.24
1	A	39	ILE	N-CA-C	-5.73	100.15	108.17
1	A	124	SER	N-CA-C	-5.72	102.44	110.50
1	A	99	ARG	N-CA-C	-5.68	105.55	112.88
1	D	12	VAL	N-CA-C	-5.66	100.26	108.87
1	A	283	ALA	N-CA-C	-5.60	105.26	111.36
1	B	88	ALA	N-CA-C	-5.58	101.59	109.96
1	C	18	THR	N-CA-C	-5.56	105.30	111.36
1	B	156	LEU	N-CA-C	-5.52	107.19	114.04
1	C	28	ILE	N-CA-C	5.51	115.50	108.12
1	A	284	HIS	CA-C-N	5.51	126.72	119.84
1	A	284	HIS	C-N-CA	5.51	126.72	119.84
1	A	315	ARG	CA-C-N	-5.50	114.71	120.38
1	A	315	ARG	C-N-CA	-5.50	114.71	120.38
1	B	12	VAL	N-CA-C	-5.50	99.82	108.23
1	C	298	ASP	N-CA-C	-5.46	101.33	109.42
1	A	195	PRO	CA-C-N	5.42	124.87	119.24
1	A	195	PRO	C-N-CA	5.42	124.87	119.24
1	B	258	PHE	N-CA-C	5.41	117.27	109.04
1	C	55	GLY	N-CA-C	-5.41	107.46	113.79
1	A	216	LEU	N-CA-C	-5.38	105.58	111.82
1	D	65	VAL	N-CA-C	-5.31	105.20	110.62
1	B	153	CYS	N-CA-C	-5.20	106.25	112.59
1	B	55	GLY	N-CA-C	-5.18	108.08	115.64
1	C	47	TRP	N-CA-C	-5.01	105.47	111.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2631	0	2509	235	0
1	B	2631	0	2509	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2631	0	2509	236	0
1	D	2631	0	2509	244	0
2	A	9	0	0	7	0
2	B	12	0	0	10	0
2	C	9	0	0	8	0
2	D	10	0	0	9	0
3	A	77	0	0	3	0
3	B	59	0	0	5	0
3	C	76	0	0	4	0
3	D	66	0	0	4	0
All	All	10842	0	10036	888	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 43.

All (888) 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:107:ARG:HH22	1:A:161:THR:HB	1.12	1.09
1:A:319:ILE:HD13	1:A:319:ILE:H	1.17	1.08
1:B:250:LYS:HD2	1:B:329:ASN:HD21	1.24	1.02
1:D:149:ASP:HB3	1:D:152:GLU:HG2	1.38	1.01
1:D:274:ILE:HG13	1:D:332:PHE:HZ	1.24	1.01
1:D:93:ARG:HH12	1:D:106:PHE:HD1	1.03	0.98
1:A:10:ALA:HB2	1:B:313:GLU:HG3	1.42	0.98
1:A:108:ILE:H	1:A:108:ILE:HD12	1.30	0.96
1:A:71:MET:HE2	1:A:312:MET:HE2	1.45	0.96
1:C:250:LYS:HE3	1:C:327:GLU:HG3	1.46	0.95
1:A:50:ASN:H	1:A:50:ASN:HD22	1.01	0.94
1:A:115:ASN:H	1:A:120:ASN:HB3	1.31	0.94
1:C:137:PRO:HG2	1:C:162:PRO:HB3	1.49	0.94
1:A:313:GLU:HG3	1:B:10:ALA:HB2	1.48	0.93
1:D:37:ILE:HD12	1:D:276:THR:HG22	1.49	0.92
1:A:232:GLN:HE21	1:B:286:ASN:HA	1.35	0.91
1:C:50:ASN:HD22	1:C:50:ASN:N	1.70	0.89
1:C:77:GLY:HA2	1:C:299:PRO:HD3	1.54	0.89
1:C:50:ASN:HD22	1:C:50:ASN:H	0.93	0.89
1:A:115:ASN:N	1:A:120:ASN:HB3	1.87	0.89
1:C:214:GLU:HG2	2:C:339:BR:BR	2.28	0.89
1:C:117:ALA:H	1:C:120:ASN:HD21	1.20	0.88
1:C:50:ASN:H	1:C:50:ASN:ND2	1.70	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:ARG:HH22	1:D:106:PHE:HE1	1.22	0.88
1:A:107:ARG:NH2	1:A:161:THR:HB	1.88	0.87
1:C:108:ILE:H	1:C:108:ILE:HD12	1.39	0.87
1:B:214:GLU:HB3	2:B:344:BR:BR	2.30	0.86
1:B:282:LYS:HE2	1:B:303:MET:HE1	1.58	0.86
1:D:104:TYR:HB2	2:D:336:BR:BR	2.30	0.86
1:C:254:ASP:HB3	1:C:256:VAL:HG12	1.57	0.85
1:C:132:ARG:HH21	1:C:132:ARG:HG3	1.41	0.84
1:D:313:GLU:OE1	1:D:315:ARG:HD3	1.77	0.84
1:D:274:ILE:HG13	1:D:332:PHE:CZ	2.12	0.84
1:C:37:ILE:HD11	1:C:81:VAL:HG11	1.57	0.84
1:B:37:ILE:HG22	1:B:276:THR:HG22	1.58	0.83
1:A:260:GLU:HG2	1:A:261:ALA:H	1.41	0.83
1:A:76:MET:HE2	1:A:261:ALA:HB1	1.61	0.83
1:A:113:VAL:HG22	1:A:130:VAL:HG22	1.60	0.83
1:D:137:PRO:HG3	1:D:185:GLY:HA3	1.61	0.82
1:B:115:ASN:H	1:B:120:ASN:HB3	1.44	0.82
1:C:11:ILE:HD12	1:C:11:ILE:O	1.79	0.82
1:D:267:LYS:HB3	1:D:270:ARG:HH22	1.44	0.81
1:B:151:ASP:HA	1:B:154:LEU:HD23	1.63	0.81
1:B:137:PRO:HG2	1:B:162:PRO:HB3	1.61	0.81
1:D:258:PHE:HD2	1:D:261:ALA:HB3	1.46	0.81
1:B:321:ALA:HB3	1:B:324:GLN:HB2	1.64	0.79
1:A:82:LEU:H	1:A:85:MET:HE3	1.49	0.78
1:D:192:PHE:CD2	1:D:238:LEU:HD21	2.19	0.78
1:A:108:ILE:HD12	1:A:108:ILE:N	1.98	0.78
1:D:250:LYS:HD2	1:D:329:ASN:HD21	1.47	0.77
1:D:80:LYS:HE3	1:D:293:GLU:O	1.84	0.77
1:A:132:ARG:HH21	1:A:132:ARG:HG3	1.49	0.77
1:B:43:ARG:HD3	1:B:270:ARG:HD2	1.66	0.77
1:C:229:LEU:HD22	1:C:232:GLN:NE2	1.98	0.77
1:B:21:MET:HE3	1:B:245:ASN:HA	1.67	0.77
1:C:147:LEU:HD11	1:C:156:LEU:HD12	1.67	0.77
1:C:229:LEU:HD22	1:C:232:GLN:HE22	1.49	0.76
1:D:95:TRP:CD2	1:D:169:PRO:HB3	2.19	0.76
1:A:108:ILE:H	1:A:108:ILE:CD1	1.99	0.76
1:A:205:ASN:OD1	1:A:206:GLU:HG2	1.86	0.76
1:B:21:MET:HE3	1:B:245:ASN:CA	2.16	0.76
1:C:231:TRP:NE1	1:C:232:GLN:HG3	2.01	0.75
1:B:136:VAL:HB	1:B:137:PRO:HD2	1.66	0.75
1:B:225:TYR:HE2	1:B:241:ARG:HH22	1.31	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:PRO:HD2	2:A:335:BR:BR	2.41	0.75
1:B:93:ARG:HH22	1:B:106:PHE:HE1	1.34	0.75
1:B:135:ASP:HB3	1:B:187:VAL:CG2	2.17	0.75
1:B:115:ASN:N	1:B:120:ASN:HB3	2.00	0.75
1:B:282:LYS:HD3	1:B:289:ASN:HA	1.67	0.74
1:C:132:ARG:HE	1:C:134:LEU:HD23	1.51	0.74
1:A:198:VAL:HG13	1:A:202:ARG:HG3	1.69	0.74
1:B:37:ILE:HG13	1:B:81:VAL:HB	1.69	0.73
1:B:43:ARG:HD2	1:B:270:ARG:HB2	1.69	0.73
1:C:282:LYS:HE3	1:C:303:MET:HE1	1.69	0.73
1:D:252:TYR:HB3	1:D:325:THR:HG21	1.70	0.73
1:B:120:ASN:O	1:B:122:THR:HG23	1.88	0.73
1:D:254:ASP:OD2	1:D:256:VAL:HB	1.89	0.72
1:D:113:VAL:HG22	1:D:130:VAL:HG22	1.68	0.72
1:A:279:LEU:HG	1:A:306:SER:HB2	1.71	0.72
1:B:39:ILE:HD13	1:B:40:THR:N	2.04	0.72
1:D:92:ARG:HB2	1:D:208:ILE:HG23	1.70	0.72
1:C:40:THR:HG22	1:C:78:THR:HG22	1.72	0.71
1:C:205:ASN:OD1	1:C:206:GLU:HG3	1.89	0.71
1:A:50:ASN:HD22	1:A:50:ASN:N	1.81	0.71
1:C:120:ASN:O	1:C:122:THR:HG23	1.90	0.71
1:C:117:ALA:H	1:C:120:ASN:ND2	1.88	0.71
1:B:279:LEU:HD13	1:B:289:ASN:HB3	1.72	0.71
1:C:117:ALA:N	1:C:120:ASN:HD21	1.86	0.71
1:C:116:SER:H	1:C:120:ASN:ND2	1.89	0.71
1:A:47:TRP:CZ2	1:A:314:ASN:HB3	2.26	0.70
1:B:7:ILE:HG12	2:B:346:BR:BR	2.47	0.70
1:D:250:LYS:HD2	1:D:329:ASN:ND2	2.06	0.70
1:B:214:GLU:HB2	2:B:339:BR:BR	2.46	0.70
1:A:260:GLU:HG2	1:A:261:ALA:N	2.05	0.70
1:C:8:TYR:CE2	1:D:315:ARG:HD2	2.27	0.70
1:D:183:GLY:C	1:D:185:GLY:H	2.00	0.69
1:D:321:ALA:HB3	1:D:324:GLN:HE21	1.55	0.69
1:A:21:MET:HG3	1:A:247:ILE:HG13	1.73	0.69
1:B:153:CYS:C	1:B:154:LEU:HD22	2.17	0.69
1:C:270:ARG:HG3	1:C:270:ARG:HH11	1.57	0.69
1:A:278:PRO:C	1:A:279:LEU:HD23	2.17	0.69
1:C:47:TRP:HH2	1:C:271:GLN:HE21	1.38	0.69
1:A:184:ASP:OD1	1:A:186:TYR:HB2	1.93	0.69
1:C:141:MET:HE2	1:C:161:THR:OG1	1.92	0.69
1:C:39:ILE:HD13	1:C:39:ILE:C	2.18	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:SER:HB2	1:A:144:ILE:HD12	1.76	0.68
1:C:20:LYS:HD3	1:D:20:LYS:HD3	1.74	0.68
1:D:137:PRO:HG3	1:D:185:GLY:CA	2.24	0.68
1:A:120:ASN:O	1:A:122:THR:HG23	1.94	0.68
1:B:287:ASP:HB3	1:B:288:PRO:HD2	1.76	0.67
1:A:321:ALA:HB3	1:A:324:GLN:CD	2.19	0.67
1:C:132:ARG:HB2	1:C:191:LEU:HD11	1.75	0.67
1:B:22:LEU:HD22	1:B:239:ILE:HD11	1.77	0.67
1:C:44:SER:HB2	1:C:267:LYS:HB2	1.77	0.67
1:D:175:ASP:C	1:D:177:GLU:H	2.00	0.67
1:B:93:ARG:NH2	1:B:106:PHE:HE1	1.92	0.67
1:B:98:THR:HA	1:B:103:PRO:HG2	1.76	0.67
1:B:178:GLY:O	1:B:189:GLU:HA	1.95	0.67
1:B:274:ILE:HG13	1:B:332:PHE:HZ	1.60	0.66
1:A:333:THR:HB	1:D:145:ALA:HB1	1.77	0.66
1:B:44:SER:HA	1:B:270:ARG:HH12	1.61	0.66
1:C:72:TRP:HA	1:C:75:MET:HE3	1.78	0.66
1:C:292:ALA:HB1	1:C:297:TYR:CE2	2.30	0.66
1:D:311:TYR:OH	1:D:313:GLU:OE2	2.10	0.65
1:D:144:ILE:N	1:D:144:ILE:HD12	2.11	0.65
1:A:269:PHE:HE1	1:A:272:ILE:HD11	1.61	0.65
1:B:95:TRP:CD2	1:B:169:PRO:HG3	2.32	0.65
1:D:21:MET:HG3	1:D:247:ILE:HG13	1.78	0.65
1:D:37:ILE:CD1	1:D:276:THR:HG22	2.26	0.65
1:D:90:ILE:HD11	1:D:208:ILE:HD11	1.79	0.65
1:B:9:ARG:HG3	1:B:9:ARG:HH11	1.63	0.64
1:C:128:TRP:HB2	1:C:194:ILE:HB	1.79	0.64
1:D:175:ASP:CB	1:D:179:THR:HB	2.27	0.64
1:C:71:MET:HE1	3:C:411:HOH:O	1.96	0.64
1:C:47:TRP:CD1	1:C:270:ARG:HD3	2.32	0.64
1:C:132:ARG:HG3	1:C:132:ARG:NH2	2.11	0.64
1:C:269:PHE:HE1	1:C:272:ILE:HD11	1.62	0.64
1:D:26:ASN:O	1:D:34:LYS:HE2	1.98	0.64
1:A:10:ALA:O	1:A:11:ILE:HG23	1.96	0.64
1:A:319:ILE:HD13	1:A:319:ILE:N	2.02	0.64
1:B:145:ALA:HB1	1:D:11:ILE:HG13	1.80	0.64
1:A:132:ARG:HG3	1:A:132:ARG:NH2	2.13	0.64
1:A:131:TYR:CD1	1:A:190:TYR:HA	2.32	0.64
1:D:95:TRP:HZ2	1:D:167:MET:O	1.81	0.64
1:B:95:TRP:CE3	1:B:169:PRO:HG3	2.32	0.64
1:A:319:ILE:H	1:A:319:ILE:CD1	1.90	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ASP:HB3	1:B:187:VAL:HG21	1.78	0.63
1:A:60:TYR:CE1	1:B:9:ARG:HD2	2.33	0.63
1:A:44:SER:HB2	1:A:267:LYS:CG	2.29	0.63
1:A:151:ASP:HA	1:A:154:LEU:HB3	1.80	0.63
1:D:252:TYR:HB3	1:D:325:THR:CG2	2.28	0.63
1:C:104:TYR:O	1:C:166:SER:N	2.28	0.63
1:A:331:LEU:O	1:A:332:PHE:HD2	1.82	0.63
1:A:17:ARG:NE	2:A:342:BR:BR	2.86	0.63
1:A:56:PHE:HD2	1:A:316:PRO:HG3	1.63	0.63
1:A:232:GLN:C	1:B:289:ASN:HD21	2.07	0.63
1:C:137:PRO:CG	1:C:162:PRO:HB3	2.26	0.63
1:C:246:THR:HG23	1:C:332:PHE:O	1.98	0.63
1:D:271:GLN:O	1:D:272:ILE:HD13	1.99	0.63
1:A:147:LEU:HD13	1:A:156:LEU:HD12	1.81	0.63
1:D:136:VAL:HA	1:D:186:TYR:HA	1.81	0.63
1:B:38:PHE:HB3	1:B:78:THR:CG2	2.28	0.62
1:C:11:ILE:HG13	1:D:61:PRO:HG2	1.81	0.62
1:D:178:GLY:O	1:D:189:GLU:HA	1.98	0.62
1:A:50:ASN:H	1:A:50:ASN:ND2	1.81	0.62
1:A:95:TRP:CD2	1:A:169:PRO:HB3	2.33	0.62
1:B:107:ARG:HH11	1:B:159:LYS:NZ	1.95	0.62
1:D:40:THR:HG21	1:D:275:ILE:HD12	1.80	0.62
1:A:202:ARG:CB	1:A:209:VAL:HG21	2.30	0.62
1:B:84:SER:HB3	2:B:342:BR:BR	2.54	0.62
1:C:108:ILE:H	1:C:108:ILE:CD1	2.10	0.62
1:D:175:ASP:HB3	1:D:179:THR:H	1.64	0.62
1:A:76:MET:HE2	1:A:261:ALA:CB	2.29	0.62
1:C:213:PRO:HD2	2:C:339:BR:BR	2.55	0.62
1:D:228:ASN:HD21	1:D:231:TRP:N	1.98	0.62
1:B:225:TYR:O	1:B:228:ASN:HB3	1.99	0.62
1:C:100:TYR:HB3	1:C:101:PRO:HD2	1.82	0.62
1:A:252:TYR:HB3	1:A:325:THR:CG2	2.30	0.62
1:D:39:ILE:HG22	1:D:79:VAL:O	2.00	0.62
1:A:7:ILE:HD12	1:A:7:ILE:N	2.15	0.61
1:A:217:LYS:O	1:A:220:PRO:HD3	2.00	0.61
1:A:279:LEU:HD23	1:A:279:LEU:N	2.15	0.61
1:B:98:THR:HA	1:B:103:PRO:CG	2.30	0.61
1:A:277:ASN:OD1	1:A:291:LYS:HE2	1.99	0.61
1:D:98:THR:HA	1:D:103:PRO:HG3	1.82	0.61
1:B:117:ALA:H	1:B:120:ASN:HB2	1.64	0.61
1:C:182:PRO:HB2	1:C:184:ASP:OD1	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LEU:HD23	1:B:156:LEU:H	1.65	0.61
1:C:8:TYR:CD2	1:D:315:ARG:HD2	2.35	0.61
1:D:137:PRO:HD2	1:D:162:PRO:HG3	1.82	0.61
1:A:282:LYS:NZ	1:A:289:ASN:OD1	2.30	0.61
1:C:266:ASN:ND2	1:C:320:MET:SD	2.73	0.61
1:D:95:TRP:CE2	1:D:169:PRO:HB3	2.35	0.61
1:B:229:LEU:O	1:B:232:GLN:HG3	2.00	0.61
1:C:90:ILE:CD1	1:C:111:ILE:HG21	2.30	0.61
1:A:8:TYR:HD2	1:A:8:TYR:N	1.99	0.61
1:A:10:ALA:HB2	1:B:313:GLU:CG	2.26	0.61
1:B:273:SER:HA	1:B:311:TYR:O	2.00	0.61
1:C:103:PRO:HD2	2:C:335:BR:BR	2.55	0.61
1:B:107:ARG:NH1	1:B:159:LYS:NZ	2.49	0.61
1:C:140:GLY:HA2	1:C:163:SER:HB2	1.83	0.61
1:D:324:GLN:HG2	1:D:325:THR:H	1.65	0.61
1:A:144:ILE:HD12	1:A:144:ILE:H	1.66	0.60
1:B:279:LEU:HD13	1:B:289:ASN:HD22	1.66	0.60
1:B:199:SER:HA	1:B:203:CYS:SG	2.40	0.60
1:C:108:ILE:HD12	1:C:108:ILE:N	2.13	0.60
1:D:15:LYS:HE2	2:D:335:BR:BR	2.57	0.60
1:C:39:ILE:HD13	1:C:39:ILE:O	2.02	0.60
1:D:106:PHE:O	1:D:186:TYR:HE2	1.84	0.60
1:D:107:ARG:HB3	1:D:159:LYS:HE3	1.84	0.60
1:A:8:TYR:N	1:A:8:TYR:CD2	2.70	0.60
1:B:68:VAL:HG21	2:B:340:BR:BR	2.57	0.60
1:D:255:SER:HA	1:D:258:PHE:CE1	2.36	0.60
1:A:309:MET:SD	1:A:312:MET:HE3	2.41	0.60
1:B:135:ASP:HB3	1:B:187:VAL:HG23	1.83	0.60
1:A:178:GLY:O	1:A:189:GLU:HA	2.01	0.60
1:C:48:SER:OG	1:C:50:ASN:ND2	2.35	0.60
1:D:135:ASP:HB3	1:D:187:VAL:CG2	2.32	0.60
1:A:17:ARG:HD3	2:A:342:BR:BR	2.57	0.59
1:A:95:TRP:CH2	1:A:169:PRO:HD3	2.37	0.59
1:B:250:LYS:CD	1:B:329:ASN:HD21	2.07	0.59
1:C:83:PRO:HD2	2:C:341:BR:BR	2.57	0.59
1:C:144:ILE:HG22	1:C:146:SER:HB2	1.84	0.59
1:C:282:LYS:HE3	1:C:303:MET:CE	2.31	0.59
1:A:130:VAL:O	1:A:191:LEU:HB2	2.02	0.59
1:C:308:GLU:OE2	1:D:15:LYS:HD2	2.02	0.59
1:C:231:TRP:HE1	1:C:232:GLN:HE21	1.50	0.59
1:A:149:ASP:HB3	1:A:152:GLU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ARG:HH22	1:A:226:GLU:HG3	1.67	0.59
1:B:93:ARG:NH2	1:B:106:PHE:CE1	2.68	0.59
1:A:119:TYR:CE2	1:A:120:ASN:ND2	2.70	0.59
1:B:148:THR:O	1:B:149:ASP:HB2	2.02	0.59
1:C:11:ILE:CG1	1:D:61:PRO:HG2	2.32	0.59
1:C:170:PRO:HB3	1:C:188:TRP:CD1	2.38	0.59
1:D:103:PRO:HG2	1:D:104:TYR:CE2	2.38	0.59
1:D:132:ARG:HH11	1:D:241:ARG:HH21	1.51	0.58
1:D:182:PRO:HG2	1:D:183:GLY:H	1.68	0.58
1:D:202:ARG:CB	1:D:209:VAL:HG21	2.33	0.58
1:D:296:TYR:CD1	1:D:297:TYR:N	2.71	0.58
1:B:107:ARG:HH11	1:B:159:LYS:HZ2	1.51	0.58
1:B:9:ARG:HG3	1:B:9:ARG:NH1	2.17	0.58
1:D:50:ASN:O	1:D:56:PHE:CD1	2.57	0.58
1:D:50:ASN:H	1:D:50:ASN:ND2	2.00	0.58
1:D:107:ARG:HG2	1:D:107:ARG:HH21	1.66	0.58
1:A:92:ARG:HB2	1:A:208:ILE:HG23	1.85	0.58
1:B:40:THR:O	1:B:272:ILE:HA	2.04	0.58
1:D:39:ILE:HG23	1:D:39:ILE:O	2.03	0.58
1:A:144:ILE:HD12	1:A:144:ILE:N	2.19	0.58
1:C:136:VAL:HB	1:C:137:PRO:HD2	1.85	0.58
1:C:43:ARG:HB3	1:C:271:GLN:HG3	1.86	0.58
1:C:199:SER:HA	1:C:203:CYS:HB2	1.86	0.58
1:A:269:PHE:CE1	1:A:272:ILE:HD11	2.39	0.58
1:D:34:LYS:HE3	1:D:34:LYS:HA	1.86	0.58
1:A:9:ARG:HB3	1:B:60:TYR:CD2	2.38	0.57
1:A:77:GLY:HA2	1:A:299:PRO:HD3	1.86	0.57
1:A:129:LEU:HD22	1:A:190:TYR:HE1	1.69	0.57
1:D:102:ASP:CB	2:D:336:BR:BR	3.07	0.57
1:B:43:ARG:CD	1:B:270:ARG:HB2	2.35	0.57
1:C:248:ARG:HB3	1:C:248:ARG:NH1	2.19	0.57
1:D:196:PRO:O	1:D:200:ILE:HG13	2.04	0.57
1:D:39:ILE:HD13	1:D:39:ILE:C	2.29	0.57
1:A:95:TRP:HB2	1:A:112:VAL:CG1	2.34	0.57
1:B:86:LEU:HD21	1:B:249:PHE:CE2	2.40	0.57
1:C:8:TYR:CZ	1:D:315:ARG:HD2	2.40	0.57
1:B:238:LEU:HB2	1:B:241:ARG:HH21	1.70	0.57
1:B:86:LEU:HD21	1:B:249:PHE:CD2	2.39	0.57
1:D:120:ASN:O	1:D:122:THR:HG23	2.05	0.57
1:A:254:ASP:HB3	1:A:256:VAL:HG22	1.86	0.57
1:A:279:LEU:HD13	1:A:289:ASN:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ILE:HA	1:C:35:ASN:O	2.03	0.57
1:C:132:ARG:HH11	1:C:134:LEU:HD21	1.70	0.57
1:C:285:PRO:HB3	1:D:232:GLN:NE2	2.20	0.57
1:A:95:TRP:CE3	1:A:169:PRO:HB3	2.40	0.57
1:B:254:ASP:HB3	1:B:257:TYR:CD2	2.40	0.57
1:A:65:VAL:HG23	2:B:335:BR:BR	2.60	0.56
1:A:95:TRP:HB2	1:A:112:VAL:HG11	1.87	0.56
1:C:60:TYR:CE1	1:D:9:ARG:HD2	2.39	0.56
1:C:250:LYS:HE3	1:C:327:GLU:CG	2.28	0.56
1:A:173:ARG:HH22	1:A:226:GLU:CG	2.18	0.56
1:B:217:LYS:HA	1:B:236:PHE:CE1	2.40	0.56
1:C:86:LEU:HD21	1:C:249:PHE:CD2	2.40	0.56
1:C:108:ILE:O	1:C:109:ASN:HB2	2.04	0.56
1:C:258:PHE:HD1	1:C:261:ALA:HB3	1.71	0.56
1:A:320:MET:HB2	3:A:355:HOH:O	2.06	0.56
1:D:31:GLY:C	1:D:33:ASP:H	2.13	0.56
1:D:228:ASN:ND2	1:D:231:TRP:H	2.03	0.56
1:C:47:TRP:CZ2	1:C:314:ASN:HB3	2.40	0.56
1:D:113:VAL:HG21	1:D:208:ILE:HG21	1.87	0.56
1:A:17:ARG:CD	2:A:342:BR:BR	3.09	0.56
1:A:151:ASP:HA	1:A:154:LEU:CB	2.35	0.56
1:B:279:LEU:H	1:B:306:SER:HB2	1.71	0.56
1:C:270:ARG:HG3	1:C:270:ARG:NH1	2.18	0.56
1:A:111:ILE:CD1	1:A:132:ARG:HG2	2.36	0.56
1:D:95:TRP:CZ2	1:D:169:PRO:HD3	2.40	0.56
1:A:308:GLU:HG3	1:B:240:TYR:CE2	2.40	0.56
1:B:105:THR:HG22	2:B:337:BR:BR	2.61	0.56
1:D:107:ARG:CZ	1:D:161:THR:HB	2.35	0.56
1:A:97:ASP:C	1:A:99:ARG:H	2.14	0.56
1:B:44:SER:HA	1:B:270:ARG:NH1	2.21	0.56
1:D:83:PRO:C	1:D:85:MET:H	2.13	0.56
1:A:183:GLY:C	1:A:185:GLY:H	2.13	0.55
1:C:20:LYS:CD	1:D:20:LYS:HD3	2.36	0.55
1:C:165:ARG:HH21	1:C:167:MET:HA	1.71	0.55
1:D:164:ALA:O	1:D:165:ARG:C	2.50	0.55
1:C:116:SER:N	1:C:120:ASN:ND2	2.53	0.55
1:D:270:ARG:HG3	1:D:270:ARG:HH11	1.72	0.55
1:C:85:MET:HB3	1:C:250:LYS:O	2.07	0.55
1:C:240:TYR:CE2	1:D:308:GLU:HG3	2.41	0.55
1:D:108:ILE:HB	1:D:159:LYS:NZ	2.22	0.55
1:B:258:PHE:HB2	1:B:260:GLU:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:THR:HG22	1:D:78:THR:HG22	1.88	0.55
1:A:202:ARG:HB3	1:A:209:VAL:HG21	1.88	0.55
1:C:35:ASN:ND2	2:D:337:BR:BR	2.94	0.55
1:A:111:ILE:HG23	1:A:130:VAL:HG13	1.88	0.55
1:A:96:GLY:O	1:A:98:THR:N	2.39	0.55
1:C:131:TYR:CD1	1:C:190:TYR:HA	2.42	0.55
1:C:319:ILE:HD12	1:C:319:ILE:O	2.06	0.55
1:D:137:PRO:HG3	1:D:185:GLY:C	2.32	0.55
1:B:92:ARG:HB2	1:B:208:ILE:HG23	1.89	0.54
1:D:95:TRP:CH2	1:D:169:PRO:HD3	2.41	0.54
1:D:202:ARG:HB2	1:D:209:VAL:HG21	1.89	0.54
1:B:42:GLY:O	1:B:43:ARG:CB	2.55	0.54
1:A:44:SER:HB2	1:A:267:LYS:HG3	1.88	0.54
1:A:252:TYR:HB3	1:A:325:THR:HG21	1.89	0.54
1:A:255:SER:HB2	1:A:322:MET:O	2.06	0.54
1:C:7:ILE:HG22	1:C:8:TYR:CD2	2.42	0.54
1:D:180:ILE:O	1:D:182:PRO:HD3	2.08	0.54
1:A:149:ASP:HB3	1:A:152:GLU:CB	2.38	0.54
1:D:304:ARG:O	1:D:305:HIS:HB2	2.07	0.54
1:A:67:GLY:C	1:A:312:MET:HE1	2.32	0.54
1:C:131:TYR:HD1	1:C:190:TYR:HA	1.73	0.54
1:C:258:PHE:CD1	1:C:261:ALA:HB3	2.43	0.54
1:B:42:GLY:HA3	1:B:74:HIS:O	2.07	0.54
1:B:226:GLU:HG2	1:B:227:ASP:N	2.23	0.54
1:D:219:ASP:OD2	1:D:222:ARG:HB2	2.08	0.54
1:B:283:ALA:O	1:B:285:PRO:HD3	2.07	0.54
1:D:149:ASP:HB3	1:D:152:GLU:CG	2.25	0.54
1:B:136:VAL:HB	1:B:137:PRO:CD	2.37	0.54
1:C:168:THR:HG23	1:C:182:PRO:HB3	1.90	0.54
1:A:214:GLU:HB2	2:A:338:BR:BR	2.62	0.54
1:A:260:GLU:OE2	1:A:260:GLU:N	2.33	0.54
1:C:95:TRP:CH2	1:C:169:PRO:HD3	2.43	0.53
1:B:151:ASP:HB3	1:B:154:LEU:HB2	1.90	0.53
1:D:102:ASP:HB3	2:D:336:BR:BR	2.63	0.53
1:B:90:ILE:CD1	1:B:111:ILE:HG21	2.39	0.53
1:C:10:ALA:O	1:C:11:ILE:HG23	2.07	0.53
1:C:175:ASP:OD1	1:C:177:GLU:N	2.42	0.53
1:A:135:ASP:HB3	1:A:187:VAL:HG23	1.89	0.53
1:B:274:ILE:HG13	1:B:332:PHE:CZ	2.40	0.53
1:D:228:ASN:HD21	1:D:231:TRP:H	1.54	0.53
1:D:304:ARG:HB3	1:D:304:ARG:HH21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:PRO:O	1:B:200:ILE:HG13	2.08	0.53
1:D:291:LYS:O	1:D:293:GLU:HG3	2.08	0.53
1:D:304:ARG:HB3	1:D:304:ARG:NH2	2.24	0.53
1:A:99:ARG:O	1:A:100:TYR:CD2	2.62	0.53
1:A:132:ARG:HB2	1:A:191:LEU:HD11	1.90	0.53
1:A:168:THR:OG1	1:A:169:PRO:HD2	2.09	0.53
1:D:165:ARG:O	1:D:165:ARG:HD3	2.09	0.53
1:D:292:ALA:HB1	1:D:297:TYR:CE2	2.44	0.53
1:A:21:MET:HG3	1:A:247:ILE:CG1	2.39	0.53
1:A:44:SER:O	1:A:267:LYS:HB2	2.09	0.53
1:A:101:PRO:O	1:A:102:ASP:C	2.52	0.53
1:C:37:ILE:HD11	1:C:81:VAL:CG1	2.35	0.53
1:C:111:ILE:HD12	1:C:132:ARG:HG2	1.90	0.53
1:C:232:GLN:O	1:D:303:MET:HE1	2.09	0.53
1:A:193:GLU:HG2	1:A:194:ILE:N	2.24	0.53
1:B:237:GLY:O	1:B:240:TYR:HB2	2.09	0.53
1:C:78:THR:OG1	1:C:297:TYR:HB2	2.09	0.53
1:C:90:ILE:HD12	1:C:111:ILE:HG21	1.91	0.53
1:A:161:THR:HG23	1:A:161:THR:O	2.08	0.53
1:B:21:MET:HE3	1:B:245:ASN:N	2.23	0.53
1:A:10:ALA:CB	1:B:313:GLU:HG3	2.29	0.52
1:A:145:ALA:C	1:A:147:LEU:H	2.17	0.52
1:C:64:SER:O	1:C:67:GLY:N	2.42	0.52
1:C:313:GLU:OE1	1:C:315:ARG:HD2	2.09	0.52
1:D:115:ASN:N	1:D:120:ASN:OD1	2.38	0.52
1:B:148:THR:HG22	1:B:160:TRP:CZ3	2.45	0.52
1:B:184:ASP:OD1	1:B:186:TYR:HB2	2.09	0.52
1:C:109:ASN:HA	1:C:132:ARG:HD3	1.90	0.52
1:A:196:PRO:O	1:A:200:ILE:HG13	2.09	0.52
1:A:219:ASP:OD2	1:A:222:ARG:HB2	2.09	0.52
1:B:42:GLY:O	1:B:43:ARG:HB2	2.08	0.52
1:B:111:ILE:HG12	1:B:242:VAL:HB	1.90	0.52
1:C:292:ALA:HB1	1:C:297:TYR:CZ	2.44	0.52
1:D:258:PHE:CD2	1:D:261:ALA:HB3	2.37	0.52
1:B:102:ASP:N	1:B:103:PRO:HD3	2.25	0.52
1:D:85:MET:HG2	1:D:250:LYS:O	2.09	0.52
1:C:61:PRO:HG2	1:D:11:ILE:CG2	2.39	0.52
1:C:97:ASP:OD1	1:C:99:ARG:NH1	2.43	0.52
1:C:303:MET:SD	1:D:232:GLN:O	2.68	0.52
1:D:118:PRO:C	1:D:120:ASN:H	2.18	0.52
1:A:39:ILE:HG13	1:A:81:VAL:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:LEU:O	1:D:85:MET:HB2	2.09	0.52
1:D:82:LEU:HB2	1:D:85:MET:HE3	1.90	0.52
1:D:183:GLY:O	1:D:185:GLY:N	2.43	0.52
1:A:227:ASP:O	1:A:229:LEU:HD22	2.10	0.52
1:A:308:GLU:HG3	1:B:240:TYR:CZ	2.45	0.52
1:A:308:GLU:OE2	1:B:15:LYS:HD2	2.10	0.52
1:B:254:ASP:HB3	1:B:257:TYR:HD2	1.74	0.52
1:C:43:ARG:HB2	1:C:74:HIS:HB3	1.92	0.52
1:A:9:ARG:HB3	1:B:60:TYR:HD2	1.74	0.51
1:C:150:LYS:HD3	3:C:370:HOH:O	2.10	0.51
1:A:131:TYR:HD1	1:A:190:TYR:HA	1.72	0.51
1:A:134:LEU:HD11	1:A:189:GLU:HB2	1.92	0.51
1:B:39:ILE:HD11	1:B:272:ILE:HG23	1.92	0.51
1:C:291:LYS:HB2	1:C:291:LYS:NZ	2.25	0.51
1:A:175:ASP:HB2	1:A:179:THR:OG1	2.10	0.51
1:A:202:ARG:HB2	1:A:209:VAL:HG21	1.91	0.51
1:C:246:THR:HA	1:C:332:PHE:O	2.10	0.51
1:D:27:SER:O	1:D:34:LYS:HE3	2.10	0.51
1:A:27:SER:O	1:A:35:ASN:N	2.38	0.51
1:A:109:ASN:HA	1:A:132:ARG:HD3	1.93	0.51
1:B:58:PRO:HB2	1:B:59:PRO:HD2	1.93	0.51
1:B:250:LYS:HA	1:B:329:ASN:ND2	2.25	0.51
1:D:175:ASP:C	1:D:177:GLU:N	2.68	0.51
1:B:145:ALA:CB	1:D:11:ILE:HG13	2.40	0.51
1:B:151:ASP:CB	1:B:154:LEU:HB2	2.41	0.51
1:C:39:ILE:O	1:C:39:ILE:HG23	2.10	0.51
1:C:87:ASP:OD2	1:C:202:ARG:NE	2.43	0.51
1:D:114:CYS:HA	1:D:120:ASN:OD1	2.10	0.51
1:D:144:ILE:HB	1:D:147:LEU:HD12	1.92	0.51
1:D:216:LEU:HD11	1:D:225:TYR:CG	2.46	0.51
1:A:111:ILE:HD12	1:A:132:ARG:HG2	1.93	0.51
1:B:36:THR:HG22	3:B:350:HOH:O	2.10	0.51
1:B:321:ALA:HB3	1:B:324:GLN:CB	2.38	0.51
1:C:56:PHE:CG	1:C:57:ALA:N	2.79	0.51
1:D:82:LEU:HD23	2:D:344:BR:BR	2.66	0.51
1:D:35:ASN:ND2	1:D:277:ASN:HD21	2.08	0.51
1:C:77:GLY:CA	1:C:299:PRO:HD3	2.36	0.51
1:D:199:SER:HA	1:D:203:CYS:SG	2.51	0.51
1:A:233:GLN:HG3	1:A:234:ASP:H	1.76	0.51
1:B:192:PHE:CD2	1:B:238:LEU:HD21	2.45	0.51
1:C:274:ILE:HG22	1:C:310:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:LYS:HA	1:C:160:TRP:CE3	2.47	0.50
1:A:77:GLY:HA3	1:A:258:PHE:CE2	2.45	0.50
1:B:298:ASP:HA	3:B:405:HOH:O	2.10	0.50
1:C:209:VAL:HG12	1:C:210:VAL:N	2.26	0.50
1:C:213:PRO:HB2	2:C:339:BR:BR	2.67	0.50
1:A:165:ARG:NH2	1:A:166:SER:O	2.44	0.50
1:C:165:ARG:NH2	1:C:167:MET:O	2.43	0.50
1:C:263:LEU:O	1:C:264:PRO:C	2.54	0.50
1:B:282:LYS:CE	1:B:303:MET:HE1	2.36	0.50
1:B:319:ILE:HD13	1:B:319:ILE:H	1.75	0.50
1:C:118:PRO:HB2	2:C:336:BR:BR	2.67	0.50
1:B:256:VAL:HG22	1:B:323:ASP:OD2	2.12	0.50
1:A:256:VAL:HG23	1:A:257:TYR:CD2	2.47	0.50
1:B:68:VAL:O	1:B:71:MET:HB3	2.11	0.50
1:C:43:ARG:N	1:C:74:HIS:O	2.44	0.50
1:C:199:SER:HA	1:C:203:CYS:SG	2.52	0.50
1:C:270:ARG:HG2	1:C:317:PRO:HA	1.94	0.50
1:D:234:ASP:OD1	1:D:241:ARG:HD3	2.11	0.50
1:A:102:ASP:HB3	1:A:105:THR:O	2.11	0.50
1:B:43:ARG:CD	1:B:270:ARG:HD2	2.39	0.50
1:C:120:ASN:C	1:C:120:ASN:HD22	2.20	0.50
1:D:64:SER:O	1:D:68:VAL:HG23	2.12	0.50
1:B:268:GLY:HA2	1:B:320:MET:CE	2.41	0.50
1:B:304:ARG:O	1:B:305:HIS:HB2	2.12	0.50
1:A:86:LEU:HD21	1:A:249:PHE:CE2	2.47	0.49
1:C:116:SER:N	1:C:120:ASN:HD21	2.10	0.49
1:D:47:TRP:NE1	1:D:270:ARG:HB3	2.27	0.49
1:D:108:ILE:HG22	1:D:109:ASN:OD1	2.12	0.49
1:B:21:MET:HE1	1:B:244:ALA:HB1	1.92	0.49
1:C:315:ARG:HB3	1:D:8:TYR:HD2	1.77	0.49
1:B:102:ASP:HA	2:B:337:BR:BR	2.67	0.49
1:B:151:ASP:CA	1:B:154:LEU:HB2	2.42	0.49
1:D:40:THR:CG2	1:D:78:THR:HG22	2.42	0.49
1:D:43:ARG:HD3	1:D:270:ARG:HB2	1.93	0.49
1:D:250:LYS:HE3	1:D:327:GLU:OE1	2.13	0.49
1:D:271:GLN:HG2	1:D:314:ASN:OD1	2.12	0.49
1:A:47:TRP:NE1	1:A:270:ARG:HB3	2.28	0.49
1:A:135:ASP:HB3	1:A:187:VAL:CG2	2.42	0.49
1:D:304:ARG:HH21	1:D:304:ARG:CB	2.24	0.49
1:A:232:GLN:NE2	1:B:286:ASN:HA	2.16	0.49
1:C:258:PHE:CE1	1:C:320:MET:HE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:TRP:CE2	1:A:199:SER:HB2	2.48	0.49
1:A:297:TYR:CD2	1:A:302:LEU:HD21	2.48	0.49
1:A:132:ARG:HE	1:A:134:LEU:HD23	1.77	0.49
1:A:156:LEU:O	1:D:167:MET:HE2	2.13	0.49
1:C:116:SER:H	1:C:120:ASN:HD21	1.58	0.49
1:C:248:ARG:HD2	1:C:329:ASN:HD22	1.78	0.49
1:D:130:VAL:O	1:D:191:LEU:HB2	2.13	0.49
1:D:233:GLN:OE1	1:D:233:GLN:N	2.45	0.49
1:A:211:PRO:HG3	1:A:216:LEU:HD13	1.95	0.49
1:B:154:LEU:HD22	1:B:154:LEU:N	2.28	0.49
1:D:29:GLY:HA3	1:D:34:LYS:HD3	1.95	0.49
1:D:150:LYS:O	1:D:154:LEU:HG	2.13	0.49
1:B:147:LEU:HD11	1:C:60:TYR:CE2	2.48	0.48
1:D:50:ASN:ND2	1:D:50:ASN:N	2.61	0.48
1:D:139:THR:N	1:D:160:TRP:HZ2	2.11	0.48
1:D:144:ILE:N	1:D:144:ILE:CD1	2.76	0.48
1:D:255:SER:HA	1:D:258:PHE:CZ	2.48	0.48
1:D:298:ASP:O	1:D:301:ASP:N	2.46	0.48
1:C:263:LEU:CD2	1:C:322:MET:HE2	2.43	0.48
1:D:309:MET:SD	1:D:312:MET:HE3	2.53	0.48
1:A:138:ASP:HA	1:A:150:LYS:HD2	1.95	0.48
1:B:321:ALA:H	1:B:324:GLN:HE21	1.60	0.48
1:C:40:THR:HG22	1:C:78:THR:CG2	2.41	0.48
1:C:255:SER:HB2	1:C:323:ASP:HA	1.95	0.48
1:D:40:THR:HB	1:D:78:THR:HG22	1.95	0.48
1:B:38:PHE:CE2	1:B:80:LYS:HB2	2.48	0.48
1:B:261:ALA:HB3	1:B:320:MET:SD	2.54	0.48
1:D:177:GLU:HA	3:D:373:HOH:O	2.14	0.48
1:C:147:LEU:HB3	1:C:153:CYS:HB2	1.95	0.48
1:C:330:ILE:CG2	1:C:332:PHE:HE2	2.27	0.48
1:D:90:ILE:CD1	1:D:111:ILE:HG21	2.44	0.48
1:D:100:TYR:O	1:D:103:PRO:HD3	2.13	0.48
1:A:274:ILE:HD12	1:A:332:PHE:CZ	2.48	0.48
1:C:263:LEU:HD23	1:C:322:MET:HE2	1.94	0.48
1:D:95:TRP:CZ2	1:D:167:MET:O	2.65	0.48
1:D:128:TRP:HB2	1:D:194:ILE:HB	1.96	0.48
1:A:56:PHE:CD2	1:A:316:PRO:HG3	2.46	0.48
1:C:44:SER:HA	1:C:268:GLY:O	2.14	0.48
1:D:267:LYS:HB3	1:D:270:ARG:NH2	2.21	0.48
1:B:270:ARG:HB3	1:B:315:ARG:O	2.14	0.48
1:C:10:ALA:HB2	1:D:313:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:THR:HG21	1:D:248:ARG:NH2	2.28	0.48
1:B:107:ARG:O	1:B:110:ASP:HB2	2.14	0.48
1:B:256:VAL:HG13	1:B:323:ASP:OD2	2.14	0.48
1:C:214:GLU:O	1:C:217:LYS:N	2.47	0.48
1:A:22:LEU:HG	1:A:26:ASN:HD22	1.79	0.47
1:A:37:ILE:HG22	1:A:81:VAL:CG2	2.44	0.47
1:C:110:ASP:O	1:C:112:VAL:HG23	2.13	0.47
1:D:95:TRP:CG	1:D:169:PRO:HB3	2.48	0.47
1:A:84:SER:HB3	2:A:340:BR:BR	2.69	0.47
1:B:90:ILE:HD12	1:B:111:ILE:HG21	1.95	0.47
1:B:256:VAL:HG22	1:B:323:ASP:CB	2.44	0.47
1:C:85:MET:HE2	1:C:251:ALA:HA	1.97	0.47
1:D:84:SER:HB3	2:D:342:BR:BR	2.69	0.47
1:D:173:ARG:HA	1:D:190:TYR:HB2	1.95	0.47
1:D:175:ASP:HB3	1:D:179:THR:N	2.29	0.47
1:A:214:GLU:HA	1:A:214:GLU:OE1	2.12	0.47
1:D:7:ILE:HG22	3:D:408:HOH:O	2.15	0.47
1:D:173:ARG:HG2	1:D:190:TYR:CE2	2.50	0.47
1:A:248:ARG:HH11	1:A:248:ARG:HG2	1.79	0.47
1:C:13:THR:HB	1:D:63:ASP:OD2	2.13	0.47
1:D:102:ASP:CG	2:D:336:BR:BR	3.12	0.47
1:D:202:ARG:HB3	1:D:209:VAL:HG21	1.96	0.47
1:B:97:ASP:OD2	1:B:99:ARG:HG3	2.15	0.47
1:C:296:TYR:CD1	1:C:297:TYR:N	2.83	0.47
1:D:82:LEU:HD12	1:D:85:MET:CE	2.45	0.47
1:D:137:PRO:HG3	1:D:186:TYR:N	2.30	0.47
1:A:83:PRO:C	1:A:85:MET:H	2.21	0.47
1:A:136:VAL:HB	1:A:137:PRO:HD2	1.97	0.47
1:B:225:TYR:CE2	1:B:241:ARG:NH2	2.79	0.47
1:C:141:MET:HE3	1:C:141:MET:C	2.39	0.47
1:C:209:VAL:CG1	1:C:210:VAL:N	2.77	0.47
1:C:266:ASN:ND2	1:C:320:MET:H	2.12	0.47
1:D:83:PRO:C	1:D:85:MET:N	2.71	0.47
1:D:106:PHE:O	1:D:186:TYR:CE2	2.66	0.47
1:D:252:TYR:O	1:D:254:ASP:N	2.48	0.47
1:B:216:LEU:HD21	1:B:225:TYR:CE2	2.50	0.47
1:D:142:CYS:HA	1:D:159:LYS:O	2.14	0.47
1:A:112:VAL:HG12	1:A:113:VAL:N	2.29	0.47
1:B:39:ILE:HA	1:B:274:ILE:HD13	1.97	0.47
1:C:168:THR:CG2	1:C:182:PRO:HB3	2.45	0.47
1:A:51:GLU:HA	1:A:56:PHE:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:GLY:O	1:B:159:LYS:C	2.56	0.47
1:B:230:THR:HA	1:B:233:GLN:OE1	2.15	0.47
1:B:266:ASN:ND2	1:B:320:MET:HG2	2.29	0.47
1:B:279:LEU:H	1:B:306:SER:CB	2.27	0.47
1:B:319:ILE:HD13	1:B:319:ILE:N	2.30	0.47
1:C:144:ILE:C	1:C:146:SER:H	2.22	0.47
1:D:31:GLY:O	1:D:33:ASP:N	2.48	0.47
1:A:234:ASP:OD2	1:A:234:ASP:C	2.57	0.46
1:C:71:MET:HG2	1:C:309:MET:SD	2.55	0.46
1:D:195:PRO:HG2	1:D:198:VAL:CG2	2.45	0.46
1:D:259:PRO:HG2	1:D:260:GLU:H	1.81	0.46
1:C:27:SER:O	1:C:35:ASN:N	2.45	0.46
1:C:137:PRO:HD3	1:C:186:TYR:CD1	2.51	0.46
1:D:33:ASP:N	1:D:33:ASP:OD2	2.48	0.46
1:D:40:THR:CB	1:D:78:THR:HG22	2.45	0.46
1:C:10:ALA:HA	1:D:313:GLU:HA	1.98	0.46
1:C:275:ILE:HG22	1:C:278:PRO:HD3	1.98	0.46
1:D:108:ILE:HG12	1:D:134:LEU:O	2.15	0.46
1:A:44:SER:HB2	1:A:267:LYS:HG2	1.97	0.46
1:B:111:ILE:HG23	1:B:130:VAL:CG1	2.46	0.46
1:C:20:LYS:HD3	1:D:20:LYS:CD	2.42	0.46
1:C:132:ARG:HE	1:C:134:LEU:CD2	2.22	0.46
1:C:249:PHE:HB3	3:C:365:HOH:O	2.16	0.46
1:A:17:ARG:HG2	1:A:334:PHE:OXT	2.16	0.46
1:A:276:THR:HG21	1:B:19:GLU:OE2	2.14	0.46
1:B:256:VAL:HG22	1:B:323:ASP:HB3	1.96	0.46
1:C:40:THR:HG21	1:C:275:ILE:HD12	1.98	0.46
1:D:292:ALA:HB1	1:D:297:TYR:CZ	2.50	0.46
1:D:321:ALA:CB	1:D:324:GLN:HE21	2.25	0.46
1:A:51:GLU:HA	1:A:56:PHE:CG	2.50	0.46
1:A:83:PRO:C	1:A:85:MET:N	2.74	0.46
1:A:230:THR:O	1:A:233:GLN:HG3	2.16	0.46
1:B:225:TYR:OH	1:B:241:ARG:NH2	2.49	0.46
1:B:226:GLU:C	1:B:228:ASN:H	2.24	0.46
1:C:198:VAL:HG21	1:C:222:ARG:HH22	1.80	0.46
1:A:82:LEU:N	1:A:85:MET:HE3	2.25	0.46
1:A:292:ALA:HB1	1:A:297:TYR:CE2	2.51	0.46
1:B:43:ARG:HB3	1:B:270:ARG:H	1.81	0.46
1:B:54:VAL:O	1:B:54:VAL:HG13	2.16	0.46
1:D:234:ASP:OD2	1:D:234:ASP:C	2.58	0.46
1:A:260:GLU:CG	1:A:261:ALA:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:MET:HG3	1:C:247:ILE:HG13	1.98	0.46
1:C:132:ARG:HB2	1:C:191:LEU:HD21	1.97	0.46
1:C:258:PHE:CZ	1:C:320:MET:HE2	2.51	0.46
1:C:273:SER:C	1:C:274:ILE:HD12	2.40	0.46
1:D:135:ASP:OD2	1:D:150:LYS:NZ	2.41	0.46
1:D:155:LYS:HE2	1:D:155:LYS:HB3	1.67	0.46
1:D:173:ARG:HH21	1:D:227:ASP:HB2	1.80	0.46
1:D:184:ASP:OD1	1:D:186:TYR:HB2	2.16	0.46
1:D:228:ASN:ND2	1:D:231:TRP:HB3	2.30	0.46
1:A:145:ALA:O	1:A:147:LEU:N	2.49	0.46
1:B:12:VAL:HG23	1:B:12:VAL:O	2.16	0.46
1:B:37:ILE:CG1	1:B:81:VAL:HB	2.43	0.46
1:B:95:TRP:O	1:B:120:ASN:ND2	2.47	0.46
1:C:51:GLU:HA	1:C:56:PHE:CD2	2.50	0.46
1:A:262:ALA:O	1:A:263:LEU:HG	2.16	0.45
1:A:269:PHE:CE2	1:A:318:ILE:HB	2.51	0.45
1:C:144:ILE:CG2	1:C:146:SER:HB2	2.46	0.45
1:C:192:PHE:CD2	1:C:238:LEU:HD21	2.52	0.45
1:D:230:THR:HG21	1:D:241:ARG:HH12	1.81	0.45
1:D:298:ASP:O	1:D:299:PRO:C	2.57	0.45
1:B:40:THR:OG1	1:B:273:SER:OG	2.32	0.45
1:C:248:ARG:HD2	1:C:329:ASN:ND2	2.31	0.45
1:D:40:THR:HG1	1:D:273:SER:HG	1.57	0.45
1:C:25:TYR:CE1	1:C:83:PRO:HB3	2.51	0.45
1:C:258:PHE:CD1	1:C:258:PHE:O	2.69	0.45
1:C:315:ARG:CZ	1:D:8:TYR:CE2	2.98	0.45
1:D:50:ASN:N	1:D:50:ASN:HD22	2.12	0.45
1:A:309:MET:N	1:B:15:LYS:HE3	2.31	0.45
1:B:120:ASN:O	1:B:121:ALA:C	2.60	0.45
1:D:87:ASP:OD2	1:D:202:ARG:NE	2.49	0.45
1:B:21:MET:CE	1:B:244:ALA:C	2.89	0.45
1:B:212:TRP:H	1:B:215:GLU:CG	2.29	0.45
1:B:229:LEU:C	1:B:231:TRP:H	2.24	0.45
1:D:92:ARG:CB	1:D:208:ILE:HG23	2.43	0.45
1:A:25:TYR:HB2	1:A:212:TRP:CH2	2.51	0.45
1:A:49:SER:OG	1:C:53:GLU:OE1	2.31	0.45
1:A:61:PRO:HG2	1:B:11:ILE:HG12	1.98	0.45
1:A:250:LYS:HE2	1:A:327:GLU:OE2	2.16	0.45
1:B:21:MET:HE3	1:B:244:ALA:C	2.41	0.45
1:B:183:GLY:C	1:B:185:GLY:H	2.24	0.45
1:C:151:ASP:O	1:C:154:LEU:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:THR:CG2	1:D:275:ILE:HD12	2.46	0.45
1:D:143:SER:HB2	1:D:144:ILE:HD12	1.98	0.45
1:D:183:GLY:C	1:D:185:GLY:N	2.66	0.45
1:D:228:ASN:HD22	1:D:231:TRP:HB3	1.81	0.45
1:A:283:ALA:C	1:A:284:HIS:ND1	2.74	0.45
1:C:44:SER:HB2	1:C:267:LYS:CB	2.46	0.45
1:C:99:ARG:C	1:C:100:TYR:CD2	2.95	0.45
1:C:334:PHE:N	1:C:334:PHE:CD2	2.83	0.45
1:D:40:THR:HG22	1:D:78:THR:CG2	2.46	0.45
1:D:111:ILE:N	1:D:111:ILE:HD12	2.32	0.45
1:D:274:ILE:HG21	1:D:310:ILE:HD11	1.98	0.45
1:A:130:VAL:HG12	1:A:191:LEU:HD12	1.99	0.45
1:A:277:ASN:OD1	1:A:291:LYS:CE	2.65	0.45
1:C:165:ARG:NH2	1:C:167:MET:HA	2.31	0.45
1:D:72:TRP:CZ3	1:D:304:ARG:HA	2.51	0.45
1:D:107:ARG:HG2	1:D:107:ARG:NH2	2.31	0.45
1:A:157:GLY:O	1:A:158:GLY:C	2.60	0.45
1:B:72:TRP:CZ3	1:B:304:ARG:HA	2.52	0.45
1:B:202:ARG:HH21	1:B:250:LYS:HG2	1.82	0.45
1:C:134:LEU:HG	1:C:189:GLU:HB2	1.99	0.45
1:A:198:VAL:HA	1:A:202:ARG:HG2	1.99	0.45
1:A:297:TYR:CG	1:A:302:LEU:HD21	2.52	0.45
1:B:284:HIS:O	1:B:286:ASN:N	2.50	0.45
1:C:123:GLU:HB3	1:C:126:ALA:HB3	1.98	0.45
1:C:311:TYR:OH	1:C:313:GLU:OE2	2.26	0.45
1:D:217:LYS:HB2	1:D:236:PHE:CD2	2.52	0.44
1:C:174:GLY:CA	1:C:180:ILE:HG12	2.47	0.44
1:D:31:GLY:C	1:D:33:ASP:N	2.75	0.44
1:D:104:TYR:O	1:D:166:SER:N	2.49	0.44
1:A:47:TRP:HE1	1:A:270:ARG:HB3	1.81	0.44
1:A:259:PRO:O	1:A:262:ALA:O	2.36	0.44
1:B:265:GLY:O	1:B:266:ASN:O	2.36	0.44
1:C:37:ILE:HG12	1:C:81:VAL:HB	1.98	0.44
1:C:248:ARG:HG3	1:C:331:LEU:HD23	2.00	0.44
1:A:183:GLY:C	1:A:185:GLY:N	2.76	0.44
1:A:304:ARG:HD3	1:A:305:HIS:NE2	2.32	0.44
1:C:330:ILE:HG21	1:C:332:PHE:HE2	1.82	0.44
1:B:272:ILE:HB	1:B:313:GLU:HB3	1.99	0.44
1:B:197:ASP:N	1:B:197:ASP:OD2	2.50	0.44
1:B:319:ILE:H	1:B:319:ILE:CD1	2.29	0.44
1:C:61:PRO:HG2	1:D:11:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:TRP:HA	1:D:75:MET:HE3	1.99	0.44
1:B:77:GLY:HA2	1:B:299:PRO:HD3	1.99	0.44
1:B:85:MET:CE	1:B:251:ALA:HA	2.47	0.44
1:B:173:ARG:HH22	1:B:226:GLU:CD	2.26	0.44
1:B:196:PRO:HD2	3:B:370:HOH:O	2.17	0.44
1:C:102:ASP:HA	2:C:335:BR:BR	2.72	0.44
1:C:221:THR:HG22	1:C:226:GLU:OE1	2.18	0.44
1:A:75:MET:O	1:A:299:PRO:HG2	2.17	0.44
1:A:120:ASN:O	1:A:121:ALA:C	2.60	0.44
1:A:250:LYS:NZ	2:A:339:BR:BR	2.99	0.44
1:B:108:ILE:HG23	1:B:134:LEU:O	2.18	0.44
1:C:66:LEU:HD22	3:C:368:HOH:O	2.17	0.44
1:C:311:TYR:CD1	1:C:311:TYR:C	2.96	0.44
1:D:175:ASP:HB3	1:D:179:THR:HB	2.00	0.44
1:D:251:ALA:O	1:D:328:ILE:N	2.39	0.44
1:A:260:GLU:CG	1:A:261:ALA:N	2.78	0.44
1:B:64:SER:O	1:B:68:VAL:HG23	2.18	0.44
1:D:205:ASN:OD1	1:D:206:GLU:HG3	2.17	0.44
1:A:50:ASN:N	1:A:50:ASN:ND2	2.52	0.43
1:A:215:GLU:HB2	3:A:417:HOH:O	2.17	0.43
1:C:273:SER:HA	1:C:311:TYR:O	2.18	0.43
1:D:249:PHE:HB3	3:D:355:HOH:O	2.18	0.43
1:A:246:THR:HA	1:A:332:PHE:O	2.18	0.43
1:B:292:ALA:HB1	1:B:297:TYR:CE2	2.53	0.43
1:C:94:ASP:HB3	1:C:119:TYR:HE2	1.83	0.43
1:C:114:CYS:HB2	1:C:131:TYR:HE2	1.83	0.43
1:D:8:TYR:HB2	3:D:351:HOH:O	2.17	0.43
1:A:267:LYS:HD2	1:A:267:LYS:N	2.32	0.43
1:A:267:LYS:O	1:A:270:ARG:NH2	2.51	0.43
1:B:271:GLN:HG2	1:B:314:ASN:OD1	2.18	0.43
1:C:235:ASP:O	1:C:236:PHE:HB2	2.18	0.43
1:D:103:PRO:HG2	1:D:104:TYR:CD2	2.53	0.43
1:B:95:TRP:O	1:B:95:TRP:HE3	2.01	0.43
1:B:225:TYR:HE2	1:B:241:ARG:NH2	2.09	0.43
1:C:87:ASP:CG	1:C:202:ARG:HH11	2.26	0.43
1:C:144:ILE:O	1:C:145:ALA:HB3	2.18	0.43
1:C:196:PRO:O	1:C:200:ILE:HG13	2.19	0.43
1:A:141:MET:HG3	1:A:142:CYS:N	2.34	0.43
1:B:44:SER:O	1:B:270:ARG:NH1	2.51	0.43
1:C:9:ARG:HD2	1:D:58:PRO:O	2.17	0.43
1:C:150:LYS:HB2	1:C:160:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LYS:O	1:A:154:LEU:N	2.52	0.43
1:B:16:PHE:CE1	1:B:20:LYS:HE3	2.53	0.43
1:B:43:ARG:HE	1:B:271:GLN:HG3	1.83	0.43
1:B:279:LEU:HD13	1:B:289:ASN:ND2	2.31	0.43
1:C:202:ARG:HB2	1:C:209:VAL:HG21	2.01	0.43
1:D:140:GLY:N	1:D:160:TRP:CZ2	2.87	0.43
1:D:270:ARG:HG3	1:D:270:ARG:NH1	2.32	0.43
1:A:83:PRO:O	1:A:85:MET:N	2.52	0.43
1:C:102:ASP:N	1:C:103:PRO:HD3	2.34	0.43
1:C:254:ASP:CG	1:C:325:THR:HG22	2.43	0.43
1:A:116:SER:H	1:A:120:ASN:HB2	1.84	0.43
1:A:118:PRO:O	1:A:120:ASN:N	2.52	0.43
1:C:150:LYS:HA	1:C:160:TRP:CZ3	2.53	0.43
1:D:217:LYS:HG3	1:D:236:PHE:CE2	2.54	0.43
1:D:231:TRP:O	1:D:235:ASP:HA	2.19	0.43
1:D:282:LYS:HE2	1:D:287:ASP:O	2.19	0.43
1:A:263:LEU:O	1:A:265:GLY:N	2.52	0.43
1:B:261:ALA:C	1:B:263:LEU:H	2.27	0.43
1:B:286:ASN:CG	1:B:286:ASN:O	2.61	0.43
1:C:169:PRO:O	1:C:170:PRO:C	2.59	0.43
1:B:41:PHE:HA	1:B:272:ILE:HD13	2.01	0.42
1:B:90:ILE:C	1:B:207:TYR:HD1	2.26	0.42
1:B:113:VAL:HG22	1:B:130:VAL:HG22	2.01	0.42
1:B:217:LYS:HE3	3:B:362:HOH:O	2.19	0.42
1:B:226:GLU:HG2	1:B:227:ASP:H	1.84	0.42
1:C:23:ASN:ND2	2:C:337:BR:BR	3.07	0.42
1:C:117:ALA:HB1	1:C:118:PRO:HD2	2.01	0.42
1:C:142:CYS:C	1:C:144:ILE:H	2.27	0.42
1:C:234:ASP:C	1:C:234:ASP:OD2	2.59	0.42
1:D:161:THR:HG23	1:D:161:THR:O	2.19	0.42
1:D:175:ASP:O	1:D:177:GLU:N	2.52	0.42
1:A:40:THR:HG22	1:A:78:THR:HG22	2.00	0.42
1:A:45:GLU:CD	1:A:74:HIS:CD2	2.98	0.42
1:A:68:VAL:HG22	1:A:309:MET:SD	2.59	0.42
1:B:43:ARG:HG2	1:B:44:SER:N	2.34	0.42
1:B:43:ARG:HG2	1:B:270:ARG:NH2	2.34	0.42
1:B:238:LEU:HA	1:B:241:ARG:HE	1.84	0.42
1:C:29:GLY:CA	1:C:34:LYS:HB3	2.49	0.42
1:D:23:ASN:O	1:D:27:SER:HB3	2.19	0.42
1:D:92:ARG:N	1:D:206:GLU:O	2.44	0.42
1:B:231:TRP:CE2	1:B:232:GLN:HG2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:LEU:O	1:B:264:PRO:C	2.61	0.42
1:B:287:ASP:CB	1:B:288:PRO:HD2	2.47	0.42
1:C:10:ALA:HB2	1:D:313:GLU:CB	2.49	0.42
1:D:135:ASP:HB3	1:D:187:VAL:HG21	2.00	0.42
1:C:40:THR:CG2	1:C:78:THR:HG22	2.46	0.42
1:D:106:PHE:CD2	1:D:188:TRP:CZ2	3.08	0.42
1:D:160:TRP:CD1	1:D:162:PRO:HD3	2.54	0.42
1:A:85:MET:HG2	3:A:353:HOH:O	2.20	0.42
1:A:101:PRO:O	1:A:103:PRO:N	2.53	0.42
1:B:131:TYR:CD1	1:B:190:TYR:HA	2.55	0.42
1:A:274:ILE:HD12	1:A:332:PHE:HZ	1.85	0.42
1:D:108:ILE:HB	1:D:159:LYS:HZ2	1.84	0.42
1:A:9:ARG:HD2	1:B:60:TYR:CE2	2.55	0.42
1:A:173:ARG:NH2	1:A:226:GLU:HG3	2.33	0.42
1:A:287:ASP:O	1:A:288:PRO:C	2.63	0.42
1:B:167:MET:HB2	1:B:184:ASP:HB3	2.01	0.42
1:B:239:ILE:HG13	1:B:240:TYR:N	2.35	0.42
1:C:314:ASN:C	1:C:315:ARG:HG2	2.41	0.42
1:D:108:ILE:O	1:D:109:ASN:HB2	2.20	0.42
1:D:228:ASN:O	1:D:231:TRP:CD1	2.73	0.42
1:D:318:ILE:C	1:D:319:ILE:O	2.62	0.42
1:A:97:ASP:O	1:A:99:ARG:N	2.53	0.42
1:A:103:PRO:HG2	1:A:104:TYR:CD2	2.55	0.42
1:A:192:PHE:CD2	1:A:238:LEU:HD21	2.55	0.42
1:A:220:PRO:O	1:A:221:THR:C	2.62	0.42
1:A:225:TYR:O	1:A:228:ASN:HB3	2.20	0.42
1:B:9:ARG:HH11	1:B:9:ARG:CG	2.31	0.42
1:B:61:PRO:HG3	1:B:312:MET:O	2.19	0.42
1:B:284:HIS:HB2	1:B:287:ASP:OD2	2.19	0.42
1:B:298:ASP:O	1:B:299:PRO:C	2.62	0.42
1:B:298:ASP:O	1:B:301:ASP:N	2.41	0.42
1:B:83:PRO:C	1:B:85:MET:H	2.28	0.42
1:B:105:THR:HG23	1:B:105:THR:O	2.20	0.42
1:B:311:TYR:OH	1:B:330:ILE:HG23	2.19	0.42
1:C:199:SER:HA	1:C:203:CYS:CB	2.49	0.42
1:C:231:TRP:CD1	1:C:232:GLN:HG3	2.54	0.42
1:C:248:ARG:HB3	1:C:248:ARG:HH11	1.83	0.42
1:C:315:ARG:HB3	1:D:8:TYR:CD2	2.53	0.42
1:A:132:ARG:HE	1:A:134:LEU:CD2	2.33	0.41
1:B:146:SER:HB3	1:D:12:VAL:HG13	2.02	0.41
1:B:258:PHE:O	1:B:258:PHE:CD1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:TYR:CG	1:C:297:TYR:N	2.87	0.41
1:C:324:GLN:HA	1:C:324:GLN:HE21	1.85	0.41
1:A:56:PHE:CD2	1:A:56:PHE:C	2.98	0.41
1:A:211:PRO:CG	1:A:216:LEU:HD13	2.50	0.41
1:B:82:LEU:HD12	1:B:85:MET:SD	2.60	0.41
1:D:101:PRO:O	1:D:102:ASP:C	2.63	0.41
1:A:119:TYR:HE2	1:A:120:ASN:HD21	1.64	0.41
1:B:119:TYR:CD1	1:B:119:TYR:N	2.87	0.41
1:C:37:ILE:CG1	1:C:81:VAL:HB	2.50	0.41
1:C:87:ASP:HB2	1:C:248:ARG:HH12	1.85	0.41
1:C:234:ASP:OD1	1:C:241:ARG:HD2	2.20	0.41
1:C:324:GLN:HA	1:C:324:GLN:NE2	2.34	0.41
1:A:20:LYS:O	1:A:23:ASN:HB2	2.21	0.41
1:A:43:ARG:CA	1:A:74:HIS:HB3	2.50	0.41
1:B:136:VAL:HB	1:B:162:PRO:HG2	2.02	0.41
1:B:195:PRO:HA	1:B:196:PRO:HD3	1.92	0.41
1:B:248:ARG:HH12	1:B:329:ASN:CG	2.29	0.41
1:B:280:GLU:O	1:B:281:ALA:C	2.64	0.41
1:C:48:SER:CB	1:C:50:ASN:HD21	2.33	0.41
1:A:97:ASP:C	1:A:99:ARG:N	2.78	0.41
1:A:308:GLU:OE2	1:B:15:LYS:CD	2.68	0.41
1:B:47:TRP:CD1	1:B:58:PRO:HB3	2.55	0.41
1:B:148:THR:HG22	1:B:160:TRP:HZ3	1.85	0.41
1:C:39:ILE:C	1:C:39:ILE:CD1	2.89	0.41
1:C:64:SER:O	1:C:65:VAL:C	2.63	0.41
1:D:75:MET:HB3	1:D:299:PRO:CG	2.50	0.41
1:A:198:VAL:HG13	1:A:202:ARG:CG	2.44	0.41
1:D:129:LEU:HB3	1:D:131:TYR:CE2	2.56	0.41
1:B:106:PHE:C	1:B:107:ARG:HG3	2.45	0.41
1:B:239:ILE:HG23	3:B:364:HOH:O	2.20	0.41
1:C:7:ILE:HG22	1:C:8:TYR:N	2.36	0.41
1:C:99:ARG:O	1:C:100:TYR:HD2	2.03	0.41
1:C:225:TYR:HE1	1:C:236:PHE:CD1	2.39	0.41
1:A:99:ARG:O	1:A:100:TYR:HD2	2.02	0.41
1:A:101:PRO:O	1:A:103:PRO:HD3	2.21	0.41
1:A:151:ASP:O	1:A:154:LEU:HB3	2.20	0.41
1:A:173:ARG:NH1	1:A:226:GLU:OE1	2.47	0.41
1:C:240:TYR:CZ	1:D:308:GLU:HG3	2.56	0.41
1:D:152:GLU:HA	1:D:155:LYS:HE2	2.02	0.41
1:A:21:MET:HE2	1:A:21:MET:HB3	1.93	0.41
1:A:104:TYR:CB	1:A:165:ARG:HD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ALA:O	1:A:118:PRO:C	2.62	0.41
1:A:145:ALA:C	1:A:147:LEU:N	2.79	0.41
1:A:254:ASP:OD2	1:A:325:THR:OG1	2.36	0.41
1:B:39:ILE:HD13	1:B:39:ILE:C	2.45	0.41
1:B:202:ARG:NH2	1:B:250:LYS:HG2	2.36	0.41
1:B:303:MET:HE2	2:B:343:BR:BR	2.76	0.41
1:C:137:PRO:HB3	1:C:185:GLY:HA3	2.02	0.41
1:C:304:ARG:O	1:C:305:HIS:HB2	2.21	0.41
1:C:330:ILE:CG2	1:C:332:PHE:CE2	3.04	0.41
1:D:191:LEU:HD23	1:D:191:LEU:HA	1.79	0.41
1:A:199:SER:HA	1:A:203:CYS:SG	2.61	0.41
1:A:254:ASP:HB3	1:A:256:VAL:CG2	2.51	0.41
1:B:84:SER:O	1:B:202:ARG:NH1	2.54	0.41
1:C:211:PRO:HD3	1:C:223:TRP:CE3	2.55	0.41
1:C:221:THR:CG2	1:C:226:GLU:HB3	2.51	0.41
1:D:40:THR:HA	1:D:78:THR:HA	2.03	0.41
1:D:184:ASP:OD1	1:D:186:TYR:CD1	2.74	0.41
1:B:269:PHE:HA	1:B:270:ARG:NH2	2.36	0.40
1:B:281:ALA:HA	2:B:343:BR:BR	2.77	0.40
1:C:220:PRO:O	1:C:225:TYR:N	2.50	0.40
1:D:165:ARG:O	1:D:166:SER:C	2.64	0.40
1:D:173:ARG:HG2	1:D:190:TYR:CD2	2.56	0.40
1:A:8:TYR:HD1	1:B:313:GLU:OE1	2.04	0.40
1:A:71:MET:HE3	1:A:273:SER:HB3	2.03	0.40
1:A:100:TYR:HB3	1:A:101:PRO:CD	2.51	0.40
1:C:10:ALA:CB	1:D:313:GLU:HB2	2.51	0.40
1:C:21:MET:HE3	1:C:212:TRP:CZ3	2.56	0.40
1:D:23:ASN:ND2	2:D:337:BR:BR	3.07	0.40
1:D:100:TYR:HB3	1:D:101:PRO:HD2	2.01	0.40
1:A:7:ILE:N	1:A:7:ILE:CD1	2.83	0.40
1:A:87:ASP:OD2	1:A:202:ARG:NE	2.55	0.40
1:A:118:PRO:C	1:A:120:ASN:H	2.29	0.40
1:A:296:TYR:CD1	1:A:296:TYR:C	2.99	0.40
1:B:21:MET:CE	1:B:245:ASN:N	2.85	0.40
1:B:107:ARG:NH1	1:B:159:LYS:HZ1	2.19	0.40
1:B:142:CYS:O	1:B:143:SER:HB3	2.21	0.40
1:B:312:MET:HE2	1:B:312:MET:HB3	1.97	0.40
1:C:8:TYR:CG	1:D:315:ARG:HD2	2.57	0.40
1:C:274:ILE:HG21	1:C:310:ILE:HD11	2.02	0.40
1:D:41:PHE:CE2	1:D:77:GLY:HA3	2.57	0.40
1:D:192:PHE:HD1	1:D:193:GLU:O	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:LEU:HD21	1:D:225:TYR:CZ	2.57	0.40
1:A:71:MET:CE	1:A:312:MET:HE2	2.32	0.40
1:A:309:MET:H	1:B:15:LYS:HE3	1.87	0.40
1:B:334:PHE:CD2	1:B:334:PHE:N	2.89	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	326/334 (98%)	279 (86%)	30 (9%)	17 (5%)	1	5
1	B	326/334 (98%)	276 (85%)	37 (11%)	13 (4%)	2	9
1	C	326/334 (98%)	281 (86%)	35 (11%)	10 (3%)	3	14
1	D	326/334 (98%)	271 (83%)	42 (13%)	13 (4%)	2	9
All	All	1304/1336 (98%)	1107 (85%)	144 (11%)	53 (4%)	2	9

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	SER
1	A	175	ASP
1	A	322	MET
1	B	43	ARG
1	B	138	ASP
1	B	149	ASP
1	B	264	PRO
1	B	266	ASN
1	B	322	MET
1	C	175	ASP
1	A	97	ASP

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Mol	Chain	Res	Type
1	A	98	THR
1	A	150	LYS
1	A	158	GLY
1	B	147	LEU
1	B	265	GLY
1	C	261	ALA
1	C	264	PRO
1	D	165	ARG
1	D	167	MET
1	D	184	ASP
1	D	253	LEU
1	D	257	TYR
1	A	43	ARG
1	B	44	SER
1	B	50	ASN
1	D	176	ALA
1	A	102	ASP
1	A	119	TYR
1	A	184	ASP
1	A	256	VAL
1	B	316	PRO
1	C	214	GLU
1	C	233	GLN
1	D	32	PRO
1	D	285	PRO
1	A	101	PRO
1	A	182	PRO
1	A	321	ALA
1	B	47	TRP
1	C	150	LYS
1	C	283	ALA
1	D	139	THR
1	D	175	ASP
1	D	259	PRO
1	A	264	PRO
1	C	232	GLN
1	C	299	PRO
1	B	285	PRO
1	C	198	VAL
1	D	182	PRO
1	A	220	PRO
1	D	219	ASP

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	289/295 (98%)	270 (93%)	19 (7%)	15	43
1	B	289/295 (98%)	276 (96%)	13 (4%)	24	58
1	C	289/295 (98%)	265 (92%)	24 (8%)	10	32
1	D	289/295 (98%)	278 (96%)	11 (4%)	29	64
All	All	1156/1180 (98%)	1089 (94%)	67 (6%)	18	49

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	8	TYR
1	A	15	LYS
1	A	49	SER
1	A	50	ASN
1	A	108	ILE
1	A	110	ASP
1	A	137	PRO
1	A	144	ILE
1	A	175	ASP
1	A	179	THR
1	A	264	PRO
1	A	266	ASN
1	A	267	LYS
1	A	279	LEU
1	A	291	LYS
1	A	315	ARG
1	A	319	ILE
1	A	322	MET
1	B	21	MET
1	B	39	ILE
1	B	66	LEU
1	B	91	PRO
1	B	136	VAL

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Mol	Chain	Res	Type
1	B	168	THR
1	B	187	VAL
1	B	228	ASN
1	B	233	GLN
1	B	264	PRO
1	B	285	PRO
1	B	319	ILE
1	B	334	PHE
1	C	36	THR
1	C	37	ILE
1	C	39	ILE
1	C	50	ASN
1	C	54	VAL
1	C	62	THR
1	C	66	LEU
1	C	81	VAL
1	C	85	MET
1	C	108	ILE
1	C	120	ASN
1	C	141	MET
1	C	167	MET
1	C	168	THR
1	C	221	THR
1	C	233	GLN
1	C	250	LYS
1	C	264	PRO
1	C	291	LYS
1	C	300	GLU
1	C	305	HIS
1	C	311	TYR
1	C	319	ILE
1	C	320	MET
1	D	11	ILE
1	D	12	VAL
1	D	34	LYS
1	D	35	ASN
1	D	39	ILE
1	D	50	ASN
1	D	144	ILE
1	D	165	ARG
1	D	189	GLU
1	D	226	GLU

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Mol	Chain	Res	Type
1	D	304	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	26	ASN
1	A	50	ASN
1	A	109	ASN
1	A	120	ASN
1	A	232	GLN
1	A	233	GLN
1	A	266	ASN
1	A	271	GLN
1	A	324	GLN
1	A	329	ASN
1	B	120	ASN
1	B	201	ASN
1	B	289	ASN
1	B	305	HIS
1	B	324	GLN
1	B	329	ASN
1	C	23	ASN
1	C	50	ASN
1	C	52	ASN
1	C	120	ASN
1	C	232	GLN
1	C	266	ASN
1	C	271	GLN
1	C	286	ASN
1	C	324	GLN
1	C	329	ASN
1	D	35	ASN
1	D	50	ASN
1	D	228	ASN
1	D	232	GLN
1	D	245	ASN
1	D	284	HIS
1	D	305	HIS
1	D	324	GLN
1	D	329	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 40 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	328/334 (98%)	0.03	5 (1%) 72 64	16, 36, 79, 91	0
1	B	328/334 (98%)	0.31	10 (3%) 52 43	16, 56, 100, 110	0
1	C	328/334 (98%)	0.06	7 (2%) 63 54	16, 37, 84, 101	0
1	D	328/334 (98%)	0.21	9 (2%) 56 47	12, 48, 89, 103	0
All	All	1312/1336 (98%)	0.15	31 (2%) 59 50	12, 44, 91, 110	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	158	GLY	3.7
1	B	54	VAL	3.5
1	B	145	ALA	3.3
1	B	319	ILE	3.3
1	C	154	LEU	2.9
1	C	233	GLN	2.8
1	D	180	ILE	2.7
1	C	261	ALA	2.7
1	D	106	PHE	2.7
1	B	153	CYS	2.7
1	C	164	ALA	2.5
1	D	151	ASP	2.5
1	B	57	ALA	2.5
1	C	249	PHE	2.4
1	B	156	LEU	2.4
1	D	264	PRO	2.4
1	C	264	PRO	2.4
1	B	256	VAL	2.3
1	B	154	LEU	2.3
1	A	156	LEU	2.1
1	B	144	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	141	MET	2.1
1	D	161	THR	2.1
1	D	145	ALA	2.1
1	D	125	GLY	2.1
1	D	256	VAL	2.0
1	A	253	LEU	2.0
1	A	7	ILE	2.0
1	A	160	TRP	2.0
1	A	158	GLY	2.0
1	C	257	TYR	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(Å ²)	Q<0.9
2	BR	D	341	1/1	0.79	0.10	44,44,44,44	1
2	BR	B	343	1/1	0.87	0.08	76,76,76,76	1
2	BR	B	340	1/1	0.87	0.11	47,47,47,47	1
2	BR	C	343	1/1	0.88	0.09	75,75,75,75	1
2	BR	B	338	1/1	0.88	0.09	54,54,54,54	1
2	BR	B	341	1/1	0.89	0.11	40,40,40,40	1
2	BR	D	343	1/1	0.89	0.08	33,33,33,33	1
2	BR	C	337	1/1	0.90	0.14	25,25,25,25	1
2	BR	B	345	1/1	0.90	0.08	48,48,48,48	1
2	BR	A	342	1/1	0.93	0.10	40,40,40,40	1
2	BR	A	339	1/1	0.93	0.05	41,41,41,41	1
2	BR	A	338	1/1	0.94	0.08	27,27,27,27	1
2	BR	D	338	1/1	0.94	0.05	40,40,40,40	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BR	B	342	1/1	0.95	0.06	37,37,37,37	1
2	BR	C	340	1/1	0.95	0.11	46,46,46,46	1
2	BR	C	341	1/1	0.95	0.07	26,26,26,26	1
2	BR	B	337	1/1	0.95	0.05	63,63,63,63	1
2	BR	A	341	1/1	0.95	0.07	37,37,37,37	1
2	BR	D	339	1/1	0.95	0.04	25,25,25,25	1
2	BR	C	335	1/1	0.95	0.05	53,53,53,53	1
2	BR	C	336	1/1	0.95	0.09	29,29,29,29	1
2	BR	D	344	1/1	0.95	0.05	39,39,39,39	1
2	BR	B	339	1/1	0.96	0.04	24,24,24,24	1
2	BR	D	336	1/1	0.96	0.06	72,72,72,72	1
2	BR	A	336	1/1	0.96	0.07	28,28,28,28	1
2	BR	B	344	1/1	0.96	0.04	25,25,25,25	1
2	BR	D	340	1/1	0.96	0.07	29,29,29,29	1
2	BR	C	338	1/1	0.96	0.05	53,53,53,53	1
2	BR	A	343	1/1	0.96	0.05	31,31,31,31	1
2	BR	B	346	1/1	0.96	0.04	45,45,45,45	1
2	BR	A	337	1/1	0.97	0.06	32,32,32,32	1
2	BR	A	335	1/1	0.97	0.04	51,51,51,51	0
2	BR	D	335	1/1	0.97	0.05	36,36,36,36	1
2	BR	C	339	1/1	0.97	0.05	35,35,35,35	1
2	BR	B	336	1/1	0.97	0.04	29,29,29,29	1
2	BR	C	342	1/1	0.98	0.12	37,37,37,37	1
2	BR	D	342	1/1	0.98	0.04	32,32,32,32	1
2	BR	A	340	1/1	0.98	0.04	18,18,18,18	1
2	BR	D	337	1/1	0.98	0.05	28,28,28,28	1
2	BR	B	335	1/1	0.99	0.05	43,43,43,43	1

6.5 Other polymers [i](#)

There are no such residues in this entry.