



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 12:57 PM EDT

PDB ID : 2ATQ
Title : RB69 single-stranded DNA binding protein-DNA polymerase fusion
Authors : Sun, S.; Geng, L.; Shamoo, Y.
Deposited on : 2005-08-25
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

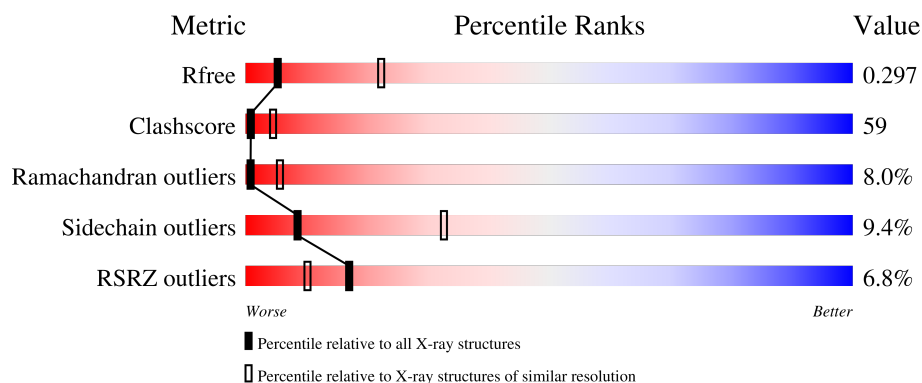
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	903	
2	B	234	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8636 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 DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	845	Total	C	N	O	S	0	0	0
			6922	4442	1148	1301	31			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	327	ALA	ASP	engineered mutation	UNP Q38087

- Molecule 2 is a protein called gp32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1685	1075	275	327	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	MET	-	initiating methionine	UNP Q7Y265

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

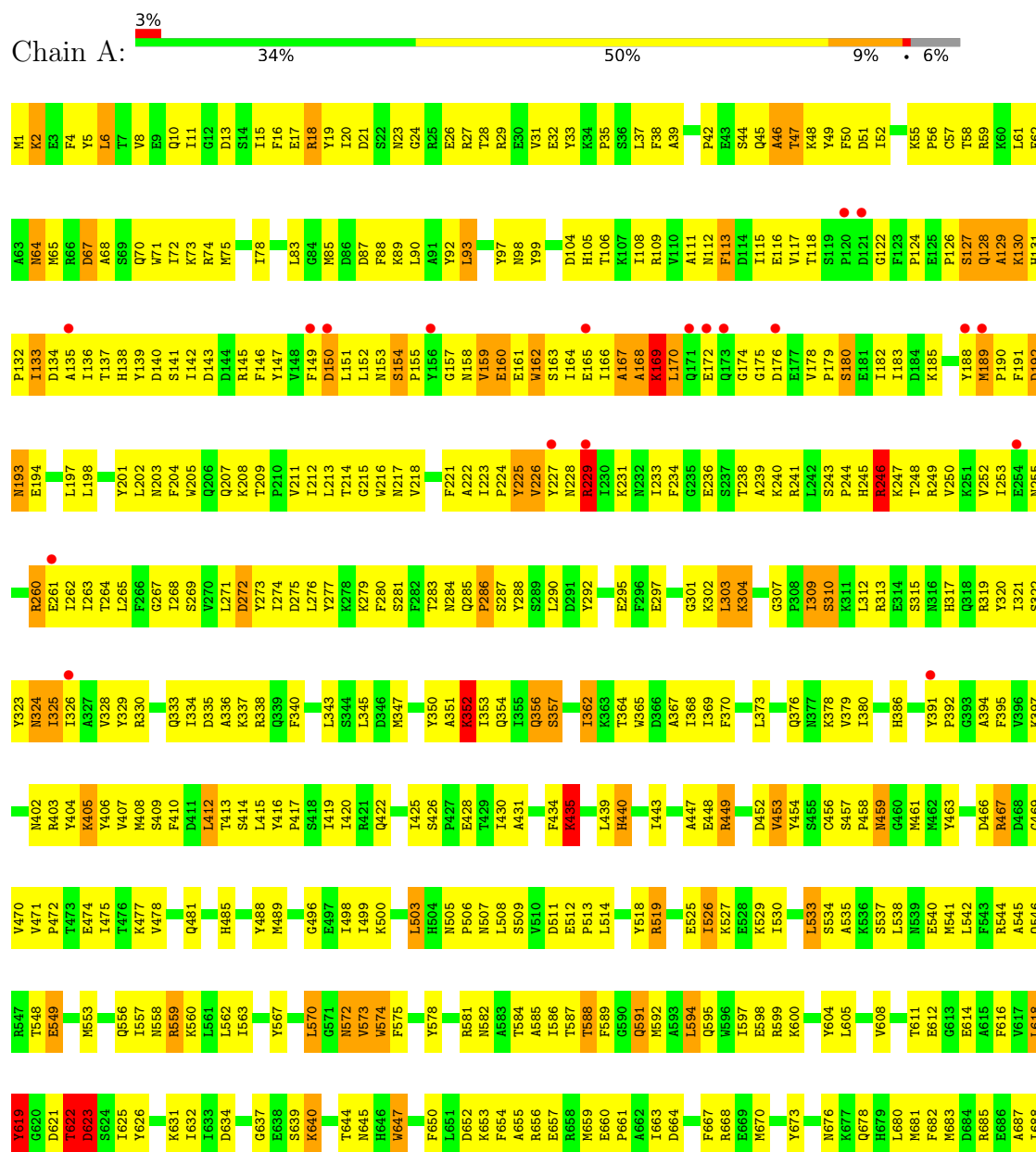
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

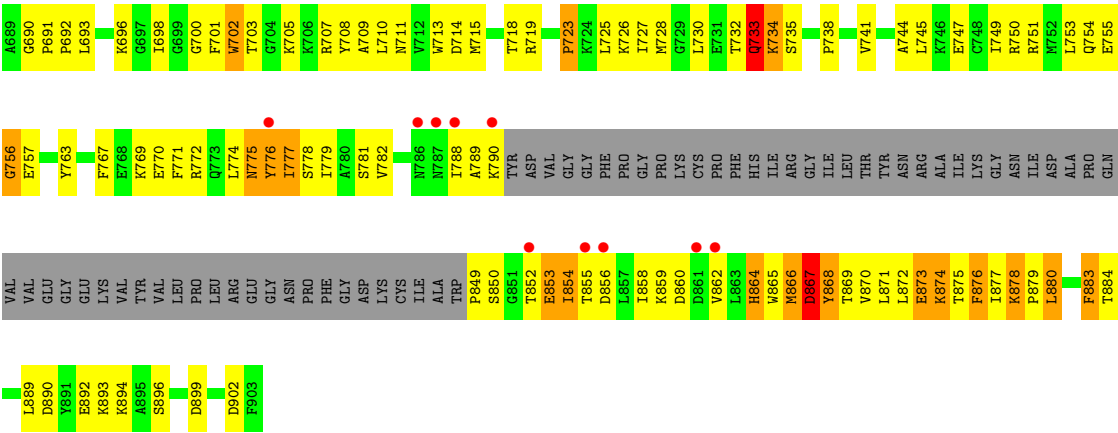
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

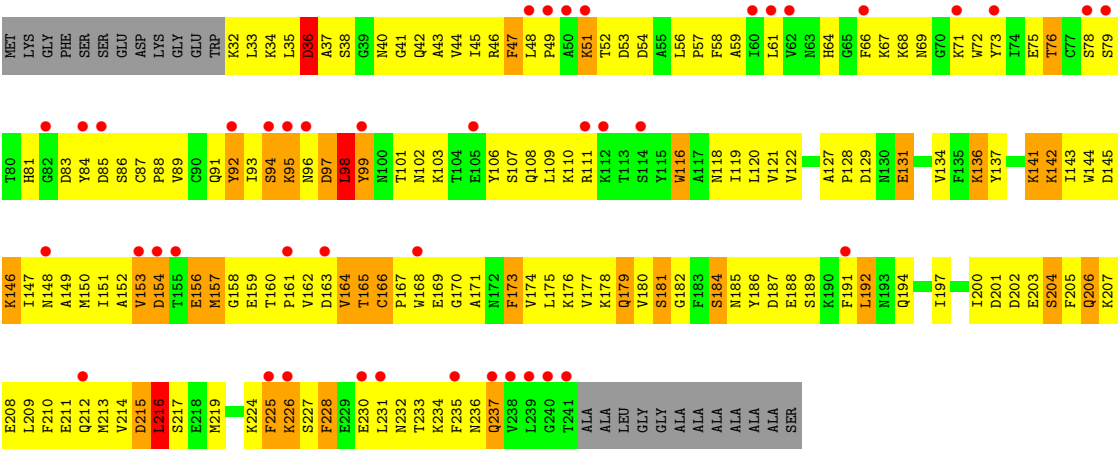
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





● Molecule 2: gp32



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	196.03Å 196.03Å 85.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.99 – 3.20 37.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.1 (37.99-3.20) 95.1 (37.99-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.284 , 0.345 0.254 , 0.297	Depositor DCC
R_{free} test set	1550 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	75.1	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8636	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: GDP, 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	0.45	0/7087	0.71	3/9568 (0.0%)
2	B	0.47	0/1723	0.83	2/2326 (0.1%)
All	All	0.45	0/8810	0.74	5/11894 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	849	PRO	CA-N-CD	-7.42	101.11	111.50
2	B	215	ASP	C-N-CA	7.30	139.95	121.70
2	B	216	LEU	N-CA-C	5.53	125.92	111.00
1	A	623	ASP	N-CA-C	5.25	125.17	111.00
1	A	756	GLY	N-CA-C	5.03	125.67	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6922	0	6818	757	0
2	B	1685	0	1643	250	0
3	A	28	0	12	1	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8636	0	8473	1007	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 59.

All (1007) 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:131:HIS:CE1	1:A:233:ILE:HD11	1.35	1.59
2:B:59:ALA:CB	2:B:216:LEU:HG	1.38	1.51
2:B:59:ALA:CB	2:B:216:LEU:CG	1.80	1.51
2:B:171:ALA:CB	2:B:191:PHE:CD1	1.94	1.49
1:A:146:PHE:CE1	1:A:185:LYS:HE3	1.49	1.47
1:A:169:LYS:HE2	1:A:319:ARG:NH2	1.22	1.46
2:B:171:ALA:CB	2:B:191:PHE:HD1	1.29	1.43
2:B:59:ALA:CA	2:B:216:LEU:HD21	1.47	1.41
1:A:146:PHE:HE1	1:A:185:LYS:CD	1.34	1.40
2:B:59:ALA:N	2:B:216:LEU:CD2	1.83	1.40
2:B:59:ALA:HB2	2:B:216:LEU:CG	0.95	1.40
2:B:67:LYS:HD2	2:B:72:TRP:NE1	1.36	1.39
2:B:67:LYS:CB	2:B:72:TRP:HD1	1.36	1.36
2:B:59:ALA:HB2	2:B:216:LEU:CD2	1.56	1.35
1:A:168:ALA:O	1:A:175:GLY:CA	1.74	1.33
1:A:146:PHE:CE1	1:A:185:LYS:CE	2.10	1.32
1:A:169:LYS:CE	1:A:319:ARG:HH21	1.43	1.31
2:B:59:ALA:CB	2:B:216:LEU:CD2	2.09	1.30
2:B:59:ALA:N	2:B:216:LEU:HD21	1.00	1.30
1:A:146:PHE:HE1	1:A:185:LYS:CE	1.44	1.29
2:B:158:GLY:O	2:B:159:GLU:HG2	1.31	1.27
2:B:163:ASP:O	2:B:164:VAL:HG23	1.38	1.22
1:A:852:THR:O	1:A:854:ILE:N	1.71	1.21
1:A:750:ARG:CG	1:A:754:GLN:HE21	1.52	1.20
1:A:154:SER:HB2	1:A:155:PRO:CD	1.72	1.20
2:B:67:LYS:CD	2:B:72:TRP:HE1	1.55	1.18
2:B:67:LYS:CD	2:B:72:TRP:NE1	2.04	1.18
1:A:131:HIS:CE1	1:A:233:ILE:CD1	2.26	1.17
2:B:94:SER:O	2:B:97:ASP:OD1	1.62	1.17
1:A:130:LYS:O	1:A:132:PRO:HD3	1.40	1.16
2:B:67:LYS:CB	2:B:72:TRP:CD1	2.27	1.16
1:A:280:PHE:CD1	1:A:343:LEU:HD23	1.80	1.16
1:A:128:GLN:HE22	1:A:130:LYS:CG	1.59	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:PHE:CE1	1:A:185:LYS:CD	2.26	1.15
1:A:169:LYS:O	1:A:170:LEU:HG	1.46	1.14
1:A:303:LEU:HD21	1:A:326:ILE:CD1	1.77	1.14
1:A:751:ARG:O	1:A:754:GLN:O	1.65	1.13
1:A:152:LEU:HD23	1:A:159:VAL:O	1.46	1.13
2:B:59:ALA:HB3	2:B:216:LEU:CD1	1.77	1.13
1:A:751:ARG:HH11	1:A:763:TYR:HB2	1.09	1.13
1:A:240:LYS:HB3	1:A:246:ARG:O	1.45	1.13
2:B:59:ALA:CB	2:B:216:LEU:CD1	2.26	1.13
2:B:59:ALA:CB	2:B:216:LEU:HD21	1.76	1.12
1:A:128:GLN:HE22	1:A:130:LYS:HG2	1.01	1.12
2:B:171:ALA:HB3	2:B:191:PHE:CD1	1.68	1.12
1:A:18:ARG:HH22	1:A:209:THR:HG22	1.08	1.11
1:A:867:ASP:CG	1:A:867:ASP:O	1.86	1.11
2:B:171:ALA:HB1	2:B:191:PHE:HD1	1.12	1.10
1:A:159:VAL:CG1	1:A:160:GLU:H	1.62	1.10
1:A:152:LEU:HD11	1:A:161:GLU:HB2	1.19	1.10
1:A:751:ARG:NH1	1:A:763:TYR:HB2	1.67	1.10
1:A:18:ARG:NH2	1:A:209:THR:HG22	1.65	1.10
2:B:59:ALA:HB3	2:B:216:LEU:HD11	1.12	1.09
1:A:159:VAL:HG12	1:A:160:GLU:N	1.67	1.09
1:A:168:ALA:O	1:A:175:GLY:HA2	1.31	1.09
2:B:59:ALA:CA	2:B:216:LEU:CD2	2.22	1.08
2:B:49:PRO:HG3	2:B:166:CYS:HA	1.32	1.08
2:B:67:LYS:HB3	2:B:72:TRP:HD1	1.08	1.08
1:A:514:LEU:H	1:A:541:MET:HE2	1.17	1.08
1:A:154:SER:HB2	1:A:155:PRO:HD2	1.30	1.07
1:A:280:PHE:CE1	1:A:343:LEU:HD23	1.88	1.07
1:A:873:GLU:HG2	1:A:877:ILE:HD12	1.25	1.07
1:A:168:ALA:O	1:A:175:GLY:HA3	1.56	1.06
1:A:146:PHE:CZ	1:A:185:LYS:HE3	1.92	1.05
1:A:152:LEU:HD11	1:A:161:GLU:CB	1.84	1.05
1:A:178:VAL:HG13	1:A:326:ILE:HG23	1.36	1.04
1:A:779:ILE:CG2	1:A:871:LEU:HD21	1.87	1.04
1:A:853:GLU:O	1:A:854:ILE:HB	1.52	1.04
1:A:303:LEU:HD21	1:A:326:ILE:HD11	1.36	1.03
2:B:71:LYS:HD2	2:B:234:LYS:HD3	1.38	1.03
2:B:67:LYS:CD	2:B:72:TRP:CD1	2.41	1.03
1:A:75:MET:HA	1:A:78:ILE:HD12	1.37	1.02
1:A:214:THR:HG22	1:A:271:LEU:O	1.60	1.02
2:B:165:THR:HG22	2:B:165:THR:O	1.57	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LYS:HD3	1:A:619:TYR:HA	1.36	1.02
1:A:159:VAL:HG12	1:A:160:GLU:H	0.88	1.02
2:B:67:LYS:HB2	2:B:72:TRP:CD1	1.94	1.02
1:A:214:THR:CG2	1:A:271:LEU:O	2.09	1.01
1:A:779:ILE:HG22	1:A:871:LEU:HD21	1.38	1.01
2:B:71:LYS:HE3	2:B:233:THR:O	1.61	1.01
2:B:163:ASP:O	2:B:164:VAL:CG2	2.09	1.00
1:A:775:ASN:ND2	1:A:776:TYR:H	1.59	1.00
1:A:214:THR:CG2	1:A:271:LEU:HB2	1.91	1.00
1:A:280:PHE:CD1	1:A:343:LEU:CD2	2.44	1.00
1:A:153:ASN:HB2	1:A:158:ASN:ND2	1.76	0.99
1:A:213:LEU:HD23	1:A:223:ILE:HD11	1.45	0.99
2:B:71:LYS:HD2	2:B:234:LYS:HA	1.45	0.99
2:B:171:ALA:HB2	2:B:191:PHE:CD1	1.95	0.99
1:A:146:PHE:HE1	1:A:185:LYS:HD2	1.27	0.98
2:B:71:LYS:CD	2:B:234:LYS:HD3	1.94	0.98
2:B:67:LYS:HB2	2:B:72:TRP:HD1	1.26	0.96
1:A:750:ARG:HG2	1:A:754:GLN:HE21	1.25	0.96
2:B:164:VAL:HG11	2:B:171:ALA:H	1.31	0.96
1:A:153:ASN:CB	1:A:158:ASN:ND2	2.28	0.96
1:A:750:ARG:HG3	1:A:754:GLN:HE21	1.30	0.95
2:B:59:ALA:H	2:B:216:LEU:HD21	1.19	0.95
2:B:59:ALA:CB	2:B:216:LEU:HD11	1.94	0.95
2:B:66:PHE:CD2	2:B:109:LEU:HG	2.00	0.95
1:A:867:ASP:O	1:A:867:ASP:OD2	1.85	0.94
1:A:126:PRO:O	1:A:127:SER:OG	1.84	0.94
1:A:128:GLN:NE2	1:A:130:LYS:CG	2.29	0.94
1:A:868:TYR:HD1	1:A:868:TYR:H	1.08	0.94
1:A:530:ILE:O	1:A:533:LEU:HB2	1.67	0.94
1:A:146:PHE:CE1	1:A:185:LYS:HD2	1.99	0.93
1:A:6:LEU:HB2	1:A:18:ARG:O	1.67	0.93
1:A:13:ASP:OD1	1:A:64:ASN:HB2	1.69	0.93
1:A:64:ASN:ND2	1:A:67:ASP:HB2	1.84	0.93
2:B:58:PHE:C	2:B:216:LEU:CD2	2.37	0.93
2:B:71:LYS:CD	2:B:234:LYS:HA	1.98	0.93
2:B:67:LYS:HB3	2:B:72:TRP:CD1	1.95	0.93
1:A:128:GLN:NE2	1:A:130:LYS:HG2	1.84	0.93
2:B:164:VAL:CG1	2:B:171:ALA:H	1.82	0.91
1:A:122:GLY:HA2	1:A:310:SER:HB2	1.53	0.91
1:A:245:HIS:O	1:A:247:LYS:N	2.03	0.91
1:A:130:LYS:O	1:A:132:PRO:CD	2.18	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:VAL:HA	1:A:229:ARG:HE	1.34	0.91
1:A:154:SER:CB	1:A:155:PRO:CD	2.48	0.90
1:A:356:GLN:H	1:A:356:GLN:HE21	1.14	0.90
1:A:854:ILE:HD11	1:A:859:LYS:HD3	1.51	0.90
1:A:150:ASP:H	1:A:190:PRO:HG3	1.37	0.90
1:A:154:SER:CB	1:A:155:PRO:HD2	2.01	0.89
1:A:394:ALA:HB1	1:A:622:THR:HG23	1.54	0.89
1:A:169:LYS:HE3	1:A:172:GLU:OE1	1.73	0.89
1:A:750:ARG:CG	1:A:754:GLN:NE2	2.36	0.88
1:A:152:LEU:CD2	1:A:159:VAL:O	2.21	0.88
1:A:18:ARG:NH2	1:A:209:THR:CG2	2.36	0.88
1:A:779:ILE:CG2	1:A:871:LEU:CD2	2.50	0.88
2:B:98:LEU:HD23	2:B:98:LEU:H	1.39	0.88
1:A:223:ILE:HA	1:A:226:VAL:HG12	1.54	0.88
1:A:169:LYS:HB2	1:A:175:GLY:CA	2.03	0.88
1:A:8:VAL:HG11	1:A:93:LEU:HD11	1.54	0.87
1:A:131:HIS:NE2	1:A:233:ILE:HD11	1.89	0.87
1:A:169:LYS:CE	1:A:319:ARG:NH2	2.16	0.87
2:B:49:PRO:HA	2:B:57:PRO:HB3	1.55	0.87
1:A:533:LEU:HB3	1:A:538:LEU:HD11	1.57	0.87
1:A:618:LEU:O	1:A:619:TYR:HB3	1.72	0.87
1:A:83:LEU:HD12	1:A:83:LEU:H	1.36	0.86
1:A:152:LEU:HD11	1:A:161:GLU:CG	2.05	0.86
1:A:159:VAL:HG12	1:A:160:GLU:HG3	1.55	0.86
2:B:88:PRO:HB2	2:B:231:LEU:HD22	1.56	0.86
1:A:163:SER:HB2	1:A:166:ILE:HB	1.57	0.86
1:A:214:THR:HG21	1:A:271:LEU:HB2	1.58	0.86
1:A:351:ALA:O	1:A:352:LYS:HB2	1.74	0.85
1:A:542:LEU:HG	1:A:546:GLN:HE21	1.39	0.85
1:A:754:GLN:O	1:A:755:GLU:HG2	1.77	0.85
2:B:71:LYS:CG	2:B:234:LYS:HA	2.06	0.85
1:A:865:TRP:O	1:A:866:MET:O	1.94	0.85
1:A:146:PHE:CZ	1:A:185:LYS:CE	2.56	0.85
1:A:618:LEU:O	1:A:619:TYR:CB	2.24	0.85
1:A:117:VAL:HG11	1:A:124:PRO:HG3	1.57	0.84
1:A:386:HIS:HB2	1:A:573:VAL:HG12	1.58	0.84
2:B:162:VAL:O	2:B:163:ASP:OD1	1.95	0.84
2:B:83:ASP:OD2	2:B:86:SER:HB3	1.75	0.84
2:B:158:GLY:O	2:B:159:GLU:CG	2.24	0.84
1:A:772:ARG:HA	1:A:868:TYR:CD2	2.12	0.83
2:B:67:LYS:HD2	2:B:72:TRP:HE1	0.71	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:SER:HB2	1:A:155:PRO:HD3	1.60	0.83
1:A:245:HIS:C	1:A:247:LYS:H	1.75	0.83
1:A:17:GLU:HG2	1:A:18:ARG:H	1.41	0.83
1:A:240:LYS:CB	1:A:246:ARG:O	2.26	0.83
1:A:394:ALA:CB	1:A:622:THR:HG23	2.08	0.83
2:B:164:VAL:HG13	2:B:170:GLY:CA	2.08	0.83
1:A:152:LEU:CD1	1:A:161:GLU:HB2	2.08	0.83
1:A:873:GLU:CG	1:A:877:ILE:HD12	2.06	0.82
1:A:64:ASN:HD22	1:A:64:ASN:H	1.26	0.82
2:B:88:PRO:HB2	2:B:231:LEU:CD2	2.09	0.82
2:B:216:LEU:O	2:B:219:MET:HG2	1.80	0.82
1:A:779:ILE:HG21	1:A:871:LEU:CD2	2.10	0.81
2:B:67:LYS:HD3	2:B:72:TRP:CD1	2.14	0.81
2:B:225:PHE:O	2:B:226:LYS:HG3	1.79	0.81
1:A:146:PHE:CD1	1:A:185:LYS:HG3	2.16	0.81
1:A:873:GLU:HA	1:A:877:ILE:HB	1.63	0.81
1:A:28:THR:HG22	1:A:28:THR:O	1.81	0.80
1:A:286:PRO:HB2	1:A:735:SER:HB2	1.62	0.80
2:B:68:LYS:O	2:B:69:ASN:HB3	1.80	0.80
1:A:133:ILE:HG21	1:A:136:ILE:HD11	1.64	0.80
2:B:67:LYS:HD2	2:B:72:TRP:CD1	2.09	0.80
1:A:241:ARG:HA	1:A:246:ARG:HH21	1.45	0.80
1:A:757:GLU:HB2	1:A:889:LEU:HD22	1.64	0.79
1:A:867:ASP:OD2	1:A:867:ASP:C	2.19	0.79
1:A:150:ASP:H	1:A:190:PRO:CG	1.95	0.79
1:A:152:LEU:O	1:A:158:ASN:HA	1.83	0.79
1:A:104:ASP:OD1	1:A:106:THR:HB	1.82	0.79
1:A:169:LYS:HB2	1:A:175:GLY:HA3	1.64	0.79
2:B:118:ASN:HD21	2:B:214:VAL:H	1.29	0.79
1:A:83:LEU:HD12	1:A:83:LEU:N	1.95	0.79
1:A:868:TYR:HD1	1:A:868:TYR:N	1.80	0.79
1:A:876:PHE:C	1:A:879:PRO:HD2	2.03	0.79
2:B:118:ASN:HD21	2:B:214:VAL:N	1.81	0.79
2:B:67:LYS:HD3	2:B:72:TRP:NE1	1.98	0.78
2:B:171:ALA:HB2	2:B:191:PHE:HD1	1.35	0.78
1:A:572:ASN:HD22	1:A:573:VAL:N	1.81	0.78
1:A:131:HIS:NE2	1:A:233:ILE:CD1	2.46	0.77
1:A:422:GLN:NE2	1:A:680:LEU:H	1.80	0.77
1:A:461:MET:CE	1:A:581:ARG:HB3	2.14	0.77
1:A:639:SER:O	1:A:640:LYS:HG3	1.83	0.77
1:A:214:THR:HG22	1:A:271:LEU:C	2.05	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:LYS:HE2	2:B:136:LYS:NZ	2.00	0.77
1:A:153:ASN:HB3	1:A:158:ASN:ND2	2.00	0.77
2:B:49:PRO:HG3	2:B:165:THR:O	1.85	0.77
2:B:171:ALA:HB1	2:B:191:PHE:CD1	1.94	0.77
1:A:159:VAL:HG12	1:A:160:GLU:CG	2.15	0.76
1:A:285:GLN:HB3	1:A:286:PRO:HD2	1.65	0.76
1:A:572:ASN:HD22	1:A:572:ASN:C	1.88	0.76
1:A:873:GLU:HG2	1:A:877:ILE:CD1	2.10	0.76
1:A:356:GLN:H	1:A:356:GLN:NE2	1.83	0.76
1:A:725:LEU:HD22	1:A:753:LEU:HD12	1.66	0.76
1:A:744:ALA:HB3	1:A:876:PHE:CE1	2.20	0.76
1:A:64:ASN:HD22	1:A:64:ASN:N	1.83	0.76
1:A:178:VAL:HG21	1:A:322:SER:HB3	1.66	0.76
1:A:309:ILE:HD13	1:A:310:SER:H	1.51	0.75
1:A:779:ILE:HG22	1:A:871:LEU:CD2	2.11	0.75
1:A:542:LEU:HG	1:A:546:GLN:NE2	2.00	0.75
1:A:189:MET:N	1:A:190:PRO:CD	2.49	0.75
2:B:92:TYR:CE2	2:B:109:LEU:HD22	2.22	0.75
2:B:153:VAL:O	2:B:154:ASP:OD1	2.05	0.75
1:A:700:GLY:HA2	1:A:753:LEU:HD22	1.67	0.74
2:B:163:ASP:C	2:B:164:VAL:HG23	2.07	0.74
1:A:159:VAL:CG1	1:A:160:GLU:HG3	2.17	0.74
1:A:741:VAL:HG13	1:A:876:PHE:HD1	1.52	0.74
1:A:775:ASN:HD22	1:A:776:TYR:H	1.34	0.74
1:A:781:SER:O	1:A:782:VAL:CG2	2.36	0.74
1:A:534:SER:O	1:A:538:LEU:HD13	1.86	0.74
1:A:852:THR:O	1:A:853:GLU:C	2.25	0.74
2:B:174:VAL:CG2	2:B:192:LEU:HD21	2.17	0.74
1:A:744:ALA:HB3	1:A:876:PHE:HE1	1.50	0.74
2:B:165:THR:O	2:B:165:THR:CG2	2.31	0.74
1:A:741:VAL:O	1:A:745:LEU:HD12	1.86	0.74
1:A:74:ARG:HG2	1:A:78:ILE:HD11	1.69	0.73
1:A:572:ASN:ND2	1:A:574:TRP:H	1.87	0.73
2:B:49:PRO:CG	2:B:165:THR:O	2.36	0.73
1:A:751:ARG:HH11	1:A:763:TYR:CB	1.94	0.73
1:A:163:SER:CB	1:A:166:ILE:HB	2.19	0.73
2:B:95:LYS:HE3	2:B:95:LYS:HA	1.70	0.73
1:A:303:LEU:CD2	1:A:326:ILE:CD1	2.64	0.73
1:A:133:ILE:CG2	1:A:136:ILE:HD11	2.19	0.73
1:A:533:LEU:HB3	1:A:538:LEU:CD1	2.18	0.73
2:B:216:LEU:HD12	2:B:219:MET:HG3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:HG23	1:A:134:ASP:OD2	1.88	0.73
1:A:145:ARG:HA	1:A:185:LYS:HB2	1.70	0.73
1:A:750:ARG:HG2	1:A:754:GLN:NE2	2.00	0.73
1:A:772:ARG:O	1:A:868:TYR:CE2	2.41	0.73
1:A:409:SER:HB3	1:A:626:TYR:CD2	2.24	0.72
1:A:500:LYS:HA	1:A:503:LEU:HD23	1.70	0.72
1:A:146:PHE:CE1	1:A:185:LYS:CG	2.72	0.72
1:A:431:ALA:HB1	1:A:454:TYR:CE2	2.24	0.72
1:A:751:ARG:NE	1:A:755:GLU:OE2	2.21	0.72
1:A:169:LYS:O	1:A:170:LEU:CG	2.33	0.72
1:A:350:TYR:HE2	1:A:368:ILE:HD13	1.54	0.72
1:A:131:HIS:HE1	1:A:233:ILE:HD11	0.92	0.71
1:A:858:ILE:HD12	1:A:859:LYS:N	2.06	0.71
1:A:35:PRO:HG3	1:A:65:MET:HG2	1.73	0.71
1:A:260:ARG:H	1:A:260:ARG:HD3	1.55	0.71
1:A:474:GLU:OE2	1:A:477:LYS:HD3	1.90	0.71
2:B:136:LYS:HD2	2:B:136:LYS:O	1.90	0.71
2:B:151:ILE:HG22	2:B:162:VAL:O	1.90	0.71
2:B:143:ILE:O	2:B:146:LYS:HB2	1.91	0.71
2:B:176:LYS:HB2	2:B:188:GLU:HB3	1.72	0.71
1:A:214:THR:CB	1:A:271:LEU:O	2.39	0.70
2:B:142:LYS:HD3	2:B:187:ASP:HB3	1.73	0.70
1:A:146:PHE:HE1	1:A:185:LYS:CG	2.04	0.70
1:A:750:ARG:HG3	1:A:754:GLN:NE2	2.05	0.70
1:A:131:HIS:HE1	1:A:233:ILE:CD1	1.86	0.70
1:A:367:ALA:O	1:A:370:PHE:HB3	1.92	0.70
1:A:639:SER:O	1:A:640:LYS:CG	2.39	0.70
1:A:772:ARG:HA	1:A:868:TYR:HD2	1.55	0.70
1:A:223:ILE:HA	1:A:226:VAL:CG1	2.22	0.70
1:A:514:LEU:HD11	1:A:533:LEU:HD21	1.72	0.70
1:A:775:ASN:ND2	1:A:776:TYR:N	2.39	0.69
1:A:152:LEU:HD11	1:A:161:GLU:HG3	1.73	0.69
1:A:419:ILE:HG12	1:A:681:MET:HE3	1.74	0.69
1:A:425:ILE:HG23	1:A:463:TYR:CE2	2.27	0.69
1:A:781:SER:O	1:A:782:VAL:HG23	1.91	0.69
1:A:271:LEU:HD21	1:A:356:GLN:HA	1.74	0.69
1:A:416:TYR:O	1:A:420:ILE:HG13	1.93	0.69
1:A:386:HIS:HB2	1:A:573:VAL:CG1	2.23	0.69
1:A:747:GLU:O	1:A:751:ARG:HG3	1.93	0.69
1:A:241:ARG:HA	1:A:246:ARG:NH2	2.07	0.69
1:A:83:LEU:H	1:A:83:LEU:CD1	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASP:HB3	1:A:90:LEU:HD12	1.75	0.69
1:A:42:PRO:C	1:A:44:SER:H	1.97	0.68
1:A:655:ALA:O	1:A:660:GLU:HG3	1.94	0.68
1:A:655:ALA:HA	1:A:659:MET:HB2	1.74	0.68
1:A:146:PHE:CE1	1:A:185:LYS:HG3	2.28	0.68
1:A:284:ASN:HA	1:A:288:TYR:OH	1.93	0.68
2:B:59:ALA:HB1	2:B:216:LEU:HG	1.65	0.68
2:B:164:VAL:HG13	2:B:170:GLY:HA3	1.76	0.68
1:A:168:ALA:C	1:A:175:GLY:HA2	2.13	0.68
1:A:214:THR:HG22	1:A:271:LEU:HB2	1.75	0.68
1:A:317:HIS:HA	1:A:320:TYR:HB3	1.75	0.68
1:A:750:ARG:O	1:A:754:GLN:HG2	1.94	0.68
1:A:214:THR:HG22	1:A:271:LEU:CA	2.23	0.68
1:A:146:PHE:HZ	1:A:185:LYS:HZ2	1.41	0.67
2:B:75:GLU:O	2:B:76:THR:C	2.31	0.67
2:B:171:ALA:HB3	2:B:191:PHE:CG	2.26	0.67
1:A:329:TYR:O	1:A:333:GLN:HG3	1.95	0.67
1:A:152:LEU:CD1	1:A:161:GLU:HG3	2.24	0.67
1:A:85:MET:HA	1:A:380:ILE:HD11	1.77	0.67
1:A:605:LEU:HD11	1:A:632:ILE:HD11	1.75	0.67
2:B:118:ASN:ND2	2:B:213:MET:HA	2.10	0.67
1:A:505:ASN:N	1:A:506:PRO:HD3	2.11	0.66
1:A:116:GLU:HB2	1:A:135:ALA:H	1.59	0.66
1:A:202:LEU:HD13	1:A:241:ARG:HB3	1.78	0.66
1:A:498:ILE:HD13	1:A:527:LYS:HD3	1.78	0.66
1:A:508:LEU:H	1:A:508:LEU:HD12	1.59	0.66
1:A:10:GLN:HG2	1:A:10:GLN:O	1.95	0.66
1:A:113:PHE:HB3	1:A:138:HIS:HA	1.78	0.66
1:A:621:ASP:O	1:A:622:THR:C	2.33	0.66
1:A:62:PHE:CE2	1:A:68:ALA:HA	2.29	0.66
1:A:214:THR:HB	1:A:271:LEU:O	1.96	0.66
1:A:858:ILE:O	1:A:862:VAL:HG23	1.96	0.66
2:B:36:ASP:OD1	2:B:41:GLY:HA2	1.96	0.66
1:A:443:ILE:HD13	1:A:595:GLN:HB2	1.78	0.66
1:A:751:ARG:C	1:A:754:GLN:O	2.35	0.66
2:B:71:LYS:HD2	2:B:234:LYS:CA	2.24	0.66
1:A:397:LYS:CD	1:A:619:TYR:HA	2.18	0.65
1:A:397:LYS:HD3	1:A:619:TYR:CA	2.22	0.65
1:A:309:ILE:HD13	1:A:310:SER:N	2.11	0.65
1:A:213:LEU:HD23	1:A:223:ILE:CD1	2.24	0.65
1:A:8:VAL:HG11	1:A:93:LEU:CD1	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:HB	1:A:16:PHE:CE2	2.31	0.65
1:A:461:MET:HE2	1:A:581:ARG:HB3	1.79	0.65
1:A:133:ILE:CD1	1:A:198:LEU:HD13	2.27	0.65
1:A:878:LYS:HB3	1:A:879:PRO:HD3	1.79	0.65
1:A:878:LYS:HA	1:A:878:LYS:HE2	1.79	0.65
2:B:96:ASN:O	2:B:98:LEU:N	2.30	0.64
2:B:99:TYR:CE2	2:B:103:LYS:NZ	2.62	0.64
2:B:164:VAL:HG22	2:B:170:GLY:HA2	1.78	0.64
1:A:64:ASN:ND2	1:A:64:ASN:H	1.94	0.64
1:A:245:HIS:C	1:A:247:LYS:N	2.46	0.64
1:A:153:ASN:HB2	1:A:158:ASN:HD22	1.61	0.64
1:A:167:ALA:O	1:A:168:ALA:C	2.34	0.64
1:A:391:TYR:HE2	1:A:587:THR:HG21	1.61	0.64
1:A:874:LYS:HE2	1:A:874:LYS:HA	1.79	0.64
1:A:189:MET:H	1:A:190:PRO:HD3	1.62	0.64
1:A:572:ASN:O	1:A:578:TYR:HB2	1.97	0.64
1:A:788:ILE:HG12	1:A:850:SER:O	1.98	0.64
2:B:119:ILE:HD13	2:B:137:TYR:HB2	1.78	0.64
2:B:167:PRO:HA	2:B:197:ILE:HD12	1.78	0.64
1:A:225:TYR:O	1:A:229:ARG:HG2	1.98	0.64
1:A:152:LEU:HD21	1:A:161:GLU:N	2.13	0.64
2:B:177:VAL:HG22	2:B:185:ASN:OD1	1.97	0.64
1:A:260:ARG:CZ	1:A:262:ILE:HD11	2.27	0.64
1:A:4:PHE:HA	1:A:97:TYR:CE2	2.33	0.63
1:A:654:PHE:O	1:A:655:ALA:HB3	1.97	0.63
1:A:223:ILE:HB	1:A:224:PRO:HD3	1.79	0.63
1:A:280:PHE:CE1	1:A:343:LEU:CD2	2.71	0.63
1:A:872:LEU:C	1:A:874:LYS:H	2.02	0.63
2:B:59:ALA:HB2	2:B:216:LEU:HG	0.63	0.63
2:B:164:VAL:CG2	2:B:194:GLN:HE22	2.12	0.63
1:A:146:PHE:CZ	1:A:185:LYS:NZ	2.66	0.63
1:A:164:ILE:HG13	1:A:165:GLU:N	2.14	0.63
1:A:223:ILE:CA	1:A:226:VAL:HG12	2.28	0.63
1:A:262:ILE:N	1:A:262:ILE:HD12	2.14	0.63
1:A:621:ASP:C	1:A:622:THR:O	2.36	0.63
1:A:458:PRO:HG3	1:A:592:MET:SD	2.39	0.63
1:A:449:ARG:HH11	1:A:449:ARG:HG2	1.64	0.63
1:A:122:GLY:CA	1:A:310:SER:HB2	2.28	0.62
1:A:713:TRP:CZ3	1:A:723:PRO:HG3	2.35	0.62
2:B:32:LYS:HE2	2:B:136:LYS:HZ3	1.64	0.62
1:A:6:LEU:HG	1:A:211:VAL:HG11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:PHE:CD2	1:A:56:PRO:HA	2.34	0.62
1:A:191:PHE:N	1:A:197:LEU:HD11	2.15	0.62
1:A:449:ARG:HG2	1:A:449:ARG:NH1	2.14	0.62
2:B:149:ALA:HA	2:B:154:ASP:OD2	1.99	0.62
2:B:214:VAL:HG13	2:B:214:VAL:O	2.00	0.62
1:A:133:ILE:HD12	1:A:198:LEU:HD13	1.81	0.62
2:B:147:ILE:HD12	2:B:148:ASN:N	2.15	0.62
1:A:350:TYR:CE2	1:A:368:ILE:HD13	2.35	0.61
2:B:205:PHE:O	2:B:209:LEU:HB2	2.00	0.61
1:A:330:ARG:O	1:A:334:ILE:HG13	2.01	0.61
2:B:49:PRO:HB3	2:B:165:THR:HG22	1.82	0.61
1:A:397:LYS:O	1:A:619:TYR:HD1	1.83	0.61
1:A:868:TYR:HA	1:A:871:LEU:HB3	1.82	0.61
2:B:34:LYS:HE2	2:B:127:ALA:CB	2.30	0.61
1:A:303:LEU:HD11	1:A:323:TYR:HB2	1.81	0.61
1:A:728:MET:HG3	1:A:728:MET:O	1.99	0.61
2:B:33:LEU:HD23	2:B:33:LEU:H	1.64	0.61
1:A:514:LEU:N	1:A:541:MET:HE2	2.02	0.61
1:A:659:MET:O	1:A:663:ILE:HG13	2.00	0.61
2:B:178:LYS:H	2:B:186:TYR:CB	2.13	0.61
1:A:594:LEU:HD11	1:A:625:ILE:CG2	2.30	0.61
1:A:745:LEU:O	1:A:749:ILE:HG13	2.00	0.61
1:A:776:TYR:CZ	1:A:852:THR:HB	2.36	0.61
1:A:145:ARG:HD2	1:A:185:LYS:HA	1.83	0.60
1:A:373:LEU:HD22	1:A:378:LYS:HD3	1.83	0.60
1:A:604:TYR:O	1:A:608:VAL:HG12	2.01	0.60
1:A:713:TRP:O	1:A:719:ARG:HD3	2.01	0.60
1:A:105:HIS:HA	1:A:108:ILE:HD12	1.82	0.60
1:A:744:ALA:CB	1:A:876:PHE:CE1	2.84	0.60
1:A:64:ASN:ND2	1:A:64:ASN:N	2.50	0.60
2:B:71:LYS:HG3	2:B:234:LYS:HA	1.80	0.60
2:B:173:PHE:HD1	2:B:191:PHE:HB3	1.65	0.60
1:A:146:PHE:HZ	1:A:185:LYS:NZ	1.99	0.60
2:B:67:LYS:CG	2:B:72:TRP:CD1	2.83	0.60
1:A:6:LEU:CB	1:A:18:ARG:O	2.47	0.60
1:A:868:TYR:N	1:A:868:TYR:CD1	2.52	0.60
1:A:216:TRP:NE1	1:A:274:ILE:HD12	2.17	0.59
1:A:325:ILE:HA	1:A:328:VAL:HG12	1.84	0.59
1:A:854:ILE:HD11	1:A:859:LYS:CD	2.29	0.59
1:A:146:PHE:HD1	1:A:185:LYS:HG3	1.66	0.59
1:A:351:ALA:O	1:A:352:LYS:CB	2.47	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:VAL:HG13	1:A:876:PHE:CD1	2.34	0.59
2:B:128:PRO:O	2:B:131:GLU:HB2	2.02	0.59
1:A:226:VAL:CA	1:A:229:ARG:HE	2.12	0.59
1:A:488:TYR:CG	1:A:519:ARG:HG2	2.38	0.59
1:A:790:LYS:HD2	1:A:790:LYS:N	2.17	0.59
1:A:150:ASP:OD2	1:A:321:ILE:HG12	2.02	0.59
2:B:171:ALA:HB2	2:B:191:PHE:CE1	2.37	0.59
1:A:741:VAL:HG11	1:A:875:THR:O	2.01	0.59
1:A:133:ILE:CD1	1:A:198:LEU:CD1	2.81	0.59
1:A:245:HIS:C	1:A:246:ARG:HG2	2.23	0.59
1:A:443:ILE:HD13	1:A:595:GLN:CB	2.32	0.59
1:A:459:ASN:HB3	1:A:588:THR:HG21	1.84	0.59
2:B:156:GLU:O	2:B:158:GLY:N	2.36	0.59
1:A:273:TYR:OH	1:A:335:ASP:HA	2.02	0.59
2:B:186:TYR:CE2	2:B:188:GLU:HB2	2.38	0.59
1:A:216:TRP:CZ3	1:A:290:LEU:HD13	2.38	0.59
1:A:250:VAL:HG22	1:A:263:ILE:CD1	2.33	0.59
1:A:866:MET:O	1:A:867:ASP:CB	2.50	0.58
1:A:62:PHE:CD2	1:A:68:ALA:HA	2.38	0.58
1:A:448:GLU:O	1:A:449:ARG:C	2.42	0.58
1:A:128:GLN:NE2	1:A:130:LYS:HG3	2.18	0.58
1:A:883:PHE:N	1:A:883:PHE:CD2	2.69	0.58
1:A:202:LEU:CD1	1:A:241:ARG:HB3	2.34	0.58
1:A:133:ILE:O	1:A:133:ILE:HG22	2.03	0.58
1:A:506:PRO:HB2	1:A:535:ALA:HB2	1.85	0.58
2:B:164:VAL:HG22	2:B:194:GLN:HE22	1.67	0.58
1:A:176:ASP:OD2	1:A:302:LYS:HG3	2.04	0.57
1:A:621:ASP:O	1:A:622:THR:O	2.22	0.57
2:B:71:LYS:HD2	2:B:234:LYS:CD	2.24	0.57
1:A:260:ARG:HG3	1:A:260:ARG:HH11	1.69	0.57
1:A:109:ARG:CZ	1:A:142:ILE:HD12	2.34	0.57
1:A:162:TRP:CZ3	1:A:164:ILE:HG22	2.39	0.57
1:A:440:HIS:HA	1:A:443:ILE:HG13	1.85	0.57
2:B:78:SER:HB3	2:B:83:ASP:CB	2.34	0.57
1:A:74:ARG:O	1:A:78:ILE:HG13	2.05	0.57
1:A:362:ILE:HG22	1:A:575:PHE:HD1	1.69	0.57
1:A:212:ILE:HD11	1:A:345:LEU:HD21	1.85	0.57
1:A:216:TRP:CE3	1:A:290:LEU:HD13	2.39	0.57
1:A:39:ALA:HB2	1:A:71:TRP:HH2	1.69	0.57
1:A:214:THR:HG22	1:A:271:LEU:CB	2.34	0.57
2:B:164:VAL:CG1	2:B:171:ALA:N	2.61	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASN:CB	1:A:158:ASN:HD21	2.18	0.57
1:A:168:ALA:HB2	1:A:322:SER:OG	2.04	0.57
1:A:883:PHE:N	1:A:883:PHE:HD2	2.02	0.57
2:B:57:PRO:HG2	2:B:58:PHE:CD1	2.40	0.57
1:A:534:SER:O	1:A:538:LEU:CD1	2.53	0.57
1:A:109:ARG:NH1	1:A:142:ILE:HD12	2.18	0.56
1:A:425:ILE:HG23	1:A:463:TYR:CZ	2.40	0.56
2:B:164:VAL:HG13	2:B:171:ALA:H	1.68	0.56
1:A:191:PHE:H	1:A:197:LEU:HD11	1.69	0.56
2:B:175:LEU:HA	2:B:189:SER:HB3	1.86	0.56
1:A:395:PHE:HB2	1:A:591:GLN:HE21	1.69	0.56
1:A:422:GLN:HG2	1:A:676:ASN:ND2	2.20	0.56
1:A:508:LEU:HD12	1:A:508:LEU:N	2.20	0.56
1:A:738:PRO:HG2	1:A:741:VAL:CG2	2.36	0.56
1:A:309:ILE:O	1:A:310:SER:CB	2.52	0.56
1:A:365:TRP:O	1:A:369:ILE:HG13	2.06	0.56
2:B:97:ASP:O	2:B:99:TYR:N	2.38	0.56
1:A:730:LEU:HB3	1:A:883:PHE:CZ	2.40	0.56
1:A:777:ILE:O	1:A:779:ILE:N	2.39	0.56
1:A:28:THR:O	1:A:28:THR:CG2	2.52	0.56
2:B:34:LYS:HE2	2:B:127:ALA:HB3	1.87	0.56
1:A:364:THR:O	1:A:368:ILE:HG13	2.05	0.55
1:A:246:ARG:HE	1:A:246:ARG:CA	2.18	0.55
1:A:391:TYR:HB2	1:A:392:PRO:HD2	1.88	0.55
1:A:478:VAL:HG13	1:A:559:ARG:HD3	1.88	0.55
1:A:13:ASP:OD2	1:A:64:ASN:OD1	2.25	0.55
1:A:634:ASP:O	1:A:637:GLY:N	2.40	0.55
1:A:128:GLN:HE22	1:A:130:LYS:CB	2.20	0.55
2:B:174:VAL:HG21	2:B:192:LEU:HD21	1.87	0.55
1:A:21:ASP:OD1	1:A:23:ASN:N	2.40	0.55
1:A:326:ILE:HB	1:A:330:ARG:NH1	2.22	0.55
2:B:47:PHE:CD1	2:B:47:PHE:N	2.74	0.55
2:B:58:PHE:C	2:B:216:LEU:HD23	2.23	0.55
1:A:17:GLU:HG2	1:A:18:ARG:N	2.16	0.55
1:A:312:LEU:O	1:A:315:SER:HB3	2.06	0.55
1:A:529:LYS:O	1:A:533:LEU:HD23	2.06	0.55
1:A:52:ILE:CG2	1:A:470:VAL:HG21	2.37	0.55
1:A:228:ASN:O	1:A:231:LYS:HB3	2.07	0.55
1:A:754:GLN:O	1:A:755:GLU:CG	2.54	0.55
1:A:425:ILE:O	1:A:472:PRO:HD3	2.07	0.54
1:A:570:LEU:HD23	1:A:570:LEU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:LEU:O	1:A:608:VAL:HG13	2.07	0.54
1:A:708:TYR:CE1	1:A:728:MET:HG2	2.42	0.54
2:B:164:VAL:HG12	2:B:165:THR:N	2.23	0.54
2:B:225:PHE:O	2:B:226:LYS:CG	2.54	0.54
1:A:351:ALA:HB3	1:A:353:ILE:HG12	1.89	0.54
1:A:320:TYR:O	1:A:323:TYR:HB3	2.07	0.54
1:A:506:PRO:CB	1:A:535:ALA:HB2	2.37	0.54
1:A:779:ILE:CG2	1:A:871:LEU:CG	2.85	0.54
2:B:144:TRP:C	2:B:146:LYS:H	2.11	0.54
1:A:74:ARG:HG2	1:A:78:ILE:CD1	2.36	0.54
1:A:189:MET:H	1:A:190:PRO:CD	2.17	0.54
1:A:286:PRO:HD2	1:A:292:TYR:HE2	1.72	0.54
1:A:605:LEU:HA	1:A:608:VAL:CG1	2.38	0.54
1:A:511:ASP:OD2	1:A:534:SER:HB3	2.08	0.54
2:B:108:GLN:HB2	2:B:109:LEU:HD12	1.88	0.54
1:A:145:ARG:HB3	1:A:185:LYS:O	2.08	0.54
1:A:272:ASP:O	1:A:275:ASP:N	2.40	0.54
1:A:876:PHE:O	1:A:879:PRO:HD2	2.07	0.54
1:A:545:ALA:O	1:A:548:THR:HB	2.08	0.54
2:B:171:ALA:HB1	2:B:191:PHE:HB2	1.90	0.54
2:B:45:ILE:CD1	2:B:121:VAL:HG22	2.37	0.54
2:B:207:LYS:C	2:B:209:LEU:H	2.11	0.54
1:A:138:HIS:ND1	1:A:201:TYR:OH	2.41	0.54
1:A:307:GLY:C	1:A:312:LEU:HD21	2.27	0.54
2:B:164:VAL:HG13	2:B:170:GLY:HA2	1.89	0.54
2:B:178:LYS:H	2:B:186:TYR:HB3	1.72	0.54
1:A:647:TRP:CD1	1:A:647:TRP:C	2.81	0.53
1:A:87:ASP:O	1:A:90:LEU:HB2	2.08	0.53
2:B:32:LYS:HE2	2:B:136:LYS:HZ2	1.73	0.53
2:B:149:ALA:CA	2:B:154:ASP:OD2	2.55	0.53
1:A:150:ASP:N	1:A:190:PRO:HG3	2.17	0.53
1:A:652:ASP:OD1	1:A:685:ARG:NH2	2.32	0.53
1:A:741:VAL:HG12	1:A:745:LEU:HD11	1.89	0.53
1:A:1:MET:O	1:A:2:LYS:C	2.47	0.53
1:A:85:MET:CA	1:A:380:ILE:HD11	2.39	0.53
1:A:111:ALA:HB3	1:A:213:LEU:HD12	1.89	0.53
1:A:373:LEU:CD2	1:A:378:LYS:HD3	2.39	0.53
1:A:701:PHE:O	1:A:708:TYR:HB2	2.08	0.53
2:B:109:LEU:HD12	2:B:109:LEU:N	2.24	0.53
1:A:16:PHE:HB3	1:A:245:HIS:CE1	2.43	0.53
1:A:274:ILE:HG23	1:A:275:ASP:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:LEU:HD23	2:B:33:LEU:N	2.23	0.53
2:B:92:TYR:HE2	2:B:109:LEU:HD22	1.67	0.53
1:A:151:LEU:HD13	1:A:194:GLU:HB2	1.89	0.53
1:A:295:GLU:HG3	1:A:301:GLY:N	2.23	0.53
1:A:705:LYS:O	1:A:707:ARG:HG3	2.09	0.53
1:A:169:LYS:HB2	1:A:175:GLY:N	2.23	0.53
1:A:471:VAL:O	1:A:475:ILE:HG13	2.09	0.53
1:A:779:ILE:HG22	1:A:871:LEU:CG	2.39	0.53
2:B:98:LEU:HD23	2:B:98:LEU:N	2.18	0.53
1:A:134:ASP:HB3	1:A:320:TYR:HE2	1.74	0.52
1:A:303:LEU:O	1:A:304:LYS:C	2.44	0.52
1:A:394:ALA:HB1	1:A:622:THR:CG2	2.34	0.52
1:A:394:ALA:CB	1:A:622:THR:CG2	2.85	0.52
1:A:660:GLU:HB2	1:A:661:PRO:HD3	1.91	0.52
1:A:854:ILE:CD1	1:A:859:LYS:HD3	2.32	0.52
2:B:79:SER:CB	2:B:111:ARG:HE	2.23	0.52
2:B:180:VAL:C	2:B:182:GLY:H	2.13	0.52
1:A:13:ASP:CG	1:A:64:ASN:HB2	2.28	0.52
1:A:412:LEU:HB2	1:A:623:ASP:O	2.10	0.52
2:B:202:ASP:OD2	2:B:204:SER:HB2	2.09	0.52
2:B:34:LYS:HD2	2:B:34:LYS:N	2.25	0.52
2:B:52:THR:HG23	2:B:53:ASP:OD2	2.09	0.52
1:A:131:HIS:CD2	1:A:198:LEU:HD22	2.44	0.52
1:A:594:LEU:HD11	1:A:625:ILE:HG23	1.89	0.52
1:A:656:ARG:HH11	1:A:656:ARG:HG2	1.73	0.52
1:A:779:ILE:CG2	1:A:871:LEU:HG	2.39	0.52
1:A:151:LEU:CD1	1:A:153:ASN:O	2.58	0.52
1:A:499:ILE:O	1:A:503:LEU:HD22	2.10	0.52
1:A:117:VAL:HG22	1:A:118:THR:N	2.24	0.52
1:A:225:TYR:C	1:A:227:TYR:H	2.13	0.52
1:A:343:LEU:HD12	1:A:558:ASN:ND2	2.25	0.52
1:A:725:LEU:HD11	1:A:750:ARG:HA	1.92	0.52
1:A:19:TYR:CD1	1:A:19:TYR:N	2.77	0.52
1:A:117:VAL:CG1	1:A:124:PRO:HG3	2.35	0.52
1:A:771:PHE:CD2	1:A:872:LEU:HD13	2.45	0.52
1:A:852:THR:O	1:A:854:ILE:CA	2.57	0.52
1:A:169:LYS:HG2	1:A:174:GLY:C	2.30	0.52
1:A:867:ASP:OD1	1:A:870:VAL:HB	2.08	0.52
2:B:179:GLN:HG2	2:B:184:SER:O	2.09	0.52
1:A:65:MET:O	1:A:68:ALA:N	2.42	0.51
1:A:169:LYS:HE2	1:A:319:ARG:HH21	0.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:LYS:NZ	2:B:146:LYS:HA	2.25	0.51
1:A:17:GLU:OE1	1:A:92:TYR:OH	2.18	0.51
1:A:189:MET:N	1:A:190:PRO:HD2	2.25	0.51
1:A:402:ASN:CG	1:A:403:ARG:H	2.14	0.51
1:A:698:ILE:HD11	1:A:701:PHE:HD1	1.75	0.51
2:B:89:VAL:O	2:B:93:ILE:HG13	2.09	0.51
1:A:249:ARG:HG2	1:A:250:VAL:N	2.26	0.51
1:A:273:TYR:CE1	1:A:335:ASP:HB2	2.45	0.51
1:A:511:ASP:OD1	1:A:534:SER:N	2.43	0.51
1:A:572:ASN:HD22	1:A:574:TRP:H	1.58	0.51
2:B:84:TYR:O	2:B:84:TYR:CD2	2.64	0.51
2:B:164:VAL:HG13	2:B:171:ALA:N	2.24	0.51
1:A:168:ALA:O	1:A:169:LYS:HB2	2.10	0.51
1:A:236:GLU:HG2	1:A:240:LYS:HE3	1.93	0.51
1:A:330:ARG:HG3	1:A:330:ARG:HH11	1.75	0.51
1:A:152:LEU:CD2	1:A:159:VAL:C	2.79	0.51
1:A:201:TYR:O	1:A:204:PHE:HB3	2.10	0.51
1:A:277:TYR:O	1:A:281:SER:HB3	2.10	0.51
1:A:485:HIS:HA	1:A:488:TYR:CD2	2.46	0.51
1:A:179:PRO:O	1:A:180:SER:C	2.49	0.51
1:A:354:GLN:HB3	1:A:356:GLN:NE2	2.26	0.51
1:A:533:LEU:HD12	1:A:537:SER:HB2	1.92	0.51
1:A:698:ILE:HD11	1:A:753:LEU:HD23	1.92	0.51
1:A:788:ILE:O	1:A:788:ILE:HD12	2.11	0.51
1:A:855:THR:O	1:A:856:ASP:HB2	2.11	0.51
1:A:115:ILE:HD13	1:A:136:ILE:HG12	1.93	0.51
1:A:309:ILE:O	1:A:310:SER:HB3	2.11	0.51
1:A:698:ILE:HG21	1:A:889:LEU:HD11	1.93	0.51
1:A:873:GLU:HA	1:A:877:ILE:CB	2.39	0.51
2:B:164:VAL:HG22	2:B:194:GLN:NE2	2.26	0.51
1:A:169:LYS:CB	1:A:175:GLY:HA3	2.39	0.50
1:A:553:MET:O	1:A:556:GLN:HG3	2.10	0.50
1:A:605:LEU:HD23	1:A:616:PHE:CB	2.41	0.50
1:A:605:LEU:HD23	1:A:616:PHE:HB3	1.93	0.50
1:A:290:LEU:HG	1:A:290:LEU:O	2.11	0.50
1:A:394:ALA:HB2	1:A:622:THR:HG23	1.91	0.50
2:B:88:PRO:CB	2:B:231:LEU:HD22	2.33	0.50
2:B:99:TYR:HE2	2:B:103:LYS:HZ3	1.51	0.50
2:B:236:ASN:O	2:B:237:GLN:HB2	2.11	0.50
1:A:128:GLN:NE2	1:A:130:LYS:CB	2.74	0.50
1:A:461:MET:HE1	1:A:581:ARG:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:LEU:HA	1:A:682:PHE:CE1	2.46	0.50
1:A:772:ARG:C	1:A:868:TYR:CE2	2.84	0.50
1:A:202:LEU:HD13	1:A:241:ARG:CB	2.41	0.50
1:A:243:SER:C	1:A:245:HIS:H	2.14	0.50
1:A:276:LEU:HG	1:A:340:PHE:HB3	1.94	0.50
1:A:869:THR:O	1:A:873:GLU:HG3	2.11	0.50
2:B:118:ASN:ND2	2:B:213:MET:CA	2.73	0.50
2:B:230:GLU:O	2:B:234:LYS:HG2	2.11	0.50
1:A:17:GLU:CG	1:A:18:ARG:H	2.18	0.50
1:A:183:ILE:HG22	1:A:183:ILE:O	2.11	0.50
1:A:781:SER:C	1:A:782:VAL:HG23	2.32	0.50
2:B:146:LYS:HG2	2:B:173:PHE:HZ	1.76	0.50
1:A:365:TRP:HZ2	1:A:562:LEU:O	1.94	0.50
1:A:496:GLY:O	1:A:499:ILE:HB	2.12	0.50
1:A:725:LEU:O	1:A:727:ILE:HG13	2.12	0.50
2:B:203:GLU:O	2:B:206:GLN:HB2	2.12	0.50
1:A:525:GLU:OE2	1:A:525:GLU:O	2.29	0.50
1:A:39:ALA:HB2	1:A:71:TRP:CH2	2.47	0.50
1:A:747:GLU:HG3	1:A:751:ARG:HD2	1.94	0.50
2:B:85:ASP:HA	2:B:91:GLN:NE2	2.27	0.50
2:B:197:ILE:O	2:B:200:ILE:HG12	2.11	0.50
2:B:207:LYS:HG3	2:B:208:GLU:N	2.27	0.49
1:A:380:ILE:HG13	1:A:380:ILE:O	2.12	0.49
1:A:526:ILE:HA	1:A:529:LYS:HB2	1.94	0.49
1:A:559:ARG:O	1:A:563:ILE:HG13	2.12	0.49
2:B:49:PRO:HD3	2:B:165:THR:O	2.12	0.49
2:B:180:VAL:O	2:B:182:GLY:N	2.45	0.49
1:A:265:LEU:HB3	1:A:268:ILE:HD12	1.93	0.49
1:A:471:VAL:O	1:A:472:PRO:C	2.49	0.49
1:A:131:HIS:CD2	1:A:198:LEU:CD2	2.95	0.49
1:A:216:TRP:HE1	1:A:274:ILE:HD12	1.77	0.49
1:A:246:ARG:HE	1:A:246:ARG:HA	1.77	0.49
1:A:347:MET:SD	1:A:562:LEU:HD13	2.53	0.49
1:A:419:ILE:HG23	1:A:589:PHE:CD2	2.47	0.49
1:A:702:TRP:CZ3	1:A:710:LEU:HD21	2.48	0.49
1:A:776:TYR:OH	1:A:852:THR:HB	2.12	0.49
2:B:174:VAL:O	2:B:176:LYS:HG3	2.11	0.49
1:A:865:TRP:C	1:A:866:MET:O	2.49	0.49
1:A:249:ARG:O	1:A:264:THR:HG22	2.13	0.49
1:A:644:THR:HG23	1:A:647:TRP:CZ3	2.48	0.49
1:A:42:PRO:C	1:A:44:SER:N	2.64	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:O	1:A:132:PRO:HG3	2.13	0.49
1:A:775:ASN:HD22	1:A:776:TYR:N	2.03	0.49
1:A:64:ASN:HD21	1:A:67:ASP:HB2	1.71	0.49
1:A:283:THR:HB	1:A:285:GLN:NE2	2.28	0.49
1:A:779:ILE:HG21	1:A:871:LEU:HD23	1.92	0.49
1:A:191:PHE:H	1:A:197:LEU:HD21	1.77	0.49
1:A:356:GLN:HE21	1:A:356:GLN:N	1.97	0.49
2:B:144:TRP:O	2:B:147:ILE:HG13	2.13	0.49
1:A:150:ASP:HB2	1:A:190:PRO:HG2	1.95	0.48
1:A:202:LEU:HD22	1:A:241:ARG:HG3	1.95	0.48
2:B:64:HIS:NE2	2:B:89:VAL:HB	2.27	0.48
2:B:164:VAL:CG1	2:B:165:THR:N	2.76	0.48
1:A:75:MET:CA	1:A:78:ILE:HD12	2.26	0.48
1:A:151:LEU:CD1	1:A:194:GLU:HB2	2.43	0.48
1:A:548:THR:O	1:A:549:GLU:C	2.51	0.48
1:A:867:ASP:OD2	1:A:869:THR:N	2.46	0.48
1:A:286:PRO:HG2	1:A:287:SER:H	1.79	0.48
1:A:769:LYS:HA	1:A:772:ARG:HD2	1.96	0.48
1:A:33:TYR:CD1	1:A:92:TYR:HD1	2.32	0.48
1:A:488:TYR:HB3	1:A:519:ARG:CG	2.44	0.48
1:A:4:PHE:HA	1:A:97:TYR:HE2	1.78	0.48
1:A:17:GLU:OE2	1:A:97:TYR:OH	2.26	0.48
1:A:304:LYS:HE3	1:A:304:LYS:HA	1.94	0.48
1:A:412:LEU:HD13	1:A:683:MET:HB2	1.94	0.48
1:A:496:GLY:HA2	1:A:499:ILE:HD12	1.95	0.48
2:B:46:ARG:NH1	2:B:197:ILE:HG12	2.28	0.48
1:A:126:PRO:O	1:A:127:SER:CB	2.60	0.48
1:A:268:ILE:HG22	1:A:269:SER:N	2.28	0.48
1:A:431:ALA:CB	1:A:454:TYR:CD2	2.96	0.48
1:A:435:LYS:NZ	1:A:435:LYS:HB3	2.29	0.48
2:B:47:PHE:H	2:B:47:PHE:HD1	1.60	0.48
1:A:89:LYS:HB2	1:A:89:LYS:NZ	2.28	0.48
1:A:354:GLN:O	1:A:357:SER:HB2	2.14	0.48
1:A:463:TYR:OH	1:A:582:ASN:ND2	2.46	0.48
1:A:574:TRP:HA	1:A:574:TRP:CE3	2.49	0.48
1:A:97:TYR:O	1:A:99:TYR:N	2.40	0.48
2:B:44:VAL:HB	2:B:122:VAL:HB	1.95	0.48
2:B:146:LYS:HA	2:B:146:LYS:HZ2	1.78	0.48
2:B:200:ILE:C	2:B:202:ASP:H	2.16	0.48
1:A:430:ILE:HD12	1:A:581:ARG:HH21	1.79	0.48
1:A:557:ILE:O	1:A:560:LYS:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:LYS:HD2	1:A:657:GLU:OE2	2.14	0.48
1:A:747:GLU:HA	1:A:747:GLU:OE2	2.13	0.48
2:B:49:PRO:CD	2:B:165:THR:O	2.62	0.48
2:B:52:THR:C	2:B:54:ASP:H	2.16	0.48
2:B:64:HIS:CE1	2:B:89:VAL:HB	2.49	0.48
2:B:235:PHE:O	2:B:236:ASN:C	2.50	0.48
1:A:231:LYS:HG3	1:A:236:GLU:HA	1.96	0.47
2:B:171:ALA:CB	2:B:191:PHE:CE1	2.79	0.47
1:A:49:TYR:CE1	1:A:59:ARG:HG3	2.49	0.47
1:A:64:ASN:ND2	1:A:67:ASP:CB	2.68	0.47
1:A:244:PRO:HD3	1:A:268:ILE:HD11	1.96	0.47
1:A:419:ILE:HG12	1:A:681:MET:CE	2.43	0.47
1:A:707:ARG:HA	1:A:728:MET:O	2.15	0.47
1:A:890:ASP:OD2	1:A:894:LYS:HD3	2.12	0.47
2:B:200:ILE:O	2:B:202:ASP:N	2.46	0.47
2:B:178:LYS:HB2	2:B:186:TYR:CG	2.49	0.47
1:A:151:LEU:HD11	1:A:153:ASN:O	2.14	0.47
1:A:725:LEU:HD11	1:A:750:ARG:CB	2.44	0.47
2:B:68:LYS:O	2:B:69:ASN:CB	2.53	0.47
1:A:403:ARG:NH2	1:A:889:LEU:CD2	2.77	0.47
1:A:407:VAL:HG11	1:A:710:LEU:HD22	1.96	0.47
1:A:687:ALA:HB2	1:A:715:MET:SD	2.54	0.47
1:A:51:ASP:OD2	1:A:55:LYS:HB2	2.14	0.47
1:A:253:ILE:HB	1:A:260:ARG:HE	1.79	0.47
1:A:572:ASN:C	1:A:572:ASN:ND2	2.60	0.47
1:A:112:ASN:H	1:A:139:TYR:HB3	1.80	0.47
1:A:174:GLY:HA3	1:A:319:ARG:CZ	2.44	0.47
1:A:191:PHE:O	1:A:192:ASP:CB	2.62	0.47
1:A:391:TYR:CE2	1:A:587:THR:HG21	2.48	0.47
1:A:589:PHE:HE2	1:A:681:MET:HE3	1.79	0.47
1:A:700:GLY:HA2	1:A:753:LEU:CD2	2.39	0.47
1:A:21:ASP:OD1	1:A:21:ASP:C	2.53	0.47
1:A:227:TYR:CD2	1:A:263:ILE:HG12	2.50	0.47
1:A:404:TYR:CD2	1:A:618:LEU:HD22	2.49	0.47
1:A:518:TYR:CE1	1:A:544:ARG:HB3	2.49	0.47
1:A:525:GLU:O	1:A:525:GLU:CD	2.53	0.47
1:A:213:LEU:CD2	1:A:223:ILE:HD11	2.32	0.47
1:A:413:THR:O	1:A:414:SER:C	2.53	0.47
2:B:134:VAL:HG23	2:B:212:GLN:OE1	2.15	0.47
1:A:31:VAL:O	1:A:33:TYR:N	2.46	0.46
1:A:402:ASN:ND2	1:A:403:ARG:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:VAL:HG22	1:A:454:TYR:CD1	2.49	0.46
1:A:654:PHE:O	1:A:655:ALA:CB	2.63	0.46
1:A:113:PHE:CB	1:A:138:HIS:HA	2.43	0.46
1:A:137:THR:CG2	1:A:328:VAL:HG11	2.45	0.46
1:A:169:LYS:HB3	1:A:170:LEU:H	1.28	0.46
1:A:774:LEU:HB2	1:A:779:ILE:HD11	1.96	0.46
2:B:49:PRO:CG	2:B:167:PRO:HD3	2.46	0.46
2:B:71:LYS:HD3	2:B:234:LYS:HD3	1.90	0.46
2:B:75:GLU:O	2:B:76:THR:O	2.33	0.46
2:B:178:LYS:N	2:B:186:TYR:HB3	2.30	0.46
1:A:365:TRP:CZ2	1:A:562:LEU:O	2.68	0.46
1:A:439:LEU:O	1:A:443:ILE:HG13	2.15	0.46
1:A:713:TRP:O	1:A:714:ASP:HB2	2.14	0.46
1:A:725:LEU:HD11	1:A:750:ARG:CA	2.45	0.46
1:A:732:THR:C	1:A:734:LYS:H	2.19	0.46
1:A:774:LEU:HB3	1:A:775:ASN:H	1.51	0.46
1:A:469:GLY:HA3	1:A:472:PRO:HG2	1.96	0.46
1:A:690:GLY:O	1:A:711:ASN:HB3	2.16	0.46
2:B:107:SER:O	2:B:110:LYS:HE2	2.15	0.46
1:A:153:ASN:HB3	1:A:158:ASN:HD21	1.78	0.46
1:A:252:VAL:HG22	1:A:261:GLU:HG3	1.97	0.46
1:A:265:LEU:CB	1:A:268:ILE:HD12	2.45	0.46
2:B:160:THR:HB	2:B:161:PRO:HD2	1.96	0.46
1:A:351:ALA:HB1	1:A:353:ILE:HG23	1.98	0.46
1:A:751:ARG:HA	1:A:755:GLU:HG2	1.98	0.46
2:B:67:LYS:HA	2:B:71:LYS:O	2.16	0.46
1:A:62:PHE:CE2	1:A:71:TRP:HB2	2.51	0.46
1:A:157:GLY:O	1:A:158:ASN:HB2	2.16	0.46
1:A:202:LEU:HD12	1:A:202:LEU:O	2.16	0.46
1:A:224:PRO:O	1:A:228:ASN:ND2	2.49	0.46
1:A:403:ARG:NH2	1:A:889:LEU:HD21	2.31	0.46
2:B:51:LYS:HG3	2:B:210:PHE:CE2	2.51	0.46
1:A:614:GLU:HG2	1:A:631:LYS:HE2	1.97	0.46
1:A:655:ALA:HA	1:A:659:MET:CB	2.44	0.46
1:A:5:TYR:CD1	1:A:93:LEU:HD21	2.51	0.46
1:A:572:ASN:ND2	1:A:573:VAL:N	2.57	0.46
2:B:56:LEU:HB3	2:B:57:PRO:HD2	1.98	0.46
1:A:295:GLU:OE2	1:A:301:GLY:HA3	2.15	0.45
1:A:471:VAL:HB	1:A:472:PRO:CD	2.46	0.45
1:A:405:LYS:HB3	1:A:406:TYR:CD1	2.51	0.45
1:A:592:MET:HE2	1:A:670:MET:SD	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ASP:CG	1:A:188:TYR:HE1	2.19	0.45
1:A:488:TYR:HB3	1:A:519:ARG:HG2	1.98	0.45
1:A:678:GLN:O	1:A:678:GLN:HG3	2.17	0.45
1:A:89:LYS:O	1:A:93:LEU:HD12	2.17	0.45
1:A:128:GLN:O	1:A:225:TYR:HE2	1.99	0.45
1:A:514:LEU:HD21	1:A:529:LYS:HB3	1.98	0.45
1:A:880:LEU:CD2	1:A:884:THR:HG23	2.46	0.45
1:A:203:ASN:O	1:A:207:GLN:HG3	2.16	0.45
1:A:217:ASN:OD1	1:A:274:ILE:HD13	2.16	0.45
1:A:260:ARG:HD3	1:A:260:ARG:N	2.27	0.45
1:A:584:THR:O	1:A:588:THR:HG22	2.17	0.45
2:B:78:SER:HB2	2:B:87:CYS:HB2	1.98	0.45
1:A:872:LEU:C	1:A:874:LYS:N	2.69	0.45
2:B:142:LYS:O	2:B:146:LYS:HD2	2.17	0.45
2:B:186:TYR:CG	2:B:187:ASP:N	2.84	0.45
1:A:33:TYR:HD2	1:A:35:PRO:HD3	1.82	0.45
1:A:57:CYS:SG	1:A:83:LEU:HD22	2.57	0.45
1:A:733:GLN:O	1:A:734:LYS:C	2.54	0.45
2:B:42:GLN:O	2:B:43:ALA:HB2	2.17	0.45
2:B:71:LYS:HB3	2:B:234:LYS:CD	2.46	0.45
1:A:111:ALA:HB1	1:A:138:HIS:CE1	2.51	0.45
1:A:420:ILE:HA	1:A:425:ILE:HD12	1.98	0.45
1:A:558:ASN:O	1:A:562:LEU:HB2	2.16	0.45
2:B:156:GLU:CD	2:B:157:MET:H	2.20	0.45
1:A:297:GLU:HA	1:A:297:GLU:OE1	2.17	0.45
1:A:338:ARG:HD2	1:A:340:PHE:CZ	2.52	0.45
1:A:449:ARG:HH11	1:A:449:ARG:CG	2.27	0.45
2:B:71:LYS:HB3	2:B:234:LYS:HB3	1.98	0.45
1:A:866:MET:SD	1:A:868:TYR:HE1	2.40	0.45
2:B:73:TYR:CE2	2:B:231:LEU:HA	2.52	0.45
2:B:178:LYS:H	2:B:186:TYR:HB2	1.80	0.45
1:A:225:TYR:C	1:A:227:TYR:N	2.69	0.44
1:A:343:LEU:HD12	1:A:558:ASN:HD21	1.81	0.44
2:B:93:ILE:O	2:B:97:ASP:HA	2.17	0.44
2:B:144:TRP:C	2:B:146:LYS:N	2.70	0.44
1:A:204:PHE:CE1	1:A:208:LYS:HD2	2.52	0.44
1:A:269:SER:OG	1:A:356:GLN:NE2	2.51	0.44
1:A:542:LEU:CG	1:A:546:GLN:HE21	2.19	0.44
1:A:8:VAL:HG23	1:A:15:ILE:HG23	2.00	0.44
1:A:619:TYR:O	1:A:619:TYR:CD2	2.70	0.44
1:A:159:VAL:CG1	1:A:160:GLU:N	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LYS:CD	1:A:319:ARG:HH21	2.20	0.44
1:A:415:LEU:O	1:A:419:ILE:HG13	2.17	0.44
1:A:431:ALA:HB1	1:A:454:TYR:CD2	2.52	0.44
1:A:158:ASN:OD1	1:A:159:VAL:N	2.48	0.44
1:A:238:THR:O	1:A:238:THR:HG22	2.17	0.44
1:A:567:TYR:OH	1:A:587:THR:CG2	2.65	0.44
2:B:178:LYS:N	2:B:186:TYR:CB	2.81	0.44
1:A:164:ILE:CG1	1:A:165:GLU:N	2.80	0.44
1:A:512:GLU:OE2	1:A:513:PRO:HD2	2.17	0.44
2:B:168:TRP:C	2:B:169:GLU:HG3	2.38	0.44
1:A:50:PHE:O	1:A:379:VAL:N	2.33	0.44
1:A:117:VAL:HG22	1:A:118:THR:H	1.80	0.44
1:A:133:ILE:HD13	1:A:198:LEU:CD1	2.48	0.44
1:A:236:GLU:O	1:A:239:ALA:HB3	2.18	0.44
1:A:439:LEU:HD21	1:A:591:GLN:HG2	2.00	0.44
1:A:853:GLU:O	1:A:854:ILE:CB	2.36	0.44
1:A:871:LEU:HG	1:A:871:LEU:O	2.18	0.44
2:B:210:PHE:HA	2:B:213:MET:SD	2.58	0.44
1:A:49:TYR:OH	3:A:999:GDP:O3A	2.33	0.44
1:A:274:ILE:CG2	1:A:275:ASP:N	2.81	0.44
1:A:323:TYR:C	1:A:325:ILE:H	2.21	0.44
1:A:466:ASP:O	1:A:467:ARG:HB2	2.17	0.44
1:A:20:ILE:HG23	1:A:24:GLY:HA2	2.00	0.44
1:A:163:SER:HB2	1:A:166:ILE:CB	2.40	0.44
1:A:605:LEU:O	1:A:608:VAL:CG1	2.66	0.44
2:B:57:PRO:HG2	2:B:58:PHE:CE1	2.53	0.44
1:A:201:TYR:O	1:A:205:TRP:N	2.43	0.43
1:A:234:PHE:O	1:A:238:THR:HB	2.18	0.43
1:A:323:TYR:HA	1:A:326:ILE:HD11	1.99	0.43
1:A:696:LYS:O	1:A:756:GLY:CA	2.66	0.43
1:A:260:ARG:HG2	1:A:261:GLU:N	2.33	0.43
2:B:81:HIS:C	2:B:83:ASP:H	2.20	0.43
1:A:178:VAL:HB	1:A:179:PRO:HD3	2.00	0.43
1:A:489:MET:SD	1:A:553:MET:CE	3.06	0.43
2:B:99:TYR:CE2	2:B:103:LYS:HD3	2.53	0.43
2:B:224:LYS:O	2:B:224:LYS:HG3	2.18	0.43
1:A:18:ARG:NH1	1:A:267:GLY:O	2.51	0.43
1:A:128:GLN:NE2	1:A:130:LYS:HB2	2.33	0.43
1:A:209:THR:CG2	1:A:244:PRO:HG3	2.47	0.43
1:A:738:PRO:HG2	1:A:741:VAL:HG23	1.99	0.43
1:A:72:ILE:O	1:A:73:LYS:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:HIS:HB3	1:A:229:ARG:HB3	2.01	0.43
1:A:425:ILE:CD1	1:A:586:ILE:HG12	2.48	0.43
1:A:727:ILE:HD13	1:A:749:ILE:HD12	2.01	0.43
1:A:767:PHE:HA	1:A:770:GLU:HB3	2.00	0.43
1:A:47:THR:HG22	1:A:48:LYS:HG2	1.99	0.43
1:A:19:TYR:O	1:A:26:GLU:HA	2.19	0.43
1:A:218:VAL:CG1	1:A:223:ILE:HG13	2.49	0.43
1:A:309:ILE:CD1	1:A:310:SER:N	2.80	0.43
1:A:698:ILE:HG12	1:A:753:LEU:HA	2.01	0.43
2:B:75:GLU:C	2:B:76:THR:O	2.56	0.43
2:B:186:TYR:HE2	2:B:188:GLU:HB2	1.82	0.43
2:B:230:GLU:O	2:B:233:THR:HG22	2.19	0.43
1:A:111:ALA:HB3	1:A:213:LEU:CD1	2.47	0.43
1:A:133:ILE:HD13	1:A:198:LEU:HD13	2.00	0.43
1:A:402:ASN:CG	1:A:403:ARG:N	2.72	0.43
1:A:709:ALA:HA	1:A:726:LYS:O	2.19	0.43
1:A:733:GLN:HE21	1:A:733:GLN:HB2	1.67	0.43
2:B:78:SER:HB3	2:B:83:ASP:HB3	2.00	0.43
1:A:129:ALA:O	1:A:131:HIS:N	2.52	0.43
1:A:214:THR:CG2	1:A:271:LEU:CB	2.76	0.43
1:A:866:MET:SD	1:A:868:TYR:CE1	3.12	0.43
2:B:95:LYS:HE3	2:B:95:LYS:CA	2.44	0.43
1:A:878:LYS:N	1:A:879:PRO:CD	2.82	0.43
1:A:457:SER:HA	1:A:458:PRO:HD3	1.91	0.42
1:A:38:PHE:CE2	1:A:59:ARG:HG2	2.54	0.42
1:A:116:GLU:HB2	1:A:135:ALA:N	2.32	0.42
1:A:899:ASP:O	1:A:902:ASP:OD2	2.37	0.42
1:A:143:ASP:OD2	1:A:208:LYS:NZ	2.50	0.42
1:A:161:GLU:HG2	1:A:188:TYR:OH	2.19	0.42
1:A:178:VAL:HB	1:A:179:PRO:CD	2.50	0.42
1:A:313:ARG:NH1	1:A:317:HIS:NE2	2.67	0.42
1:A:426:SER:HB2	1:A:472:PRO:HD2	2.00	0.42
1:A:496:GLY:O	1:A:500:LYS:HG3	2.18	0.42
2:B:49:PRO:CB	2:B:165:THR:O	2.68	0.42
1:A:408:MET:HG2	1:A:688:ILE:HG12	2.01	0.42
1:A:514:LEU:CD1	1:A:533:LEU:HD21	2.45	0.42
1:A:656:ARG:HG2	1:A:656:ARG:NH1	2.34	0.42
2:B:52:THR:C	2:B:54:ASP:N	2.72	0.42
2:B:167:PRO:HA	2:B:197:ILE:CD1	2.48	0.42
1:A:178:VAL:C	1:A:180:SER:H	2.23	0.42
1:A:192:ASP:O	1:A:193:ASN:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ILE:O	1:A:330:ARG:N	2.48	0.42
1:A:405:LYS:HD3	1:A:406:TYR:CE1	2.55	0.42
1:A:892:GLU:HG3	1:A:892:GLU:O	2.20	0.42
2:B:35:LEU:C	2:B:37:ALA:H	2.22	0.42
1:A:26:GLU:O	1:A:27:ARG:HG2	2.20	0.42
1:A:37:LEU:C	1:A:38:PHE:CD1	2.93	0.42
1:A:135:ALA:C	1:A:136:ILE:HG13	2.40	0.42
1:A:215:GLY:HA3	1:A:218:VAL:HG21	2.01	0.42
1:A:247:LYS:HG3	1:A:248:THR:N	2.35	0.42
2:B:146:LYS:HD2	2:B:146:LYS:N	2.34	0.42
2:B:176:LYS:CB	2:B:188:GLU:HB3	2.45	0.42
1:A:74:ARG:CG	1:A:78:ILE:HD11	2.42	0.42
1:A:525:GLU:O	1:A:526:ILE:HG13	2.20	0.42
1:A:781:SER:O	1:A:782:VAL:HG22	2.16	0.42
2:B:204:SER:C	2:B:206:GLN:H	2.22	0.42
1:A:37:LEU:HD23	1:A:37:LEU:HA	1.84	0.42
1:A:212:ILE:CD1	1:A:345:LEU:HD21	2.47	0.42
1:A:693:LEU:HA	1:A:693:LEU:HD12	1.73	0.42
1:A:790:LYS:HD2	1:A:790:LYS:H	1.85	0.42
2:B:171:ALA:CB	2:B:191:PHE:HB2	2.49	0.42
1:A:135:ALA:HA	1:A:149:PHE:O	2.20	0.42
1:A:225:TYR:O	1:A:227:TYR:N	2.52	0.42
1:A:253:ILE:HG12	1:A:262:ILE:HD13	2.00	0.42
1:A:376:GLN:HB2	1:A:378:LYS:HD2	2.01	0.42
1:A:584:THR:O	1:A:585:ALA:C	2.58	0.42
1:A:644:THR:HG21	1:A:713:TRP:CH2	2.54	0.42
1:A:209:THR:HG23	1:A:244:PRO:HG3	2.01	0.42
1:A:426:SER:OG	1:A:471:VAL:HG23	2.19	0.42
1:A:469:GLY:CA	1:A:472:PRO:HG2	2.50	0.42
1:A:741:VAL:HG12	1:A:745:LEU:CD1	2.50	0.42
1:A:776:TYR:CE2	1:A:852:THR:HB	2.55	0.42
2:B:36:ASP:C	2:B:38:SER:N	2.73	0.42
2:B:200:ILE:C	2:B:202:ASP:N	2.73	0.42
1:A:279:LYS:HG2	1:A:280:PHE:CE2	2.55	0.41
1:A:406:TYR:CD1	1:A:406:TYR:N	2.87	0.41
2:B:216:LEU:CD1	2:B:219:MET:HG3	2.45	0.41
1:A:725:LEU:HD11	1:A:750:ARG:HB2	2.02	0.41
2:B:180:VAL:C	2:B:182:GLY:N	2.74	0.41
2:B:216:LEU:O	2:B:219:MET:CG	2.61	0.41
1:A:260:ARG:HG3	1:A:260:ARG:NH1	2.35	0.41
1:A:503:LEU:HD13	1:A:503:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:LEU:CD1	1:A:632:ILE:HD11	2.48	0.41
1:A:619:TYR:CD2	1:A:619:TYR:C	2.91	0.41
2:B:40:ASN:HA	2:B:177:VAL:O	2.20	0.41
2:B:61:LEU:HB3	2:B:116:TRP:HZ3	1.84	0.41
1:A:88:PHE:O	1:A:89:LYS:C	2.58	0.41
1:A:104:ASP:OD1	1:A:106:THR:CB	2.59	0.41
1:A:131:HIS:NE2	1:A:198:LEU:CD2	2.84	0.41
1:A:664:ASP:O	1:A:668:ARG:HG3	2.19	0.41
2:B:48:LEU:HD21	2:B:120:LEU:HB2	2.02	0.41
2:B:61:LEU:HB3	2:B:116:TRP:CZ3	2.55	0.41
2:B:149:ALA:HB1	2:B:154:ASP:OD2	2.21	0.41
1:A:74:ARG:HD3	1:A:78:ILE:HD11	2.03	0.41
1:A:410:PHE:HB3	1:A:683:MET:HG2	2.03	0.41
1:A:611:THR:OG1	1:A:612:GLU:N	2.52	0.41
2:B:107:SER:O	2:B:110:LYS:HG2	2.20	0.41
2:B:144:TRP:O	2:B:146:LYS:N	2.53	0.41
1:A:113:PHE:C	1:A:113:PHE:CD2	2.92	0.41
1:A:402:ASN:ND2	1:A:403:ARG:H	2.18	0.41
1:A:790:LYS:N	1:A:790:LYS:CD	2.84	0.41
2:B:64:HIS:ND1	2:B:89:VAL:HG11	2.36	0.41
1:A:113:PHE:CD2	1:A:113:PHE:O	2.74	0.41
1:A:403:ARG:HH22	1:A:889:LEU:CD2	2.34	0.41
1:A:507:ASN:ND2	1:A:509:SER:OG	2.53	0.41
1:A:667:PHE:HD1	1:A:670:MET:HE2	1.85	0.41
2:B:66:PHE:CE2	2:B:109:LEU:CD2	3.03	0.41
1:A:33:TYR:CD2	1:A:35:PRO:HD3	2.56	0.41
1:A:113:PHE:HE2	1:A:218:VAL:HG11	1.86	0.41
1:A:146:PHE:CD1	1:A:146:PHE:N	2.89	0.41
1:A:647:TRP:O	1:A:650:PHE:HB3	2.20	0.41
1:A:680:LEU:HA	1:A:682:PHE:CZ	2.56	0.41
2:B:45:ILE:CG2	2:B:119:ILE:HD12	2.51	0.41
2:B:59:ALA:CA	2:B:216:LEU:HD23	2.40	0.41
2:B:71:LYS:CB	2:B:234:LYS:HD3	2.51	0.41
2:B:228:PHE:N	2:B:228:PHE:CD1	2.88	0.41
1:A:124:PRO:HG2	1:A:221:PHE:HE2	1.86	0.41
1:A:333:GLN:O	1:A:336:ALA:HB3	2.21	0.41
1:A:597:ILE:HD12	1:A:597:ILE:HA	1.96	0.41
2:B:49:PRO:HG2	2:B:167:PRO:HD3	2.02	0.41
2:B:225:PHE:O	2:B:226:LYS:CB	2.68	0.41
1:A:109:ARG:HD3	1:A:140:ASP:OD2	2.21	0.40
1:A:147:TYR:N	1:A:147:TYR:CD1	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LYS:NZ	1:A:598:GLU:OE2	2.51	0.40
1:A:481:GLN:HB3	1:A:559:ARG:HD2	2.03	0.40
1:A:713:TRP:CE3	1:A:723:PRO:HG3	2.56	0.40
2:B:71:LYS:HB3	2:B:234:LYS:CB	2.51	0.40
2:B:171:ALA:CB	2:B:191:PHE:CG	2.80	0.40
2:B:211:GLU:C	2:B:213:MET:H	2.25	0.40
1:A:233:ILE:HG22	1:A:234:PHE:CD1	2.56	0.40
1:A:397:LYS:O	1:A:619:TYR:CD1	2.70	0.40
1:A:537:SER:O	1:A:540:GLU:HB3	2.21	0.40
1:A:862:VAL:C	1:A:864:HIS:H	2.24	0.40
2:B:106:TYR:CE1	2:B:110:LYS:HB3	2.56	0.40
1:A:45:GLN:O	1:A:46:ALA:C	2.60	0.40
1:A:240:LYS:O	1:A:246:ARG:HA	2.20	0.40
1:A:280:PHE:CD1	1:A:343:LEU:HD22	2.49	0.40
1:A:409:SER:HB3	1:A:626:TYR:CE2	2.56	0.40
1:A:428:GLU:OE1	1:A:428:GLU:N	2.44	0.40
1:A:691:PRO:HA	1:A:692:PRO:HD3	2.00	0.40
1:A:202:LEU:CD2	1:A:241:ARG:HG3	2.51	0.40
1:A:447:ALA:O	1:A:673:TYR:OH	2.28	0.40
1:A:594:LEU:HD13	1:A:594:LEU:HA	1.79	0.40
1:A:870:VAL:C	1:A:872:LEU:H	2.25	0.40
2:B:49:PRO:HB3	2:B:165:THR:O	2.20	0.40
2:B:91:GLN:NE2	2:B:91:GLN:HA	2.37	0.40
2:B:153:VAL:O	2:B:153:VAL:HG23	2.21	0.40
2:B:174:VAL:CG2	2:B:192:LEU:CD2	2.96	0.40
1:A:33:TYR:HE2	1:A:35:PRO:HB3	1.87	0.40
1:A:434:PHE:HE2	1:A:456:CYS:HB3	1.87	0.40
1:A:859:LYS:O	1:A:860:ASP:C	2.60	0.40
2:B:46:ARG:O	2:B:120:LEU:N	2.54	0.40
2:B:48:LEU:HD13	2:B:209:LEU:HD21	2.03	0.40
2:B:98:LEU:H	2:B:98:LEU:CD2	2.18	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	841/903 (93%)	637 (76%)	145 (17%)	59 (7%)	1	8
2	B	208/234 (89%)	137 (66%)	46 (22%)	25 (12%)	0	2
All	All	1049/1137 (92%)	774 (74%)	191 (18%)	84 (8%)	1	6

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	ALA
1	A	154	SER
1	A	159	VAL
1	A	182	ILE
1	A	192	ASP
1	A	222	ALA
1	A	246	ARG
1	A	352	LYS
1	A	405	LYS
1	A	619	TYR
1	A	622	THR
1	A	623	ASP
1	A	640	LYS
1	A	778	SER
1	A	853	GLU
1	A	854	ILE
1	A	866	MET
1	A	867	ASP
2	B	51	LYS
2	B	97	ASP
2	B	98	LEU
2	B	142	LYS
2	B	153	VAL
2	B	157	MET
2	B	165	THR
2	B	181	SER
2	B	216	LEU
2	B	226	LYS
2	B	227	SER
1	A	46	ALA
1	A	133	ILE
1	A	160	GLU
1	A	162	TRP

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Mol	Chain	Res	Type
1	A	169	LYS
1	A	170	LEU
1	A	180	SER
1	A	193	ASN
1	A	325	ILE
1	A	599	ARG
1	A	777	ILE
1	A	896	SER
2	B	102	ASN
2	B	141	LYS
2	B	201	ASP
1	A	98	ASN
1	A	130	LYS
1	A	168	ALA
1	A	526	ILE
1	A	776	TYR
1	A	789	ALA
1	A	864	HIS
1	A	876	PHE
2	B	36	ASP
2	B	145	ASP
2	B	237	GLN
1	A	2	LYS
1	A	18	ARG
1	A	141	SER
1	A	167	ALA
1	A	229	ARG
1	A	467	ARG
1	A	600	LYS
1	A	893	LYS
2	B	192	LEU
2	B	204	SER
2	B	217	SER
1	A	127	SER
1	A	272	ASP
1	A	723	PRO
1	A	733	GLN
1	A	734	LYS
1	A	873	GLU
2	B	76	THR
2	B	152	ALA
2	B	154	ASP

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Mol	Chain	Res	Type
2	B	184	SER
1	A	29	ARG
1	A	286	PRO
1	A	324	ASN
1	A	435	LYS
1	A	189	MET
1	A	226	VAL
1	A	417	PRO
2	B	164	VAL

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	753/800 (94%)	690 (92%)	63 (8%)	11	39
2	B	188/200 (94%)	163 (87%)	25 (13%)	4	18
All	All	941/1000 (94%)	853 (91%)	88 (9%)	8	33

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	32	GLU
1	A	47	THR
1	A	58	THR
1	A	61	LEU
1	A	64	ASN
1	A	67	ASP
1	A	70	GLN
1	A	93	LEU
1	A	113	PHE
1	A	128	GLN
1	A	150	ASP
1	A	169	LYS
1	A	225	TYR

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Mol	Chain	Res	Type
1	A	229	ARG
1	A	246	ARG
1	A	255	ASN
1	A	260	ARG
1	A	303	LEU
1	A	304	LYS
1	A	309	ILE
1	A	310	SER
1	A	324	ASN
1	A	337	LYS
1	A	352	LYS
1	A	356	GLN
1	A	357	SER
1	A	362	ILE
1	A	412	LEU
1	A	435	LYS
1	A	440	HIS
1	A	449	ARG
1	A	452	ASP
1	A	453	VAL
1	A	459	ASN
1	A	503	LEU
1	A	519	ARG
1	A	533	LEU
1	A	549	GLU
1	A	559	ARG
1	A	570	LEU
1	A	572	ASN
1	A	573	VAL
1	A	574	TRP
1	A	588	THR
1	A	591	GLN
1	A	594	LEU
1	A	618	LEU
1	A	619	TYR
1	A	622	THR
1	A	645	ASN
1	A	647	TRP
1	A	702	TRP
1	A	703	THR
1	A	718	THR
1	A	733	GLN

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Mol	Chain	Res	Type
1	A	775	ASN
1	A	867	ASP
1	A	868	TYR
1	A	874	LYS
1	A	878	LYS
1	A	880	LEU
1	A	883	PHE
2	B	36	ASP
2	B	47	PHE
2	B	92	TYR
2	B	94	SER
2	B	95	LYS
2	B	98	LEU
2	B	99	TYR
2	B	101	THR
2	B	116	TRP
2	B	129	ASP
2	B	131	GLU
2	B	136	LYS
2	B	141	LYS
2	B	146	LYS
2	B	150	MET
2	B	156	GLU
2	B	166	CYS
2	B	173	PHE
2	B	179	GLN
2	B	181	SER
2	B	206	GLN
2	B	215	ASP
2	B	225	PHE
2	B	228	PHE
2	B	232	ASN

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	64	ASN
1	A	70	GLN
1	A	128	GLN
1	A	203	ASN
1	A	228	ASN
1	A	245	HIS

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Mol	Chain	Res	Type
1	A	285	GLN
1	A	356	GLN
1	A	386	HIS
1	A	402	ASN
1	A	422	GLN
1	A	459	ASN
1	A	507	ASN
1	A	546	GLN
1	A	572	ASN
1	A	582	ASN
1	A	591	GLN
1	A	676	ASN
1	A	733	GLN
1	A	754	GLN
1	A	775	ASN
2	B	42	GLN
2	B	91	GLN
2	B	102	ASN
2	B	118	ASN
2	B	130	ASN
2	B	194	GLN
2	B	232	ASN
2	B	236	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GDP	A	999	-	24,30,30	1.57	5 (20%)	31,47,47	2.84	13 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GDP	A	999	-	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	GDP	O4'-C1'	4.33	1.47	1.41
3	A	999	GDP	C6-N1	2.77	1.37	1.33
3	A	999	GDP	PB-O3B	2.21	1.63	1.54
3	A	999	GDP	C8-N7	-2.14	1.30	1.34
3	A	999	GDP	C2-N2	2.05	1.38	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	GDP	O2B-PB-O3A	-6.75	82.01	104.64
3	A	999	GDP	C2-N3-C4	5.49	121.62	115.36
3	A	999	GDP	O3B-PB-O3A	-5.42	86.45	104.64
3	A	999	GDP	PA-O3A-PB	-4.83	116.25	132.83
3	A	999	GDP	N3-C2-N1	-4.62	121.06	127.22
3	A	999	GDP	O3A-PB-O1B	-4.53	86.06	111.19
3	A	999	GDP	C5-C6-N1	-3.45	118.71	123.43
3	A	999	GDP	O2B-PB-O1B	3.12	122.89	110.68
3	A	999	GDP	C6-C5-C4	-3.07	117.87	120.80
3	A	999	GDP	C6-N1-C2	3.02	120.73	115.93
3	A	999	GDP	PA-O5'-C5'	-2.82	105.17	121.68
3	A	999	GDP	C3'-C2'-C1'	2.61	104.91	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	GDP	O3B-PB-O2B	2.34	116.60	107.64

There are no chirality outliers.

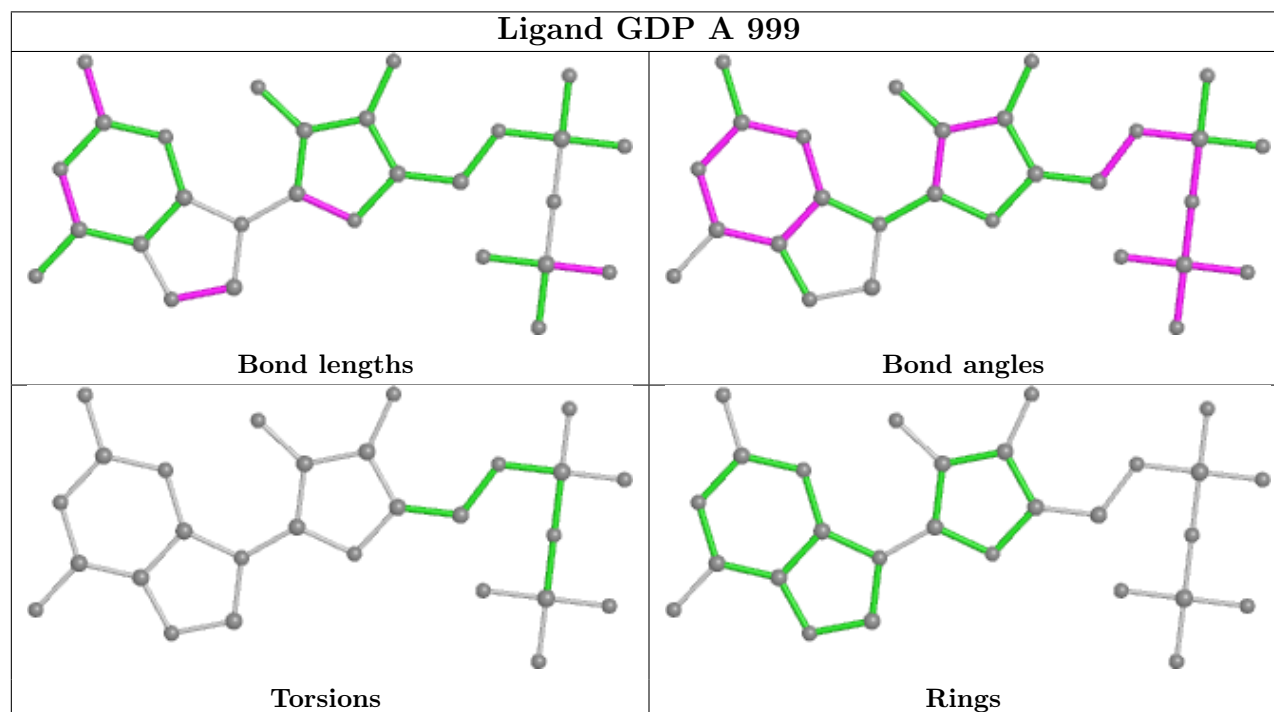
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	845/903 (93%)	-0.04	29 (3%) 45 29	13, 61, 157, 171	0
2	B	210/234 (89%)	1.05	43 (20%) 1 1	55, 133, 171, 198	0
All	All	1055/1137 (92%)	0.18	72 (6%) 17 10	13, 74, 162, 198	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	240	GLY	9.8
2	B	238	VAL	9.4
2	B	82	GLY	8.5
2	B	241	THR	6.7
2	B	114	SER	6.0
1	A	150	ASP	5.5
2	B	62	VAL	5.4
1	A	120	PRO	5.3
2	B	66	PHE	5.2
2	B	239	LEU	5.1
2	B	51	LYS	5.1
2	B	154	ASP	4.8
1	A	135	ALA	4.7
2	B	226	LYS	4.4
2	B	153	VAL	4.3
1	A	787	ASN	4.1
2	B	50	ALA	4.1
2	B	49	PRO	3.8
2	B	73	TYR	3.7
1	A	171	GLN	3.6
2	B	96	ASN	3.2
1	A	776	TYR	3.2
2	B	94	SER	3.1
2	B	163	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	105	GLU	3.1
1	A	261	GLU	3.1
2	B	237	GLN	3.1
2	B	161	PRO	3.1
1	A	149	PHE	3.1
1	A	326	ILE	3.1
2	B	85	ASP	3.0
2	B	168	TRP	3.0
2	B	60	ILE	3.0
2	B	78	SER	3.0
1	A	786	ASN	3.0
1	A	852	THR	2.9
1	A	173	GLN	2.9
2	B	212	GLN	2.8
1	A	176	ASP	2.8
2	B	225	PHE	2.8
1	A	861	ASP	2.7
2	B	191	PHE	2.7
2	B	230	GLU	2.7
2	B	92	TYR	2.6
1	A	188	TYR	2.6
2	B	48	LEU	2.6
2	B	111	ARG	2.6
2	B	99	TYR	2.6
2	B	95	LYS	2.6
1	A	121	ASP	2.6
2	B	155	THR	2.6
1	A	856	ASP	2.6
2	B	235	PHE	2.4
1	A	189	MET	2.4
1	A	227	TYR	2.4
2	B	61	LEU	2.4
1	A	229	ARG	2.3
1	A	855	THR	2.3
1	A	790	LYS	2.3
1	A	391	TYR	2.3
2	B	79	SER	2.3
1	A	172	GLU	2.2
1	A	862	VAL	2.2
1	A	254	GLU	2.2
2	B	231	LEU	2.2
1	A	165	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	788	ILE	2.2
2	B	148	ASN	2.1
1	A	156	TYR	2.1
2	B	71	LYS	2.1
2	B	112	LYS	2.1
2	B	84	TYR	2.1

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 monosaccharides in this entry.

6.4 Ligands [i](#)

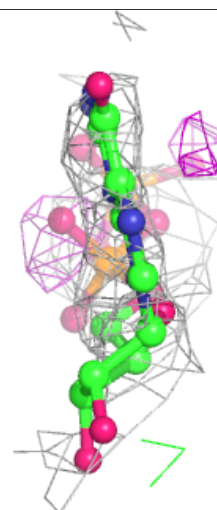
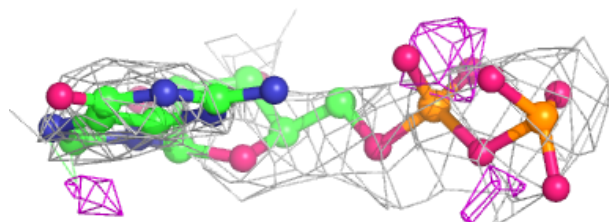
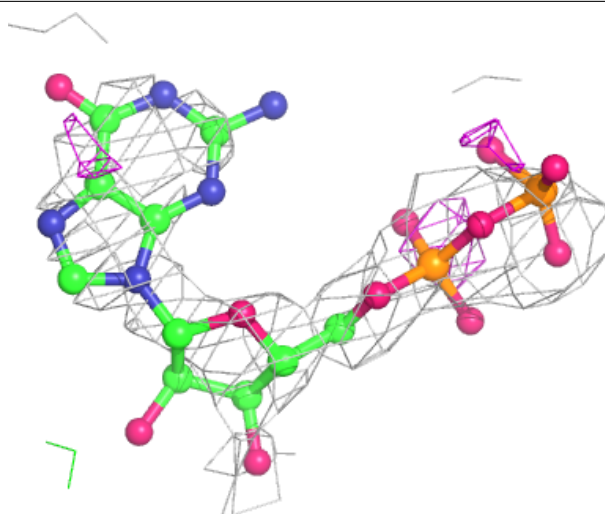
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GDP	A	999	28/28	0.82	0.55	141,146,158,158	0
4	ZN	B	1	1/1	0.92	0.03	125,125,125,125	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 GDP A 999:

$2mF_o-DF_c$ (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.