Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 01:53 PM EST

PDB ID	:	1IBR
Title	:	COMPLEX OF RAN WITH IMPORTIN BETA
Authors	:	Vetter, I.R.; Arndt, A.; Kutay, U.; Goerlich, D.; Wittinghofer, A.
Deposited on	:	1999-05-14
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

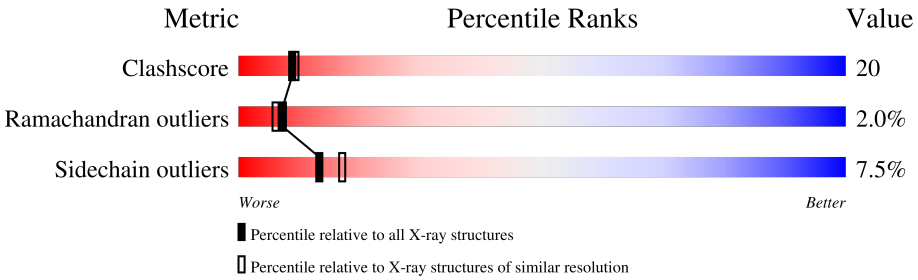
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	216	56% 20% · 22%
1	C	216	54% 22% · 22%
2	B	462	63% 29% 7% ·
2	D	462	56% 31% 7% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10117 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 GTP-binding nuclear protein RAN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	1
			1371	890	242	235	4			
1	C	169	Total	C	N	O	S	0	0	1
			1371	890	242	235	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ARG	SER	conflict	UNP P62826
C	129	ARG	SER	conflict	UNP P62826

- Molecule 2 is a protein called Importin beta-1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	458	Total	C	N	O	S	0	0	0
			3573	2255	595	698	25			
2	D	438	Total	C	N	O	S	0	0	0
			3424	2158	573	669	24			

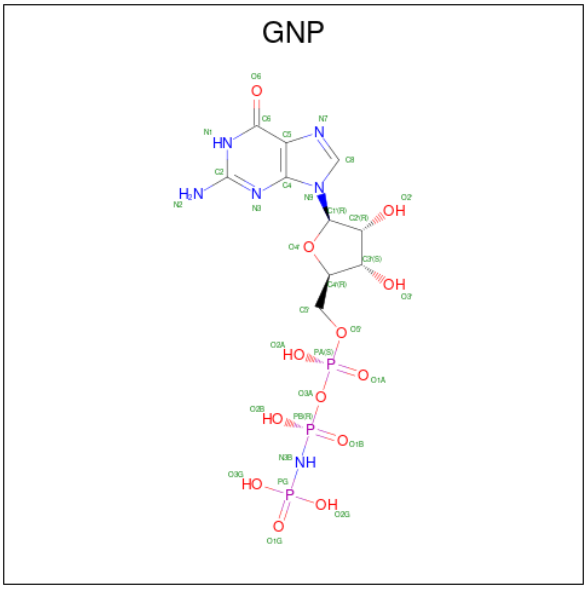
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	97	GLN	HIS	conflict	UNP Q14974
D	97	GLN	HIS	conflict	UNP Q14974

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	77	Total	O	0	0
			77	77		
5	B	121	Total	O	0	0
			121	121		
5	C	29	Total	O	0	0
			29	29		
5	D	85	Total	O	0	0
			85	85		

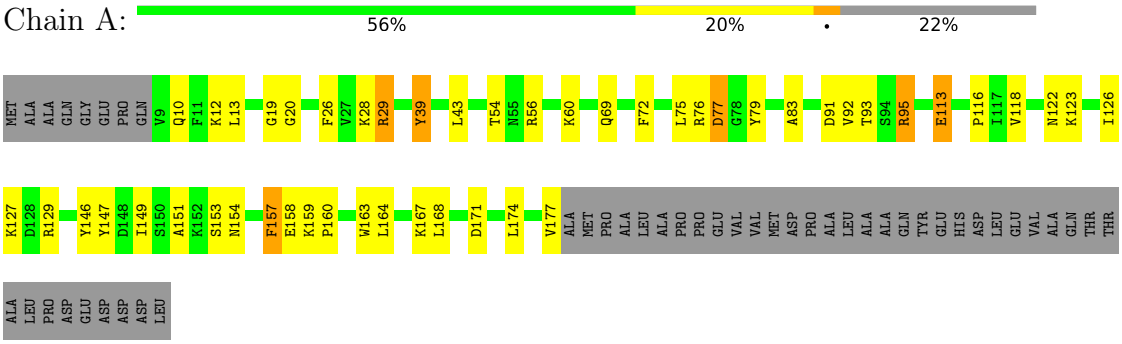
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

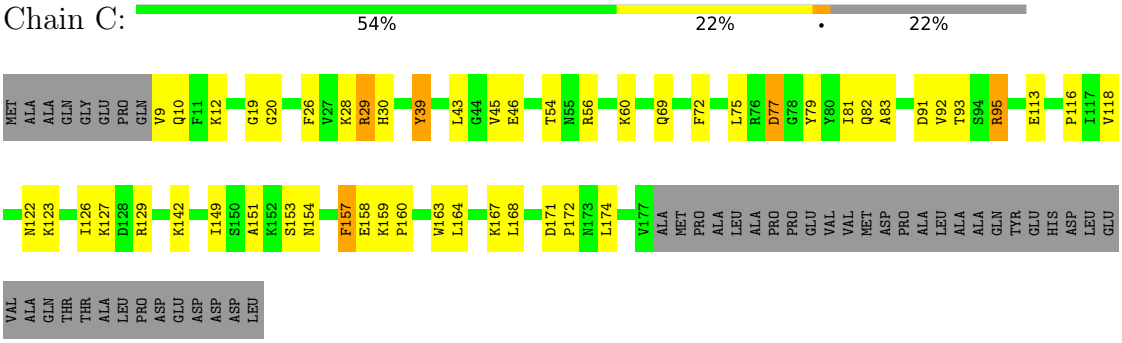
• Molecule 1: GTP-binding nuclear protein RAN

Chain A:



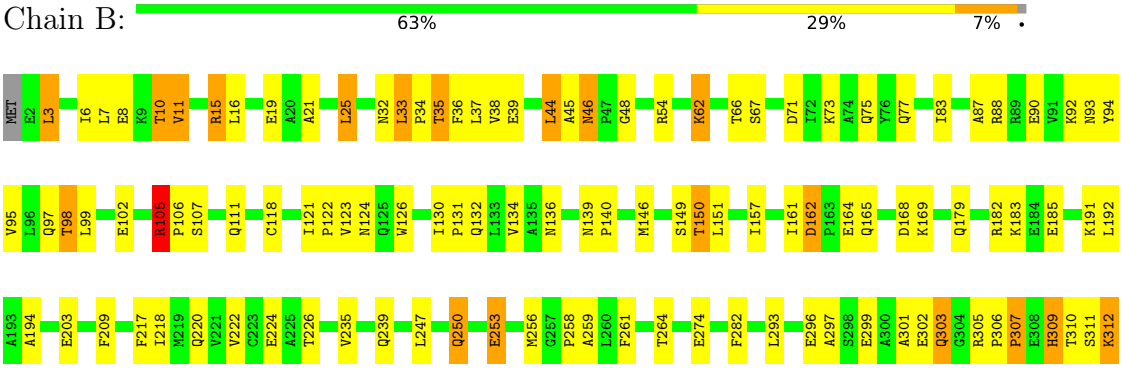
• Molecule 1: GTP-binding nuclear protein RAN

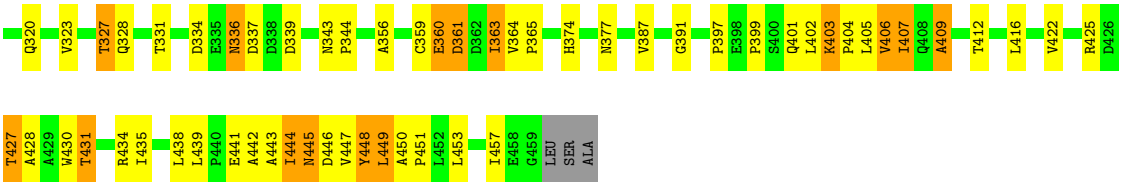
Chain C:



• Molecule 2: Importin beta-1 subunit

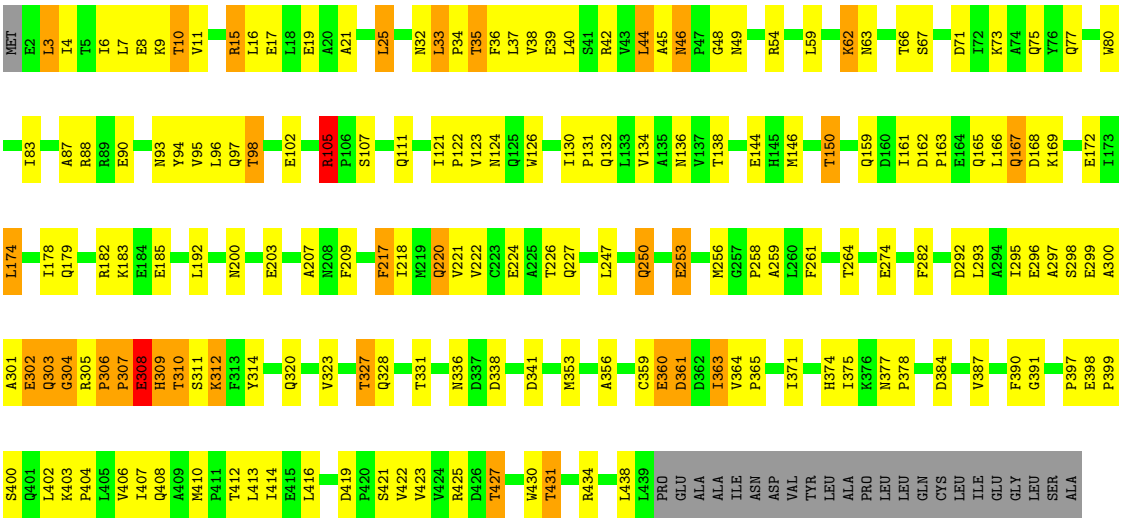
Chain B:





• Molecule 2: Importin beta-1 subunit

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.70Å 108.95Å 114.05Å 90.00° 100.66° 90.00°	Depositor
Resolution (Å)	28.70 – 2.30	Depositor
% Data completeness (in resolution range)	96.7 (28.70-2.30)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.245 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10117	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.42	0/1405	0.64	0/1897
1	C	0.41	0/1405	0.63	0/1897
2	B	0.36	0/3638	0.63	1/4954 (0.0%)
2	D	0.36	0/3486	0.63	4/4744 (0.1%)
All	All	0.38	0/9934	0.63	5/13492 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	306	PRO	C-N-CD	-7.15	104.87	120.60
2	D	306	PRO	N-CA-C	-7.15	93.51	112.10
2	D	312	LYS	N-CA-C	-6.19	94.29	111.00
2	D	310	THR	N-CA-C	-6.00	94.80	111.00
2	B	302	GLU	N-CA-C	5.42	125.64	111.00

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	1371	0	1393	49	0
1	C	1371	0	1393	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3573	0	3564	154	1
2	D	3424	0	3413	158	1
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	32	0	13	4	0
4	C	32	0	13	2	0
5	A	77	0	0	5	0
5	B	121	0	0	6	0
5	C	29	0	0	3	0
5	D	85	0	0	3	0
All	All	10117	0	9789	400	1

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 20.

All (400) 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)
2:D:250:GLN:HE22	2:D:308:GLU:HB3	1.17	1.07
1:C:75:LEU:HD13	2:D:10:THR:HG22	1.37	1.05
2:B:406:VAL:HG23	2:B:407:ILE:H	1.25	0.99
2:D:250:GLN:HE22	2:D:308:GLU:CB	1.77	0.98
2:B:310:THR:HG22	2:B:312:LYS:HD3	1.51	0.92
2:D:307:PRO:HB2	2:D:308:GLU:OE1	1.74	0.87
2:D:297:ALA:HB2	2:D:309:HIS:CD2	2.12	0.84
1:A:75:LEU:HD13	2:B:10:THR:HG22	1.60	0.81
2:B:406:VAL:HG23	2:B:407:ILE:N	1.96	0.80
2:B:403:LYS:HE2	2:B:444:ILE:HD11	1.64	0.79
2:D:302:GLU:C	2:D:304:GLY:H	1.83	0.78
2:D:146:MET:O	2:D:150:THR:HG23	1.84	0.77
2:B:162:ASP:OD2	2:B:164:GLU:HB2	1.83	0.77
2:D:46:ASN:ND2	2:D:48:GLY:H	1.83	0.76
2:B:299:GLU:C	2:B:301:ALA:H	1.89	0.75
2:D:323:VAL:O	2:D:327:THR:HG23	1.86	0.75
2:B:46:ASN:ND2	2:B:48:GLY:H	1.83	0.75
2:B:397:PRO:HB2	2:B:402:LEU:HG	1.69	0.74
2:B:253:GLU:OE2	2:B:312:LYS:HG3	1.88	0.74
2:B:146:MET:O	2:B:150:THR:HG23	1.87	0.74
2:D:250:GLN:NE2	2:D:308:GLU:HB3	1.99	0.74
2:B:102:GLU:OE1	2:B:107:SER:HB2	1.87	0.73
2:B:405:LEU:HA	2:B:409:ALA:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:297:ALA:HB2	2:D:309:HIS:NE2	2.04	0.73
2:B:323:VAL:O	2:B:327:THR:HG23	1.88	0.73
1:A:26:PHE:CE1	1:A:149:ILE:HD11	2.23	0.73
2:D:174:LEU:HD11	2:D:218:ILE:HD11	1.70	0.72
2:D:94:TYR:O	2:D:98:THR:HG22	1.89	0.72
2:B:444:ILE:O	2:B:444:ILE:HG13	1.90	0.72
2:D:364:VAL:HB	2:D:365:PRO:HD3	1.71	0.72
2:B:118:CYS:SG	2:B:161:ILE:HG23	2.30	0.72
2:B:364:VAL:HB	2:B:365:PRO:HD3	1.72	0.72
2:B:399:PRO:HA	2:B:402:LEU:HB2	1.71	0.72
1:C:75:LEU:CD1	2:D:10:THR:HG22	2.17	0.72
2:D:66:THR:HG22	2:D:67:SER:H	1.55	0.71
2:B:95:VAL:O	2:B:98:THR:HG23	1.90	0.71
2:B:94:TYR:O	2:B:98:THR:HG22	1.90	0.70
2:D:95:VAL:O	2:D:98:THR:HG23	1.92	0.70
2:B:399:PRO:HG3	2:B:441:GLU:HB3	1.73	0.69
2:D:102:GLU:OE1	2:D:107:SER:HB2	1.93	0.69
2:B:406:VAL:CG2	2:B:407:ILE:H	2.03	0.69
2:B:444:ILE:O	2:B:445:ASN:HB2	1.91	0.69
2:B:66:THR:HG22	2:B:67:SER:H	1.57	0.69
2:B:157:ILE:O	2:B:161:ILE:HG13	1.93	0.69
2:B:44:LEU:HD13	2:B:98:THR:HG21	1.76	0.68
1:C:116:PRO:HB3	1:C:167:LYS:HG2	1.77	0.67
2:B:336:ASN:ND2	5:B:607:HOH:O	2.19	0.67
2:B:402:LEU:C	2:B:404:PRO:HD2	2.14	0.67
2:D:384:ASP:OD2	2:D:423:VAL:HG12	1.93	0.67
1:A:116:PRO:HB3	1:A:167:LYS:HG2	1.76	0.67
2:B:256:MET:O	2:B:258:PRO:HD2	1.94	0.67
2:D:256:MET:O	2:D:258:PRO:HD2	1.95	0.67
2:D:203:GLU:HG2	2:D:247:LEU:HD11	1.77	0.66
2:B:334:ASP:OD2	5:B:607:HOH:O	2.13	0.66
2:D:293:LEU:HD13	2:D:311:SER:CB	2.26	0.66
2:D:309:HIS:ND1	2:D:309:HIS:C	2.49	0.66
1:C:26:PHE:CE1	1:C:149:ILE:HD11	2.31	0.66
2:B:403:LYS:O	2:B:406:VAL:HG22	1.96	0.65
2:D:256:MET:HE3	2:D:261:PHE:HB2	1.79	0.65
1:C:95:ARG:NE	1:C:95:ARG:H	1.94	0.65
2:B:168:ASP:OD1	2:B:169:LYS:HG3	1.96	0.65
2:B:309:HIS:HE1	2:B:311:SER:HB3	1.62	0.65
2:B:123:VAL:HG12	2:B:123:VAL:O	1.97	0.65
1:C:19:GLY:HA3	1:C:69:GLN:HE21	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LYS:NZ	1:A:28:LYS:HB3	2.12	0.64
1:A:95:ARG:NE	1:A:95:ARG:H	1.95	0.64
1:C:172:PRO:HB2	2:D:336:ASN:HD21	1.63	0.64
2:D:132:GLN:HE21	2:D:136:ASN:HD21	1.45	0.64
1:C:122:ASN:HA	1:C:149:ILE:HG22	1.80	0.64
2:D:44:LEU:O	2:D:54:ARG:NH1	2.31	0.64
2:B:256:MET:HE3	2:B:261:PHE:HB2	1.80	0.63
2:D:328:GLN:O	2:D:331:THR:HB	1.97	0.63
2:B:445:ASN:OD1	2:B:448:TYR:HB2	1.99	0.63
1:A:28:LYS:HG2	5:A:697:HOH:O	1.99	0.63
2:D:338:ASP:HB3	2:D:341:ASP:CG	2.19	0.63
2:B:161:ILE:HD12	2:B:161:ILE:O	1.98	0.63
2:B:328:GLN:O	2:B:331:THR:HB	1.98	0.62
1:A:19:GLY:HA3	1:A:69:GLN:HE21	1.65	0.62
2:D:7:LEU:O	2:D:10:THR:OG1	2.18	0.62
2:D:302:GLU:C	2:D:304:GLY:N	2.52	0.62
1:A:29:ARG:HD3	1:A:154:ASN:OD1	1.99	0.62
1:C:29:ARG:HD3	1:C:154:ASN:OD1	1.99	0.62
1:C:28:LYS:NZ	1:C:28:LYS:HB3	2.15	0.62
2:D:123:VAL:HG12	2:D:123:VAL:O	1.99	0.62
2:B:401:GLN:O	2:B:404:PRO:HD3	2.00	0.62
2:B:403:LYS:HD3	2:B:442:ALA:HB1	1.81	0.61
2:D:15:ARG:O	2:D:19:GLU:HG3	2.00	0.61
2:D:124:ASN:CG	2:D:124:ASN:O	2.38	0.61
2:B:297:ALA:HB2	2:B:309:HIS:CD2	2.35	0.61
2:D:15:ARG:HG3	2:D:16:LEU:N	2.15	0.61
1:C:19:GLY:HA3	1:C:69:GLN:NE2	2.15	0.61
2:B:309:HIS:CE1	2:B:311:SER:H	2.18	0.61
2:D:44:LEU:HD13	2:D:98:THR:HG21	1.83	0.61
1:A:122:ASN:HA	1:A:149:ILE:HG22	1.80	0.61
2:B:124:ASN:O	2:B:124:ASN:CG	2.39	0.60
1:C:29:ARG:HD2	1:C:151:ALA:O	2.01	0.60
2:B:297:ALA:O	2:B:299:GLU:N	2.34	0.60
2:B:403:LYS:NZ	2:B:406:VAL:HG11	2.16	0.60
2:D:71:ASP:O	2:D:75:GLN:HG3	2.00	0.60
2:B:15:ARG:HG3	2:B:16:LEU:N	2.17	0.60
2:D:391:GLY:HA3	2:D:431:THR:HG23	1.83	0.60
2:B:71:ASP:O	2:B:75:GLN:HG3	2.00	0.60
2:B:406:VAL:HG23	2:B:407:ILE:HG13	1.82	0.60
2:D:178:ILE:HD12	2:D:221:VAL:HG11	1.84	0.60
2:D:360:GLU:O	2:D:397:PRO:HA	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ARG:HD2	1:A:151:ALA:O	2.02	0.60
1:A:118:VAL:HG22	1:A:163:TRP:CE3	2.37	0.60
2:B:15:ARG:O	2:B:19:GLU:HG3	2.02	0.60
2:B:7:LEU:O	2:B:10:THR:OG1	2.20	0.59
1:C:93:THR:HG22	1:C:93:THR:O	2.02	0.59
2:D:163:PRO:O	2:D:167:GLN:OE1	2.19	0.59
1:C:43:LEU:HD13	1:C:72:PHE:HB3	1.84	0.59
2:D:356:ALA:HA	2:D:363:ILE:HG12	1.84	0.59
2:D:136:ASN:HB3	2:D:150:THR:HG21	1.85	0.59
1:A:93:THR:HG22	1:A:93:THR:O	2.02	0.59
2:B:374:HIS:HD2	2:B:377:ASN:HD22	1.51	0.58
2:B:253:GLU:CD	2:B:312:LYS:HE3	2.23	0.58
1:A:19:GLY:HA3	1:A:69:GLN:NE2	2.18	0.58
2:B:132:GLN:HE21	2:B:136:ASN:HD21	1.49	0.58
1:A:118:VAL:HG23	1:A:164:LEU:HD21	1.85	0.58
2:D:293:LEU:HD13	2:D:311:SER:HB2	1.85	0.58
2:B:105:ARG:HH11	2:B:105:ARG:HG2	1.67	0.58
1:C:118:VAL:HG22	1:C:163:TRP:CE3	2.39	0.58
2:D:83:ILE:HB	2:D:88:ARG:HD2	1.85	0.58
2:D:356:ALA:O	2:D:360:GLU:HA	2.04	0.58
1:A:43:LEU:HD13	1:A:72:PHE:HB3	1.84	0.57
2:B:93:ASN:O	2:B:97:GLN:HG3	2.04	0.57
2:B:387:VAL:HG11	2:B:428:ALA:HA	1.86	0.57
2:D:132:GLN:HE21	2:D:136:ASN:ND2	2.01	0.57
2:B:405:LEU:HD13	2:B:435:ILE:CG2	2.34	0.57
1:A:54:THR:CB	1:A:174:LEU:HD11	2.35	0.57
2:B:356:ALA:HA	2:B:363:ILE:HG12	1.85	0.57
2:D:174:LEU:O	2:D:178:ILE:HG12	2.04	0.57
2:D:93:ASN:O	2:D:97:GLN:HG3	2.05	0.57
2:D:353:MET:O	2:D:356:ALA:HB3	2.05	0.57
2:D:138:THR:HA	2:D:179:GLN:HE22	1.70	0.57
1:C:54:THR:CB	1:C:174:LEU:HD11	2.35	0.57
2:D:250:GLN:NE2	2:D:308:GLU:CB	2.59	0.57
2:B:122:PRO:HB3	2:B:165:GLN:HG3	1.86	0.56
2:B:405:LEU:HD13	2:B:435:ILE:HG21	1.87	0.56
2:D:399:PRO:O	2:D:403:LYS:HG3	2.05	0.56
1:A:177:VAL:N	5:A:514:HOH:O	2.38	0.56
1:C:118:VAL:HG23	1:C:164:LEU:HD21	1.88	0.56
2:D:374:HIS:HD2	2:D:377:ASN:HD22	1.52	0.56
2:D:402:LEU:O	2:D:406:VAL:HG22	2.06	0.56
2:B:403:LYS:N	2:B:404:PRO:CD	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLU:OE2	2:B:105:ARG:HG3	2.06	0.56
2:B:132:GLN:HE21	2:B:136:ASN:ND2	2.04	0.56
2:B:356:ALA:O	2:B:360:GLU:HA	2.05	0.56
2:B:105:ARG:HG2	2:B:105:ARG:NH1	2.21	0.55
1:A:20:GLY:H	4:A:250:GNP:HNB3	1.53	0.55
2:B:21:ALA:O	2:B:25:LEU:HD22	2.07	0.55
2:B:337:ASP:OD1	5:B:607:HOH:O	2.18	0.55
2:B:391:GLY:HA3	2:B:431:THR:HG23	1.89	0.55
2:B:256:MET:C	2:B:258:PRO:HD2	2.27	0.55
1:A:164:LEU:O	1:A:168:LEU:HD22	2.07	0.55
2:B:309:HIS:HE1	2:B:311:SER:CB	2.20	0.55
2:B:203:GLU:HG2	2:B:247:LEU:HD11	1.90	0.54
2:B:299:GLU:C	2:B:301:ALA:N	2.59	0.54
2:D:34:PRO:HG3	2:D:83:ILE:HD12	1.90	0.54
2:D:203:GLU:HG2	2:D:247:LEU:CD1	2.37	0.54
2:D:207:ALA:HB3	5:D:753:HOH:O	2.07	0.54
2:D:264:THR:HG21	2:D:282:PHE:CD2	2.43	0.54
2:B:3:LEU:HD12	2:B:39:GLU:HG2	1.89	0.54
2:D:3:LEU:HD12	2:D:39:GLU:HG2	1.90	0.54
2:D:73:LYS:O	2:D:77:GLN:HG3	2.08	0.54
2:B:66:THR:HG22	2:B:67:SER:N	2.21	0.54
2:B:264:THR:HG21	2:B:282:PHE:CD2	2.43	0.54
2:D:300:ALA:O	2:D:301:ALA:HB3	2.07	0.54
2:D:359:CYS:O	2:D:361:ASP:N	2.42	0.53
2:D:410:MET:CE	2:D:414:ILE:HD11	2.38	0.53
2:B:44:LEU:O	2:B:54:ARG:NH1	2.42	0.53
2:D:21:ALA:O	2:D:25:LEU:HD22	2.08	0.53
2:D:66:THR:HG22	2:D:67:SER:N	2.22	0.53
2:D:256:MET:C	2:D:258:PRO:HD2	2.29	0.53
1:C:12:LYS:NZ	1:C:79:TYR:O	2.39	0.53
1:C:142:LYS:HE2	5:C:755:HOH:O	2.08	0.53
1:C:164:LEU:O	1:C:168:LEU:HD22	2.09	0.53
2:B:73:LYS:O	2:B:77:GLN:HG3	2.09	0.53
2:D:122:PRO:HA	2:D:165:GLN:NE2	2.23	0.52
2:D:253:GLU:CD	2:D:312:LYS:HZ2	2.11	0.52
2:B:403:LYS:CE	2:B:444:ILE:HD11	2.36	0.52
2:D:303:GLN:O	2:D:305:ARG:N	2.42	0.52
2:B:62:LYS:HG3	2:B:111:GLN:HB3	1.91	0.52
2:B:359:CYS:O	2:B:361:ASP:N	2.42	0.52
1:C:20:GLY:H	4:C:252:GNP:HNB3	1.57	0.52
2:B:336:ASN:C	2:B:336:ASN:HD22	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:THR:HG22	5:B:538:HOH:O	2.09	0.52
2:D:105:ARG:HH11	2:D:105:ARG:HG2	1.74	0.52
2:D:159:GLN:HB2	2:D:200:ASN:HB3	1.92	0.52
2:D:308:GLU:OE1	2:D:308:GLU:N	2.43	0.52
2:B:179:GLN:O	2:B:182:ARG:HG2	2.10	0.52
1:C:10:GLN:HA	1:C:60:LYS:O	2.10	0.52
1:A:113:GLU:CD	2:B:105:ARG:HG3	2.31	0.51
2:D:398:GLU:OE1	2:D:399:PRO:HD2	2.10	0.51
2:B:33:LEU:HD22	2:B:37:LEU:HG	1.91	0.51
2:B:306:PRO:O	2:B:307:PRO:C	2.49	0.51
2:D:45:ALA:HA	2:D:98:THR:HB	1.92	0.51
2:D:256:MET:HG2	2:D:314:TYR:CD1	2.46	0.51
2:B:99:LEU:HD22	2:B:149:SER:HB3	1.91	0.51
2:B:363:ILE:HD12	2:B:363:ILE:H	1.76	0.51
2:D:178:ILE:HG22	2:D:182:ARG:HD3	1.92	0.51
2:D:300:ALA:HB1	2:D:303:GLN:HB2	1.91	0.51
2:D:227:GLN:HG3	5:D:575:HOH:O	2.11	0.51
2:D:302:GLU:O	2:D:302:GLU:HG3	2.10	0.51
2:D:80:TRP:O	2:D:88:ARG:HD2	2.11	0.51
2:B:183:LYS:N	2:B:224:GLU:OE2	2.42	0.50
2:D:136:ASN:CB	2:D:150:THR:HG21	2.42	0.50
1:A:10:GLN:HA	1:A:60:LYS:O	2.11	0.50
2:D:33:LEU:HD22	2:D:37:LEU:HG	1.92	0.50
2:D:25:LEU:HD12	2:D:36:PHE:HZ	1.77	0.50
2:D:363:ILE:HD12	2:D:363:ILE:H	1.77	0.50
1:A:91:ASP:CG	1:A:123:LYS:HD2	2.32	0.50
1:A:54:THR:HB	1:A:174:LEU:HD11	1.93	0.50
1:A:12:LYS:NZ	1:A:79:TYR:O	2.39	0.50
1:C:159:LYS:HB2	1:C:160:PRO:HD3	1.92	0.50
2:B:3:LEU:HD23	2:B:6:ILE:HD11	1.93	0.50
2:B:6:ILE:HD12	2:B:7:LEU:N	2.27	0.50
2:D:293:LEU:O	2:D:309:HIS:CD2	2.65	0.50
2:D:105:ARG:HG2	2:D:105:ARG:NH1	2.27	0.49
1:A:159:LYS:HB2	1:A:160:PRO:HD3	1.94	0.49
1:C:92:VAL:HG11	1:C:129:ARG:NE	2.27	0.49
1:C:54:THR:HB	1:C:174:LEU:HD11	1.93	0.49
1:A:92:VAL:HG11	1:A:129:ARG:NE	2.27	0.49
4:A:250:GNP:O1G	5:A:597:HOH:O	2.20	0.49
2:B:446:ASP:O	2:B:447:VAL:HG12	2.12	0.49
2:B:444:ILE:O	2:B:445:ASN:CB	2.57	0.49
2:D:122:PRO:HA	2:D:165:GLN:CD	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:CYS:HA	2:B:161:ILE:CG2	2.43	0.49
2:D:3:LEU:HD23	2:D:6:ILE:HD11	1.95	0.49
2:D:302:GLU:O	2:D:304:GLY:N	2.46	0.49
2:D:42:ARG:NH2	2:D:94:TYR:OH	2.46	0.48
2:D:222:VAL:O	2:D:226:THR:HG23	2.13	0.48
2:D:387:VAL:HG22	2:D:416:LEU:HD13	1.95	0.48
2:B:296:GLU:OE2	2:B:309:HIS:HB2	2.13	0.48
1:A:75:LEU:CD1	2:B:10:THR:HG22	2.39	0.48
2:B:453:LEU:O	2:B:457:ILE:HG13	2.14	0.48
2:D:360:GLU:O	2:D:397:PRO:HG3	2.13	0.48
2:D:404:PRO:HA	2:D:407:ILE:HG22	1.96	0.48
2:B:87:ALA:O	2:B:90:GLU:HB2	2.14	0.48
1:A:56:ARG:HD2	1:A:171:ASP:OD2	2.14	0.48
2:B:11:VAL:HG22	5:B:612:HOH:O	2.12	0.48
1:C:56:ARG:HD2	1:C:171:ASP:OD2	2.14	0.48
1:C:91:ASP:CG	1:C:123:LYS:HD2	2.33	0.48
2:B:310:THR:O	2:B:311:SER:C	2.51	0.48
2:D:66:THR:HG23	2:D:73:LYS:CD	2.44	0.48
2:D:309:HIS:ND1	2:D:310:THR:N	2.61	0.47
2:B:183:LYS:HB2	2:B:224:GLU:OE2	2.14	0.47
2:B:405:LEU:CA	2:B:409:ALA:HB3	2.43	0.47
2:B:274:GLU:H	2:B:274:GLU:CD	2.17	0.47
1:C:77:ASP:HB3	2:D:59:LEU:HD13	1.96	0.47
2:D:274:GLU:H	2:D:274:GLU:CD	2.16	0.47
2:D:3:LEU:O	2:D:6:ILE:HG13	2.14	0.47
1:A:28:LYS:HB3	1:A:28:LYS:HZ2	1.79	0.47
2:D:9:LYS:HD3	2:D:17:GLU:OE1	2.15	0.47
2:D:410:MET:HE1	2:D:414:ILE:HD11	1.97	0.47
2:D:403:LYS:HB2	2:D:404:PRO:CD	2.45	0.47
2:B:185:GLU:O	2:B:191:LYS:NZ	2.30	0.47
2:B:25:LEU:HD12	2:B:36:PHE:CZ	2.51	0.46
2:B:443:ALA:HA	2:B:449:LEU:CD1	2.46	0.46
2:D:360:GLU:C	2:D:363:ILE:HD11	2.36	0.46
1:A:12:LYS:HD3	1:A:83:ALA:HA	1.97	0.46
2:B:402:LEU:C	2:B:404:PRO:CD	2.81	0.46
2:D:121:ILE:N	2:D:122:PRO:HD2	2.31	0.46
2:D:398:GLU:OE1	2:D:398:GLU:HA	2.16	0.46
2:B:45:ALA:HA	2:B:98:THR:HB	1.97	0.46
2:D:6:ILE:HD12	2:D:7:LEU:N	2.30	0.46
2:B:222:VAL:O	2:B:226:THR:HG23	2.16	0.45
2:D:138:THR:HA	2:D:179:GLN:NE2	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:302:GLU:OE1	2:D:304:GLY:HA2	2.16	0.45
2:B:92:LYS:HD2	2:B:126:TRP:CE2	2.52	0.45
2:B:360:GLU:C	2:B:363:ILE:HD11	2.36	0.45
2:D:122:PRO:HB3	2:D:165:GLN:HG2	1.98	0.45
2:D:296:GLU:OE2	2:D:308:GLU:HG2	2.16	0.45
1:A:54:THR:C	1:A:56:ARG:H	2.20	0.45
1:C:95:ARG:NH1	1:C:95:ARG:HB2	2.31	0.45
1:C:12:LYS:HD3	1:C:83:ALA:HA	1.97	0.45
2:D:62:LYS:HG3	2:D:111:GLN:HB3	1.97	0.45
2:D:83:ILE:HB	2:D:88:ARG:CD	2.46	0.45
1:C:157:PHE:CE1	1:C:158:GLU:HG3	2.52	0.45
2:D:293:LEU:HD13	2:D:311:SER:HB3	1.97	0.45
1:A:39:TYR:CD1	1:A:39:TYR:C	2.90	0.45
2:B:121:ILE:N	2:B:122:PRO:HD2	2.32	0.45
2:D:4:ILE:HD13	2:D:49:ASN:OD1	2.17	0.45
2:D:375:ILE:HD11	2:D:416:LEU:HD11	1.98	0.45
1:A:95:ARG:NH1	1:A:95:ARG:HB2	2.32	0.45
2:D:390:PHE:CE2	2:D:413:LEU:HD11	2.52	0.45
2:B:343:ASN:HB2	2:B:344:PRO:CD	2.47	0.45
2:B:312:LYS:NZ	2:B:312:LYS:HB3	2.32	0.45
2:B:427:THR:O	2:B:431:THR:OG1	2.34	0.45
1:C:28:LYS:HB3	1:C:28:LYS:HZ2	1.81	0.45
1:C:82:GLN:OE1	2:D:11:VAL:HG21	2.17	0.45
2:D:295:ILE:O	2:D:299:GLU:HG3	2.17	0.45
2:D:25:LEU:HD12	2:D:36:PHE:CZ	2.52	0.44
1:A:113:GLU:HG3	2:B:106:PRO:HD3	1.99	0.44
2:B:130:ILE:HB	2:B:131:PRO:HD3	1.99	0.44
2:D:427:THR:O	2:D:431:THR:OG1	2.35	0.44
1:A:157:PHE:CE1	1:A:158:GLU:HG3	2.51	0.44
1:C:54:THR:OG1	1:C:174:LEU:HD11	2.17	0.44
2:D:161:ILE:HG12	2:D:162:ASP:N	2.32	0.44
1:A:122:ASN:CA	1:A:149:ILE:HG22	2.47	0.44
2:B:136:ASN:HB3	2:B:150:THR:HG21	1.98	0.44
1:C:9:VAL:HG13	5:C:766:HOH:O	2.18	0.44
1:C:54:THR:C	1:C:56:ARG:H	2.19	0.44
1:C:122:ASN:OD1	1:C:149:ILE:HG23	2.17	0.44
1:C:126:ILE:HD11	4:C:252:GNP:N2	2.33	0.44
2:B:130:ILE:HG12	5:B:617:HOH:O	2.16	0.44
2:D:87:ALA:O	2:D:90:GLU:HB2	2.16	0.44
2:B:402:LEU:HB3	2:B:438:LEU:HD21	2.00	0.44
2:D:96:LEU:HG	2:D:126:TRP:HZ2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:402:LEU:O	2:D:406:VAL:HG13	2.18	0.44
1:C:39:TYR:CD1	1:C:39:TYR:C	2.90	0.43
2:B:6:ILE:CD1	2:B:25:LEU:HD11	2.48	0.43
2:B:402:LEU:O	2:B:405:LEU:HD23	2.17	0.43
1:C:122:ASN:CA	1:C:149:ILE:HG22	2.47	0.43
1:A:91:ASP:OD1	1:A:123:LYS:HD2	2.18	0.43
2:D:168:ASP:OD2	2:D:169:LYS:HG3	2.18	0.43
2:B:130:ILE:O	2:B:134:VAL:HG23	2.19	0.43
1:A:153:SER:O	1:A:154:ASN:HB2	2.19	0.43
1:C:91:ASP:OD1	1:C:123:LYS:HD2	2.18	0.43
2:D:130:ILE:HG13	2:D:166:LEU:HD11	2.01	0.43
2:D:217:PHE:O	2:D:220:GLN:HB3	2.19	0.43
1:A:92:VAL:O	1:A:92:VAL:CG1	2.67	0.43
1:A:177:VAL:N	5:A:608:HOH:O	2.52	0.43
4:A:250:GNP:O2B	5:A:597:HOH:O	2.21	0.43
2:B:253:GLU:OE1	2:B:312:LYS:HE3	2.18	0.43
2:D:11:VAL:O	2:D:11:VAL:HG22	2.19	0.43
2:D:306:PRO:HG2	2:D:309:HIS:HB3	2.01	0.43
2:B:3:LEU:HD12	2:B:39:GLU:CG	2.48	0.42
2:B:25:LEU:HD12	2:B:36:PHE:HZ	1.84	0.42
2:B:387:VAL:CG2	2:B:416:LEU:HD13	2.49	0.42
1:A:26:PHE:HE1	1:A:149:ILE:HD11	1.78	0.42
1:C:77:ASP:HB2	2:D:63:ASN:HD21	1.84	0.42
2:D:253:GLU:CG	2:D:312:LYS:HZ3	2.32	0.42
2:B:310:THR:HG22	2:B:312:LYS:CD	2.37	0.42
2:B:363:ILE:H	2:B:363:ILE:CD1	2.32	0.42
1:A:13:LEU:HD23	1:A:13:LEU:C	2.39	0.42
2:B:32:ASN:OD1	2:B:34:PRO:HD2	2.19	0.42
2:B:83:ILE:HB	2:B:88:ARG:HD2	2.02	0.42
2:B:218:ILE:O	2:B:222:VAL:HG23	2.19	0.42
2:D:11:VAL:HG22	5:D:580:HOH:O	2.19	0.42
2:D:253:GLU:CG	2:D:312:LYS:NZ	2.83	0.42
1:A:54:THR:OG1	1:A:174:LEU:HD11	2.20	0.42
2:D:132:GLN:NE2	2:D:136:ASN:HD21	2.16	0.42
1:A:126:ILE:HD11	4:A:250:GNP:N2	2.34	0.42
2:D:169:LYS:O	2:D:172:GLU:HG3	2.19	0.42
2:B:105:ARG:HH11	2:B:105:ARG:CG	2.33	0.42
1:A:122:ASN:O	1:A:123:LYS:HB2	2.20	0.42
2:B:250:GLN:H	2:B:250:GLN:HG2	1.62	0.42
1:C:9:VAL:CG1	5:C:766:HOH:O	2.67	0.42
2:D:299:GLU:O	2:D:300:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:391:GLY:CA	2:D:431:THR:HG23	2.49	0.42
2:B:360:GLU:O	2:B:397:PRO:HA	2.19	0.41
2:B:403:LYS:CE	2:B:406:VAL:HG11	2.51	0.41
2:B:405:LEU:HD13	2:B:435:ILE:HG23	2.02	0.41
2:D:15:ARG:HG3	2:D:16:LEU:H	1.84	0.41
2:D:130:ILE:O	2:D:134:VAL:HG23	2.21	0.41
2:D:387:VAL:CG2	2:D:416:LEU:HD13	2.49	0.41
2:D:130:ILE:HB	2:D:131:PRO:HD3	2.01	0.41
2:D:400:SER:O	2:D:404:PRO:CD	2.68	0.41
2:B:151:LEU:HD13	2:B:194:ALA:HB2	2.01	0.41
2:B:235:VAL:O	2:B:239:GLN:HG3	2.20	0.41
2:B:343:ASN:HB2	2:B:344:PRO:HD2	2.02	0.41
2:B:405:LEU:HA	2:B:409:ALA:CB	2.42	0.41
2:D:32:ASN:CG	2:D:35:THR:OG1	2.59	0.41
1:A:28:LYS:HB3	1:A:28:LYS:HZ3	1.85	0.41
1:C:92:VAL:O	1:C:92:VAL:CG1	2.68	0.41
2:D:34:PRO:O	2:D:38:VAL:HG23	2.20	0.41
2:B:34:PRO:O	2:B:38:VAL:HG23	2.20	0.41
2:B:123:VAL:O	2:B:123:VAL:CG1	2.66	0.41
2:D:323:VAL:O	2:D:327:THR:CG2	2.62	0.41
2:B:34:PRO:HG3	2:B:83:ILE:HG23	2.03	0.41
2:D:377:ASN:HA	2:D:378:PRO:HD3	1.91	0.41
2:D:361:ASP:N	2:D:361:ASP:OD1	2.54	0.41
1:A:76:ARG:HB2	1:A:77:ASP:H	1.48	0.41
2:B:139:ASN:HA	2:B:140:PRO:HD3	1.94	0.41
2:B:293:LEU:HB3	2:B:311:SER:HB2	2.02	0.41
2:B:422:VAL:HG12	2:B:425:ARG:NH1	2.36	0.41
2:B:430:TRP:CZ2	2:B:434:ARG:HD2	2.56	0.41
1:C:153:SER:O	1:C:154:ASN:HB2	2.20	0.41
2:D:419:ASP:OD2	2:D:421:SER:HB3	2.21	0.41
2:D:422:VAL:HG12	2:D:425:ARG:NH1	2.36	0.41
1:A:146:TYR:CG	1:A:147:TYR:N	2.89	0.41
2:B:397:PRO:HB2	2:B:402:LEU:CG	2.45	0.41
2:B:305:ARG:O	2:B:306:PRO:C	2.59	0.40
2:B:447:VAL:O	2:B:447:VAL:HG22	2.21	0.40
1:C:30:HIS:CE1	1:C:157:PHE:O	2.75	0.40
1:C:81:ILE:HG22	1:C:82:GLN:HG3	2.03	0.40
2:D:183:LYS:HG2	2:D:224:GLU:OE2	2.21	0.40
2:D:253:GLU:HG2	2:D:312:LYS:HZ3	1.86	0.40
2:D:403:LYS:N	2:D:404:PRO:HD2	2.36	0.40
2:B:402:LEU:HA	2:B:402:LEU:HD23	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:VAL:CG2	2:B:407:ILE:N	2.67	0.40
1:C:45:VAL:HG22	1:C:46:GLU:N	2.36	0.40
2:D:161:ILE:HG12	2:D:162:ASP:H	1.86	0.40
2:D:403:LYS:HB2	2:D:404:PRO:HD3	2.03	0.40
2:D:371:ILE:O	2:D:375:ILE:HB	2.22	0.40
2:D:430:TRP:CZ2	2:D:434:ARG:HD2	2.57	0.40
2:B:450:ALA:HB3	2:B:451:PRO:CD	2.52	0.40
2:D:36:PHE:CZ	2:D:40:LEU:HD11	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:GLU:OE1	2:D:144:GLU:OE2[2_645]	2.04	0.16

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	167/216 (77%)	157 (94%)	8 (5%)	2 (1%)	13	14
1	C	167/216 (77%)	156 (93%)	9 (5%)	2 (1%)	13	14
2	B	456/462 (99%)	415 (91%)	30 (7%)	11 (2%)	6	4
2	D	436/462 (94%)	403 (92%)	24 (6%)	9 (2%)	7	5
All	All	1226/1356 (90%)	1131 (92%)	71 (6%)	24 (2%)	7	6

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	303	GLN
2	B	307	PRO

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Mol	Chain	Res	Type
2	B	360	GLU
2	B	407	ILE
2	B	444	ILE
2	B	445	ASN
2	D	302	GLU
2	D	307	PRO
2	D	360	GLU
1	A	127	LYS
1	C	127	LYS
2	D	304	GLY
2	D	308	GLU
2	B	409	ALA
2	D	105	ARG
1	A	113	GLU
2	B	403	LYS
1	C	113	GLU
2	D	303	GLN
2	B	105	ARG
2	B	259	ALA
2	D	259	ALA
2	D	298	SER
2	B	406	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	148/185 (80%)	143 (97%)	5 (3%)	37 51
1	C	148/185 (80%)	143 (97%)	5 (3%)	37 51
2	B	395/398 (99%)	359 (91%)	36 (9%)	9 11
2	D	379/398 (95%)	345 (91%)	34 (9%)	9 11
All	All	1070/1166 (92%)	990 (92%)	80 (8%)	13 17

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	39	TYR
1	A	77	ASP
1	A	95	ARG
1	A	157	PHE
2	B	3	LEU
2	B	8	GLU
2	B	10	THR
2	B	11	VAL
2	B	15	ARG
2	B	25	LEU
2	B	33	LEU
2	B	35	THR
2	B	44	LEU
2	B	46	ASN
2	B	62	LYS
2	B	98	THR
2	B	105	ARG
2	B	150	THR
2	B	162	ASP
2	B	192	LEU
2	B	209	PHE
2	B	217	PHE
2	B	220	GLN
2	B	250	GLN
2	B	253	GLU
2	B	303	GLN
2	B	309	HIS
2	B	312	LYS
2	B	320	GLN
2	B	327	THR
2	B	336	ASN
2	B	339	ASP
2	B	361	ASP
2	B	363	ILE
2	B	412	THR
2	B	427	THR
2	B	431	THR
2	B	439	LEU
2	B	448	TYR
2	B	449	LEU
1	C	29	ARG
1	C	39	TYR

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Mol	Chain	Res	Type
1	C	77	ASP
1	C	95	ARG
1	C	157	PHE
2	D	3	LEU
2	D	8	GLU
2	D	10	THR
2	D	15	ARG
2	D	25	LEU
2	D	33	LEU
2	D	35	THR
2	D	44	LEU
2	D	46	ASN
2	D	62	LYS
2	D	98	THR
2	D	105	ARG
2	D	150	THR
2	D	167	GLN
2	D	174	LEU
2	D	185	GLU
2	D	192	LEU
2	D	209	PHE
2	D	217	PHE
2	D	220	GLN
2	D	250	GLN
2	D	253	GLU
2	D	292	ASP
2	D	308	GLU
2	D	309	HIS
2	D	320	GLN
2	D	327	THR
2	D	361	ASP
2	D	363	ILE
2	D	408	GLN
2	D	412	THR
2	D	427	THR
2	D	431	THR
2	D	438	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN

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Mol	Chain	Res	Type
1	A	100	ASN
1	A	105	HIS
1	A	114	ASN
1	A	156	ASN
2	B	22	GLN
2	B	46	ASN
2	B	75	GLN
2	B	86	ASN
2	B	93	ASN
2	B	136	ASN
2	B	171	ASN
2	B	196	ASN
2	B	285	ASN
2	B	309	HIS
2	B	320	GLN
2	B	328	GLN
2	B	336	ASN
2	B	374	HIS
1	C	69	GLN
1	C	100	ASN
1	C	105	HIS
1	C	114	ASN
1	C	156	ASN
1	C	173	ASN
2	D	22	GLN
2	D	46	ASN
2	D	75	GLN
2	D	86	ASN
2	D	93	ASN
2	D	136	ASN
2	D	179	GLN
2	D	196	ASN
2	D	250	GLN
2	D	278	GLN
2	D	285	ASN
2	D	320	GLN
2	D	328	GLN
2	D	336	ASN
2	D	374	HIS
2	D	408	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	GNP	A	250	3	29,34,34	1.70	6 (20%)	33,54,54	2.22	5 (15%)
4	GNP	C	252	3	29,34,34	1.71	6 (20%)	33,54,54	2.18	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GNP	A	250	3	-	3/14/38/38	0/3/3/3
4	GNP	C	252	3	-	3/14/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	252	GNP	C6-N1	4.53	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	250	GNP	C6-N1	4.46	1.40	1.33
4	C	252	GNP	PG-O2G	-3.80	1.46	1.56
4	A	250	GNP	PG-O2G	-3.70	1.46	1.56
4	A	250	GNP	PB-O2B	-3.50	1.47	1.56
4	C	252	GNP	PB-O2B	-3.50	1.47	1.56
4	C	252	GNP	C5-C6	2.98	1.46	1.41
4	A	250	GNP	C5-C6	2.96	1.46	1.41
4	A	250	GNP	C8-N7	-2.77	1.29	1.34
4	C	252	GNP	C8-N7	-2.74	1.29	1.34
4	C	252	GNP	C4-N3	2.08	1.38	1.35
4	A	250	GNP	PB-O3A	2.00	1.61	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	250	GNP	C5-C6-N1	-7.96	112.55	123.43
4	C	252	GNP	C5-C6-N1	-7.93	112.58	123.43
4	A	250	GNP	C2-N1-C6	6.29	125.92	115.93
4	C	252	GNP	C2-N1-C6	6.23	125.82	115.93
4	A	250	GNP	O3G-PG-O1G	-4.18	102.93	113.45
4	A	250	GNP	N3-C2-N1	-3.89	122.04	127.22
4	C	252	GNP	N3-C2-N1	-3.72	122.26	127.22
4	C	252	GNP	O3G-PG-O1G	-3.72	104.10	113.45
4	C	252	GNP	C4-C5-C6	-2.30	118.60	120.80
4	A	250	GNP	C4-C5-C6	-2.24	118.66	120.80

There are no chirality outliers.

All (6) torsion outliers are listed below:

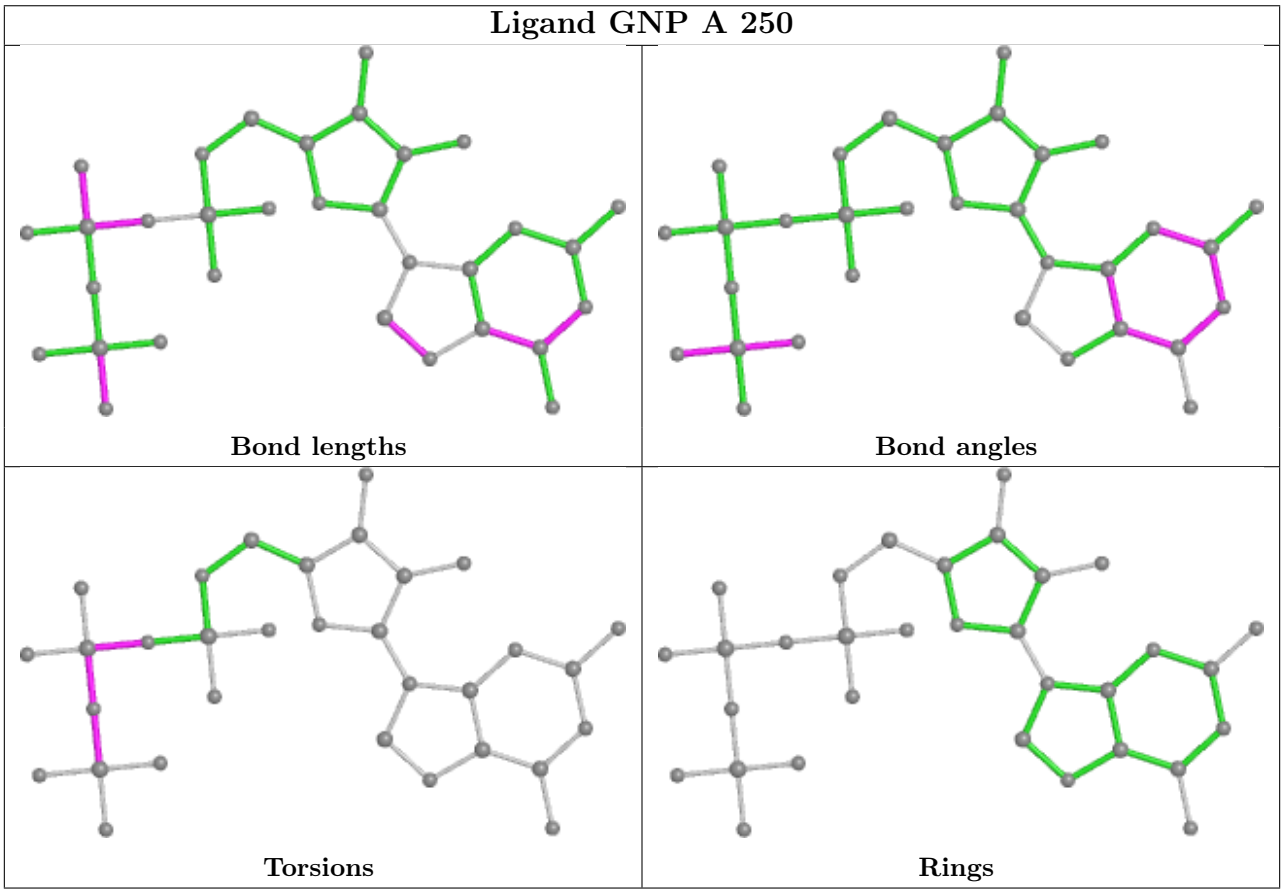
Mol	Chain	Res	Type	Atoms
4	A	250	GNP	PB-N3B-PG-O1G
4	A	250	GNP	PG-N3B-PB-O1B
4	A	250	GNP	PA-O3A-PB-O1B
4	C	252	GNP	PB-N3B-PG-O1G
4	C	252	GNP	PG-N3B-PB-O1B
4	C	252	GNP	PA-O3A-PB-O1B

There are no ring outliers.

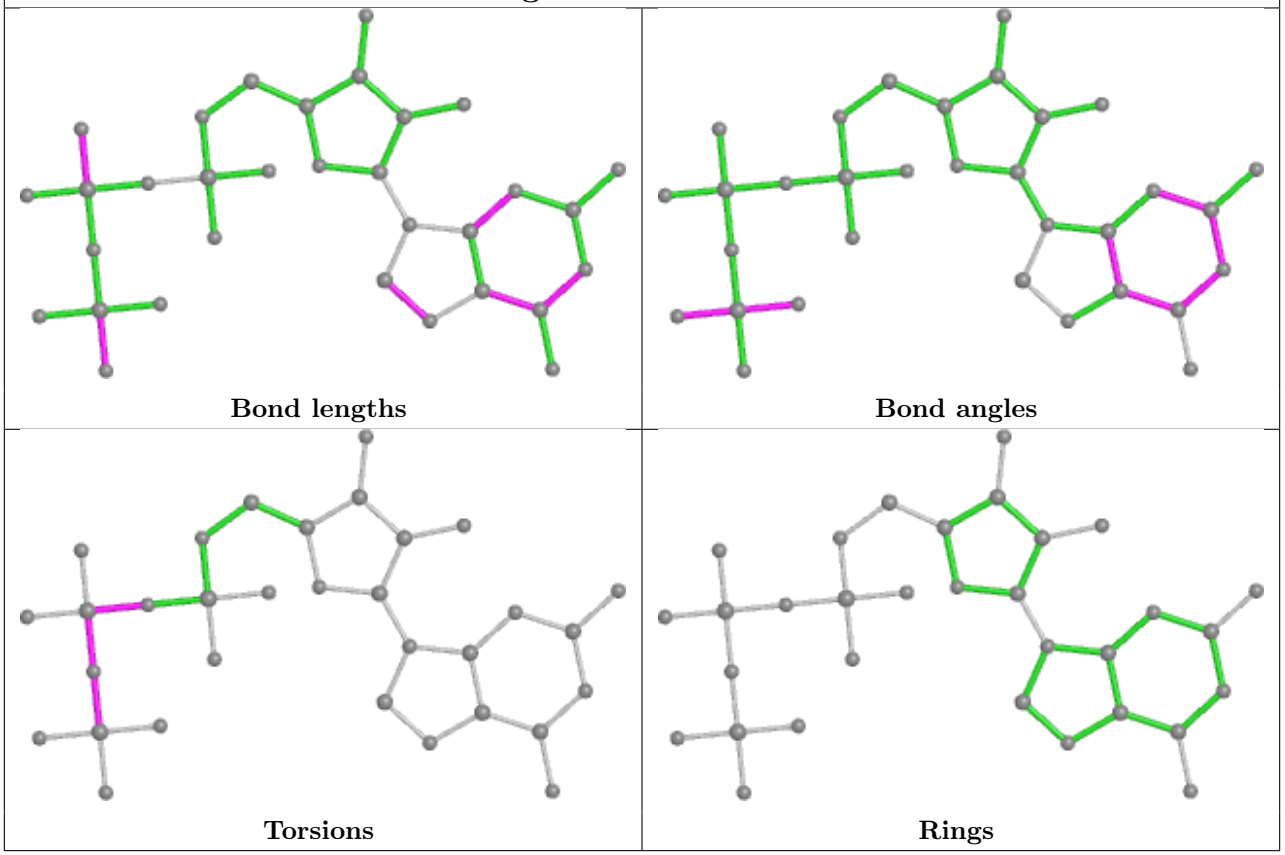
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	250	GNP	4	0
4	C	252	GNP	2	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 then 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.



Ligand GNP C 252



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.