



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:55 AM UTC

PDB ID : 1VG9 / pdb_00001vg9
Title : The crystal structures of the REP-1 protein in complex with C-terminally truncated Rab7 protein
Authors : Rak, A.; Pylypenko, O.; Niculae, A.; Pyatkov, K.; Goody, R.S.; Alexandrov, K.
Deposited on : 2004-04-23
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

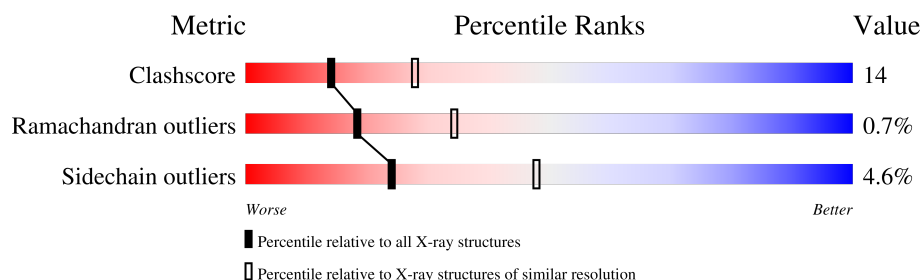
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	650	
1	C	650	
1	E	650	
1	G	650	
2	B	185	
2	D	185	
2	F	185	
2	H	185	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22604 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 Rab proteins geranylgeranyltransferase component A 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3993	2524	672	767	30			
1	C	502	Total	C	N	O	S	0	0	0
			3980	2516	670	764	30			
1	E	500	Total	C	N	O	S	0	0	0
			3988	2521	671	766	30			
1	G	502	Total	C	N	O	S	0	0	0
			3984	2518	670	766	30			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	LYS	GLN	engineered mutation	UNP P37727
A	462	ARG	LYS	engineered mutation	UNP P37727
A	473	THR	ALA	engineered mutation	UNP P37727
A	483	ALA	GLY	engineered mutation	UNP P37727
C	231	LYS	GLN	engineered mutation	UNP P37727
C	462	ARG	LYS	engineered mutation	UNP P37727
C	473	THR	ALA	engineered mutation	UNP P37727
C	483	ALA	GLY	engineered mutation	UNP P37727
E	231	LYS	GLN	engineered mutation	UNP P37727
E	462	ARG	LYS	engineered mutation	UNP P37727
E	473	THR	ALA	engineered mutation	UNP P37727
E	483	ALA	GLY	engineered mutation	UNP P37727
G	231	LYS	GLN	engineered mutation	UNP P37727
G	462	ARG	LYS	engineered mutation	UNP P37727
G	473	THR	ALA	engineered mutation	UNP P37727
G	483	ALA	GLY	engineered mutation	UNP P37727

- Molecule 2 is a protein called Ras-related protein Rab-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1335	849	225	255	6			
2	D	173	Total	C	N	O	S	0	0	0
			1371	870	233	262	6			
2	F	168	Total	C	N	O	S	0	0	0
			1332	847	227	252	6			
2	H	173	Total	C	N	O	S	0	0	0
			1371	870	233	262	6			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

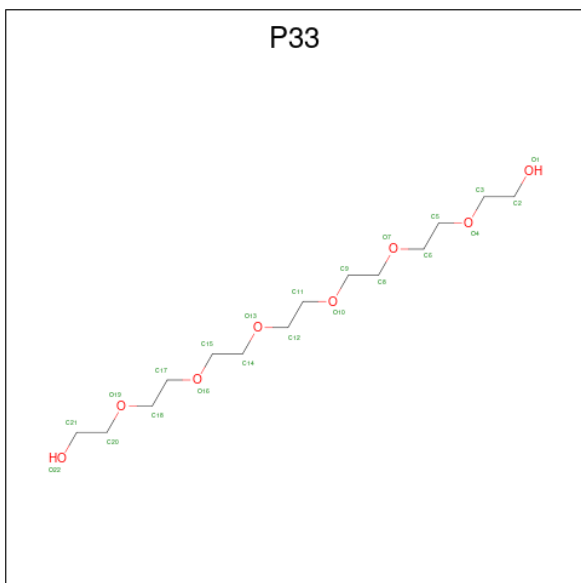
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		
4	F	1	Total	K	0	0
			1	1		
4	H	1	Total	K	0	0
			1	1		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
5	D	1	Total 28	C 10	N 5	O 11	P 2	0	0
5	F	1	Total 28	C 10	N 5	O 11	P 2	0	0
5	H	1	Total 28	C 10	N 5	O 11	P 2	0	0

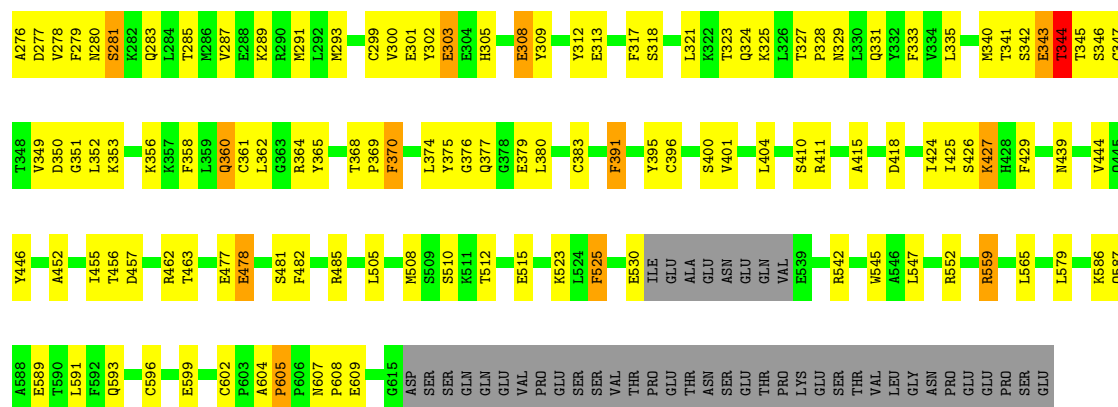
- Molecule 6 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (CCD ID: P33) (formula: $C_{14}H_{30}O_8$).



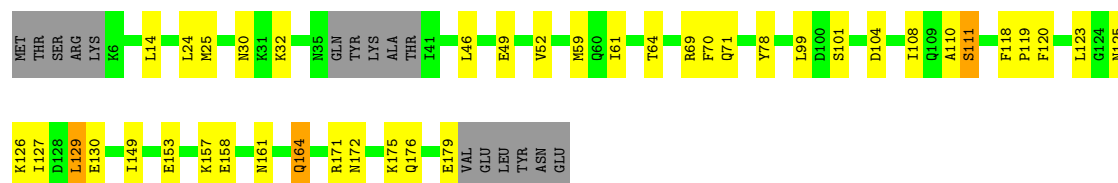
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			22	14	8		
6	D	1	Total	C	O	0	0
			22	14	8		
6	F	1	Total	C	O	0	0
			22	14	8		
6	H	1	Total	C	O	0	0
			22	14	8		

- Molecule 7 is water.

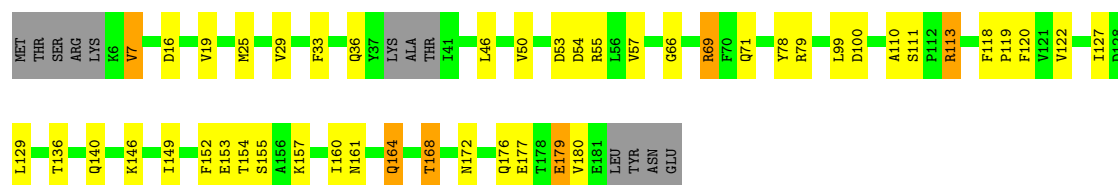
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	223	Total	O	0	0
			223	223		
7	B	62	Total	O	0	0
			62	62		
7	C	164	Total	O	0	0
			164	164		
7	D	63	Total	O	0	0
			63	63		
7	E	222	Total	O	0	0
			222	222		
7	F	69	Total	O	0	0
			69	69		
7	G	171	Total	O	0	0
			171	171		
7	H	68	Total	O	0	0
			68	68		



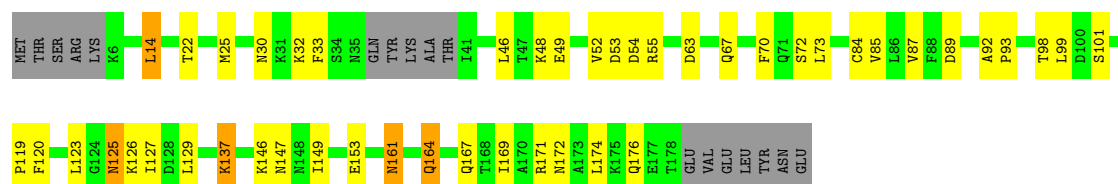
- Molecule 2: Ras-related protein Rab-7



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L99	D100		A110	S111	P112	R113		F118	P119	F120	V121	V122	L123	G124	N125	K126	I127	D128	L129		K137	R138		K146	N147	R148	I149		F152	E153	T154	S155	A156	K157		I160	N161		Q164	A165	F166	Q167	T168	I169	A170	R171	N172		Q176		E179	V180	E181	LEU	TYR	ASN	GLU
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4 Data and refinement statistics

Xtrriage (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	66.39Å 144.69Å 200.09Å 90.00° 90.13° 90.00°	Depositor
Resolution (Å)	19.42 – 2.50	Depositor
% Data completeness (in resolution range)	99.7 (19.42-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.206 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	22604	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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: P33, MG, GDP, K

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	0.55	0/4071	0.95	9/5508 (0.2%)
1	C	0.54	0/4058	0.97	7/5493 (0.1%)
1	E	0.54	0/4066	0.97	10/5501 (0.2%)
1	G	0.54	0/4062	0.98	14/5498 (0.3%)
2	B	0.53	0/1359	0.97	3/1840 (0.2%)
2	D	0.53	0/1395	0.92	2/1888 (0.1%)
2	F	0.49	0/1356	0.90	2/1835 (0.1%)
2	H	0.53	0/1395	0.93	2/1888 (0.1%)
All	All	0.54	0/21762	0.96	49/29451 (0.2%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	376	GLY	N-CA-C	8.85	120.36	111.95
1	C	64	GLU	N-CA-C	7.77	120.14	107.32
1	C	376	GLY	N-CA-C	7.68	120.90	112.29
1	E	51	SER	N-CA-C	-7.11	101.37	110.19
1	E	376	GLY	N-CA-C	6.95	119.13	112.04
1	G	510	SER	N-CA-C	-6.81	102.80	112.13
1	C	614	ASP	N-CA-C	6.66	120.14	110.28
1	E	370	PHE	N-CA-C	6.62	120.47	109.95
1	A	376	GLY	N-CA-C	6.55	118.72	112.04
1	C	370	PHE	N-CA-C	6.54	120.19	109.72
1	G	257	ILE	N-CA-C	-6.44	101.27	109.58
1	G	34	VAL	N-CA-C	6.34	117.73	108.53
1	A	51	SER	N-CA-C	-6.18	102.81	110.41
1	E	384	PHE	CA-CB-CG	-6.15	107.65	113.80
1	C	257	ILE	N-CA-C	-6.14	101.66	109.58
1	G	391	PHE	CA-CB-CG	-6.09	107.71	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	370	PHE	N-CA-C	6.06	119.41	109.72
1	A	257	ILE	N-CA-C	-6.05	101.78	109.58
1	E	257	ILE	N-CA-C	-5.96	101.10	109.21
1	C	34	VAL	N-CA-C	5.92	117.12	108.53
2	H	29	VAL	N-CA-C	5.80	116.44	110.82
1	A	228	LEU	N-CA-C	-5.75	105.76	112.89
1	A	370	PHE	N-CA-C	5.64	118.75	109.72
1	G	248	VAL	N-CA-C	-5.62	105.69	113.00
1	E	447	ARG	N-CA-C	-5.61	101.88	109.95
1	G	525	PHE	N-CA-C	5.53	118.09	109.52
1	E	517	LEU	N-CA-C	5.53	120.68	113.88
2	D	29	VAL	N-CA-C	5.49	115.58	110.42
1	E	228	LEU	N-CA-C	-5.46	106.12	112.89
2	F	70	PHE	CA-CB-CG	-5.46	108.34	113.80
1	A	466	ASP	N-CA-C	5.45	116.91	110.97
2	B	130	GLU	N-CA-C	5.45	118.15	111.82
1	G	271	VAL	CA-C-N	5.41	125.17	119.76
1	G	271	VAL	C-N-CA	5.41	125.17	119.76
2	H	125	ASN	N-CA-C	5.24	117.29	110.53
1	A	403	CYS	N-CA-C	5.23	116.24	108.60
2	B	125	ASN	N-CA-C	5.23	118.18	110.59
1	A	493	THR	N-CA-C	-5.21	106.90	113.20
2	F	125	ASN	N-CA-C	5.20	118.15	110.46
1	E	586	LYS	N-CA-C	5.19	116.93	111.28
1	E	510	SER	N-CA-C	-5.17	105.19	112.12
1	G	605	PRO	N-CA-C	-5.12	104.46	110.70
1	G	380	LEU	CA-C-N	-5.11	113.28	118.85
1	G	380	LEU	C-N-CA	-5.11	113.28	118.85
2	D	154	THR	N-CA-C	5.10	117.62	109.81
2	B	70	PHE	CA-CB-CG	-5.10	108.70	113.80
1	G	228	LEU	N-CA-C	-5.05	105.87	112.23
1	C	51	SER	N-CA-C	-5.04	103.40	110.35
1	A	517	LEU	N-CA-C	5.03	120.06	113.88

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	3993	0	3934	125	0
1	C	3980	0	3912	102	0
1	E	3988	0	3929	132	0
1	G	3984	0	3916	112	0
2	B	1335	0	1306	26	0
2	D	1371	0	1342	32	0
2	F	1332	0	1311	31	0
2	H	1371	0	1342	54	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
5	B	28	0	12	1	0
5	D	28	0	12	0	0
5	F	28	0	12	0	0
5	H	28	0	12	2	0
6	B	22	0	30	5	0
6	D	22	0	30	1	0
6	F	22	0	30	2	0
6	H	22	0	30	1	0
7	A	223	0	0	3	0
7	B	62	0	0	1	0
7	C	164	0	0	0	0
7	D	63	0	0	0	0
7	E	222	0	0	3	0
7	F	69	0	0	2	0
7	G	171	0	0	2	0
7	H	68	0	0	2	0
All	All	22604	0	21160	609	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 14.

All (609) 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:316:THR:HA	1:A:347:CYS:HA	1.29	1.05
1:E:288:GLU:HA	1:E:291:MET:HE2	1.36	1.02
1:A:600:ASP:HB3	1:A:603:PRO:HG3	1.43	1.00
1:A:291:MET:HE1	1:A:327:THR:HG23	1.48	0.96
1:E:600:ASP:HB3	1:E:603:PRO:HG3	1.54	0.89
1:E:316:THR:HA	1:E:347:CYS:HA	1.56	0.87
1:A:327:THR:HB	1:A:328:PRO:HD2	1.56	0.85
1:G:264:ARG:HD3	1:G:265:GLU:HG3	1.60	0.82
1:E:329:ASN:C	1:E:329:ASN:HD22	1.88	0.81
1:E:607:ASN:HD21	1:E:609:GLU:HB2	1.43	0.81
1:E:78:GLN:HB2	1:E:417:ILE:HD13	1.62	0.80
1:E:291:MET:HE1	1:E:327:THR:HG23	1.64	0.80
2:B:157:LYS:HG2	2:B:158:GLU:OE2	1.81	0.79
1:E:236:ARG:HH11	1:E:364:ARG:HD3	1.46	0.79
1:G:264:ARG:HG2	1:G:283:GLN:OE1	1.84	0.78
2:D:7:VAL:HB	2:D:57:VAL:HG12	1.66	0.78
1:A:79:ILE:HD11	1:A:85:ALA:HB2	1.64	0.78
1:A:78:GLN:HB2	1:A:417:ILE:HD13	1.65	0.77
2:H:113:ARG:HH22	2:H:179:GLU:HB2	1.49	0.77
1:A:327:THR:O	1:A:331:GLN:HB2	1.85	0.76
2:B:119:PRO:HG2	2:B:176:GLN:HB2	1.67	0.76
1:C:457:ASP:OD2	1:C:542:ARG:HB2	1.85	0.76
2:F:25:MET:HE3	2:F:46:LEU:HG	1.67	0.76
2:F:137:LYS:HE3	2:F:137:LYS:HA	1.68	0.76
1:E:243:LEU:HD23	1:E:248:VAL:HG13	1.68	0.75
1:E:243:LEU:HD23	1:E:248:VAL:CG1	2.18	0.74
1:C:73:SER:O	1:C:74:MET:HB2	1.87	0.74
1:E:264:ARG:HG2	1:E:265:GLU:HG3	1.69	0.74
1:E:288:GLU:HB3	1:E:330:LEU:HD11	1.70	0.74
1:C:264:ARG:HG2	1:C:283:GLN:OE1	1.88	0.73
1:A:288:GLU:HB3	1:A:330:LEU:HD11	1.71	0.73
2:D:176:GLN:O	2:D:180:VAL:HG23	1.89	0.73
2:D:113:ARG:HG2	2:D:180:VAL:HG22	1.68	0.72
1:C:76:GLN:H	1:C:76:GLN:NE2	1.87	0.72
1:E:321:LEU:HG	1:E:331:GLN:HG2	1.72	0.72
2:H:113:ARG:HE	2:H:180:VAL:CG2	2.02	0.72
1:A:5:LEU:HD12	1:A:6:PRO:HD2	1.72	0.72
2:F:119:PRO:HG2	2:F:176:GLN:HB2	1.73	0.71
1:A:410:SER:O	1:A:411:ARG:HB2	1.91	0.70
1:C:37:VAL:HG12	1:C:396:CYS:HB2	1.73	0.70
1:E:322:LYS:HA	1:E:331:GLN:NE2	2.06	0.70
2:B:164:GLN:CD	2:B:164:GLN:H	2.00	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:587:GLN:O	1:G:591:LEU:HD13	1.91	0.70
2:B:175:LYS:O	2:B:179:GLU:HG2	1.92	0.70
1:G:291:MET:HG2	1:G:325:LYS:HE2	1.74	0.69
1:E:407:ASP:HB2	1:E:414:LYS:HD2	1.74	0.69
2:H:176:GLN:O	2:H:180:VAL:HG23	1.92	0.69
1:E:329:ASN:HD22	1:E:330:LEU:N	1.91	0.69
2:F:161:ASN:ND2	2:F:164:GLN:HG3	2.08	0.69
1:G:264:ARG:NH2	1:G:329:ASN:OD1	2.27	0.68
1:E:288:GLU:HA	1:E:291:MET:CE	2.20	0.68
2:F:164:GLN:H	2:F:164:GLN:CD	2.00	0.68
1:C:340:MET:HE1	1:C:370:PHE:HZ	1.57	0.68
1:G:275:ARG:HG3	1:G:276:ALA:N	2.07	0.68
1:C:287:VAL:O	1:C:291:MET:HG3	1.94	0.68
1:C:327:THR:O	1:C:331:GLN:HG3	1.94	0.68
1:C:327:THR:C	1:C:331:GLN:HE21	2.00	0.67
1:A:340:MET:HE1	1:A:579:LEU:HD22	1.76	0.67
2:H:120:PHE:O	2:H:149:ILE:HG23	1.94	0.67
1:E:236:ARG:NH1	1:E:364:ARG:HD3	2.09	0.66
1:A:316:THR:CA	1:A:347:CYS:HA	2.17	0.66
1:G:343:GLU:HG3	1:G:344:THR:H	1.59	0.66
1:G:275:ARG:HG3	1:G:276:ALA:H	1.60	0.66
1:G:356:LYS:HE2	1:G:360:GLN:OE1	1.96	0.66
2:D:122:VAL:HG23	2:D:149:ILE:HG21	1.78	0.65
2:H:119:PRO:HB3	2:H:172:ASN:HB3	1.79	0.65
2:D:119:PRO:HB3	2:D:172:ASN:HB3	1.78	0.65
1:A:291:MET:HE3	1:A:330:LEU:HD12	1.79	0.65
1:E:287:VAL:O	1:E:291:MET:HG3	1.96	0.65
1:C:587:GLN:O	1:C:591:LEU:HD13	1.97	0.65
1:E:29:ARG:HB2	1:E:387:MET:HE2	1.79	0.65
1:E:264:ARG:NH1	1:E:264:ARG:HB3	2.11	0.65
1:G:477:GLU:O	1:G:477:GLU:HG2	1.95	0.65
1:C:462:ARG:H	1:C:462:ARG:NE	1.94	0.65
1:E:457:ASP:OD2	1:E:542:ARG:HB2	1.96	0.65
1:E:294:LYS:HB2	1:E:294:LYS:NZ	2.12	0.65
1:G:415:ALA:HB1	1:G:424:ILE:O	1.96	0.65
2:D:113:ARG:CZ	2:D:179:GLU:HB3	2.27	0.65
2:D:161:ASN:OD1	2:D:164:GLN:HG3	1.96	0.64
2:H:53:ASP:O	2:H:54:ASP:HB2	1.95	0.64
1:A:81:GLU:CD	1:A:81:GLU:H	2.06	0.64
1:C:322:LYS:HA	1:C:331:GLN:OE1	1.97	0.64
1:A:315:THR:O	1:A:347:CYS:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ASN:HD21	1:A:365:TYR:HB3	1.62	0.64
2:B:25:MET:HE3	2:B:46:LEU:HG	1.79	0.64
1:E:327:THR:HB	1:E:328:PRO:HD2	1.79	0.64
1:G:559:ARG:HH12	1:G:565:LEU:HB2	1.61	0.64
2:H:113:ARG:HE	2:H:180:VAL:HG22	1.63	0.64
2:B:101:SER:HB3	6:B:3302:P33:H121	1.79	0.63
1:C:317:PHE:CG	1:C:351:GLY:HA3	2.33	0.63
1:E:291:MET:HE3	1:E:330:LEU:HD12	1.81	0.63
2:D:161:ASN:HA	2:D:164:GLN:CG	2.29	0.63
1:E:340:MET:HE1	1:E:370:PHE:HZ	1.63	0.63
1:C:9:PHE:O	1:C:426:SER:HA	1.98	0.63
1:C:61:GLU:HA	1:C:65:ASN:ND2	2.13	0.63
1:G:37:VAL:HG12	1:G:396:CYS:HB2	1.79	0.63
1:G:76:GLN:H	1:G:76:GLN:NE2	1.96	0.63
1:G:277:ASP:C	1:G:279:PHE:H	2.06	0.63
1:A:407:ASP:HB2	1:A:414:LYS:HD2	1.81	0.62
1:A:327:THR:HB	1:A:328:PRO:CD	2.29	0.62
1:E:467:GLN:NE2	1:E:492:SER:H	1.95	0.62
1:C:263:PHE:HE1	1:C:268:VAL:HG23	1.65	0.62
1:G:586:LYS:HD2	1:G:586:LYS:C	2.24	0.62
1:C:65:ASN:O	1:C:66:ASN:HB2	1.98	0.62
1:C:374:LEU:O	1:C:375:TYR:HB2	2.00	0.62
1:A:294:LYS:HB2	1:A:294:LYS:NZ	2.15	0.62
1:E:591:LEU:HD13	7:E:9118:HOH:O	2.00	0.62
1:E:485:ARG:HD2	1:E:579:LEU:HD13	1.81	0.61
1:G:281:SER:HB2	1:G:289:LYS:HE2	1.82	0.61
1:C:415:ALA:HB1	1:C:424:ILE:O	1.99	0.61
1:E:74:MET:N	1:E:76:GLN:HE21	1.98	0.61
1:E:512:THR:OG1	1:E:515:GLU:HG3	2.00	0.61
1:C:276:ALA:O	1:C:279:PHE:HB2	2.01	0.61
1:A:600:ASP:HB3	1:A:603:PRO:CG	2.24	0.61
2:B:120:PHE:HB2	2:B:149:ILE:HG21	1.83	0.61
1:E:410:SER:O	1:E:411:ARG:HB2	2.01	0.61
1:G:340:MET:HE1	1:G:370:PHE:HZ	1.66	0.61
1:A:236:ARG:NH2	1:A:364:ARG:HE	1.99	0.60
1:C:88:LEU:HD21	1:C:404:LEU:CD1	2.32	0.60
1:G:589:GLU:O	1:G:593:GLN:HG3	2.02	0.60
1:E:248:VAL:CG2	1:E:383:CYS:HB3	2.31	0.60
2:H:78:TYR:HB3	2:H:110:ALA:HB2	1.82	0.60
2:B:59:MET:HE3	2:B:61:ILE:HD11	1.84	0.60
1:A:317:PHE:CG	1:A:351:GLY:HA3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:PHE:CE1	1:C:308:GLU:HG2	2.37	0.59
1:A:591:LEU:HD13	7:A:8118:HOH:O	2.02	0.59
1:E:322:LYS:HA	1:E:331:GLN:HE22	1.67	0.59
2:D:119:PRO:HG2	2:D:176:GLN:HB2	1.85	0.59
1:E:79:ILE:HD11	1:E:85:ALA:HB2	1.84	0.59
1:G:287:VAL:O	1:G:291:MET:HG3	2.02	0.59
1:G:327:THR:C	1:G:331:GLN:HE21	2.11	0.59
1:C:263:PHE:CE2	1:C:523:LYS:HD3	2.37	0.59
1:E:268:VAL:HG12	1:E:461:LEU:HD12	1.84	0.59
1:G:236:ARG:CZ	1:G:364:ARG:HD2	2.33	0.59
1:A:467:GLN:NE2	1:A:492:SER:H	2.00	0.58
2:D:120:PHE:O	2:D:149:ILE:HG23	2.03	0.58
1:E:457:ASP:CG	1:E:542:ARG:HB2	2.28	0.58
1:A:246:SER:O	1:A:247:ASN:HB2	2.01	0.58
1:A:284:LEU:HD13	1:A:292:LEU:HD11	1.85	0.58
1:C:277:ASP:C	1:C:279:PHE:H	2.10	0.58
1:E:5:LEU:HD12	1:E:6:PRO:HD2	1.85	0.58
1:E:220:GLU:HG3	1:E:497:MET:HE3	1.85	0.57
2:H:113:ARG:NH2	2:H:179:GLU:HB2	2.18	0.57
1:C:232:LEU:HB2	1:C:579:LEU:HD11	1.85	0.57
1:G:9:PHE:O	1:G:426:SER:HA	2.04	0.57
1:G:457:ASP:OD2	1:G:542:ARG:HB2	2.04	0.57
1:E:243:LEU:HA	1:E:248:VAL:CG1	2.34	0.57
1:E:467:GLN:HE21	1:E:492:SER:CB	2.18	0.57
1:G:401:VAL:HA	1:G:418:ASP:HA	1.85	0.57
1:A:2:ALA:C	1:A:4:ASN:H	2.12	0.57
1:C:88:LEU:HD21	1:C:404:LEU:HD13	1.87	0.57
1:G:596:CYS:O	1:G:599:GLU:HB2	2.04	0.57
1:E:335:LEU:HD11	1:E:343:GLU:HB2	1.85	0.56
1:C:76:GLN:H	1:C:76:GLN:HE21	1.52	0.56
1:G:317:PHE:CG	1:G:351:GLY:HA3	2.40	0.56
1:E:374:LEU:O	1:E:375:TYR:HB2	2.05	0.56
2:H:113:ARG:HE	2:H:180:VAL:HG23	1.70	0.56
1:E:342:SER:C	1:E:344:THR:H	2.13	0.56
2:H:67:GLN:HB2	2:H:73:LEU:HD23	1.86	0.56
2:H:161:ASN:OD1	2:H:164:GLN:HG3	2.05	0.56
1:G:235:SER:OG	1:G:361:CYS:HB3	2.06	0.56
1:E:340:MET:HE1	1:E:370:PHE:CZ	2.40	0.56
2:H:119:PRO:HG2	2:H:176:GLN:HB2	1.88	0.56
1:G:452:ALA:HB3	1:G:505:LEU:HB2	1.87	0.56
1:A:336:HIS:HB2	7:A:8468:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:ASN:C	1:E:329:ASN:ND2	2.56	0.55
1:E:359:LEU:O	1:E:362:LEU:HB2	2.07	0.55
2:F:119:PRO:HB3	2:F:172:ASN:HB3	1.87	0.55
1:A:312:TYR:HA	1:A:315:THR:HG22	1.88	0.55
1:E:214:TYR:CE1	1:E:218:ILE:HD11	2.41	0.55
1:A:5:LEU:HD12	1:A:6:PRO:CD	2.35	0.55
1:A:46:ASN:CG	1:A:551:MET:HE2	2.31	0.55
1:C:239:LEU:HD21	1:C:380:LEU:HD13	1.89	0.55
1:C:245:LYS:O	1:C:604:ALA:HB2	2.07	0.55
1:G:245:LYS:O	1:G:604:ALA:HB2	2.07	0.55
2:D:78:TYR:HB3	2:D:110:ALA:HB2	1.88	0.55
2:H:24:LEU:HD23	2:H:156:ALA:HB2	1.89	0.55
1:C:236:ARG:HH11	1:C:236:ARG:HG2	1.71	0.55
1:E:37:VAL:HG12	1:E:396:CYS:HB2	1.89	0.55
1:A:320:TYR:CD2	1:A:348:THR:HG23	2.42	0.55
1:G:16:THR:HG23	1:G:38:ASP:HB2	1.89	0.55
1:A:248:VAL:CG1	1:A:383:CYS:HB3	2.36	0.55
1:E:467:GLN:HE22	1:E:492:SER:H	1.52	0.54
1:E:243:LEU:CD2	1:E:248:VAL:HG13	2.36	0.54
1:A:305:HIS:C	1:A:307:ASP:H	2.16	0.54
2:D:113:ARG:NH2	2:D:179:GLU:HB3	2.23	0.54
1:A:288:GLU:HA	1:A:291:MET:HE2	1.89	0.54
2:B:127:ILE:HG21	2:B:153:GLU:HB3	1.89	0.54
1:G:368:THR:HB	1:G:369:PRO:HD2	1.89	0.54
1:A:322:LYS:HA	1:A:331:GLN:HE22	1.73	0.54
1:E:377:GLN:HE22	1:E:581:ASN:HD21	1.55	0.54
1:C:486:VAL:HG22	1:C:505:LEU:HG	1.89	0.54
1:C:586:LYS:C	1:C:586:LYS:HD2	2.33	0.54
1:E:415:ALA:HB1	1:E:424:ILE:O	2.08	0.54
1:A:485:ARG:HD2	1:A:579:LEU:HD13	1.90	0.53
2:B:71:GLN:NE2	6:B:3302:P33:H111	2.23	0.53
1:C:401:VAL:HA	1:C:418:ASP:HA	1.89	0.53
1:G:66:ASN:N	1:G:66:ASN:ND2	2.56	0.53
1:G:340:MET:HE1	1:G:370:PHE:CZ	2.42	0.53
1:E:74:MET:N	1:E:76:GLN:NE2	2.57	0.53
1:E:284:LEU:CD2	1:E:330:LEU:HD21	2.38	0.53
2:F:89:ASP:HB3	2:F:92:ALA:HB3	1.89	0.53
1:G:410:SER:O	1:G:411:ARG:HB2	2.08	0.53
1:C:596:CYS:O	1:C:599:GLU:HB2	2.08	0.53
2:D:53:ASP:O	2:D:54:ASP:HB2	2.08	0.53
2:B:101:SER:CB	6:B:3302:P33:H121	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:ARG:O	1:E:267:THR:HG23	2.09	0.53
1:A:247:ASN:HD22	1:A:605:PRO:HD2	1.74	0.53
1:C:18:LEU:HB3	1:C:19:PRO:HD3	1.91	0.53
1:C:456:THR:HG21	1:C:525:PHE:CE2	2.44	0.53
1:E:246:SER:O	1:E:247:ASN:HB2	2.07	0.53
1:G:263:PHE:CE2	1:G:523:LYS:HD3	2.44	0.53
1:G:285:THR:O	1:G:289:LYS:HG3	2.09	0.53
2:H:33:PHE:CD1	2:H:157:LYS:HA	2.44	0.53
1:E:275:ARG:HD2	1:E:293:MET:CE	2.39	0.53
2:H:89:ASP:CG	2:H:126:LYS:HD2	2.34	0.53
1:C:62:TYR:CD2	1:C:95:ILE:HB	2.44	0.52
1:E:285:THR:OG1	1:E:287:VAL:HG12	2.09	0.52
2:H:11:VAL:HG21	2:H:59:MET:HE3	1.91	0.52
2:D:79:ARG:HG2	2:D:79:ARG:HH11	1.75	0.52
1:A:296:LEU:O	1:A:300:VAL:HG23	2.09	0.52
1:A:320:TYR:HB2	1:A:348:THR:OG1	2.08	0.52
1:C:56:LEU:HA	1:C:59:LEU:HD12	1.91	0.52
1:G:18:LEU:HB3	1:G:19:PRO:HD3	1.91	0.52
2:H:64:THR:HG23	7:H:9162:HOH:O	2.08	0.52
2:B:104:ASP:O	2:B:108:ILE:HG12	2.10	0.52
1:G:341:THR:HB	1:G:346:SER:OG	2.08	0.52
1:C:519:ARG:HD3	1:C:519:ARG:C	2.34	0.52
1:E:81:GLU:H	1:E:81:GLU:CD	2.18	0.52
1:E:264:ARG:HB3	1:E:264:ARG:HH11	1.72	0.52
1:G:318:SER:HB3	1:G:335:LEU:HD21	1.92	0.52
2:H:152:PHE:HZ	2:H:168:THR:HG21	1.75	0.52
1:E:59:LEU:HD22	1:E:98:VAL:HG11	1.92	0.52
1:A:245:LYS:HE2	1:A:602:CYS:O	2.10	0.52
1:A:307:ASP:HA	1:A:310:ARG:HG3	1.92	0.52
1:E:294:LYS:HB2	1:E:294:LYS:HZ3	1.73	0.52
1:E:452:ALA:HB3	1:E:505:LEU:HB2	1.92	0.52
1:A:62:TYR:CD2	1:A:95:ILE:HB	2.45	0.52
1:C:589:GLU:HG3	1:C:601:PHE:CD2	2.45	0.52
1:G:607:ASN:ND2	1:G:609:GLU:H	2.08	0.52
1:C:302:TYR:O	1:C:309:TYR:CE2	2.64	0.51
2:B:52:VAL:HG11	2:B:171:ARG:HA	1.91	0.51
1:C:340:MET:HE1	1:C:370:PHE:CZ	2.40	0.51
1:C:452:ALA:HB3	1:C:505:LEU:HB2	1.90	0.51
1:E:301:GLU:HB2	1:E:304:GLU:HG3	1.92	0.51
1:C:106:GLN:O	1:C:107:ASP:CG	2.54	0.51
1:G:455:ILE:HD12	1:G:545:TRP:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:GLU:HB2	1:E:267:THR:HG23	1.93	0.51
2:H:59:MET:SD	2:H:170:ALA:HB2	2.51	0.51
1:E:243:LEU:HA	1:E:248:VAL:HG12	1.92	0.51
1:G:361:CYS:HB2	1:G:369:PRO:CB	2.41	0.51
2:D:127:ILE:HG21	2:D:153:GLU:HB3	1.93	0.51
1:G:76:GLN:H	1:G:76:GLN:HE21	1.57	0.50
2:D:136:THR:O	2:D:140:GLN:HG3	2.10	0.50
1:E:467:GLN:HE21	1:E:492:SER:HB3	1.74	0.50
1:E:243:LEU:HD23	1:E:248:VAL:HG11	1.92	0.50
1:G:301:GLU:HA	1:G:303:GLU:OE1	2.11	0.50
1:A:412:LYS:HE2	1:A:567:SER:OG	2.12	0.50
1:E:264:ARG:HH11	1:E:264:ARG:CB	2.24	0.50
1:G:586:LYS:HD2	1:G:586:LYS:O	2.11	0.50
1:A:282:LYS:HE2	1:A:286:MET:CE	2.41	0.50
1:G:278:VAL:HG12	1:G:278:VAL:O	2.11	0.50
1:C:512:THR:OG1	1:C:515:GLU:HG3	2.11	0.50
1:G:232:LEU:HB2	1:G:579:LEU:HD11	1.94	0.50
1:C:291:MET:HG2	1:C:325:LYS:HE3	1.94	0.50
1:C:318:SER:HB3	1:C:335:LEU:HD21	1.93	0.50
1:C:347:CYS:SG	1:C:350:ASP:HB2	2.52	0.50
1:C:362:LEU:C	1:C:362:LEU:HD23	2.37	0.50
1:G:246:SER:O	1:G:247:ASN:HB2	2.12	0.50
2:H:97:LYS:NZ	2:H:138:ARG:HH22	2.10	0.50
1:C:283:GLN:HA	1:C:283:GLN:HE21	1.77	0.50
1:E:284:LEU:N	1:E:284:LEU:HD12	2.27	0.50
1:G:66:ASN:N	1:G:66:ASN:HD22	2.09	0.50
1:G:374:LEU:O	1:G:375:TYR:HB2	2.12	0.50
1:C:462:ARG:H	1:C:462:ARG:CD	2.25	0.49
1:G:312:TYR:CE2	1:G:323:THR:HG21	2.47	0.49
1:A:415:ALA:HB1	1:A:424:ILE:O	2.12	0.49
1:G:362:LEU:C	1:G:362:LEU:HD23	2.37	0.49
1:A:264:ARG:NH1	1:A:264:ARG:HB3	2.27	0.49
1:E:296:LEU:O	1:E:300:VAL:HG23	2.12	0.49
1:E:343:GLU:OE2	1:E:343:GLU:N	2.46	0.49
2:F:33:PHE:HA	7:F:9371:HOH:O	2.13	0.49
1:G:64:GLU:OE2	1:G:64:GLU:HA	2.12	0.49
1:E:456:THR:OG1	1:E:501:TYR:HB2	2.12	0.49
1:A:329:ASN:O	1:A:332:TYR:HB3	2.12	0.49
1:C:236:ARG:HG2	1:C:236:ARG:NH1	2.28	0.49
1:E:287:VAL:HG13	1:E:288:GLU:N	2.27	0.49
1:E:289:LYS:O	1:E:292:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:120:PHE:HB2	2:F:149:ILE:HG21	1.93	0.49
1:A:83:GLU:OE2	1:A:414:LYS:NZ	2.44	0.49
1:C:305:HIS:N	1:C:306:PRO:HD3	2.28	0.49
1:E:312:TYR:HA	1:E:315:THR:HG22	1.93	0.49
1:E:358:PHE:O	1:E:362:LEU:HD13	2.12	0.49
1:C:263:PHE:HE2	1:C:523:LYS:HD3	1.76	0.49
1:G:65:ASN:HD22	1:G:91:LYS:NZ	2.11	0.49
2:H:155:SER:HB3	2:H:160:ILE:HB	1.95	0.49
1:A:265:GLU:HB2	1:A:267:THR:CG2	2.42	0.49
2:H:126:LYS:HG2	5:H:2303:GDP:C6	2.48	0.49
1:A:448:GLN:HB2	1:A:509:SER:HB2	1.95	0.48
2:F:161:ASN:HD22	2:F:164:GLN:HG3	1.76	0.48
1:G:248:VAL:CG1	1:G:383:CYS:HB3	2.42	0.48
2:H:137:LYS:HG2	7:H:9111:HOH:O	2.13	0.48
1:G:377:GLN:HB3	7:G:9170:HOH:O	2.14	0.48
1:G:415:ALA:HB2	1:G:425:ILE:HA	1.95	0.48
1:A:525:PHE:CD2	1:A:541:PRO:HG2	2.48	0.48
1:G:106:GLN:O	1:G:107:ASP:CG	2.56	0.48
2:H:113:ARG:HG2	2:H:180:VAL:HG22	1.95	0.48
1:G:277:ASP:C	1:G:279:PHE:N	2.71	0.48
2:D:25:MET:HG2	2:D:46:LEU:HD12	1.95	0.48
1:E:62:TYR:CD2	1:E:95:ILE:HB	2.49	0.48
1:C:246:SER:O	1:C:247:ASN:HB2	2.13	0.48
1:G:342:SER:OG	1:G:345:THR:HB	2.13	0.48
1:A:264:ARG:O	1:A:267:THR:HG23	2.14	0.48
2:B:30:ASN:O	2:B:32:LYS:HG3	2.13	0.48
2:B:64:THR:HG23	7:B:8127:HOH:O	2.13	0.48
2:H:20:GLY:HA2	5:H:2303:GDP:O3A	2.14	0.48
1:C:275:ARG:HB3	1:C:293:MET:CE	2.44	0.48
2:F:87:VAL:HG22	2:F:123:LEU:HB2	1.95	0.48
2:F:101:SER:HB3	6:F:3306:P33:H121	1.95	0.48
1:A:322:LYS:HA	1:A:331:GLN:NE2	2.29	0.48
1:G:356:LYS:O	1:G:360:GLN:HG3	2.14	0.48
1:G:444:VAL:HG11	1:G:446:TYR:CE2	2.49	0.48
2:H:56:LEU:C	2:H:56:LEU:HD23	2.38	0.48
1:C:410:SER:O	1:C:411:ARG:HB2	2.14	0.48
1:G:36:HIS:HB3	1:G:395:TYR:CE1	2.48	0.48
1:A:358:PHE:O	1:A:362:LEU:HD13	2.14	0.47
2:D:155:SER:HB3	2:D:160:ILE:HB	1.96	0.47
1:A:59:LEU:HD22	1:A:98:VAL:HG11	1.96	0.47
1:A:452:ALA:HB3	1:A:505:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:407:ASP:HB2	1:E:414:LYS:CD	2.42	0.47
1:E:412:LYS:HE3	1:E:567:SER:OG	2.13	0.47
1:A:538:VAL:HG12	1:A:538:VAL:O	2.13	0.47
1:E:305:HIS:C	1:E:307:ASP:H	2.22	0.47
1:G:462:ARG:N	1:G:462:ARG:HD2	2.29	0.47
1:E:248:VAL:HG22	1:E:383:CYS:HB3	1.94	0.47
2:B:71:GLN:HB3	6:B:3302:P33:H151	1.97	0.47
1:C:391:PHE:CZ	1:C:605:PRO:HB3	2.49	0.47
2:F:127:ILE:HG21	2:F:153:GLU:HB3	1.97	0.47
2:H:113:ARG:HH22	2:H:179:GLU:CB	2.25	0.47
1:A:3:ASP:HA	2:B:69:ARG:HE	1.80	0.47
1:A:239:LEU:HD21	1:A:380:LEU:HD13	1.97	0.47
1:A:264:ARG:C	1:A:266:GLY:N	2.72	0.47
1:A:338:ILE:CG2	1:A:355:THR:HG23	2.45	0.47
1:A:451:ARG:NH2	1:A:504:HIS:ND1	2.57	0.47
1:C:275:ARG:HB3	1:C:293:MET:SD	2.55	0.47
2:D:110:ALA:O	2:D:111:SER:C	2.57	0.47
1:G:59:LEU:HD22	1:G:98:VAL:HG11	1.96	0.47
1:A:368:THR:HB	1:A:369:PRO:HD2	1.96	0.47
1:A:457:ASP:CG	1:A:542:ARG:HB2	2.40	0.47
1:E:600:ASP:HB3	1:E:603:PRO:CG	2.36	0.47
1:A:236:ARG:CZ	1:A:364:ARG:HE	2.28	0.47
1:E:302:TYR:OH	1:E:353:LYS:HG2	2.14	0.47
1:A:358:PHE:CE2	1:A:362:LEU:HD11	2.50	0.47
1:C:292:LEU:O	1:C:296:LEU:HG	2.15	0.47
1:G:391:PHE:CZ	1:G:605:PRO:HB3	2.50	0.47
1:A:377:GLN:HG2	7:A:8157:HOH:O	2.14	0.46
2:D:16:ASP:O	2:D:19:VAL:HG22	2.15	0.46
1:G:327:THR:HB	1:G:328:PRO:HD2	1.97	0.46
1:A:289:LYS:O	1:A:292:LEU:HB2	2.16	0.46
1:C:280:ASN:O	1:C:282:LYS:HG3	2.16	0.46
1:C:519:ARG:CZ	1:C:523:LYS:HZ3	2.29	0.46
1:E:284:LEU:HD12	1:E:284:LEU:H	1.80	0.46
1:E:401:VAL:HA	1:E:418:ASP:HA	1.97	0.46
1:G:276:ALA:O	1:G:279:PHE:HB2	2.15	0.46
2:D:161:ASN:C	2:D:164:GLN:HG2	2.41	0.46
1:E:18:LEU:HB3	1:E:19:PRO:HD3	1.97	0.46
1:E:320:TYR:CE1	1:E:324:GLN:NE2	2.84	0.46
1:E:446:TYR:CE2	1:E:552:ARG:HD3	2.51	0.46
1:G:65:ASN:HD22	1:G:91:LYS:HZ1	1.63	0.46
1:C:248:VAL:CG1	1:C:383:CYS:HB3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:TYR:O	1:C:309:TYR:HE2	1.98	0.46
1:E:223:ARG:HA	1:E:223:ARG:NE	2.31	0.46
1:G:485:ARG:HD2	1:G:579:LEU:HD13	1.98	0.46
1:G:62:TYR:CD2	1:G:95:ILE:HB	2.51	0.46
1:A:264:ARG:HG2	1:A:265:GLU:HG3	1.97	0.46
1:A:220:GLU:HG3	1:A:497:MET:HE3	1.98	0.45
1:A:235:SER:HB3	1:A:364:ARG:HD2	1.98	0.45
1:A:374:LEU:O	1:A:375:TYR:HB2	2.15	0.45
1:A:401:VAL:HA	1:A:418:ASP:HA	1.98	0.45
1:A:410:SER:O	1:A:411:ARG:CB	2.63	0.45
1:E:275:ARG:CD	1:E:293:MET:HE3	2.46	0.45
1:G:212:ILE:HA	1:G:216:GLN:OE1	2.15	0.45
1:E:76:GLN:CD	1:E:76:GLN:H	2.23	0.45
1:E:538:VAL:HG12	1:E:538:VAL:O	2.16	0.45
1:G:280:ASN:O	1:G:281:SER:C	2.58	0.45
1:A:294:LYS:HB2	1:A:294:LYS:HZ3	1.80	0.45
1:A:307:ASP:HA	1:A:310:ARG:CG	2.46	0.45
2:B:110:ALA:O	2:B:111:SER:C	2.59	0.45
1:A:288:GLU:CB	1:A:330:LEU:HD11	2.45	0.45
1:C:285:THR:O	1:C:289:LYS:HG3	2.16	0.45
1:A:305:HIS:ND1	1:A:305:HIS:N	2.64	0.45
1:C:82:ASN:HA	1:C:408:LYS:HD2	1.98	0.45
2:H:127:ILE:HG21	2:H:153:GLU:HB3	1.99	0.45
1:A:223:ARG:HA	1:A:223:ARG:HD3	1.57	0.45
1:E:238:LEU:HB3	1:E:585:VAL:HG11	1.99	0.45
1:E:448:GLN:HB2	1:E:509:SER:HB2	1.98	0.45
2:F:161:ASN:HD22	2:F:161:ASN:HA	1.57	0.45
1:G:302:TYR:O	1:G:309:TYR:HE2	2.00	0.45
1:E:84:GLU:HB3	1:E:408:LYS:NZ	2.31	0.45
2:H:24:LEU:HD13	2:H:123:LEU:HD12	1.97	0.45
1:C:280:ASN:O	1:C:281:SER:C	2.60	0.45
1:E:292:LEU:HG	1:E:330:LEU:HD13	1.99	0.45
1:A:59:LEU:HD13	1:A:100:VAL:HG21	1.98	0.44
1:A:345:THR:O	1:A:345:THR:HG22	2.16	0.44
1:C:16:THR:HG23	1:C:38:ASP:HB2	1.99	0.44
1:G:343:GLU:HG3	1:G:344:THR:N	2.28	0.44
1:G:358:PHE:C	1:G:358:PHE:CD2	2.95	0.44
1:G:364:ARG:NH1	1:G:365:TYR:OH	2.50	0.44
1:A:23:ILE:HG12	1:A:430:ILE:HD13	2.00	0.44
2:D:33:PHE:CG	2:D:157:LYS:HA	2.52	0.44
1:A:340:MET:CE	1:A:579:LEU:HD22	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:LEU:HD12	1:E:579:LEU:HD11	1.99	0.44
1:G:360:GLN:HE21	1:G:360:GLN:HB3	1.59	0.44
1:G:478:GLU:HG2	1:G:481:SER:HB2	1.99	0.44
1:A:264:ARG:C	1:A:266:GLY:H	2.25	0.44
1:A:317:PHE:HA	1:A:348:THR:HA	2.00	0.44
1:A:456:THR:OG1	1:A:501:TYR:HB2	2.18	0.44
1:C:61:GLU:HB2	1:C:65:ASN:HD22	1.81	0.44
1:C:307:ASP:HA	1:C:310:ARG:HH12	1.81	0.44
1:E:607:ASN:HA	1:E:608:PRO:HD3	1.82	0.44
1:E:401:VAL:CG1	1:E:416:VAL:HB	2.48	0.44
1:E:525:PHE:CD2	1:E:541:PRO:HG2	2.52	0.44
2:F:30:ASN:O	2:F:32:LYS:HG3	2.18	0.44
2:B:129:LEU:HD12	2:B:129:LEU:HA	1.84	0.44
2:D:100:ASP:OD1	2:D:146:LYS:HE3	2.18	0.44
1:G:379:GLU:CD	2:H:79:ARG:HE	2.26	0.44
1:G:321:LEU:O	1:G:324:GLN:HB2	2.17	0.44
1:C:88:LEU:HD21	1:C:404:LEU:HD11	1.99	0.44
1:C:478:GLU:N	1:C:478:GLU:CD	2.76	0.44
2:D:146:LYS:O	2:D:149:ILE:HG13	2.18	0.44
1:E:319:GLU:O	1:E:322:LYS:HB2	2.17	0.44
1:C:356:LYS:O	1:C:360:GLN:HG3	2.17	0.44
1:C:478:GLU:HG2	1:C:481:SER:OG	2.18	0.44
1:G:279:PHE:C	1:G:279:PHE:CD2	2.96	0.44
1:A:526:THR:CG2	1:A:542:ARG:HD3	2.48	0.43
2:F:53:ASP:O	2:F:54:ASP:HB2	2.18	0.43
2:H:100:ASP:OD1	2:H:146:LYS:HE3	2.17	0.43
2:H:113:ARG:CG	2:H:180:VAL:HG22	2.48	0.43
2:B:71:GLN:HE22	6:B:3302:P33:H111	1.82	0.43
2:H:11:VAL:HG21	2:H:59:MET:CE	2.47	0.43
2:H:47:THR:HA	2:H:59:MET:O	2.18	0.43
1:A:305:HIS:O	1:A:307:ASP:N	2.51	0.43
1:A:359:LEU:O	1:A:362:LEU:HB2	2.18	0.43
2:F:48:LYS:HE3	7:F:9165:HOH:O	2.17	0.43
2:F:55:ARG:HD3	2:F:174:LEU:HD21	2.00	0.43
1:G:361:CYS:HB2	1:G:369:PRO:HB3	2.00	0.43
2:B:119:PRO:HB3	2:B:172:ASN:HB3	1.99	0.43
2:D:33:PHE:CD1	2:D:157:LYS:HA	2.53	0.43
2:D:161:ASN:HA	2:D:164:GLN:HG3	2.00	0.43
1:E:397:LEU:HG	2:F:72:SER:HB3	2.01	0.43
1:G:305:HIS:HB3	1:G:308:GLU:OE1	2.18	0.43
1:A:602:CYS:N	1:A:603:PRO:HD3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:TYR:CE1	1:A:218:ILE:HD11	2.54	0.43
1:E:607:ASN:HD21	1:E:609:GLU:CB	2.21	0.43
1:A:343:GLU:CD	1:A:344:THR:HG23	2.43	0.43
1:C:242:LEU:HD11	1:C:602:CYS:HB2	2.01	0.43
1:C:299:CYS:O	1:C:300:VAL:C	2.61	0.43
2:F:22:THR:OG1	2:F:63:ASP:OD1	2.37	0.43
2:F:52:VAL:HG11	2:F:171:ARG:HA	1.99	0.43
2:H:36:GLN:HB2	2:H:37:TYR:H	1.66	0.43
1:C:418:ASP:OD1	1:C:418:ASP:C	2.61	0.43
1:E:343:GLU:OE2	1:E:344:THR:HG23	2.19	0.43
2:F:146:LYS:O	2:F:147:ASN:HB3	2.19	0.43
2:H:71:GLN:HB3	6:H:3308:P33:H151	2.01	0.43
1:A:287:VAL:O	1:A:291:MET:HG3	2.18	0.43
1:C:29:ARG:NH2	1:C:606:PRO:HD3	2.34	0.43
1:E:239:LEU:HD21	1:E:380:LEU:HD13	2.01	0.43
2:F:14:LEU:HD22	2:F:84:CYS:SG	2.58	0.43
2:F:98:THR:HG22	6:F:3306:P33:H92	2.01	0.43
2:H:14:LEU:HD12	2:H:84:CYS:SG	2.58	0.43
2:H:67:GLN:HB2	2:H:73:LEU:CD2	2.48	0.43
1:E:300:VAL:HG12	1:E:300:VAL:O	2.18	0.43
1:E:302:TYR:HB2	1:E:352:LEU:HD13	2.01	0.43
1:E:312:TYR:CA	1:E:315:THR:HG22	2.49	0.43
1:E:377:GLN:HG2	7:E:9157:HOH:O	2.18	0.43
1:A:273:CYS:O	1:A:274:SER:C	2.62	0.42
2:B:164:GLN:CD	2:B:164:GLN:N	2.74	0.42
1:A:106:GLN:O	1:A:107:ASP:HB3	2.19	0.42
1:A:282:LYS:HE2	1:A:286:MET:HE2	2.00	0.42
1:C:462:ARG:CD	1:C:462:ARG:N	2.81	0.42
1:E:79:ILE:CD1	1:E:85:ALA:HB2	2.49	0.42
1:E:302:TYR:O	1:E:309:TYR:HE2	2.02	0.42
2:H:161:ASN:HA	2:H:164:GLN:CG	2.49	0.42
1:A:284:LEU:HD22	1:A:330:LEU:HD21	2.01	0.42
2:D:152:PHE:HZ	2:D:168:THR:HG21	1.84	0.42
1:E:255:LYS:HE2	1:E:492:SER:OG	2.19	0.42
1:E:411:ARG:HD3	7:E:9303:HOH:O	2.18	0.42
2:F:161:ASN:HD22	2:F:164:GLN:CG	2.32	0.42
2:H:122:VAL:HG23	2:H:149:ILE:HG21	2.02	0.42
1:A:329:ASN:OD1	1:A:329:ASN:C	2.62	0.42
1:A:467:GLN:HE21	1:A:492:SER:CB	2.32	0.42
1:E:284:LEU:HD23	1:E:330:LEU:HD21	2.01	0.42
1:A:299:CYS:C	1:A:301:GLU:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:PRO:HA	1:C:309:TYR:CE2	2.55	0.42
1:E:59:LEU:HD23	1:E:59:LEU:HA	1.87	0.42
1:G:86:ILE:HB	1:G:404:LEU:HB2	2.02	0.42
1:G:263:PHE:HE1	1:G:268:VAL:HG22	1.84	0.42
2:H:7:VAL:HB	2:H:57:VAL:HG12	2.02	0.42
1:A:274:SER:C	1:A:276:ALA:N	2.76	0.42
1:A:292:LEU:O	1:A:293:MET:C	2.62	0.42
1:A:312:TYR:CA	1:A:315:THR:HG22	2.49	0.42
1:C:278:VAL:HG12	1:C:278:VAL:O	2.19	0.42
1:C:301:GLU:C	1:C:303:GLU:H	2.26	0.42
1:C:333:PHE:O	1:C:337:SER:HB2	2.20	0.42
1:C:444:VAL:HG11	1:C:446:TYR:CE2	2.55	0.42
2:D:118:PHE:HA	2:D:119:PRO:HD3	1.76	0.42
1:G:462:ARG:O	1:G:463:THR:HG23	2.19	0.42
2:H:51:MET:SD	2:H:55:ARG:O	2.78	0.42
1:E:539:GLU:HG2	1:E:542:ARG:HH21	1.84	0.42
2:H:146:LYS:HA	2:H:146:LYS:HD3	1.86	0.42
2:H:166:PHE:HA	2:H:169:ILE:HB	2.01	0.42
1:A:607:ASN:HA	1:A:608:PRO:HD3	1.90	0.42
2:F:125:ASN:CG	2:F:126:LYS:N	2.78	0.42
1:G:317:PHE:O	1:G:321:LEU:HG	2.19	0.42
1:G:349:VAL:HA	1:G:352:LEU:HD12	2.02	0.42
2:H:161:ASN:HA	2:H:164:GLN:CD	2.44	0.42
1:A:268:VAL:HG12	1:A:461:LEU:HD12	2.01	0.42
1:C:310:ARG:NH1	1:C:310:ARG:HB3	2.34	0.42
1:C:477:GLU:HG2	1:C:477:GLU:O	2.20	0.42
2:H:110:ALA:O	2:H:111:SER:C	2.63	0.42
2:H:165:ALA:O	2:H:169:ILE:HG13	2.20	0.42
1:A:291:MET:O	1:A:295:PHE:HB2	2.19	0.42
1:A:526:THR:HG23	1:A:542:ARG:HD3	2.01	0.42
2:B:118:PHE:HA	2:B:119:PRO:HD3	1.79	0.42
1:C:368:THR:HB	1:C:369:PRO:HD2	2.02	0.42
1:C:452:ALA:HA	1:C:547:LEU:O	2.20	0.42
1:E:5:LEU:HD12	1:E:6:PRO:CD	2.50	0.42
1:E:245:LYS:HE2	1:E:602:CYS:O	2.20	0.42
1:E:607:ASN:CG	1:E:609:GLU:H	2.28	0.42
2:F:125:ASN:CG	2:F:126:LYS:H	2.28	0.42
1:G:478:GLU:CD	1:G:478:GLU:N	2.78	0.42
2:H:176:GLN:O	2:H:180:VAL:CG2	2.66	0.42
1:A:454:LEU:HD22	1:A:543:LEU:HD11	2.01	0.41
2:D:71:GLN:HB3	6:D:3304:P33:H151	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:343:GLU:OE2	1:G:344:THR:HG23	2.20	0.41
1:G:607:ASN:HD21	1:G:609:GLU:HB2	1.85	0.41
1:A:86:ILE:HB	1:A:404:LEU:HB2	2.02	0.41
1:A:317:PHE:CE2	1:A:321:LEU:HD11	2.55	0.41
1:C:273:CYS:H	1:C:277:ASP:CB	2.34	0.41
1:E:532:GLU:OE2	1:E:532:GLU:HA	2.20	0.41
2:F:92:ALA:HA	2:F:93:PRO:HD2	1.94	0.41
1:G:271:VAL:HB	1:G:333:PHE:CE1	2.55	0.41
1:G:361:CYS:HB2	1:G:369:PRO:HB2	2.02	0.41
1:G:456:THR:HG21	1:G:525:PHE:CE2	2.55	0.41
1:A:312:TYR:O	1:A:315:THR:HG22	2.20	0.41
1:A:452:ALA:HA	1:A:547:LEU:O	2.20	0.41
1:E:236:ARG:HD2	1:E:364:ARG:CZ	2.50	0.41
2:F:67:GLN:HB2	2:F:73:LEU:HD23	2.03	0.41
1:G:275:ARG:HB3	1:G:293:MET:CE	2.50	0.41
2:H:25:MET:HG2	2:H:46:LEU:HD12	2.02	0.41
1:A:339:ALA:O	1:A:340:MET:HB2	2.20	0.41
2:F:161:ASN:ND2	2:F:164:GLN:CG	2.80	0.41
1:C:44:GLY:O	1:C:45:GLY:C	2.62	0.41
1:C:358:PHE:CD2	1:C:358:PHE:C	2.98	0.41
1:G:343:GLU:C	1:G:345:THR:H	2.27	0.41
1:G:426:SER:HB3	1:G:429:PHE:CZ	2.56	0.41
1:G:427:LYS:HD2	7:G:9225:HOH:O	2.21	0.41
1:A:466:ASP:O	1:A:468:GLN:N	2.54	0.41
1:C:224:PHE:HB3	1:C:226:ILE:CD1	2.51	0.41
1:C:277:ASP:C	1:C:279:PHE:N	2.77	0.41
1:C:519:ARG:CZ	1:C:523:LYS:NZ	2.84	0.41
1:E:236:ARG:HD2	1:E:364:ARG:NE	2.34	0.41
1:G:375:TYR:CG	2:H:79:ARG:HD3	2.56	0.41
2:H:118:PHE:HA	2:H:119:PRO:HD3	1.77	0.41
1:A:9:PHE:O	1:A:426:SER:HA	2.20	0.41
1:A:457:ASP:OD1	1:A:542:ARG:HB2	2.20	0.41
1:C:438:GLU:H	1:C:438:GLU:CD	2.27	0.41
2:D:113:ARG:CG	2:D:180:VAL:HG22	2.46	0.41
1:A:512:THR:OG1	1:A:515:GLU:HG3	2.21	0.41
2:D:113:ARG:NH2	2:D:179:GLU:CB	2.83	0.41
1:E:248:VAL:HG22	1:E:248:VAL:O	2.20	0.41
1:E:299:CYS:C	1:E:301:GLU:H	2.29	0.41
1:G:299:CYS:O	1:G:300:VAL:C	2.63	0.41
1:A:238:LEU:HD11	1:A:586:LYS:HE3	2.03	0.41
2:B:24:LEU:HD13	2:B:123:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:PHE:HE1	1:C:268:VAL:CG2	2.32	0.41
1:C:579:LEU:O	1:C:579:LEU:HD12	2.20	0.41
1:G:242:LEU:HD11	1:G:602:CYS:HB2	2.03	0.41
1:G:353:LYS:HE2	1:G:353:LYS:HB3	1.84	0.41
1:A:5:LEU:HA	1:A:6:PRO:HD3	1.92	0.41
1:E:565:LEU:HA	1:E:565:LEU:HD12	1.85	0.41
1:G:512:THR:OG1	1:G:515:GLU:HG3	2.21	0.41
1:C:26:ALA:HB2	1:C:602:CYS:SG	2.61	0.40
1:C:273:CYS:HB3	1:C:362:LEU:CD1	2.50	0.40
1:E:211:ARG:NH1	1:E:528:TYR:OH	2.54	0.40
2:H:164:GLN:CD	2:H:164:GLN:H	2.28	0.40
1:A:264:ARG:HB2	1:A:332:TYR:CE2	2.56	0.40
1:A:300:VAL:O	1:A:300:VAL:HG12	2.20	0.40
1:E:260:ILE:O	1:E:271:VAL:HG12	2.21	0.40
1:G:39:SER:HB3	1:G:400:SER:HB3	2.03	0.40
1:G:446:TYR:CE2	1:G:552:ARG:HD3	2.56	0.40
1:A:416:VAL:HG13	1:A:429:PHE:HE1	1.87	0.40
2:B:126:LYS:HG2	5:B:2302:GDP:C6	2.56	0.40
1:C:275:ARG:HG3	1:C:276:ALA:N	2.36	0.40
1:C:462:ARG:O	1:C:463:THR:HG23	2.22	0.40
2:D:66:GLY:O	2:D:69:ARG:HB2	2.21	0.40
1:E:320:TYR:CG	1:E:348:THR:HG23	2.55	0.40
1:E:321:LEU:HD11	1:E:326:LEU:HD13	2.03	0.40
1:G:59:LEU:HD22	1:G:98:VAL:CG1	2.51	0.40
2:B:78:TYR:HB3	2:B:110:ALA:HB2	2.02	0.40
1:C:415:ALA:HB2	1:C:425:ILE:HA	2.03	0.40
1:E:364:ARG:NH2	1:G:608:PRO:HB3	2.37	0.40
1:A:288:GLU:HA	1:A:291:MET:CE	2.51	0.40
1:A:290:ARG:HD2	1:A:294:LYS:NZ	2.36	0.40
2:F:85:VAL:CG2	2:F:169:ILE:HD13	2.51	0.40
1:G:247:ASN:C	1:G:249:SER:N	2.76	0.40
1:G:418:ASP:OD1	1:G:418:ASP:C	2.64	0.40
1:G:482:PHE:CD1	1:G:508:MET:HB2	2.56	0.40
2:H:89:ASP:OD2	2:H:126:LYS:HD2	2.22	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	495/650 (76%)	456 (92%)	32 (6%)	7 (1%)	9	17
1	C	496/650 (76%)	454 (92%)	38 (8%)	4 (1%)	16	31
1	E	494/650 (76%)	461 (93%)	30 (6%)	3 (1%)	21	38
1	G	496/650 (76%)	462 (93%)	32 (6%)	2 (0%)	30	49
2	B	165/185 (89%)	160 (97%)	5 (3%)	0	100	100
2	D	169/185 (91%)	160 (95%)	9 (5%)	0	100	100
2	F	164/185 (89%)	156 (95%)	8 (5%)	0	100	100
2	H	169/185 (91%)	159 (94%)	8 (5%)	2 (1%)	10	20
All	All	2648/3340 (79%)	2468 (93%)	162 (6%)	18 (1%)	18	34

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	ARG
1	A	467	GLN
1	A	3	ASP
1	C	309	TYR
1	E	310	ARG
1	E	343	GLU
1	G	281	SER
2	H	36	GLN
1	A	292	LEU
1	A	306	PRO
1	A	598	ASN
1	C	60	LYS
1	C	65	ASN
2	H	35	ASN
1	A	275	ARG
1	C	278	VAL
1	G	344	THR

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Mol	Chain	Res	Type
1	E	292	LEU

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	452/581 (78%)	435 (96%)	17 (4%)	29	56
1	C	450/581 (78%)	437 (97%)	13 (3%)	37	65
1	E	452/581 (78%)	429 (95%)	23 (5%)	21	43
1	G	451/581 (78%)	428 (95%)	23 (5%)	21	43
2	B	144/162 (89%)	137 (95%)	7 (5%)	22	45
2	D	148/162 (91%)	136 (92%)	12 (8%)	11	23
2	F	144/162 (89%)	136 (94%)	8 (6%)	19	39
2	H	148/162 (91%)	140 (95%)	8 (5%)	20	41
All	All	2389/2972 (80%)	2278 (95%)	111 (5%)	24	48

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	GLU
1	A	235	SER
1	A	255	LYS
1	A	267	THR
1	A	283	GLN
1	A	294	LYS
1	A	301	GLU
1	A	305	HIS
1	A	310	ARG
1	A	343	GLU
1	A	347	CYS
1	A	404	LEU
1	A	466	ASP
1	A	559	ARG

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Mol	Chain	Res	Type
1	A	565	LEU
1	A	591	LEU
1	A	599	GLU
2	B	14	LEU
2	B	49	GLU
2	B	99	LEU
2	B	111	SER
2	B	129	LEU
2	B	161	ASN
2	B	164	GLN
1	C	68	VAL
1	C	71	GLU
1	C	76	GLN
1	C	99	GLU
1	C	263	PHE
1	C	275	ARG
1	C	359	LEU
1	C	364	ARG
1	C	439	ASN
1	C	445	GLN
1	C	462	ARG
1	C	473	THR
1	C	560	ASP
2	D	7	VAL
2	D	36	GLN
2	D	50	VAL
2	D	55	ARG
2	D	69	ARG
2	D	99	LEU
2	D	113	ARG
2	D	129	LEU
2	D	164	GLN
2	D	168	THR
2	D	177	GLU
2	D	179	GLU
1	E	74	MET
1	E	76	GLN
1	E	106	GLN
1	E	236	ARG
1	E	255	LYS
1	E	257	ILE
1	E	267	THR

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Mol	Chain	Res	Type
1	E	271	VAL
1	E	283	GLN
1	E	284	LEU
1	E	286	MET
1	E	290	ARG
1	E	294	LYS
1	E	329	ASN
1	E	347	CYS
1	E	374	LEU
1	E	404	LEU
1	E	466	ASP
1	E	470	SER
1	E	532	GLU
1	E	559	ARG
1	E	565	LEU
1	E	591	LEU
2	F	14	LEU
2	F	49	GLU
2	F	99	LEU
2	F	129	LEU
2	F	137	LYS
2	F	161	ASN
2	F	164	GLN
2	F	167	GLN
1	G	66	ASN
1	G	71	GLU
1	G	73	SER
1	G	76	GLN
1	G	99	GLU
1	G	233	LEU
1	G	240	ILE
1	G	263	PHE
1	G	265	GLU
1	G	303	GLU
1	G	308	GLU
1	G	313	GLU
1	G	343	GLU
1	G	344	THR
1	G	347	CYS
1	G	350	ASP
1	G	360	GLN
1	G	427	LYS

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Mol	Chain	Res	Type
1	G	439	ASN
1	G	478	GLU
1	G	530	GLU
1	G	547	LEU
1	G	559	ARG
2	H	36	GLN
2	H	50	VAL
2	H	55	ARG
2	H	99	LEU
2	H	129	LEU
2	H	147	ASN
2	H	164	GLN
2	H	168	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	A	247	ASN
1	A	256	ASN
1	A	270	GLN
1	A	280	ASN
1	A	283	GLN
1	A	331	GLN
1	A	336	HIS
1	A	360	GLN
1	A	448	GLN
1	A	467	GLN
1	A	583	ASN
1	A	594	GLN
2	B	26	ASN
2	B	30	ASN
2	B	60	GLN
2	B	161	ASN
2	B	172	ASN
1	C	63	GLN
1	C	65	ASN
1	C	76	GLN
1	C	78	GLN
1	C	225	ASN
1	C	247	ASN
1	C	270	GLN

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Mol	Chain	Res	Type
1	C	305	HIS
1	C	324	GLN
1	C	331	GLN
1	C	336	HIS
1	C	448	GLN
1	C	581	ASN
1	C	593	GLN
1	C	594	GLN
2	D	26	ASN
2	D	140	GLN
2	D	148	ASN
2	D	164	GLN
2	D	172	ASN
1	E	210	ASN
1	E	247	ASN
1	E	270	GLN
1	E	329	ASN
1	E	336	HIS
1	E	402	GLN
1	E	467	GLN
1	E	535	ASN
1	E	581	ASN
1	E	594	GLN
2	F	26	ASN
2	F	133	GLN
2	F	147	ASN
2	F	161	ASN
2	F	172	ASN
1	G	4	ASN
1	G	63	GLN
1	G	65	ASN
1	G	66	ASN
1	G	76	GLN
1	G	78	GLN
1	G	270	GLN
1	G	428	HIS
1	G	439	ASN
1	G	448	GLN
1	G	581	ASN
1	G	583	ASN
1	G	607	ASN
2	H	26	ASN

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Mol	Chain	Res	Type
2	H	36	GLN
2	H	117	ASN
2	H	140	GLN
2	H	148	ASN
2	H	172	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\# Z > 2$
5	GDP	B	2302	3	29,30,30	1.22	4 (13%)	45,47,47	1.66	10 (22%)
5	GDP	F	2305	3	29,30,30	1.28	2 (6%)	45,47,47	1.65	9 (20%)
6	P33	F	3306	4	21,21,21	0.51	0	20,20,20	0.58	0
6	P33	B	3302	4	21,21,21	0.51	0	20,20,20	0.58	0
6	P33	H	3308	4	21,21,21	0.54	0	20,20,20	0.54	0
5	GDP	D	2300	3	29,30,30	1.37	1 (3%)	45,47,47	1.57	5 (11%)
6	P33	D	3304	4	21,21,21	0.51	0	20,20,20	0.54	0
5	GDP	H	2303	3	29,30,30	1.43	1 (3%)	45,47,47	1.63	8 (17%)

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
5	GDP	B	2302	3	-	1/16/32/32	0/3/3/3
5	GDP	F	2305	3	-	1/16/32/32	0/3/3/3
6	P33	F	3306	4	-	6/19/19/19	-
6	P33	B	3302	4	-	8/19/19/19	-
6	P33	H	3308	4	-	7/19/19/19	-
5	GDP	D	2300	3	-	1/16/32/32	0/3/3/3
6	P33	D	3304	4	-	7/19/19/19	-
5	GDP	H	2303	3	-	1/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	2303	GDP	PA-O3A	5.89	1.65	1.59
5	D	2300	GDP	PA-O3A	5.23	1.65	1.59
5	F	2305	GDP	PA-O3A	3.93	1.63	1.59
5	B	2302	GDP	PA-O3A	3.36	1.63	1.59
5	B	2302	GDP	C6-N1	2.33	1.43	1.38
5	F	2305	GDP	C6-N1	2.28	1.43	1.38
5	B	2302	GDP	C2-N3	2.17	1.38	1.33
5	B	2302	GDP	C3'-C4'	2.03	1.58	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	2303	GDP	O2A-PA-O3A	5.80	122.94	107.27
5	F	2305	GDP	O2A-PA-O3A	5.72	122.74	107.27
5	B	2302	GDP	O3A-PA-O1A	-5.62	93.79	110.70
5	D	2300	GDP	O2A-PA-O3A	5.56	122.30	107.27
5	B	2302	GDP	O2A-PA-O3A	5.51	122.18	107.27
5	F	2305	GDP	O3A-PA-O1A	-5.22	95.00	110.70
5	H	2303	GDP	O3A-PA-O1A	-4.92	95.89	110.70
5	D	2300	GDP	O3A-PA-O1A	-4.80	96.28	110.70
5	F	2305	GDP	O3B-PB-O2B	-2.60	98.05	107.80
5	D	2300	GDP	O3B-PB-O2B	-2.57	98.18	107.80
5	H	2303	GDP	O3B-PB-O2B	-2.43	98.70	107.80
5	D	2300	GDP	O3B-PB-O3A	2.40	112.68	104.64
5	B	2302	GDP	O3B-PB-O2B	-2.38	98.89	107.80
5	F	2305	GDP	C1'-N9-C8	2.37	133.47	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2302	GDP	O3'-C3'-C4'	-2.37	104.27	111.08
5	H	2303	GDP	O3B-PB-O3A	2.33	112.45	104.64
5	H	2303	GDP	C1'-N9-C8	2.32	133.33	126.73
5	B	2302	GDP	O4'-C4'-C3'	-2.31	100.56	105.15
5	B	2302	GDP	C1'-N9-C8	2.27	133.18	126.73
5	F	2305	GDP	O4'-C4'-C5'	2.22	116.45	109.33
5	H	2303	GDP	O3'-C3'-C4'	-2.20	104.75	111.08
5	H	2303	GDP	O4'-C4'-C5'	2.18	116.31	109.33
5	B	2302	GDP	O4'-C4'-C5'	2.17	116.29	109.33
5	F	2305	GDP	O3B-PB-O3A	2.16	111.89	104.64
5	F	2305	GDP	C1'-N9-C4	-2.14	120.16	126.49
5	D	2300	GDP	C1'-N9-C8	2.13	132.79	126.73
5	F	2305	GDP	O4'-C4'-C3'	-2.11	100.96	105.15
5	B	2302	GDP	C1'-N9-C4	-2.07	120.38	126.49
5	H	2303	GDP	C1'-N9-C4	-2.07	120.38	126.49
5	F	2305	GDP	O3'-C3'-C4'	-2.04	105.23	111.08
5	B	2302	GDP	O3B-PB-O3A	2.03	111.44	104.64
5	B	2302	GDP	O2A-PA-O5'	2.00	116.63	107.57

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	3302	P33	O13-C14-C15-O16
6	F	3306	P33	O7-C8-C9-O10
6	H	3308	P33	O13-C14-C15-O16
6	H	3308	P33	O7-C8-C9-O10
6	D	3304	P33	O13-C14-C15-O16
6	B	3302	P33	O19-C20-C21-O22
6	F	3306	P33	O1-C2-C3-O4
6	D	3304	P33	O7-C8-C9-O10
6	B	3302	P33	O7-C8-C9-O10
6	H	3308	P33	C18-C17-O16-C15
6	D	3304	P33	C18-C17-O16-C15
6	D	3304	P33	C2-C3-O4-C5
6	H	3308	P33	C15-C14-O13-C12
6	D	3304	P33	C15-C14-O13-C12
5	B	2302	GDP	PB-O3A-PA-O2A
5	D	2300	GDP	PB-O3A-PA-O2A
5	F	2305	GDP	PB-O3A-PA-O2A
5	H	2303	GDP	PB-O3A-PA-O2A
6	D	3304	P33	C8-C9-O10-C11

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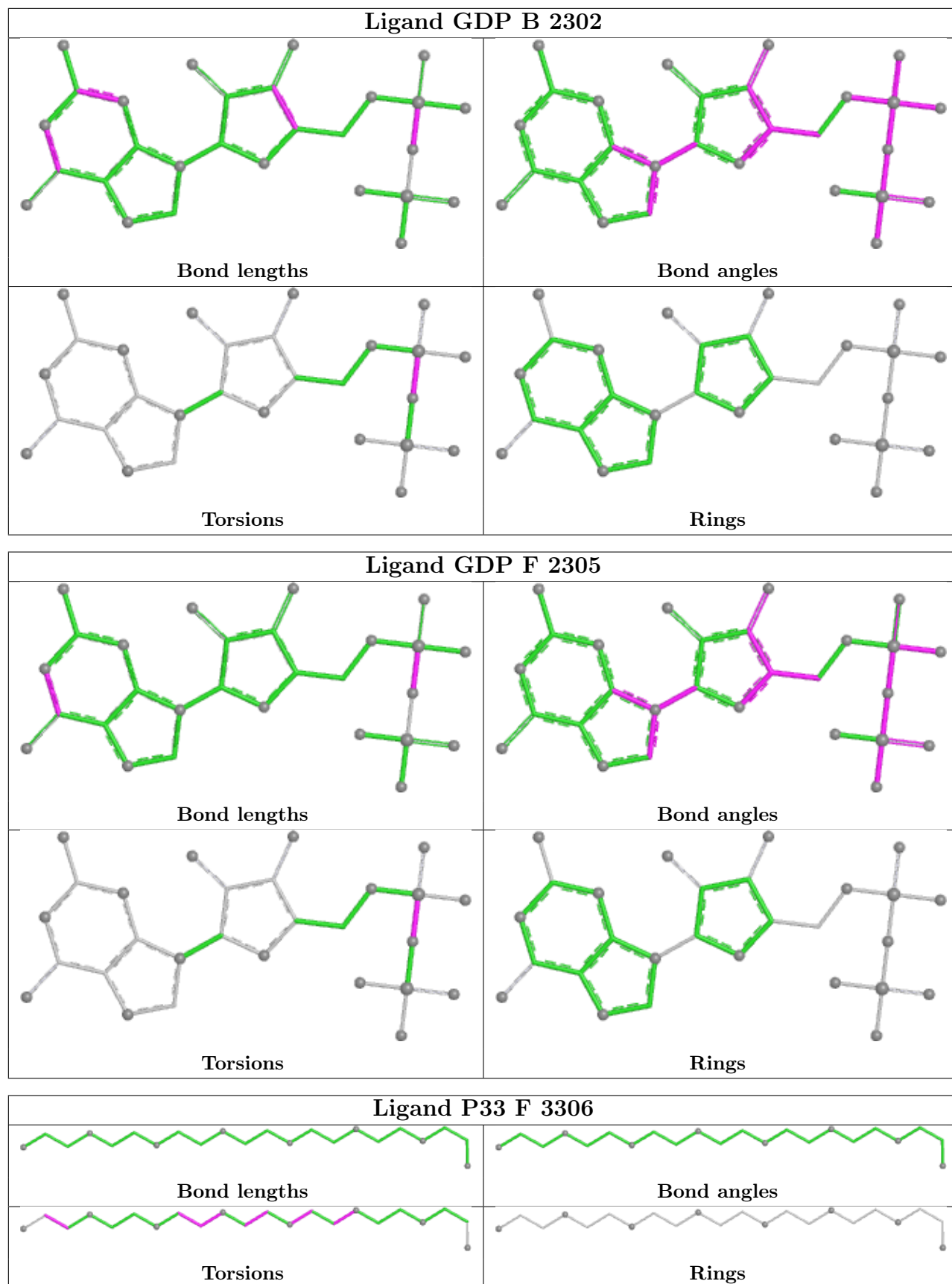
Mol	Chain	Res	Type	Atoms
6	F	3306	P33	C8-C9-O10-C11
6	H	3308	P33	C8-C9-O10-C11
6	F	3306	P33	C15-C14-O13-C12
6	B	3302	P33	C15-C14-O13-C12
6	B	3302	P33	C2-C3-O4-C5
6	F	3306	P33	C14-C15-O16-C17
6	B	3302	P33	C18-C17-O16-C15
6	B	3302	P33	C8-C9-O10-C11
6	H	3308	P33	C11-C12-O13-C14
6	H	3308	P33	O10-C11-C12-O13
6	B	3302	P33	O10-C11-C12-O13
6	F	3306	P33	O10-C11-C12-O13
6	D	3304	P33	O10-C11-C12-O13

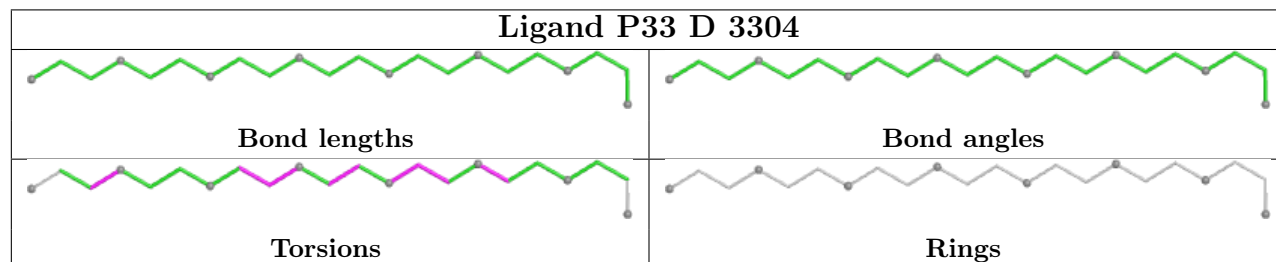
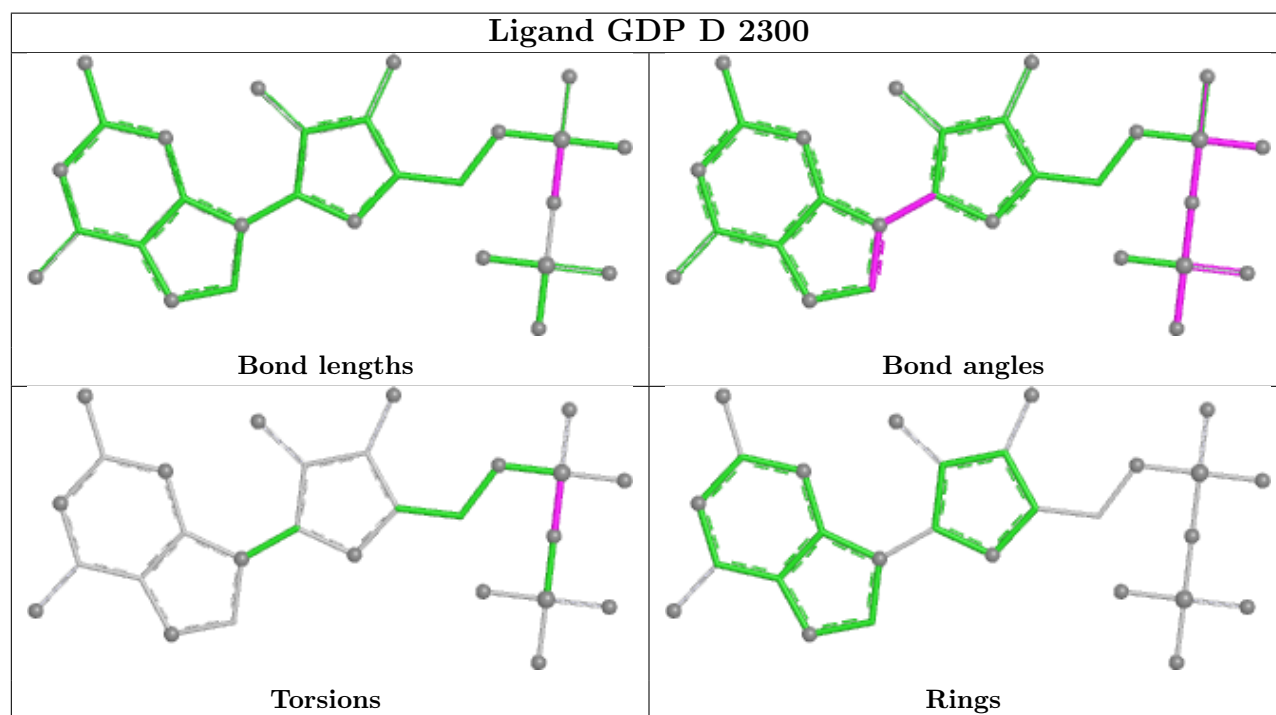
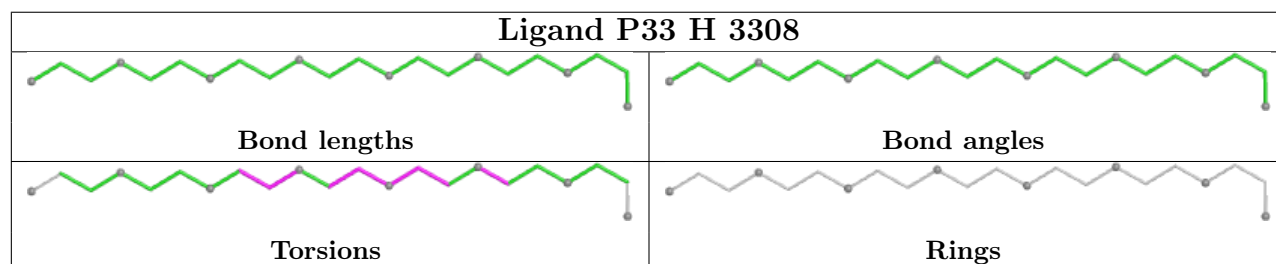
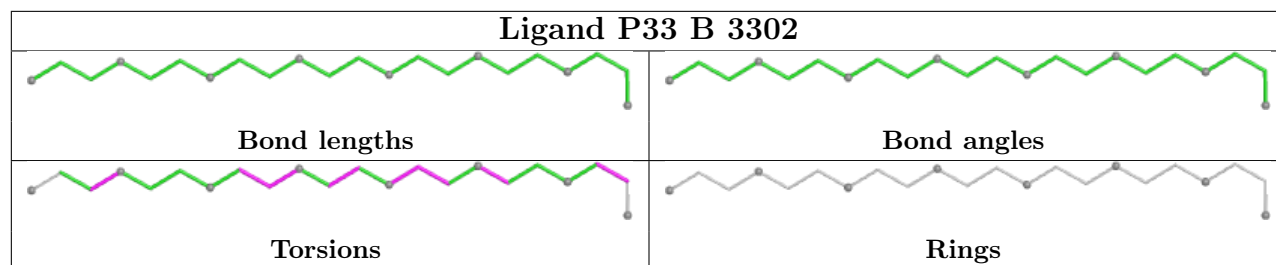
There are no ring outliers.

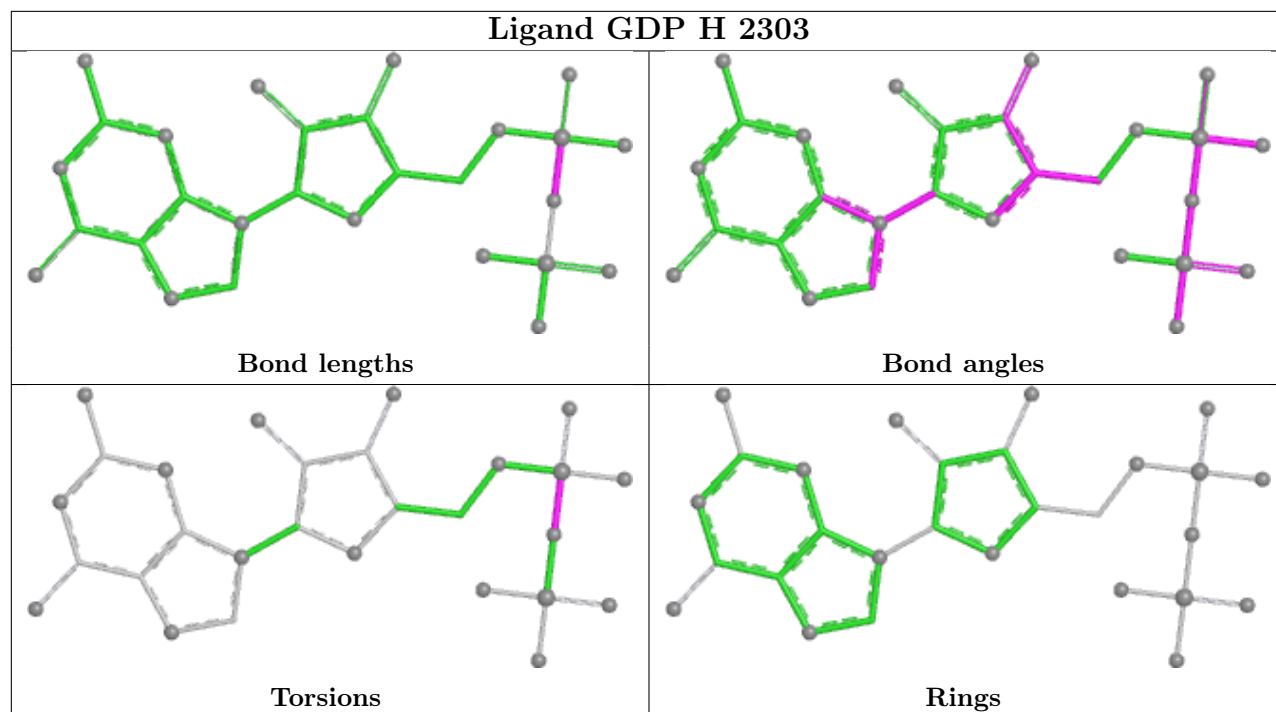
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2302	GDP	1	0
6	F	3306	P33	2	0
6	B	3302	P33	5	0
6	H	3308	P33	1	0
6	D	3304	P33	1	0
5	H	2303	GDP	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 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

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.