



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:33 PM UTC

PDB ID : 3TJZ / pdb_00003tjz
Title : Crystal Structure of Arf1 Bound to the gamma/zeta-COP Core Complex
Authors : Goldberg, J.; Yu, X.; Breitman, M.
Deposited on : 2011-08-25
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

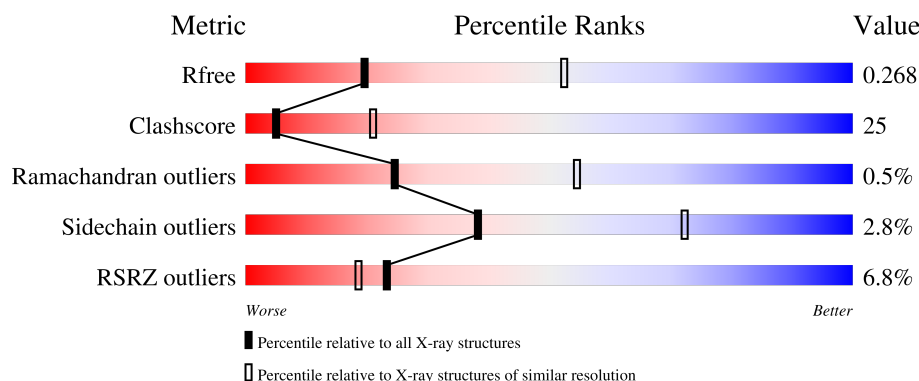
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	164	0% 73% 24% ..
1	D	164	3% 61% 35% ..
2	B	355	6% 47% 24% . 26%
2	E	355	8% 41% 30% . 27%
3	C	153	4% 62% 26% . . 8%

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Mol	Chain	Length	Quality of chain
3	F	153	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a red segment at the beginning labeled '8%', a green segment labeled '40%', a yellow segment labeled '48%', and a small red segment at the end labeled '8%'. There are two dots between the yellow and red segments.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8970 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 ADP-ribosylation factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1273	805	224	238	6			
1	D	159	Total	C	N	O	S	0	0	0
			1273	805	224	238	6			

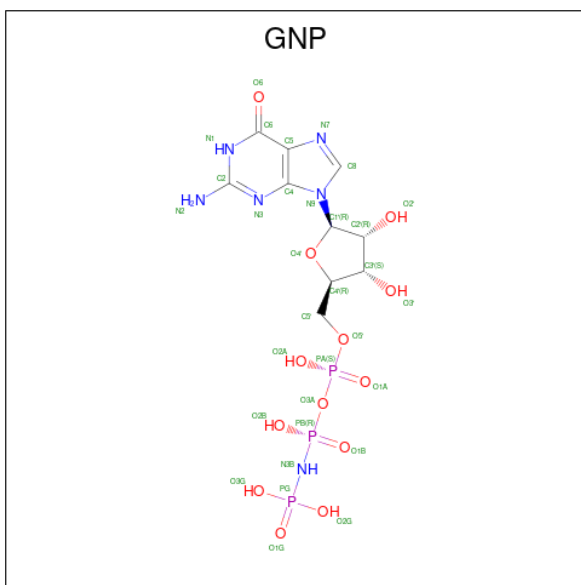
- Molecule 2 is a protein called Coatomer subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	264	Total	C	N	O	S	0	0	0
			2069	1305	366	379	19			
2	E	260	Total	C	N	O	S	0	0	0
			2033	1283	359	372	19			

- Molecule 3 is a protein called Coatomer subunit zeta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	140	Total	C	N	O	S	0	0	0
			1128	723	179	221	5			
3	F	140	Total	C	N	O	S	0	0	0
			1128	723	179	221	5			

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



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

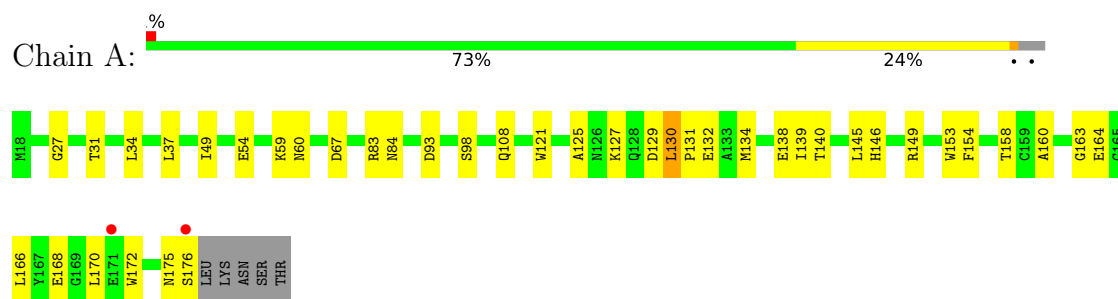
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0

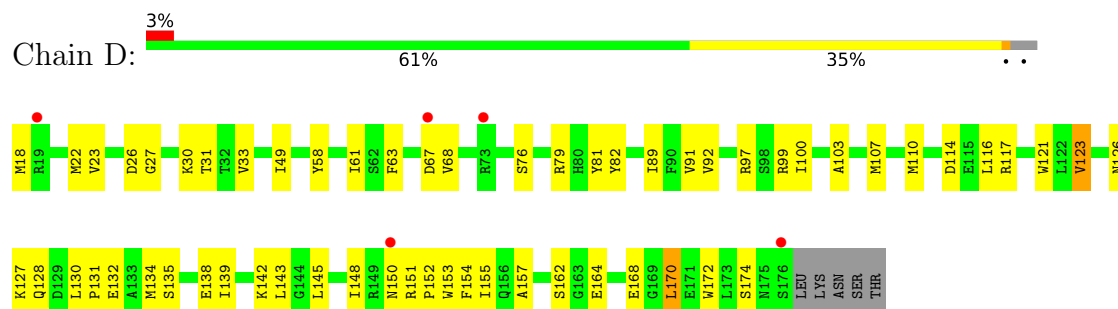
3 Residue-property plots [i](#)

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 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.

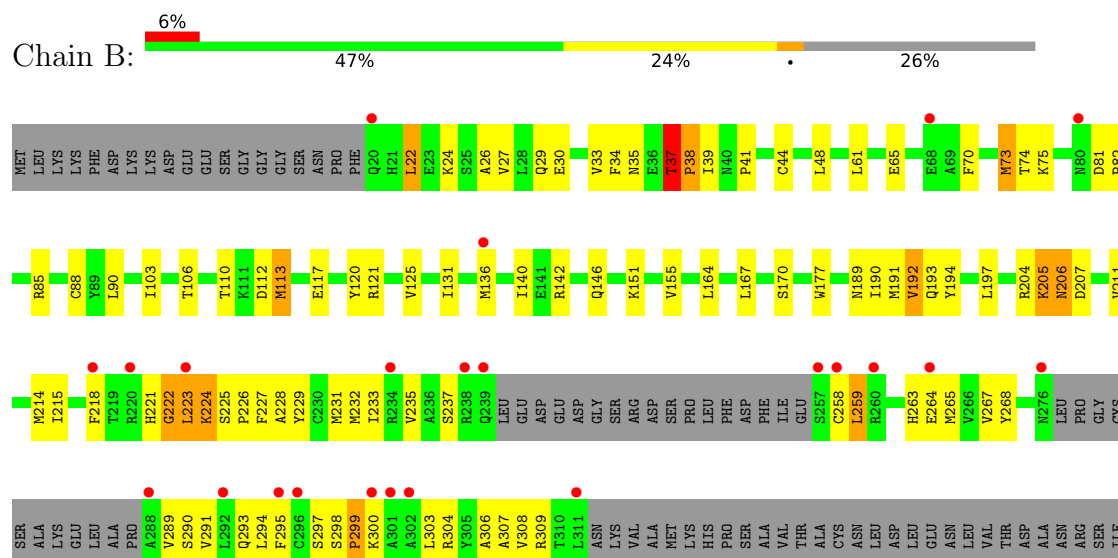
• Molecule 1: ADP-ribosylation factor 1



• Molecule 1: ADP-ribosylation factor 1



• Molecule 2: Coatomer subunit gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	163.58Å 163.58Å 145.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.90 45.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.00-2.90) 96.4 (45.00-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.64 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.206 , 0.260 0.224 , 0.268	Depositor DCC
R_{free} test set	2000 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8970	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.62	0/1297	1.04	3/1755 (0.2%)
1	D	0.55	0/1297	0.99	2/1755 (0.1%)
2	B	0.57	1/2100 (0.0%)	1.01	12/2831 (0.4%)
2	E	0.53	0/2063	1.03	6/2781 (0.2%)
3	C	0.60	0/1146	1.00	4/1549 (0.3%)
3	F	0.44	0/1146	0.92	5/1549 (0.3%)
All	All	0.56	1/9049 (0.0%)	1.00	32/12220 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	38	PRO	N-CD	-5.90	1.39	1.47

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	37	THR	N-CA-C	9.69	125.93	112.75
2	B	223	LEU	N-CA-C	9.54	124.58	110.46
2	B	206	ASN	CB-CA-C	-9.44	91.64	110.42
1	A	108	GLN	N-CA-C	8.83	122.02	111.33
2	B	37	THR	CB-CA-C	-8.04	97.81	112.76
3	C	35	TYR	CA-C-N	7.90	127.45	119.24
3	C	35	TYR	C-N-CA	7.90	127.45	119.24
2	E	275	VAL	N-CA-C	7.77	119.09	108.84
3	C	57	SER	N-CA-C	-7.46	99.60	110.64
2	E	37	THR	CA-C-N	-6.59	112.98	119.90
2	E	37	THR	C-N-CA	-6.59	112.98	119.90
1	D	130	LEU	CA-C-N	6.38	125.60	118.97
1	D	130	LEU	C-N-CA	6.38	125.60	118.97
2	B	192	VAL	CB-CA-C	-6.16	104.09	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	38	PRO	N-CA-C	-6.11	99.89	112.47
3	C	57	SER	CB-CA-C	5.78	116.90	109.80
2	B	140	ILE	N-CA-C	5.71	118.49	112.83
2	B	206	ASN	N-CA-C	5.62	122.78	110.80
2	B	170	SER	N-CA-C	5.49	119.18	107.70
2	E	294	LEU	N-CA-CB	5.48	118.17	110.12
2	E	219	THR	N-CA-C	-5.47	105.40	111.36
3	F	35	TYR	CA-C-N	5.39	125.21	119.28
3	F	35	TYR	C-N-CA	5.39	125.21	119.28
2	E	260	ARG	N-CA-C	5.38	117.90	111.71
3	F	138	ASP	CA-C-N	5.36	125.17	119.28
3	F	138	ASP	C-N-CA	5.36	125.17	119.28
3	F	128	ILE	N-CA-C	5.25	115.91	110.82
1	A	130	LEU	CA-C-N	5.17	124.61	119.24
1	A	130	LEU	C-N-CA	5.17	124.61	119.24
2	B	224	LYS	N-CA-CB	5.16	118.49	110.80
2	B	224	LYS	N-CA-C	-5.09	105.97	113.61
2	B	237	SER	N-CA-C	5.03	121.51	110.80

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	1273	0	1263	23	0
1	D	1273	0	1263	54	0
2	B	2069	0	2127	130	0
2	E	2033	0	2095	131	0
3	C	1128	0	1127	50	0
3	F	1128	0	1127	77	0
4	A	32	0	13	1	0
4	D	32	0	13	1	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
All	All	8970	0	9028	448	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 25.

All (448) 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:B:37:THR:CG2	2:B:38:PRO:HD3	1.35	1.57
2:B:37:THR:HG22	2:B:38:PRO:CD	1.46	1.45
1:D:150:ASN:OD1	1:D:151:ARG:HG2	1.25	1.33
2:B:299:PRO:O	2:B:300:LYS:HG3	1.23	1.29
1:D:150:ASN:OD1	1:D:151:ARG:CG	1.88	1.22
2:B:37:THR:CG2	2:B:38:PRO:CD	2.09	1.20
2:B:259:LEU:HD23	2:B:259:LEU:N	1.55	1.16
2:E:70:PHE:O	2:E:73:MET:HG2	1.47	1.14
2:B:204:ARG:HD2	2:B:214:MET:CE	1.78	1.13
2:B:103:ILE:CD1	2:B:136:MET:HE1	1.79	1.12
2:B:103:ILE:HD11	2:B:136:MET:CE	1.78	1.12
3:F:68:VAL:CG1	3:F:91:MET:SD	2.39	1.11
2:B:113:MET:HE2	2:B:125:VAL:HG22	1.11	1.10
2:B:204:ARG:HD2	2:B:214:MET:HE3	1.34	1.10
3:F:68:VAL:HG11	3:F:91:MET:SD	1.90	1.10
2:B:103:ILE:HD11	2:B:136:MET:HE1	1.19	1.09
3:C:48:ILE:HG12	3:C:62:LEU:HD23	1.11	1.08
3:C:44:PHE:CZ	3:C:48:ILE:HD11	1.89	1.06
2:B:205:LYS:O	2:B:206:ASN:HB2	1.53	1.06
2:B:299:PRO:O	2:B:300:LYS:CG	2.04	1.05
3:C:48:ILE:CG1	3:C:62:LEU:HD23	1.87	1.04
2:B:121:ARG:NH1	2:B:155:VAL:HG21	1.72	1.03
2:B:197:LEU:HD13	2:B:223:LEU:HD11	1.42	1.01
2:E:193:GLN:NE2	2:E:223:LEU:HB3	1.76	1.00
2:B:291:VAL:HG12	2:B:291:VAL:O	1.60	1.00
2:B:113:MET:CE	2:B:125:VAL:HG22	1.91	0.99
3:C:44:PHE:CZ	3:C:48:ILE:CD1	2.46	0.99
2:E:35:ASN:O	2:E:75:LYS:HE2	1.64	0.98
2:E:35:ASN:HA	2:E:75:LYS:CD	1.94	0.97
2:E:113:MET:SD	2:E:125:VAL:HG22	2.09	0.93
3:F:68:VAL:HG12	3:F:94:LEU:HD12	1.50	0.93
2:E:113:MET:HE3	2:E:125:VAL:HG21	1.50	0.92
2:B:37:THR:HG23	2:B:38:PRO:N	1.81	0.92
2:B:259:LEU:N	2:B:259:LEU:CD2	2.30	0.91
3:F:128:ILE:HG22	3:F:129:VAL:HG23	1.50	0.91
1:A:31:THR:HG22	1:A:67:ASP:OD2	1.69	0.91
1:D:22:MET:HE1	1:D:33:VAL:HG11	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:70:PHE:O	2:E:73:MET:CG	2.20	0.90
3:F:68:VAL:HG13	3:F:91:MET:SD	2.09	0.90
2:B:197:LEU:CD1	2:B:223:LEU:HD11	2.02	0.90
2:E:113:MET:HE3	2:E:125:VAL:CG2	2.01	0.89
2:B:259:LEU:HD23	2:B:259:LEU:H	1.32	0.89
2:E:35:ASN:HA	2:E:75:LYS:HD3	1.55	0.88
2:E:257:SER:O	2:E:258:CYS:SG	2.33	0.86
1:D:27:GLY:H	4:D:201:GNP:HNB3	1.21	0.85
3:F:26:LEU:HD21	3:F:114:LEU:HD23	1.59	0.85
2:B:204:ARG:CD	2:B:214:MET:HE3	2.06	0.84
2:E:193:GLN:HE22	2:E:223:LEU:HB3	1.32	0.84
2:B:103:ILE:CG1	2:B:136:MET:HE1	2.07	0.83
2:B:193:GLN:OE1	2:B:223:LEU:HD22	1.79	0.83
2:B:113:MET:HE2	2:B:125:VAL:CG2	2.02	0.83
1:D:61:ILE:HD11	1:D:174:SER:OG	1.78	0.83
2:B:37:THR:CG2	2:B:38:PRO:N	2.33	0.82
2:E:113:MET:O	2:E:121:ARG:HD2	1.79	0.82
2:E:293:GLN:HG2	2:E:294:LEU:N	1.94	0.81
3:F:21:ASN:HB2	3:F:74:ASP:OD1	1.80	0.81
2:E:34:PHE:O	2:E:75:LYS:HD3	1.79	0.81
2:B:37:THR:HG23	2:B:38:PRO:CD	2.08	0.81
3:C:82:SER:OG	3:C:85:GLU:HG2	1.79	0.80
2:B:291:VAL:O	2:B:291:VAL:CG1	2.30	0.80
3:F:105:LEU:HD23	3:F:113:ALA:HB1	1.61	0.80
3:C:44:PHE:CE1	3:C:48:ILE:HD11	2.17	0.80
2:B:70:PHE:O	2:B:73:MET:HG3	1.81	0.79
1:A:27:GLY:H	4:A:201:GNP:HNB3	1.31	0.79
3:F:68:VAL:HG12	3:F:94:LEU:CD1	2.12	0.79
2:B:197:LEU:CD1	2:B:223:LEU:CD1	2.61	0.78
2:B:197:LEU:HD11	2:B:223:LEU:HD21	1.65	0.78
2:E:75:LYS:HG2	2:E:78:GLN:HE21	1.48	0.77
1:D:150:ASN:OD1	1:D:151:ARG:HG3	1.84	0.77
2:E:35:ASN:HA	2:E:75:LYS:HD2	1.65	0.77
2:B:103:ILE:CD1	2:B:136:MET:CE	2.49	0.77
3:C:48:ILE:HG12	3:C:62:LEU:CD2	2.06	0.76
2:B:190:ILE:HG23	2:B:225:SER:CB	2.15	0.76
3:F:55:THR:HG22	3:F:56:ASP:H	1.50	0.75
2:B:191:MET:HE1	2:B:227:PHE:CE2	2.20	0.75
2:B:299:PRO:C	2:B:300:LYS:HG3	2.11	0.75
2:B:193:GLN:HE22	2:B:224:LYS:H	1.35	0.75
2:B:190:ILE:HG21	2:B:226:PRO:HD2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:LYS:HD2	2:B:61:LEU:HD23	1.69	0.74
2:E:90:LEU:HD21	3:F:123:LEU:HD23	1.68	0.74
2:E:305:TYR:CZ	2:E:309:ARG:HD2	2.22	0.73
2:B:291:VAL:HG13	2:B:294:LEU:HD12	1.70	0.73
1:A:146:HIS:O	1:A:149:ARG:NH1	2.22	0.72
2:E:51:ILE:O	2:E:55:ILE:HG13	1.89	0.72
3:C:139:PRO:O	3:C:143:VAL:HG23	1.89	0.72
2:B:204:ARG:HD2	2:B:214:MET:HE1	1.71	0.72
2:E:305:TYR:CE2	2:E:309:ARG:HD2	2.24	0.72
3:F:61:LEU:C	3:F:62:LEU:HD12	2.15	0.72
2:B:218:PHE:O	2:B:222:GLY:HA2	1.91	0.71
2:E:113:MET:CE	2:E:125:VAL:HG22	2.20	0.71
2:E:117:GLU:HG2	2:E:120:TYR:CE2	2.25	0.71
3:F:124:ALA:O	3:F:128:ILE:HD12	1.89	0.71
2:B:190:ILE:HG23	2:B:225:SER:HA	1.73	0.71
2:B:197:LEU:HD13	2:B:223:LEU:CD1	2.18	0.71
2:B:258:CYS:C	2:B:259:LEU:HD23	2.15	0.71
2:B:113:MET:HE3	2:B:125:VAL:HA	1.73	0.70
2:E:113:MET:CE	2:E:125:VAL:CG2	2.69	0.70
2:B:113:MET:CE	2:B:125:VAL:HA	2.22	0.70
1:D:154:PHE:HB2	1:D:172:TRP:CE2	2.26	0.70
2:E:70:PHE:C	2:E:73:MET:HG2	2.16	0.70
2:E:231:MET:O	2:E:235:VAL:HG23	1.91	0.70
2:B:309:ARG:NH2	3:C:87:GLU:OE2	2.23	0.69
2:E:37:THR:HB	2:E:38:PRO:HD3	1.74	0.69
2:E:90:LEU:CD2	3:F:123:LEU:HD23	2.22	0.69
2:E:293:GLN:HG2	2:E:294:LEU:H	1.56	0.69
3:C:70:LYS:HG2	3:C:71:SER:H	1.56	0.69
1:D:61:ILE:CD1	1:D:174:SER:OG	2.41	0.69
2:E:86:ARG:O	2:E:90:LEU:HD13	1.93	0.69
2:B:223:LEU:HD13	2:B:228:ALA:HB1	1.74	0.68
2:B:30:GLU:O	2:B:33:VAL:HG12	1.94	0.68
2:B:291:VAL:HA	2:B:293:GLN:HE22	1.59	0.68
2:B:205:LYS:O	2:B:206:ASN:CB	2.38	0.68
1:D:151:ARG:HB2	1:D:152:PRO:HD2	1.76	0.67
2:B:289:VAL:CG1	2:B:290:SER:N	2.58	0.67
2:B:289:VAL:HG12	2:B:290:SER:N	2.08	0.67
3:C:44:PHE:CZ	3:C:48:ILE:HD12	2.27	0.67
2:B:142:ARG:O	2:B:146:GLN:HG3	1.94	0.67
1:D:162:SER:OG	1:D:164:GLU:HG3	1.95	0.67
2:B:298:SER:N	2:B:299:PRO:HD2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:289:VAL:HG12	2:E:291:VAL:HG23	1.75	0.67
3:F:92:THR:CG2	3:F:137:SER:HB2	2.26	0.66
1:D:150:ASN:OD1	1:D:151:ARG:N	2.29	0.66
3:C:56:ASP:O	3:C:57:SER:C	2.37	0.66
3:F:15:ALA:O	3:F:16:ILE:HD13	1.96	0.66
1:D:107:MET:HE1	1:D:143:LEU:HB3	1.78	0.66
2:E:191:MET:HE3	2:E:191:MET:HA	1.78	0.65
3:C:74:ASP:OD2	3:C:111:LYS:HB3	1.96	0.65
1:D:81:TYR:HE2	2:E:104:ILE:HD11	1.61	0.65
1:D:134:MET:HE3	1:D:139:ILE:CD1	2.26	0.65
3:C:57:SER:O	3:C:69:TYR:CZ	2.49	0.65
2:E:294:LEU:HD13	2:E:310:THR:OG1	1.97	0.65
3:C:74:ASP:OD2	3:C:111:LYS:CB	2.45	0.64
2:E:208:ARG:HA	2:E:211:VAL:HG22	1.80	0.64
2:B:221:HIS:O	2:B:222:GLY:O	2.16	0.64
2:E:201:TYR:CE2	3:F:8:PRO:HG2	2.32	0.64
1:D:22:MET:HE1	1:D:33:VAL:CG1	2.27	0.64
2:E:161:VAL:O	2:E:164:LEU:HB3	1.98	0.63
2:B:190:ILE:HG23	2:B:225:SER:CA	2.28	0.63
2:E:26:ALA:O	2:E:30:GLU:HG3	1.98	0.63
3:F:88:LEU:HD12	3:F:88:LEU:O	1.97	0.63
1:D:22:MET:HE2	1:D:91:VAL:HG21	1.81	0.63
1:D:23:VAL:HG12	1:D:68:VAL:HG22	1.81	0.63
1:D:150:ASN:CG	1:D:151:ARG:HG2	2.20	0.63
2:E:75:LYS:HG2	2:E:78:GLN:NE2	2.14	0.63
2:B:229:TYR:O	2:B:233:ILE:HG13	1.99	0.62
3:C:68:VAL:HG22	3:C:91:MET:HE1	1.80	0.62
2:E:75:LYS:O	2:E:78:GLN:HG2	2.00	0.62
2:B:121:ARG:HH12	2:B:155:VAL:HG21	1.62	0.62
1:D:134:MET:HE3	1:D:139:ILE:HD11	1.81	0.62
3:F:41:GLN:O	3:F:45:GLU:HG3	1.99	0.62
1:D:128:GLN:HG3	1:D:157:ALA:HB1	1.81	0.62
2:E:39:ILE:O	2:E:41:PRO:HD3	1.99	0.62
3:F:55:THR:HG22	3:F:56:ASP:N	2.15	0.62
2:E:205:LYS:O	2:E:206:ASN:HB2	2.00	0.61
2:E:198:GLY:HA3	3:F:10:LEU:HD11	1.80	0.61
2:B:197:LEU:HD11	2:B:223:LEU:CD2	2.28	0.61
2:B:289:VAL:CG1	2:B:291:VAL:HG23	2.31	0.61
2:E:149:VAL:HG13	2:E:180:GLU:HB3	1.83	0.61
1:D:30:LYS:HB3	1:D:67:ASP:OD1	2.01	0.60
2:E:88:CYS:O	2:E:92:ILE:HG13	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PHE:HB2	1:A:172:TRP:CE2	2.37	0.60
2:E:193:GLN:HE22	2:E:223:LEU:CB	2.11	0.60
2:E:264:GLU:O	2:E:267:VAL:HG22	2.02	0.60
2:E:24:LYS:HD2	2:E:24:LYS:N	2.16	0.60
2:E:35:ASN:C	2:E:75:LYS:HE2	2.25	0.60
3:F:21:ASN:CB	3:F:74:ASP:OD1	2.48	0.60
2:B:136:MET:O	2:B:136:MET:HG2	2.02	0.60
1:A:131:PRO:HB2	1:A:132:GLU:OE2	2.02	0.60
1:A:168:GLU:N	1:A:168:GLU:OE1	2.32	0.60
3:C:44:PHE:CE2	3:C:48:ILE:HD12	2.37	0.59
3:F:62:LEU:HD12	3:F:62:LEU:N	2.17	0.59
2:B:90:LEU:HD11	3:C:123:LEU:HD23	1.83	0.59
2:E:229:TYR:O	2:E:230:CYS:C	2.43	0.59
2:E:271:ALA:O	2:E:274:ILE:HG13	2.03	0.59
1:D:31:THR:HA	1:D:67:ASP:OD2	2.02	0.59
3:C:21:ASN:O	3:C:49:PHE:CZ	2.55	0.59
3:C:88:LEU:O	3:C:92:THR:HG23	2.03	0.59
3:C:70:LYS:HG2	3:C:71:SER:N	2.17	0.59
1:D:168:GLU:N	1:D:168:GLU:OE1	2.34	0.59
3:F:25:ARG:HB2	3:F:45:GLU:OE1	2.03	0.59
3:C:57:SER:O	3:C:69:TYR:CE1	2.55	0.58
2:E:113:MET:HB2	2:E:125:VAL:HG23	1.83	0.58
2:B:90:LEU:CD1	3:C:123:LEU:HD23	2.33	0.58
2:B:298:SER:N	2:B:299:PRO:CD	2.67	0.58
3:C:48:ILE:CG1	3:C:62:LEU:CD2	2.75	0.58
1:D:123:VAL:HG22	1:D:155:ILE:HG13	1.85	0.58
2:E:231:MET:HG2	2:E:232:MET:HE2	1.85	0.58
2:E:113:MET:HB2	2:E:125:VAL:CG2	2.33	0.58
2:E:309:ARG:HH22	3:F:61:LEU:HD22	1.68	0.58
2:B:289:VAL:HG11	2:B:291:VAL:HG23	1.85	0.58
2:B:121:ARG:HH11	2:B:155:VAL:HG21	1.63	0.57
2:E:292:LEU:O	2:E:295:PHE:HB2	2.03	0.57
1:A:125:ALA:HB1	1:A:139:ILE:HD12	1.85	0.57
2:E:73:MET:HE1	2:E:91:THR:HB	1.86	0.57
1:D:23:VAL:HG12	1:D:68:VAL:CG2	2.35	0.57
2:B:193:GLN:CD	2:B:223:LEU:HD22	2.30	0.57
3:C:34:THR:O	3:C:36:PRO:HD3	2.05	0.57
3:C:68:VAL:HG22	3:C:91:MET:CE	2.34	0.57
1:D:81:TYR:HE2	2:E:104:ILE:CD1	2.17	0.57
2:E:264:GLU:CD	2:E:264:GLU:H	2.13	0.57
2:E:222:GLY:HA2	2:E:229:TYR:OH	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:LEU:O	1:D:151:ARG:NH2	2.38	0.56
3:F:70:LYS:HB3	3:F:94:LEU:HD21	1.87	0.56
3:C:99:ASP:O	3:C:103:GLN:HG3	2.05	0.56
2:E:217:LYS:O	2:E:220:ARG:HB3	2.06	0.56
3:F:82:SER:OG	3:F:85:GLU:HG2	2.05	0.56
2:B:117:GLU:OE1	2:B:120:TYR:CE2	2.59	0.56
2:E:193:GLN:HE21	2:E:223:LEU:HD22	1.71	0.56
1:D:138:GLU:HG2	1:D:142:LYS:HZ2	1.70	0.56
2:E:274:ILE:HD12	2:E:275:VAL:N	2.21	0.55
3:C:73:ILE:N	3:C:73:ILE:HD13	2.20	0.55
2:E:300:LYS:HG2	2:E:301:ALA:N	2.21	0.55
2:B:70:PHE:O	2:B:73:MET:CG	2.51	0.55
2:E:293:GLN:CG	2:E:294:LEU:N	2.69	0.55
2:B:193:GLN:NE2	2:B:224:LYS:H	2.04	0.55
2:B:304:ARG:O	2:B:308:VAL:HG23	2.07	0.55
2:B:103:ILE:HG13	2:B:136:MET:HE1	1.86	0.55
2:E:221:HIS:NE2	2:E:222:GLY:O	2.40	0.55
2:B:303:LEU:HD23	2:B:303:LEU:O	2.07	0.55
1:D:81:TYR:CE2	2:E:104:ILE:HD11	2.42	0.55
2:E:301:ALA:O	2:E:302:ALA:HB3	2.07	0.55
2:E:85:ARG:NH1	2:E:112:ASP:OD2	2.40	0.54
2:E:94:GLU:OE2	3:F:29:LYS:NZ	2.34	0.54
1:D:135:SER:O	1:D:139:ILE:HG12	2.07	0.54
2:B:293:GLN:H	2:B:293:GLN:CD	2.15	0.54
2:B:295:PHE:O	2:B:298:SER:HB2	2.07	0.54
2:B:22:LEU:HD13	2:B:27:VAL:HG21	1.90	0.54
1:A:93:ASP:CG	1:A:127:LYS:HD2	2.32	0.54
2:E:274:ILE:HD12	2:E:275:VAL:HG13	1.89	0.54
2:E:300:LYS:O	2:E:304:ARG:HG3	2.08	0.54
2:B:26:ALA:O	2:B:29:GLN:HB3	2.07	0.54
2:E:81:ASP:OD2	2:E:83:THR:OG1	2.20	0.54
2:E:289:VAL:HG12	2:E:291:VAL:CG2	2.38	0.54
2:B:290:SER:O	2:B:293:GLN:OE1	2.26	0.53
2:E:300:LYS:HG2	2:E:301:ALA:H	1.74	0.53
2:B:264:GLU:HG3	3:C:88:LEU:HD23	1.89	0.53
3:F:26:LEU:CD2	3:F:114:LEU:HD23	2.37	0.53
2:B:24:LYS:HD2	2:B:61:LEU:CD2	2.39	0.53
2:B:190:ILE:CG2	2:B:226:PRO:HD2	2.39	0.53
1:D:26:ASP:OD1	1:D:99:ARG:NH1	2.38	0.53
1:D:97:ARG:O	1:D:100:ILE:HG22	2.07	0.53
3:F:21:ASN:CG	3:F:74:ASP:OD1	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:THR:O	2:B:110:THR:HG23	2.09	0.53
2:B:22:LEU:CD1	2:B:27:VAL:HG21	2.39	0.52
2:B:85:ARG:NH1	2:B:112:ASP:OD2	2.41	0.52
2:E:268:TYR:CD1	2:E:268:TYR:C	2.86	0.52
3:F:75:LEU:HD21	3:F:111:LYS:HB2	1.91	0.52
2:B:293:GLN:HE21	2:B:294:LEU:HG	1.73	0.52
3:C:124:ALA:O	3:C:128:ILE:HG13	2.10	0.52
2:E:201:TYR:HE2	3:F:8:PRO:HG2	1.74	0.52
2:E:193:GLN:NE2	2:E:223:LEU:CB	2.64	0.52
2:E:53:TYR:CE2	2:E:57:GLN:HG3	2.44	0.52
2:E:275:VAL:O	2:E:276:ASN:HB2	2.10	0.52
3:F:21:ASN:ND2	3:F:74:ASP:OD1	2.43	0.51
2:E:47:ILE:O	2:E:51:ILE:HD12	2.09	0.51
1:D:22:MET:HE3	1:D:89:ILE:HG21	1.91	0.51
3:C:70:LYS:CG	3:C:71:SER:H	2.23	0.51
1:A:59:LYS:O	1:A:60:ASN:HB3	2.11	0.51
2:B:177:TRP:N	2:B:177:TRP:CD1	2.79	0.51
2:E:117:GLU:CG	2:E:120:TYR:CD2	2.94	0.51
2:E:197:LEU:HD13	2:E:223:LEU:HD13	1.93	0.51
2:E:222:GLY:CA	2:E:229:TYR:OH	2.58	0.51
2:E:113:MET:O	2:E:121:ARG:CD	2.53	0.51
3:F:43:ALA:HA	3:F:46:LYS:HE3	1.92	0.51
1:D:145:LEU:O	1:D:148:ILE:HG12	2.11	0.51
2:E:299:PRO:O	2:E:300:LYS:HB2	2.11	0.51
3:F:19:LEU:HD22	3:F:24:ASP:O	2.11	0.51
2:E:296:CYS:O	2:E:299:PRO:HD2	2.10	0.50
3:C:68:VAL:CG2	3:C:91:MET:HE2	2.41	0.50
2:B:22:LEU:HD13	2:B:27:VAL:CG2	2.42	0.50
2:E:35:ASN:CA	2:E:75:LYS:HD3	2.34	0.50
3:C:68:VAL:HG21	3:C:91:MET:HE2	1.92	0.50
1:D:22:MET:HE2	1:D:91:VAL:CG2	2.42	0.50
1:D:154:PHE:HB2	1:D:172:TRP:NE1	2.27	0.50
2:B:297:SER:HB3	2:B:303:LEU:HD22	1.92	0.50
2:E:117:GLU:HG2	2:E:120:TYR:CD2	2.47	0.50
2:B:103:ILE:HD11	2:B:136:MET:HE3	1.85	0.50
2:B:190:ILE:HG21	2:B:226:PRO:CD	2.41	0.50
2:B:193:GLN:OE1	2:B:223:LEU:CD2	2.56	0.50
3:F:55:THR:CG2	3:F:56:ASP:H	2.22	0.50
2:E:221:HIS:CD2	2:E:222:GLY:O	2.65	0.49
2:B:39:ILE:O	2:B:41:PRO:HD3	2.13	0.49
1:A:140:THR:HG23	1:A:145:LEU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:ASN:OD1	2:B:75:LYS:HD2	2.12	0.49
3:F:136:GLU:HG3	3:F:138:ASP:H	1.77	0.49
1:D:18:MET:HE3	1:D:63:PHE:CE1	2.48	0.49
1:D:49:ILE:HG22	2:E:106:THR:HB	1.95	0.49
1:D:58:TYR:HB3	1:D:63:PHE:HE2	1.78	0.49
2:E:300:LYS:CG	2:E:301:ALA:H	2.25	0.49
3:F:74:ASP:OD2	3:F:75:LEU:HD23	2.13	0.49
3:F:26:LEU:HD13	3:F:115:LEU:HD11	1.94	0.49
2:B:121:ARG:O	2:B:125:VAL:HG23	2.13	0.49
3:F:20:ASP:OD1	3:F:111:LYS:NZ	2.37	0.49
3:C:106:ARG:O	3:C:107:LYS:HB2	2.13	0.48
1:D:138:GLU:HG2	1:D:142:LYS:NZ	2.27	0.48
3:C:104:MET:HE1	3:C:120:GLY:HA3	1.94	0.48
3:C:74:ASP:OD2	3:C:111:LYS:HB2	2.12	0.48
3:C:68:VAL:CG2	3:C:91:MET:CE	2.92	0.48
3:F:77:PHE:HZ	3:F:109:VAL:HG21	1.78	0.48
3:F:92:THR:CG2	3:F:137:SER:CB	2.90	0.48
3:F:101:LEU:HD23	3:F:104:MET:HE3	1.94	0.48
1:D:170:LEU:HD12	1:D:170:LEU:HA	1.69	0.48
2:E:293:GLN:CG	2:E:294:LEU:H	2.25	0.48
2:B:34:PHE:HD1	2:B:44:CYS:HG	1.62	0.48
3:F:92:THR:HG21	3:F:137:SER:HB2	1.94	0.48
1:D:151:ARG:HB2	1:D:152:PRO:CD	2.44	0.48
2:B:231:MET:O	2:B:235:VAL:HG23	2.14	0.47
2:B:289:VAL:CG1	2:B:290:SER:H	2.26	0.47
1:A:163:GLY:HA2	1:A:166:LEU:HD12	1.96	0.47
2:E:205:LYS:O	2:E:206:ASN:CB	2.62	0.47
2:B:197:LEU:CD1	2:B:223:LEU:HD13	2.44	0.47
2:E:35:ASN:CA	2:E:75:LYS:CD	2.82	0.47
3:F:13:VAL:HG12	3:F:31:TYR:CD2	2.50	0.47
3:F:141:GLN:NE2	3:F:141:GLN:HA	2.30	0.47
3:F:141:GLN:HA	3:F:141:GLN:HE21	1.79	0.47
2:B:293:GLN:CD	2:B:293:GLN:N	2.72	0.47
1:D:23:VAL:C	1:D:30:LYS:HD3	2.40	0.47
2:B:164:LEU:O	2:B:167:LEU:HB2	2.15	0.47
1:D:107:MET:O	1:D:110:MET:HB2	2.15	0.47
2:B:82:PRO:HB3	2:B:120:TYR:OH	2.15	0.46
3:F:16:ILE:HG12	3:F:31:TYR:HE2	1.79	0.46
2:B:73:MET:HG3	2:B:74:THR:N	2.31	0.46
2:E:259:LEU:HD21	2:E:271:ALA:HB2	1.97	0.46
3:F:66:THR:OG1	3:F:83:SER:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HG22	1:A:49:ILE:O	2.15	0.46
3:F:14:LYS:HB2	3:F:81:GLY:HA2	1.98	0.46
2:B:24:LYS:HE3	2:B:65:GLU:OE1	2.15	0.46
2:B:264:GLU:HG3	2:B:265:MET:N	2.31	0.46
1:A:134:MET:HE2	1:A:138:GLU:HG2	1.98	0.46
2:B:190:ILE:HG23	2:B:225:SER:HB2	1.98	0.46
2:B:211:VAL:O	2:B:214:MET:HB3	2.16	0.46
2:E:300:LYS:CG	2:E:301:ALA:N	2.79	0.46
1:A:121:TRP:O	1:A:153:TRP:HA	2.16	0.46
3:C:32:ASP:C	3:C:32:ASP:OD1	2.58	0.46
3:F:127:GLU:O	3:F:135:LEU:HB3	2.16	0.46
2:B:73:MET:HB2	2:B:73:MET:HE3	1.60	0.45
3:F:7:GLU:OE1	3:F:7:GLU:N	2.49	0.45
2:B:113:MET:CE	2:B:125:VAL:CG2	2.78	0.45
3:F:42:LYS:O	3:F:46:LYS:HG3	2.17	0.45
2:E:305:TYR:OH	2:E:309:ARG:NH1	2.49	0.45
1:D:151:ARG:CB	1:D:152:PRO:HD2	2.46	0.45
3:F:92:THR:HG21	3:F:137:SER:CB	2.46	0.45
3:F:121:LEU:O	3:F:125:VAL:HG23	2.16	0.45
1:D:114:ASP:O	1:D:117:ARG:HB2	2.16	0.45
2:E:271:ALA:O	2:E:274:ILE:CG1	2.64	0.45
3:F:72:SER:O	3:F:73:ILE:C	2.59	0.45
2:E:81:ASP:HA	2:E:82:PRO:HD2	1.84	0.45
3:F:27:PHE:CD1	3:F:121:LEU:HD21	2.52	0.44
2:E:71:PHE:HA	2:E:74:THR:HG23	1.99	0.44
3:F:35:TYR:CZ	3:F:44:PHE:CD1	3.06	0.44
3:F:53:HIS:C	3:F:55:THR:H	2.26	0.44
2:B:85:ARG:O	2:B:88:CYS:HB2	2.18	0.44
3:C:141:GLN:O	3:C:145:ARG:HG3	2.17	0.44
1:D:100:ILE:O	1:D:103:ALA:HB3	2.18	0.44
2:E:259:LEU:CD2	2:E:271:ALA:HB2	2.47	0.44
3:F:89:MET:O	3:F:93:VAL:HG23	2.17	0.44
1:A:34:LEU:HD11	1:A:54:GLU:HB2	1.99	0.44
1:D:126:ASN:CG	1:D:127:LYS:H	2.25	0.44
3:F:48:ILE:HG12	3:F:62:LEU:HD22	2.00	0.44
2:B:189:ASN:OD1	2:B:192:VAL:HG23	2.18	0.44
2:B:215:ILE:HA	2:B:218:PHE:CE2	2.52	0.44
2:B:215:ILE:HD11	2:B:235:VAL:HG12	1.98	0.44
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.90	0.44
3:F:48:ILE:O	3:F:52:THR:HG22	2.18	0.44
1:A:83:ARG:O	1:A:84:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ASP:OD1	1:A:130:LEU:HG	2.18	0.44
1:A:175:ASN:O	1:A:176:SER:C	2.60	0.44
2:B:151:LYS:HA	2:B:151:LYS:HD3	1.70	0.44
1:D:131:PRO:HB2	1:D:132:GLU:OE2	2.18	0.44
2:E:225:SER:HB3	2:E:228:ALA:HB3	2.00	0.43
2:B:81:ASP:HA	2:B:82:PRO:HD3	1.88	0.43
2:B:263:HIS:O	2:B:267:VAL:HG23	2.18	0.43
3:C:103:GLN:HB2	3:C:143:VAL:HG21	1.99	0.43
2:E:257:SER:C	2:E:258:CYS:SG	3.01	0.43
1:A:160:ALA:HA	1:A:166:LEU:HD11	2.00	0.43
2:B:48:LEU:HD23	2:B:48:LEU:HA	1.82	0.43
2:B:136:MET:O	2:B:136:MET:CG	2.66	0.43
2:B:204:ARG:HH11	2:B:214:MET:CE	2.30	0.43
2:E:76:LEU:HD13	2:E:84:LEU:HD11	1.99	0.43
3:F:72:SER:HB2	3:F:75:LEU:O	2.17	0.43
2:B:190:ILE:HG23	2:B:225:SER:OG	2.18	0.43
2:E:208:ARG:HA	2:E:211:VAL:CG2	2.48	0.43
2:E:259:LEU:HD21	2:E:271:ALA:N	2.34	0.43
1:A:158:THR:HA	1:A:164:GLU:O	2.17	0.43
2:E:189:ASN:OD1	2:E:192:VAL:HG23	2.18	0.43
2:B:205:LYS:O	2:B:205:LYS:HG3	2.15	0.43
3:F:20:ASP:HB3	3:F:23:GLY:H	1.84	0.43
2:E:199:LEU:O	2:E:203:VAL:HG23	2.19	0.43
2:E:217:LYS:HA	2:E:220:ARG:NH2	2.34	0.43
2:E:261:ASN:OD1	2:E:263:HIS:HB2	2.19	0.43
1:A:131:PRO:HB2	1:A:132:GLU:CD	2.44	0.43
3:F:23:GLY:HA3	3:F:49:PHE:CE2	2.54	0.43
1:D:79:ARG:HA	1:D:82:TYR:CD2	2.54	0.43
1:D:138:GLU:CG	1:D:142:LYS:NZ	2.81	0.43
2:E:175:LYS:O	2:E:178:VAL:HG13	2.18	0.43
2:E:270:ALA:O	2:E:274:ILE:HG23	2.18	0.43
3:F:77:PHE:CZ	3:F:109:VAL:HG21	2.53	0.43
2:E:24:LYS:N	2:E:24:LYS:CD	2.80	0.42
2:E:117:GLU:HG2	2:E:120:TYR:HE2	1.82	0.42
3:F:16:ILE:HD12	3:F:79:VAL:HG22	2.01	0.42
3:C:138:ASP:C	3:C:138:ASP:OD1	2.62	0.42
2:E:269:GLU:OE1	3:F:86:ASN:HB2	2.19	0.42
3:C:21:ASN:O	3:C:49:PHE:HZ	1.99	0.42
3:F:69:TYR:HA	3:F:77:PHE:O	2.20	0.42
2:E:75:LYS:CG	2:E:78:GLN:NE2	2.82	0.42
2:E:215:ILE:HA	2:E:218:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:20:ASP:HB3	3:F:24:ASP:H	1.84	0.42
1:D:26:ASP:OD1	1:D:26:ASP:O	2.36	0.42
2:B:113:MET:CE	2:B:125:VAL:CA	2.96	0.42
2:B:164:LEU:HD22	3:C:10:LEU:HD12	2.02	0.42
3:C:34:THR:C	3:C:36:PRO:HD3	2.44	0.42
2:B:258:CYS:CA	2:B:259:LEU:HD23	2.50	0.42
1:D:121:TRP:O	1:D:153:TRP:HA	2.19	0.42
2:B:268:TYR:CZ	2:B:306:ALA:HB1	2.55	0.42
3:C:62:LEU:HD12	3:C:63:GLU:H	1.85	0.42
3:C:70:LYS:CG	3:C:71:SER:N	2.81	0.42
2:E:259:LEU:HD21	2:E:271:ALA:CA	2.50	0.42
3:F:52:THR:HG21	3:F:78:TYR:OH	2.20	0.42
3:C:113:ALA:O	3:C:116:GLU:HB2	2.20	0.42
2:E:70:PHE:CA	2:E:73:MET:HG2	2.49	0.42
2:E:215:ILE:O	2:E:219:THR:OG1	2.33	0.42
3:F:27:PHE:C	3:F:27:PHE:CD2	2.98	0.41
2:B:103:ILE:CD1	2:B:136:MET:HE3	2.43	0.41
3:C:14:LYS:HE3	3:C:32:ASP:OD2	2.20	0.41
1:D:145:LEU:HD23	1:D:145:LEU:HA	1.92	0.41
2:B:191:MET:O	2:B:194:TYR:HB3	2.20	0.41
2:E:151:LYS:HA	2:E:151:LYS:HD3	1.87	0.41
3:F:40:GLU:O	3:F:43:ALA:HB3	2.19	0.41
3:C:59:ILE:O	3:C:59:ILE:HG23	2.21	0.41
1:A:37:LEU:HD13	1:A:170:LEU:HD11	2.02	0.41
2:E:53:TYR:CZ	2:E:57:GLN:OE1	2.73	0.41
3:C:138:ASP:HA	3:C:139:PRO:HD3	1.88	0.41
3:F:37:SER:HB2	3:F:40:GLU:OE1	2.21	0.41
3:F:77:PHE:HZ	3:F:109:VAL:CG2	2.33	0.41
2:B:37:THR:HG22	2:B:38:PRO:HD3	0.50	0.41
2:E:137:LEU:HD23	2:E:173:VAL:HG11	2.03	0.41
2:E:291:VAL:HG12	2:E:291:VAL:O	2.20	0.41
2:E:131:ILE:C	2:E:131:ILE:HD12	2.46	0.41
2:E:274:ILE:HD12	2:E:275:VAL:CG1	2.51	0.41
3:F:98:PHE:CE2	3:F:109:VAL:HG11	2.56	0.40
2:E:36:GLU:OE1	2:E:36:GLU:HA	2.21	0.40
2:B:207:ASP:OD1	2:B:207:ASP:C	2.63	0.40
2:E:191:MET:HA	2:E:191:MET:CE	2.50	0.40
2:E:221:HIS:CE1	2:E:222:GLY:O	2.75	0.40
3:F:111:LYS:CG	3:F:115:LEU:HD22	2.52	0.40
2:E:70:PHE:HA	2:E:73:MET:SD	2.61	0.40
2:E:225:SER:HA	2:E:226:PRO:HD2	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:LEU:HB3	2:B:232:MET:HE3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	157/164 (96%)	153 (98%)	4 (2%)	0	100	100
1	D	157/164 (96%)	152 (97%)	5 (3%)	0	100	100
2	B	258/355 (73%)	243 (94%)	12 (5%)	3 (1%)	10	34
2	E	254/355 (72%)	237 (93%)	16 (6%)	1 (0%)	30	59
3	C	138/153 (90%)	132 (96%)	5 (4%)	1 (1%)	18	48
3	F	138/153 (90%)	127 (92%)	11 (8%)	0	100	100
All	All	1102/1344 (82%)	1044 (95%)	53 (5%)	5 (0%)	24	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	222	GLY
2	E	291	VAL
2	B	307	ALA
2	B	299	PRO
3	C	73	ILE

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	136/141 (96%)	135 (99%)	1 (1%)	76	92
1	D	136/141 (96%)	132 (97%)	4 (3%)	37	71
2	B	231/307 (75%)	224 (97%)	7 (3%)	36	70
2	E	227/307 (74%)	222 (98%)	5 (2%)	45	77
3	C	128/138 (93%)	123 (96%)	5 (4%)	28	63
3	F	128/138 (93%)	122 (95%)	6 (5%)	23	56
All	All	986/1172 (84%)	958 (97%)	28 (3%)	38	72

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	SER
2	B	22	LEU
2	B	37	THR
2	B	73	MET
2	B	113	MET
2	B	131	ILE
2	B	205	LYS
2	B	259	LEU
3	C	58	GLU
3	C	68	VAL
3	C	73	ILE
3	C	104	MET
3	C	106	ARG
1	D	76	SER
1	D	92	VAL
1	D	123	VAL
1	D	170	LEU
2	E	51	ILE
2	E	132	THR
2	E	134	SER
2	E	265	MET
2	E	267	VAL
3	F	38	VAL
3	F	46	LYS
3	F	71	SER
3	F	88	LEU
3	F	109	VAL

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Mol	Chain	Res	Type
3	F	128	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
2	B	40	ASN
2	B	130	GLN
2	B	182	GLN
2	B	193	GLN
2	B	293	GLN
3	C	141	GLN
2	E	46	HIS
2	E	78	GLN
2	E	193	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	201	5	34,34,34	1.39	5 (14%)	47,54,54	1.28	4 (8%)
4	GNP	D	201	5	34,34,34	1.16	4 (11%)	47,54,54	1.24	4 (8%)

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	201	5	-	7/18/38/38	0/3/3/3
4	GNP	D	201	5	-	3/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	GNP	PB-O3A	-3.81	1.54	1.59
4	A	201	GNP	PA-O3A	-3.80	1.55	1.59
4	A	201	GNP	PG-O1G	3.07	1.50	1.46
4	D	201	GNP	PG-O1G	3.06	1.50	1.46
4	D	201	GNP	PB-O3A	-3.01	1.55	1.59
4	D	201	GNP	PA-O3A	-2.84	1.56	1.59
4	A	201	GNP	PB-O2B	-2.64	1.49	1.56
4	A	201	GNP	PG-O3G	-2.29	1.50	1.56
4	D	201	GNP	PB-O2B	-2.22	1.50	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	201	GNP	O3G-PG-O1G	-5.04	100.83	113.45
4	A	201	GNP	O1G-PG-N3B	-4.15	105.66	111.77
4	A	201	GNP	O3G-PG-O1G	-4.13	103.09	113.45
4	A	201	GNP	O2G-PG-O3G	3.44	116.83	107.59
4	D	201	GNP	O2B-PB-O1B	2.87	116.03	109.87
4	A	201	GNP	O2B-PB-O1B	2.59	115.43	109.87
4	D	201	GNP	O2G-PG-O3G	2.54	114.42	107.59
4	D	201	GNP	C3'-C2'-C1'	-2.15	97.40	101.46

There are no chirality outliers.

All (10) torsion outliers are listed below:

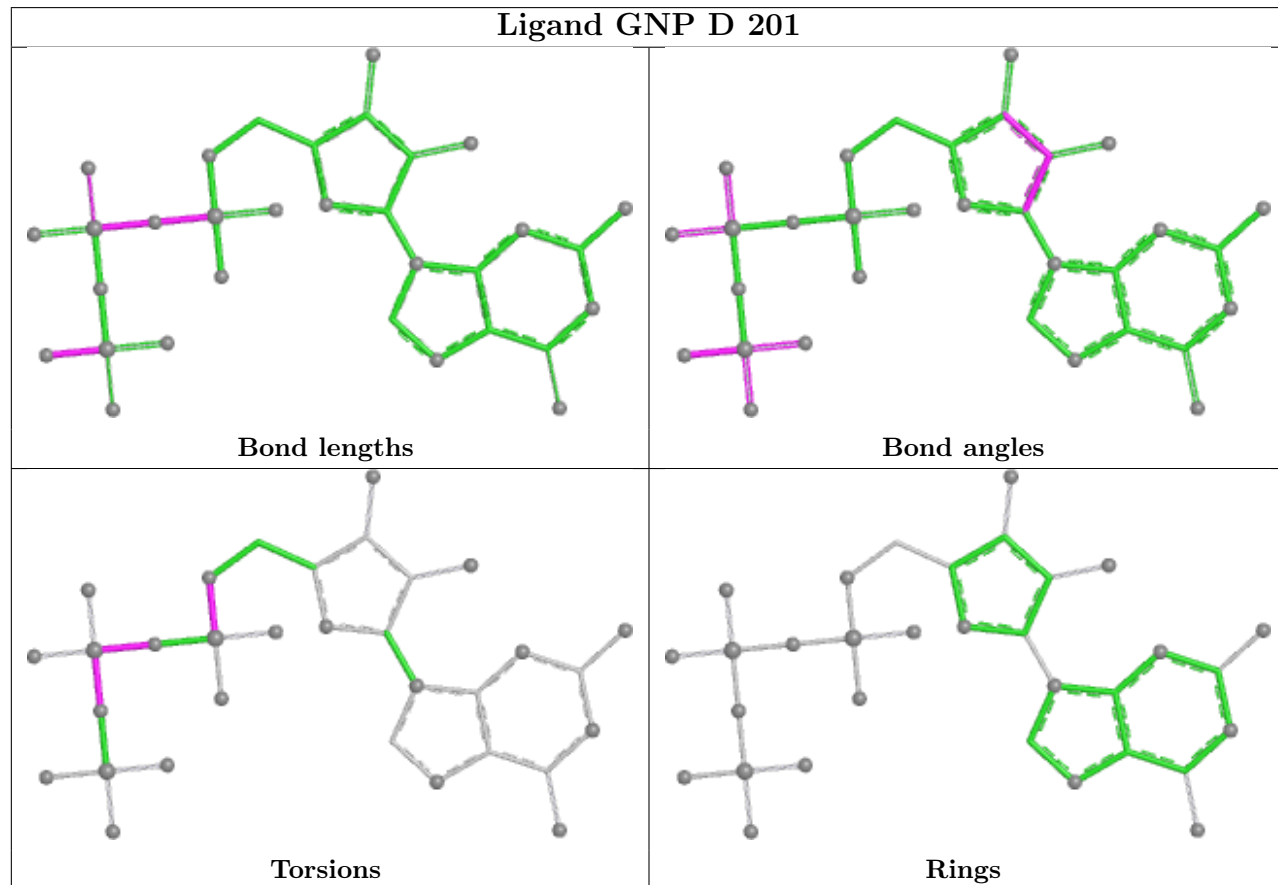
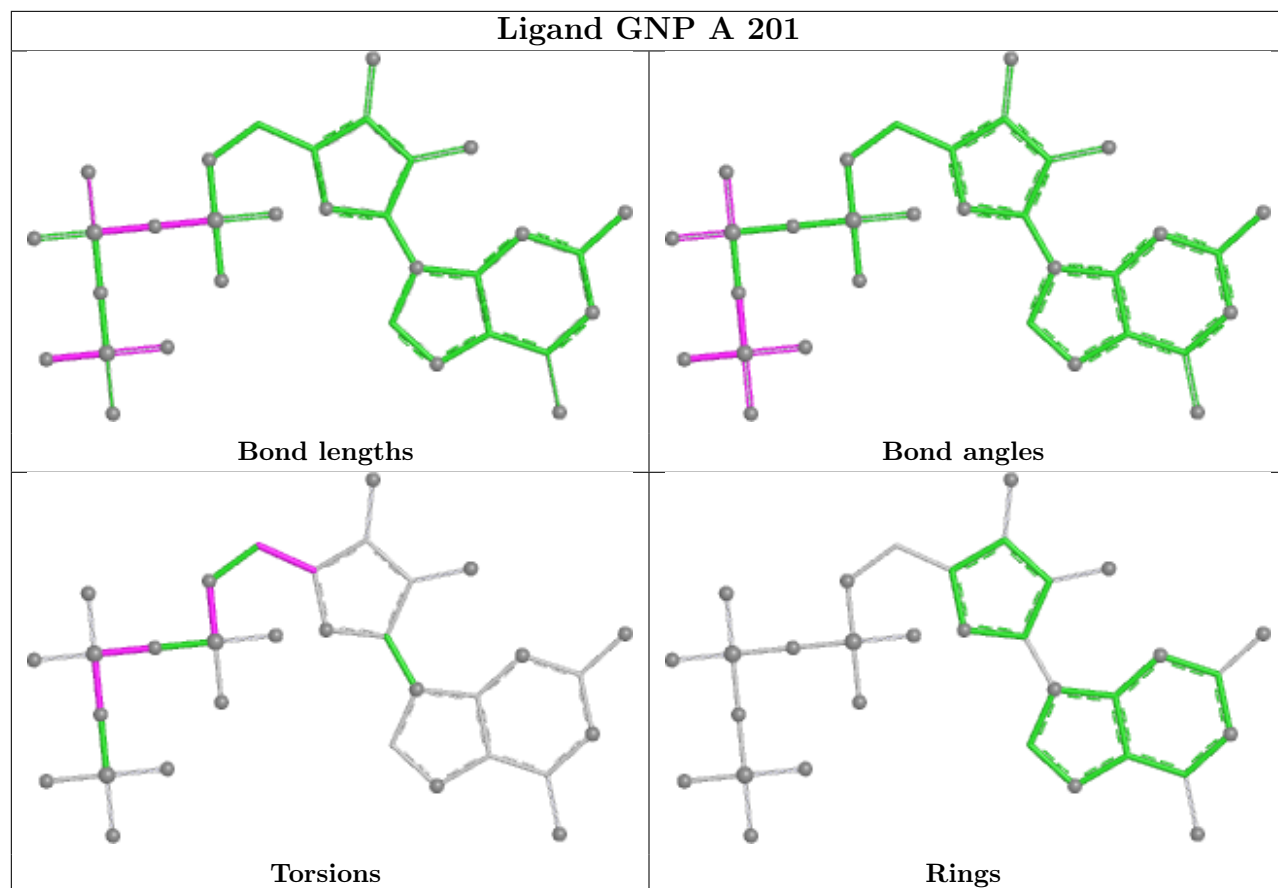
Mol	Chain	Res	Type	Atoms
4	A	201	GNP	PG-N3B-PB-O1B
4	A	201	GNP	PA-O3A-PB-O2B
4	A	201	GNP	C5'-O5'-PA-O3A
4	A	201	GNP	C5'-O5'-PA-O1A
4	D	201	GNP	PG-N3B-PB-O1B
4	D	201	GNP	PA-O3A-PB-O2B
4	A	201	GNP	O4'-C4'-C5'-O5'
4	A	201	GNP	C3'-C4'-C5'-O5'
4	D	201	GNP	C5'-O5'-PA-O3A
4	A	201	GNP	PA-O3A-PB-O1B

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	201	GNP	1	0
4	D	201	GNP	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

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

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	159/164 (96%)	-0.28	2 (1%) 75 67	35, 51, 75, 96	0
1	D	159/164 (96%)	-0.00	5 (3%) 51 42	37, 66, 95, 123	0
2	B	264/355 (74%)	0.32	23 (8%) 16 13	41, 67, 106, 137	0
2	E	260/355 (73%)	0.52	27 (10%) 11 10	45, 76, 120, 136	0
3	C	140/153 (91%)	0.05	6 (4%) 40 31	36, 56, 87, 110	0
3	F	140/153 (91%)	0.89	13 (9%) 14 12	44, 98, 136, 154	0
All	All	1122/1344 (83%)	0.27	76 (6%) 23 18	35, 67, 116, 154	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	50	ASN	6.5
2	E	257	SER	6.2
2	B	257	SER	5.9
2	E	258	CYS	5.3
2	E	73	MET	5.2
2	B	311	LEU	5.2
2	B	300	LYS	5.0
2	E	311	LEU	4.7
2	E	219	THR	4.6
2	B	302	ALA	4.6
3	F	146	VAL	4.4
2	B	258	CYS	4.4
2	B	223	LEU	4.3
2	E	288	ALA	4.2
2	B	301	ALA	4.2
2	B	292	LEU	4.0
3	F	21	ASN	4.0
3	F	136	GLU	4.0
3	C	146	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	264	GLU	3.6
2	E	80	ASN	3.6
2	B	276	ASN	3.5
2	B	218	PHE	3.4
2	B	288	ALA	3.3
2	E	24	LYS	3.2
2	B	136	MET	3.2
2	E	268	TYR	3.1
2	B	80	ASN	3.1
2	B	220	ARG	3.1
2	E	236	ALA	3.0
3	C	21	ASN	3.0
2	E	294	LEU	3.0
3	C	57	SER	2.9
3	F	91	MET	2.9
1	D	73	ARG	2.9
2	E	275	VAL	2.9
2	B	260	ARG	2.8
3	C	117	ASN	2.8
2	E	223	LEU	2.8
3	C	48	ILE	2.8
2	B	234	ARG	2.7
3	F	88	LEU	2.7
1	D	19	ARG	2.7
1	D	150	ASN	2.7
2	E	301	ALA	2.7
2	B	239	GLN	2.7
1	D	67	ASP	2.6
2	B	68	GLU	2.6
1	A	176	SER	2.6
2	E	290	SER	2.6
2	E	297	SER	2.5
2	E	310	THR	2.5
2	E	292	LEU	2.4
2	E	303	LEU	2.4
3	C	40	GLU	2.4
2	E	222	GLY	2.4
3	F	109	VAL	2.4
2	B	238	ARG	2.4
3	F	74	ASP	2.4
2	B	20	GLN	2.4
2	E	138	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	69	TYR	2.4
2	E	305	TYR	2.3
1	D	176	SER	2.3
3	F	56	ASP	2.3
2	B	296	CYS	2.3
2	B	295	PHE	2.2
2	E	302	ALA	2.2
2	E	272	SER	2.2
1	A	171	GLU	2.1
3	F	9	SER	2.1
2	E	289	VAL	2.1
2	E	300	LYS	2.1
2	E	271	ALA	2.1
3	F	58	GLU	2.1
3	F	105	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

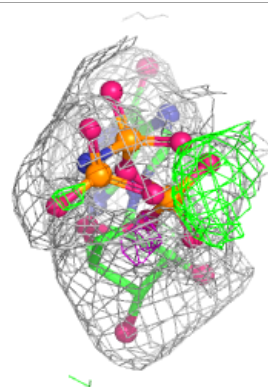
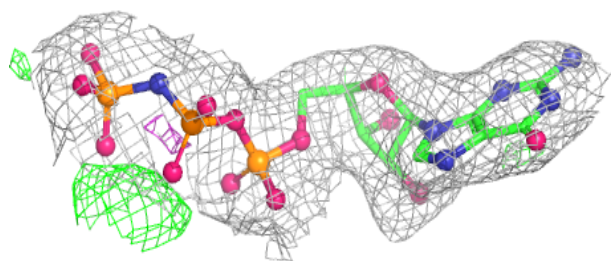
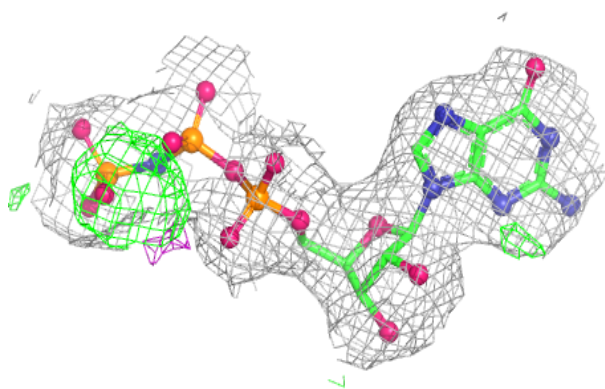
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	D	202	1/1	0.95	0.17	51,51,51,51	0
4	GNP	D	201	32/32	0.97	0.06	32,53,63,71	0
5	MG	A	202	1/1	0.97	0.22	47,47,47,47	0
4	GNP	A	201	32/32	0.97	0.06	30,49,68,70	0

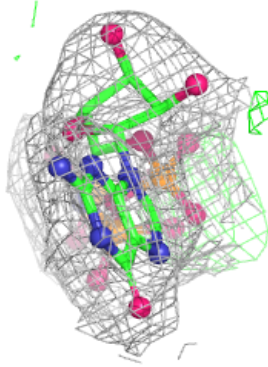
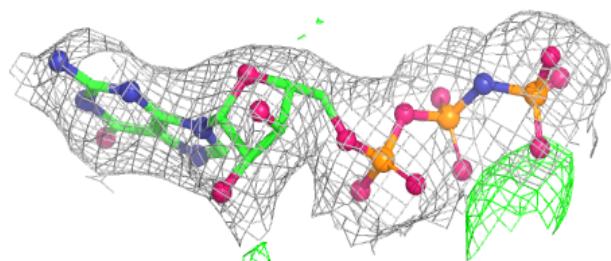
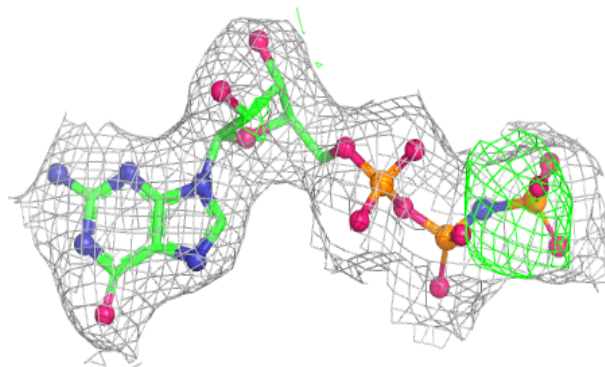
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GNP D 201:

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

**Electron density around GNP A 201:**

$2mF_o-DF_c$ (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.