



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:37 PM UTC

PDB ID : 8YER / pdb_00008yer
Title : Tubulin-RB3_SLD-TTL in complex with compound 4
Authors : Wu, C.Y.; Wang, Y.X.
Deposited on : 2024-02-23
Resolution : 2.71 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

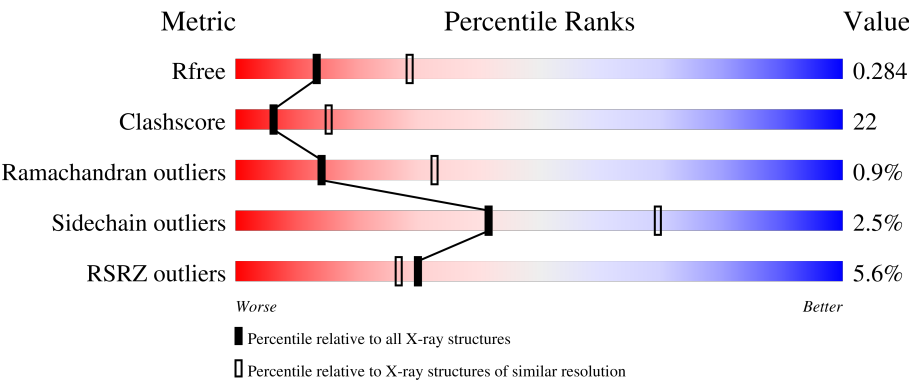
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	440	60%37%..
1	C	440	72%26%.
2	B	431	63%35%..
2	D	431	10% 53%43%..
3	E	143	4% 50%32%.15%

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Mol	Chain	Length	Quality of chain
4	F	380	16% 48% 37% 13%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 17484 atoms, of which 52 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 Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3405	2154	580	649	22			
1	C	440	Total	C	N	O	S	0	0	0
			3433	2172	583	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3351	2104	572	649	26			
2	D	421	Total	C	N	O	S	0	0	0
			3300	2076	559	638	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

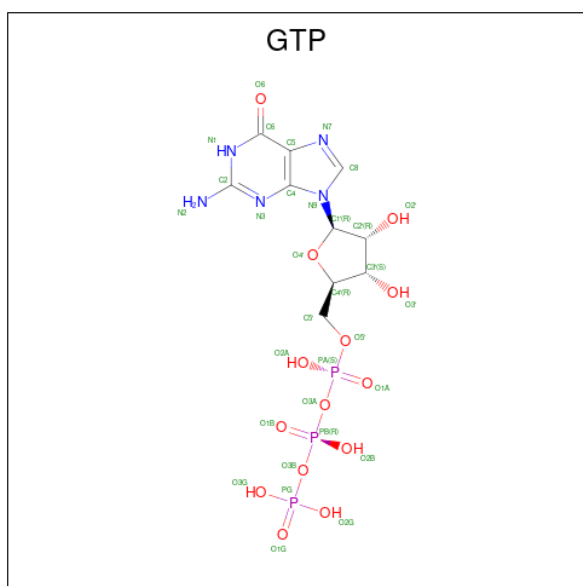
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	332	Total	C	N	O	S	0	0	0
			2713	1740	466	493	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP A0A8C9FGJ1
F	380	HIS	-	expression tag	UNP A0A8C9FGJ1

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	32	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	32	0
			32	10	5	14	3		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	1	0
			1	1		
6	C	1	Total	Ca	1	0
			1	1		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

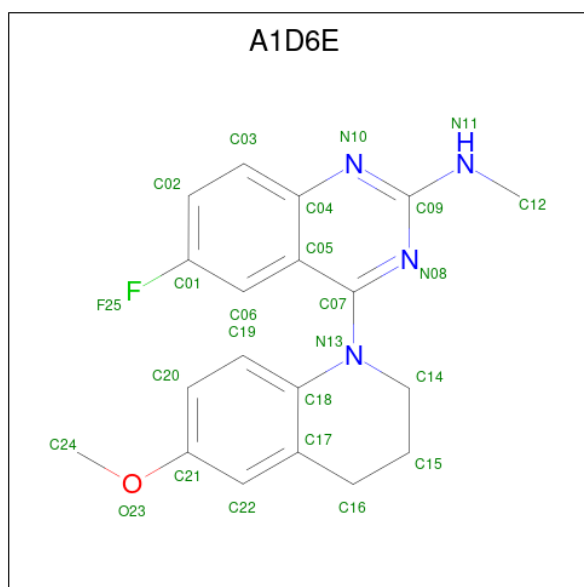
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	1	0
			1	1		
7	B	1	Total	Mg	1	0
			1	1		

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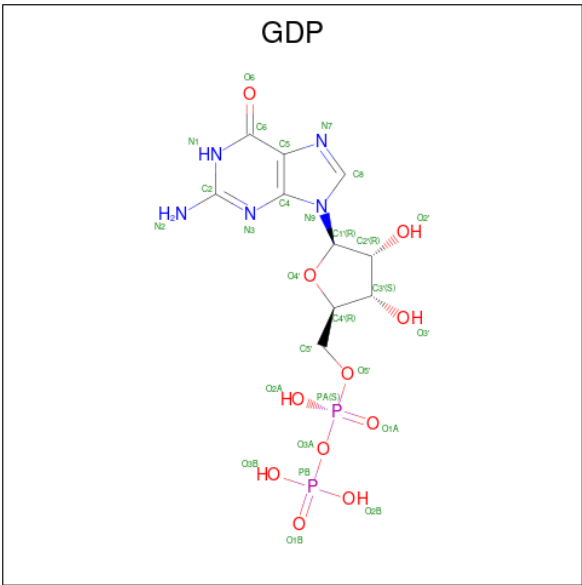
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg	1	0
			1	1		

- Molecule 8 is 6-fluoranyl-4-(6-methoxy-3,4-dihydro-2 {H}-quinolin-1-yl)- {N}-methyl-quinazolin-2-amine (CCD ID: A1D6E) (formula: C₁₉H₁₉FN₄O) (labeled as "Ligand of Interest" by depositor).



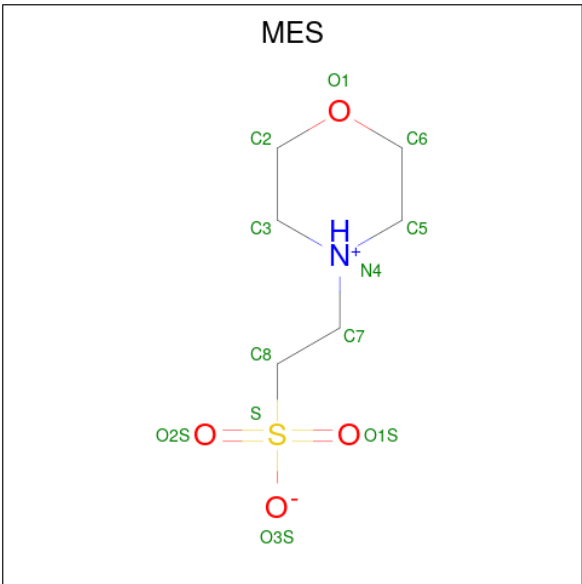
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	F	H	N	O	0	0
			44	19	1	19	4	1		
8	D	1	Total	C	F	H	N	O	0	0
			44	19	1	19	4	1		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



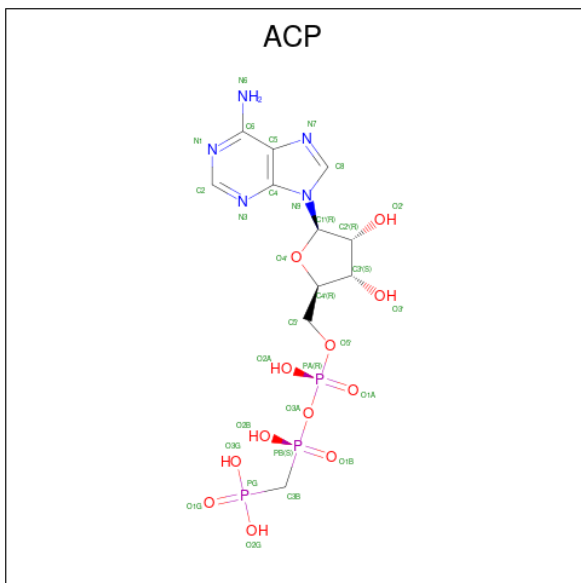
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	12	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	12	0
			12	6	1	4	1		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



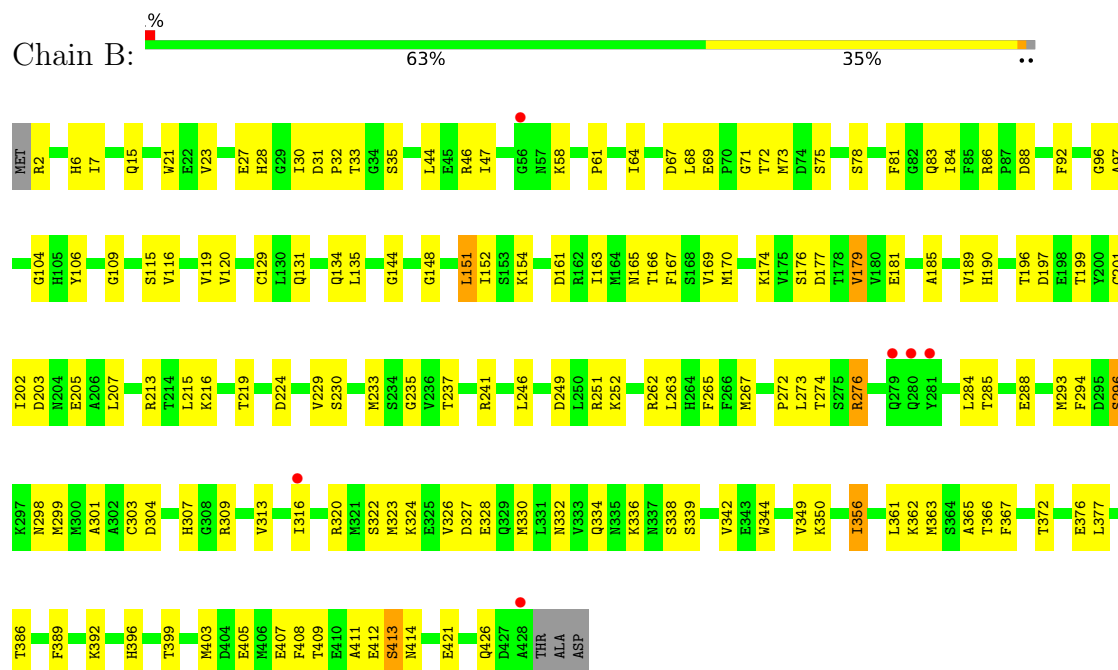
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	F	1	Total	C	H	N	O	P	45	0
			45	11	14	5	12	3		

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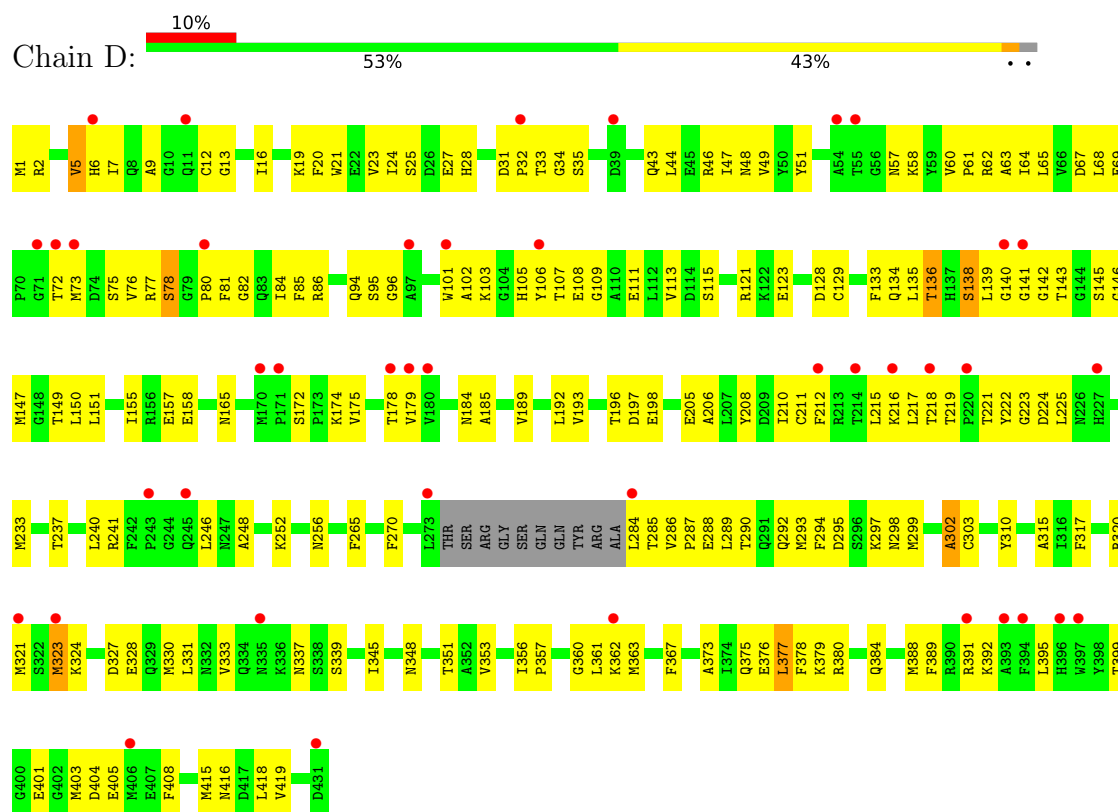
- Molecule 1: Detyrosinated tubulin alpha-1B chain



- Molecule 2: Tubulin beta chain

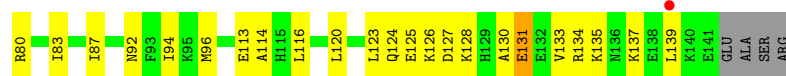
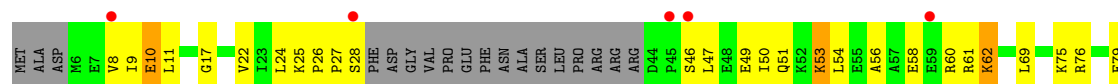


- Molecule 2: Tubulin beta chain

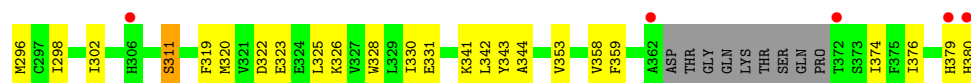
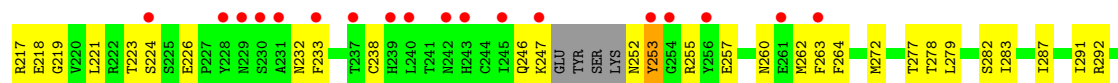
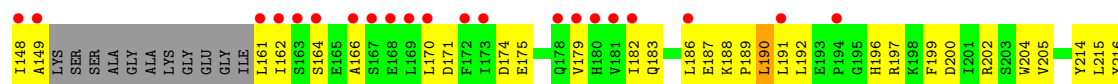
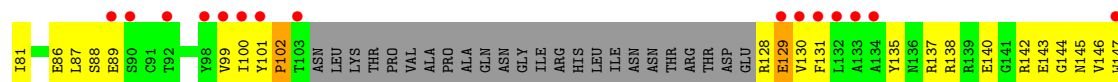
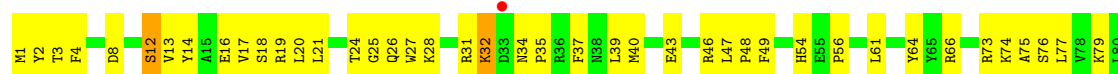


- Molecule 3: Stathmin-4





● Molecule 4: Tubulin-tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.15Å 157.26Å 181.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.70 – 2.71 39.70 – 2.71	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.70-2.71) 99.9 (39.70-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.222 , 0.286 0.222 , 0.284	Depositor DCC
R_{free} test set	2000 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17484	wwPDB-VP
Average B, all atoms (Å ²)	61.0	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, A1D6E, GDP, MES, GTP, ACP, 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	0.41	0/3482	0.60	0/4728
1	C	0.44	0/3511	0.62	0/4768
2	B	0.42	0/3426	0.60	0/4643
2	D	0.35	0/3373	0.53	0/4570
3	E	0.41	0/1008	0.57	0/1337
4	F	0.30	0/2775	0.50	0/3752
All	All	0.39	0/17575	0.58	0/23798

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
4	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	217	LEU	Peptide
4	F	311	SER	Peptide

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	3405	0	3313	149	0
1	C	3433	0	3337	86	0
2	B	3351	0	3216	136	0
2	D	3300	0	3175	198	0
3	E	1000	0	1018	48	0
4	F	2713	0	2659	171	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	25	19	0	2	0
8	D	25	19	0	1	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	24	0	24	0	0
11	F	31	14	14	0	0
All	All	17432	52	16804	756	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 22.

All (756) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:285:THR:HG22	2:D:288:GLU:HG3	1.20	1.16
2:B:73:MET:HE2	2:B:92:PHE:HB3	1.32	1.10
2:D:290:THR:HG23	2:D:330:MET:HE3	1.47	0.95
2:D:285:THR:HG22	2:D:288:GLU:CG	1.96	0.95
2:D:294:PHE:HE1	2:D:330:MET:HE1	1.31	0.93
4:F:192:LEU:CD2	4:F:262:MET:HE1	1.99	0.92
4:F:100:ILE:HD12	4:F:128:ARG:N	1.85	0.91
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:190:LEU:HD12	4:F:323:GLU:HA	1.53	0.91
2:B:81:PHE:O	2:B:84:ILE:HG22	1.71	0.91
2:D:21:TRP:O	2:D:25:SER:OG	1.89	0.90
2:D:134:GLN:HA	2:D:165:ASN:O	1.71	0.90
4:F:137:ARG:O	4:F:137:ARG:NH1	2.04	0.89
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.55	0.88
3:E:92:ASN:HD21	3:E:96:MET:HE3	1.39	0.88
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.55	0.87
3:E:116:LEU:O	3:E:120:LEU:HD23	1.74	0.87
2:D:77:ARG:HA	2:D:82:GLY:HA3	1.57	0.86
1:A:88:HIS:N	1:A:91:GLN:OE1	2.07	0.86
2:D:19:LYS:O	2:D:23:VAL:HG23	1.75	0.86
4:F:149:ALA:HB3	4:F:161:LEU:HB3	1.54	0.86
3:E:51:GLN:OE1	3:E:51:GLN:HA	1.76	0.85
2:D:378:PHE:HD1	2:D:415:MET:HE2	1.42	0.85
2:D:401:GLU:HA	3:E:137:LYS:HD2	1.58	0.85
3:E:53:LYS:HG3	3:E:54:LEU:N	1.90	0.84
4:F:24:THR:HG23	4:F:26:GLN:H	1.41	0.84
4:F:16:GLU:O	4:F:20:LEU:HD12	1.77	0.84
2:B:392:LYS:HE2	2:B:405:GLU:OE2	1.78	0.83
4:F:218:GLU:HG3	4:F:342:LEU:HD22	1.58	0.83
1:C:287:SER:OG	1:C:290:GLU:HG3	1.78	0.83
2:D:179:VAL:O	2:D:388:MET:HE1	1.77	0.82
4:F:226:GLU:OE2	4:F:252:ASN:ND2	2.13	0.82
2:D:60:VAL:HG11	2:D:86:ARG:HG3	1.62	0.81
2:D:321:MET:HB3	2:D:363:MET:HE1	1.61	0.81
2:D:285:THR:HG23	2:D:287:PRO:HD2	1.62	0.81
1:A:154:MET:HG3	1:A:194:THR:HG23	1.62	0.81
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.61	0.80
2:D:67:ASP:OD2	2:D:72:THR:OG1	1.98	0.80
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.16	0.80
2:D:151:LEU:O	2:D:155:ILE:HG13	1.80	0.80
4:F:215:LEU:HD23	4:F:376:ILE:HD12	1.63	0.80
4:F:135:TYR:OH	4:F:164:SER:O	2.01	0.79
2:D:211:CYS:HA	2:D:215:LEU:HD23	1.63	0.79
2:D:211:CYS:HB3	2:D:217:LEU:HD12	1.65	0.79
2:B:224:ASP:OD1	2:B:276:ARG:NH2	2.16	0.79
2:D:65:LEU:HD21	2:D:85:PHE:CE2	2.18	0.78
2:B:161:ASP:O	2:B:251:ARG:NH2	2.16	0.78
3:E:25:LYS:HD3	3:E:26:PRO:O	1.82	0.78
2:D:65:LEU:HD21	2:D:85:PHE:HE2	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:21:LEU:O	4:F:24:THR:HG22	1.84	0.78
4:F:31:ARG:HE	4:F:32:LYS:H	1.33	0.77
2:D:288:GLU:O	2:D:292:GLN:HG3	1.85	0.77
4:F:148:ILE:HD13	4:F:162:ILE:HG12	1.65	0.77
4:F:199:PHE:O	4:F:320:MET:HE1	1.85	0.77
2:D:294:PHE:CE1	2:D:330:MET:HE1	2.19	0.76
2:D:395:LEU:O	2:D:399:THR:HG22	1.85	0.76
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.68	0.75
1:C:248:LEU:HD12	1:C:357:TYR:OH	1.86	0.75
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.21	0.74
4:F:263:PHE:HE2	4:F:341:LYS:HD3	1.52	0.74
4:F:149:ALA:CB	4:F:161:LEU:HB3	2.18	0.74
4:F:296:MET:HE3	4:F:380:HIS:CB	2.18	0.73
1:A:97:GLU:HG3	2:B:2:ARG:NH1	2.04	0.73
1:A:2:ARG:O	1:A:51:THR:HG22	1.87	0.73
4:F:135:TYR:CD2	4:F:166:ALA:HB2	2.23	0.73
2:D:1:MET:HE3	2:D:128:ASP:HB2	1.70	0.73
2:D:106:TYR:CD1	3:E:133:VAL:HG11	2.24	0.73
4:F:73:ARG:HG2	4:F:76:SER:HB2	1.70	0.73
1:A:72:PRO:HB3	1:A:94:THR:HG21	1.71	0.73
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.22	0.73
4:F:188:LYS:HD3	4:F:323:GLU:CD	2.13	0.72
2:B:309:ARG:NH2	2:B:342:VAL:HA	2.04	0.72
2:B:23:VAL:HG21	2:B:230:SER:HB3	1.70	0.72
1:A:81:GLY:O	1:A:84:ARG:HG2	1.89	0.72
2:D:73:MET:HE2	2:D:77:ARG:HH22	1.53	0.72
2:B:2:ARG:HB3	2:B:131:GLN:HG2	1.71	0.72
2:D:31:ASP:OD1	2:D:33:THR:HG22	1.88	0.72
1:C:220:GLU:OE2	1:C:220:GLU:N	2.23	0.72
3:E:47:LEU:HD12	3:E:47:LEU:O	1.90	0.71
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.24	0.71
2:D:290:THR:HG23	2:D:330:MET:CE	2.19	0.71
1:A:101:ASN:HD21	2:B:252:LYS:HD3	1.55	0.71
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.26	0.71
2:D:145:SER:O	2:D:149:THR:HG23	1.91	0.70
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.73	0.70
2:D:324:LYS:HE2	2:D:328:GLU:OE2	1.91	0.70
2:B:46:ARG:HG3	2:B:46:ARG:HH11	1.54	0.70
1:A:1:MET:HE2	1:A:50:ASN:HB2	1.72	0.70
2:B:176:SER:HB2	2:B:181:GLU:OE1	1.92	0.70
2:B:330:MET:HE3	2:B:330:MET:HA	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:VAL:HG12	2:B:233:MET:HE2	1.72	0.70
2:D:1:MET:HG3	2:D:128:ASP:HB3	1.73	0.70
3:E:131:GLU:OE1	3:E:134:ARG:NH2	2.23	0.70
2:B:2:ARG:HB3	2:B:131:GLN:CG	2.22	0.69
1:A:9:VAL:HG22	1:A:68:VAL:CG1	2.22	0.69
2:B:307:HIS:ND1	2:B:376:GLU:OE2	2.24	0.69
4:F:149:ALA:HB3	4:F:161:LEU:CD2	2.22	0.69
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.73	0.69
4:F:149:ALA:HB3	4:F:161:LEU:HD23	1.73	0.69
4:F:89:GLU:OE2	4:F:89:GLU:N	2.23	0.69
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.28	0.69
2:D:285:THR:CG2	2:D:288:GLU:HG3	2.12	0.69
2:D:63:ALA:O	2:D:64:ILE:HD13	1.93	0.68
4:F:148:ILE:HD13	4:F:162:ILE:CG1	2.21	0.68
4:F:147:TRP:O	4:F:162:ILE:HG23	1.93	0.68
2:D:327:ASP:O	2:D:331:LEU:HD13	1.94	0.68
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.29	0.68
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.30	0.67
1:A:163:LYS:H	1:A:164:LYS:HZ2	1.43	0.67
2:D:23:VAL:O	2:D:27:GLU:HG3	1.94	0.67
2:D:377:LEU:HD23	2:D:378:PHE:N	2.09	0.67
1:A:370:LYS:HD2	1:A:371:VAL:H	1.59	0.67
2:B:177:ASP:O	1:C:352:LYS:HE2	1.94	0.67
4:F:296:MET:HE3	4:F:380:HIS:CG	2.29	0.67
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.77	0.67
4:F:75:ALA:O	4:F:79:LYS:HG3	1.93	0.66
2:B:293:MET:CE	2:B:365:ALA:HB1	2.25	0.66
1:C:4:CYS:HB3	1:C:136:LEU:CD1	2.25	0.66
2:D:377:LEU:HD23	2:D:377:LEU:C	2.21	0.66
4:F:31:ARG:NE	4:F:32:LYS:H	1.93	0.66
4:F:192:LEU:HD12	4:F:192:LEU:H	1.58	0.66
2:D:7:ILE:HG22	2:D:135:LEU:HD12	1.78	0.66
1:A:71:GLU:OE2	1:A:73:THR:HB	1.96	0.66
2:D:65:LEU:HD11	2:D:85:PHE:CD2	2.31	0.66
2:D:375:GLN:O	2:D:379:LYS:HG3	1.95	0.66
2:D:44:LEU:HA	2:D:47:ILE:HB	1.76	0.66
1:C:209:ILE:HD11	1:C:302:MET:SD	2.36	0.66
1:A:187:SER:CB	1:A:391:LEU:HD21	2.27	0.65
2:D:34:GLY:O	2:D:58:LYS:HA	1.97	0.65
4:F:102:PRO:HB3	4:F:174:ASP:HA	1.78	0.65
4:F:171:ASP:O	4:F:175:GLU:HG2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:12:SER:HB2	4:F:343:TYR:OH	1.96	0.65
2:D:172:SER:OG	2:D:205:GLU:HB2	1.97	0.65
2:D:77:ARG:HA	2:D:82:GLY:CA	2.25	0.65
2:D:81:PHE:O	2:D:84:ILE:HG22	1.97	0.65
4:F:188:LYS:HD3	4:F:323:GLU:OE2	1.96	0.64
2:B:135:LEU:CD2	2:B:152:ILE:HD11	2.27	0.64
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.28	0.64
1:A:1:MET:HE2	1:A:50:ASN:CB	2.26	0.64
2:D:80:PRO:O	2:D:81:PHE:HB2	1.97	0.64
2:D:65:LEU:HD22	2:D:76:VAL:HG11	1.80	0.64
2:D:32:PRO:HB3	2:D:81:PHE:HA	1.79	0.63
4:F:246:GLN:O	4:F:253:TYR:HD2	1.81	0.63
1:A:88:HIS:NE2	1:A:90:GLU:HG3	2.13	0.63
2:B:293:MET:HE3	2:B:365:ALA:HB1	1.81	0.63
4:F:296:MET:CE	4:F:380:HIS:CG	2.82	0.63
2:B:166:THR:OG1	2:B:199:THR:HG22	1.99	0.63
2:D:73:MET:HE2	2:D:77:ARG:HH12	1.64	0.63
4:F:192:LEU:HD11	4:F:199:PHE:CD1	2.34	0.63
2:B:134:GLN:HA	2:B:165:ASN:O	1.99	0.63
4:F:218:GLU:HG3	4:F:342:LEU:CD2	2.29	0.63
2:D:404:ASP:OD1	2:D:405:GLU:N	2.32	0.63
2:D:73:MET:HE2	2:D:77:ARG:NH2	2.12	0.62
4:F:263:PHE:HE2	4:F:341:LYS:CD	2.13	0.62
1:A:94:THR:HG22	1:A:95:GLY:O	1.98	0.62
2:B:73:MET:HE2	2:B:92:PHE:CB	2.22	0.62
1:C:221:ARG:NH2	2:D:323:MET:HB3	2.15	0.62
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.35	0.62
2:D:151:LEU:CD2	2:D:155:ILE:HD11	2.30	0.62
2:D:1:MET:HE3	2:D:128:ASP:CB	2.30	0.61
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.82	0.61
1:A:214:ARG:HG2	1:A:219:ILE:O	2.00	0.61
4:F:100:ILE:CG2	4:F:128:ARG:HD2	2.30	0.61
2:D:293:MET:CG	2:D:367:PHE:HB2	2.30	0.61
2:D:9:ALA:O	2:D:13:GLY:HA3	2.00	0.61
4:F:135:TYR:HE2	4:F:166:ALA:H	1.48	0.61
1:A:93:ILE:HD12	1:A:118:VAL:HG22	1.83	0.60
2:D:206:ALA:O	2:D:210:ILE:HG13	2.01	0.60
2:D:6:HIS:CE1	2:D:21:TRP:HE1	2.18	0.60
1:A:333:ALA:O	1:A:336:LYS:HG3	2.01	0.60
4:F:148:ILE:HD12	4:F:149:ALA:H	1.66	0.60
2:D:20:PHE:O	2:D:24:ILE:HG12	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:HG13	1:A:68:VAL:O	2.02	0.60
2:B:304:ASP:HB3	2:B:307:HIS:ND1	2.16	0.60
4:F:137:ARG:NH1	4:F:140:GLU:HB3	2.16	0.60
2:D:2:ARG:NH1	2:D:129:CYS:SG	2.74	0.60
2:D:315:ALA:HB3	2:D:351:THR:HG22	1.83	0.60
2:D:378:PHE:CD1	2:D:415:MET:HE2	2.30	0.60
4:F:46:ARG:HB3	4:F:46:ARG:CZ	2.30	0.60
4:F:86:GLU:C	4:F:87:LEU:HD23	2.27	0.60
2:D:20:PHE:CD1	2:D:233:MET:HE2	2.37	0.60
4:F:4:PHE:HB3	4:F:27:TRP:CZ3	2.37	0.60
2:D:72:THR:O	2:D:76:VAL:HG23	2.02	0.60
1:A:298:PRO:HA	1:A:301:GLN:HG3	1.84	0.59
2:B:2:ARG:HA	2:B:129:CYS:O	2.01	0.59
4:F:128:ARG:NE	4:F:170:LEU:HD22	2.17	0.59
2:D:360:GLY:C	2:D:361:LEU:HD23	2.26	0.59
4:F:217:ARG:HG3	4:F:218:GLU:N	2.17	0.59
2:D:284:LEU:N	2:D:362:LYS:HZ1	1.99	0.59
4:F:3:THR:OG1	4:F:37:PHE:HA	2.02	0.59
1:A:27:GLU:OE1	1:A:243:ARG:NH2	2.35	0.59
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.33	0.59
1:A:298:PRO:O	1:A:301:GLN:HG3	2.02	0.59
2:B:64:ILE:HD13	2:B:120:VAL:HG22	1.83	0.59
4:F:77:LEU:HD12	4:F:77:LEU:O	2.02	0.59
4:F:138:ARG:NH1	4:F:144:GLY:O	2.35	0.59
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.38	0.59
1:A:88:HIS:HD2	1:A:90:GLU:HB2	1.67	0.59
4:F:128:ARG:HE	4:F:170:LEU:HD22	1.67	0.59
4:F:148:ILE:O	4:F:182:ILE:HA	2.02	0.59
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.84	0.59
2:B:154:LYS:HZ2	3:E:76:ARG:CZ	2.16	0.59
4:F:138:ARG:HB3	4:F:145:ASN:HD21	1.67	0.59
1:A:285:GLN:HG3	1:A:372:GLN:CD	2.28	0.58
3:E:130:ALA:HA	3:E:133:VAL:HG12	1.84	0.58
2:B:293:MET:HE2	2:B:367:PHE:HB2	1.86	0.58
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.33	0.58
2:D:65:LEU:HD11	2:D:85:PHE:HD2	1.68	0.58
2:D:107:THR:OG1	2:D:108:GLU:N	2.35	0.58
1:A:370:LYS:HD2	1:A:371:VAL:N	2.17	0.58
2:B:68:LEU:HD12	2:B:97:ALA:HB2	1.84	0.58
4:F:192:LEU:HD23	4:F:262:MET:HE1	1.84	0.58
4:F:144:GLY:HA3	4:F:187:GLU:OE1	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:TRP:H	1:A:346:TRP:CD1	2.22	0.58
2:B:284:LEU:N	2:B:284:LEU:HD12	2.19	0.58
1:A:154:MET:HG3	1:A:194:THR:CG2	2.33	0.58
2:D:388:MET:HG2	2:D:391:ARG:HH21	1.68	0.58
1:A:223:THR:O	1:A:227:LEU:HG	2.04	0.57
1:A:395:PHE:CD1	1:A:422:ARG:HD3	2.39	0.57
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.86	0.57
2:D:356:ILE:N	2:D:356:ILE:HD12	2.17	0.57
2:B:72:THR:O	2:B:75:SER:HB2	2.05	0.57
1:A:402:ARG:HH11	1:A:402:ARG:HG3	1.69	0.57
2:B:35:SER:OG	2:B:58:LYS:HE2	2.04	0.57
4:F:128:ARG:N	4:F:128:ARG:HD2	2.19	0.57
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.40	0.57
2:B:69:GLU:HG3	2:B:96:GLY:HA2	1.85	0.57
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.33	0.57
2:B:309:ARG:HH21	2:B:342:VAL:HA	1.69	0.57
2:D:73:MET:HE2	2:D:77:ARG:NH1	2.20	0.57
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.38	0.56
1:A:28:HIS:O	1:A:36:MET:HE3	2.04	0.56
2:D:46:ARG:HH12	2:D:48:ASN:HD21	1.53	0.56
2:D:215:LEU:N	2:D:215:LEU:HD22	2.20	0.56
2:D:285:THR:HG23	2:D:287:PRO:CD	2.34	0.56
1:A:103:TYR:CD2	1:A:189:LEU:HD13	2.40	0.56
2:B:46:ARG:HG3	2:B:46:ARG:NH1	2.17	0.56
2:B:135:LEU:HD22	2:B:152:ILE:HD11	1.88	0.56
2:D:210:ILE:HG22	2:D:215:LEU:CD2	2.35	0.56
2:B:294:PHE:CE1	2:B:330:MET:HE1	2.40	0.56
2:B:377:LEU:C	2:B:377:LEU:HD23	2.31	0.56
4:F:47:LEU:C	4:F:47:LEU:HD23	2.31	0.56
4:F:192:LEU:HD21	4:F:262:MET:HE1	1.87	0.56
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.40	0.56
2:D:289:LEU:HD12	2:D:289:LEU:H	1.71	0.56
1:C:119:LEU:HD12	1:C:156:ARG:NH2	2.21	0.56
1:A:102:ASN:HB3	1:A:105:ARG:HB3	1.86	0.55
1:A:298:PRO:HA	1:A:301:GLN:CD	2.31	0.55
2:D:1:MET:CE	2:D:128:ASP:HB2	2.35	0.55
2:D:63:ALA:C	2:D:64:ILE:HD13	2.31	0.55
1:C:101:ASN:ND2	2:D:252:LYS:HE2	2.22	0.55
1:C:101:ASN:HD21	2:D:252:LYS:HE2	1.71	0.55
4:F:138:ARG:HB3	4:F:145:ASN:OD1	2.07	0.55
2:D:286:VAL:HB	2:D:287:PRO:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:O	1:A:238:ILE:HG13	2.06	0.55
2:B:31:ASP:CG	2:B:33:THR:HG22	2.31	0.55
1:C:219:ILE:HG21	1:C:222:PRO:HA	1.89	0.55
2:D:20:PHE:CE1	2:D:24:ILE:HD13	2.41	0.55
1:A:88:HIS:CD2	1:A:90:GLU:H	2.25	0.55
2:D:330:MET:HA	2:D:330:MET:HE2	1.89	0.55
2:D:12:CYS:HB3	2:D:138:SER:OG	2.07	0.55
1:A:413:MET:HE2	1:A:418:PHE:CE1	2.42	0.54
2:B:350:LYS:HG3	8:B:501:A1D6E:O23	2.06	0.54
2:D:7:ILE:HG22	2:D:135:LEU:CD1	2.36	0.54
2:D:189:VAL:HG11	2:D:415:MET:HE3	1.89	0.54
2:D:323:MET:SD	2:D:353:VAL:HG11	2.47	0.54
1:A:165:SER:OG	1:A:256:GLN:NE2	2.40	0.54
2:B:179:VAL:HG12	1:C:348:PRO:CG	2.35	0.54
2:B:215:LEU:HD23	2:B:215:LEU:N	2.21	0.54
1:C:288:VAL:HG22	1:C:323:VAL:HG22	1.89	0.54
2:D:24:ILE:HG22	2:D:241:ARG:CZ	2.38	0.54
1:A:402:ARG:HG3	1:A:402:ARG:NH1	2.23	0.54
2:B:61:PRO:CD	2:B:84:ILE:HG12	2.37	0.54
2:D:77:ARG:CA	2:D:82:GLY:HA3	2.34	0.54
4:F:100:ILE:HG21	4:F:128:ARG:HD2	1.89	0.54
4:F:191:LEU:H	4:F:191:LEU:HD12	1.73	0.54
2:D:211:CYS:HA	2:D:215:LEU:HB2	1.89	0.54
4:F:190:LEU:CD1	4:F:323:GLU:HA	2.32	0.54
1:A:159:VAL:HG12	1:A:160:ASP:OD1	2.08	0.53
4:F:298:ILE:HD12	4:F:302:ILE:HD13	1.89	0.53
1:A:2:ARG:HB3	1:A:133:GLN:HG3	1.90	0.53
1:A:97:GLU:HG3	2:B:2:ARG:HH12	1.73	0.53
1:A:176:GLN:NE2	4:F:56:PRO:HB3	2.23	0.53
2:B:362:LYS:O	2:B:363:MET:HG2	2.07	0.53
3:E:56:ALA:HB1	3:E:60:ARG:HH12	1.73	0.53
4:F:101:TYR:CD1	4:F:179:VAL:HG22	2.43	0.53
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.90	0.53
1:A:101:ASN:ND2	2:B:252:LYS:HD3	2.22	0.53
2:D:28:HIS:HA	2:D:43:GLN:HB3	1.90	0.53
2:D:221:THR:HG23	2:D:224:ASP:H	1.71	0.53
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.43	0.53
1:A:16:ILE:O	1:A:19:ALA:HB3	2.09	0.53
1:A:239:THR:OG1	1:A:243:ARG:NH1	2.41	0.53
2:B:262:ARG:NH1	2:B:421:GLU:OE1	2.35	0.53
2:B:324:LYS:O	2:B:328:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1:MET:HE3	4:F:25:GLY:O	2.09	0.53
2:B:235:GLY:HA3	2:B:366:THR:OG1	2.08	0.53
2:D:174:LYS:HD2	2:D:208:TYR:HD2	1.73	0.53
1:C:209:ILE:HG22	1:C:227:LEU:CD2	2.34	0.53
2:D:68:LEU:HD12	2:D:143:THR:HG23	1.90	0.53
1:C:399:TYR:O	1:C:402:ARG:HD3	2.09	0.53
3:E:139:LEU:HD12	3:E:139:LEU:O	2.08	0.53
4:F:190:LEU:HD13	4:F:322:ASP:O	2.09	0.53
1:A:221:ARG:HD3	2:B:323:MET:HE2	1.91	0.53
1:C:68:VAL:HG11	1:C:118:VAL:HG21	1.91	0.52
3:E:53:LYS:HG3	3:E:54:LEU:H	1.69	0.52
1:A:71:GLU:HG2	1:A:72:PRO:N	2.23	0.52
1:A:323:VAL:HG12	1:A:355:ILE:CD1	2.40	0.52
4:F:218:GLU:CG	4:F:342:LEU:HD22	2.35	0.52
1:C:320:ARG:HA	1:C:356:ASN:O	2.08	0.52
2:D:321:MET:HE2	2:D:363:MET:HE2	1.90	0.52
1:A:18:ASN:ND2	1:A:78:VAL:HG22	2.16	0.52
1:C:252:LEU:HD12	1:C:252:LEU:O	2.10	0.52
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.40	0.52
2:B:316:ILE:CG2	2:B:366:THR:HB	2.39	0.52
1:A:90:GLU:O	1:A:121:ARG:HD2	2.09	0.52
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.74	0.52
1:A:357:TYR:CD2	3:E:17:GLY:HA2	2.45	0.52
2:B:116:VAL:CG1	2:B:151:LEU:HD21	2.40	0.52
2:D:7:ILE:O	2:D:135:LEU:HD12	2.10	0.52
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.28	0.52
2:D:101:TRP:NE1	2:D:146:GLY:HA2	2.25	0.52
1:A:401:LYS:HG3	2:B:344:TRP:CD2	2.45	0.52
2:B:219:THR:HG22	2:B:219:THR:O	2.10	0.52
2:D:373:ALA:O	2:D:376:GLU:HB2	2.10	0.52
4:F:61:LEU:HD22	4:F:358:VAL:HG21	1.92	0.52
1:A:34:GLY:O	1:A:61:HIS:N	2.35	0.51
1:A:234:ILE:HG12	1:A:302:MET:HE3	1.92	0.51
4:F:16:GLU:OE2	4:F:19:ARG:HD3	2.09	0.51
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.45	0.51
2:B:31:ASP:OD1	2:B:33:THR:HG22	2.10	0.51
2:D:31:ASP:OD1	2:D:33:THR:CG2	2.58	0.51
2:D:68:LEU:O	2:D:96:GLY:HA2	2.11	0.51
1:C:209:ILE:CG2	1:C:227:LEU:HD22	2.34	0.51
2:D:20:PHE:CZ	2:D:24:ILE:CD1	2.94	0.51
1:A:351:PHE:HB2	3:E:22:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:ARG:NH1	2:D:48:ASN:HD21	2.08	0.51
4:F:218:GLU:HA	4:F:218:GLU:OE1	2.10	0.51
1:A:120:ASP:O	1:A:124:LYS:HG2	2.11	0.51
2:B:69:GLU:HG3	2:B:96:GLY:CA	2.41	0.51
2:D:1:MET:HE3	2:D:128:ASP:CG	2.36	0.51
1:A:260:VAL:HG11	1:A:266:HIS:HB3	1.93	0.51
2:B:86:ARG:HE	2:B:88:ASP:HB2	1.75	0.51
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.45	0.51
2:D:7:ILE:O	2:D:135:LEU:HA	2.11	0.51
3:E:22:VAL:HG13	3:E:22:VAL:O	2.11	0.51
4:F:137:ARG:HH11	4:F:140:GLU:HB3	1.75	0.51
1:A:414:GLU:O	1:A:416:GLY:N	2.44	0.51
2:D:140:GLY:O	2:D:184:ASN:ND2	2.39	0.51
1:A:316:CYS:HA	1:A:352:LYS:O	2.11	0.51
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.92	0.51
2:D:60:VAL:CG1	2:D:86:ARG:HG3	2.37	0.51
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.45	0.50
1:C:216:ASN:HB3	1:C:275:VAL:O	2.10	0.50
2:B:174:LYS:HE3	2:B:205:GLU:CD	2.35	0.50
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.46	0.50
1:A:221:ARG:NE	2:B:327:ASP:OD2	2.44	0.50
2:B:356:ILE:HD13	2:B:356:ILE:N	2.27	0.50
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.12	0.50
1:A:285:GLN:HG3	1:A:372:GLN:NE2	2.26	0.50
1:A:314:ALA:O	1:A:315:CYS:HB2	2.11	0.50
2:B:190:HIS:CE1	2:B:414:ASN:HD22	2.28	0.50
2:D:416:ASN:O	2:D:419:VAL:HG22	2.11	0.50
1:A:323:VAL:HG12	1:A:355:ILE:HD13	1.94	0.50
3:E:75:LYS:HD3	3:E:79:GLU:OE2	2.11	0.50
4:F:64:TYR:O	4:F:311:SER:HB3	2.12	0.50
4:F:135:TYR:HD2	4:F:166:ALA:HB2	1.74	0.50
1:A:192:HIS:CG	1:A:421:ALA:HA	2.45	0.50
2:D:211:CYS:CA	2:D:215:LEU:HD23	2.35	0.50
1:A:2:ARG:CB	1:A:133:GLN:HG3	2.42	0.50
2:B:263:LEU:HD23	2:B:263:LEU:N	2.27	0.50
4:F:138:ARG:HB3	4:F:145:ASN:ND2	2.26	0.49
1:A:156:ARG:O	1:A:159:VAL:N	2.44	0.49
1:A:195:LEU:HD12	1:A:266:HIS:CE1	2.46	0.49
1:A:414:GLU:C	1:A:416:GLY:N	2.67	0.49
2:B:30:ILE:HD12	2:B:30:ILE:N	2.27	0.49
4:F:216:TYR:CD1	4:F:374:ILE:HD12	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:HIS:CD2	2:B:411:ALA:HA	2.47	0.49
4:F:197:ARG:HB3	4:F:224:SER:O	2.12	0.49
2:B:179:VAL:HG22	1:C:258:ASN:OD1	2.12	0.49
1:C:285:GLN:NE2	1:C:285:GLN:HA	2.27	0.49
2:D:2:ARG:O	2:D:49:VAL:HG22	2.11	0.49
4:F:128:ARG:N	4:F:128:ARG:CD	2.75	0.49
2:B:28:HIS:HB3	2:B:47:ILE:CD1	2.42	0.49
2:B:73:MET:CE	2:B:92:PHE:HB3	2.23	0.49
2:D:157:GLU:HA	3:E:123:LEU:HD13	1.95	0.49
4:F:191:LEU:HD12	4:F:191:LEU:N	2.28	0.49
4:F:200:ASP:O	4:F:221:LEU:HA	2.13	0.49
2:B:362:LYS:C	2:B:363:MET:HG2	2.38	0.49
2:D:174:LYS:HB3	2:D:208:TYR:CD2	2.48	0.49
2:D:212:PHE:O	2:D:216:LYS:HA	2.13	0.49
1:A:116:ASP:OD1	1:A:156:ARG:NH2	2.43	0.49
1:C:392:ASP:OD2	1:C:429:GLU:OE2	2.30	0.49
2:D:47:ILE:HD11	2:D:51:TYR:CD2	2.47	0.49
2:D:330:MET:HE2	2:D:333:VAL:HG11	1.94	0.49
4:F:223:THR:O	4:F:260:ASN:HB3	2.13	0.49
2:B:237:THR:O	2:B:241:ARG:HG3	2.13	0.48
4:F:31:ARG:HE	4:F:32:LYS:N	2.04	0.48
1:A:213:CYS:O	1:A:217:LEU:HB2	2.13	0.48
1:A:413:MET:CE	1:A:418:PHE:CE1	2.96	0.48
4:F:148:ILE:CD1	4:F:149:ALA:H	2.26	0.48
4:F:191:LEU:HD22	4:F:196:HIS:CD2	2.48	0.48
1:A:63:PRO:C	1:A:65:ALA:H	2.21	0.48
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.42	0.48
2:D:330:MET:O	2:D:333:VAL:HG12	2.12	0.48
1:C:333:ALA:HA	1:C:336:LYS:HE2	1.95	0.48
2:D:24:ILE:HA	2:D:27:GLU:HG3	1.94	0.48
2:B:330:MET:HE3	2:B:330:MET:CA	2.41	0.48
2:D:380:ARG:O	2:D:384:GLN:HG3	2.13	0.48
4:F:138:ARG:CB	4:F:145:ASN:OD1	2.62	0.48
2:B:28:HIS:HB3	2:B:47:ILE:HD11	1.95	0.48
3:E:123:LEU:O	3:E:126:LYS:HB2	2.12	0.48
1:A:339:ARG:HB2	1:A:341:ILE:CD1	2.43	0.48
2:B:83:GLN:HA	2:B:83:GLN:OE1	2.13	0.48
1:C:292:THR:HG22	1:C:335:ILE:HD13	1.96	0.48
2:D:356:ILE:HD12	2:D:356:ILE:H	1.78	0.48
4:F:135:TYR:CE1	4:F:145:ASN:HB3	2.48	0.48
4:F:186:LEU:HD12	4:F:320:MET:CG	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LYS:HG3	2:B:344:TRP:CE3	2.48	0.48
1:C:115:ILE:HG23	1:C:116:ASP:N	2.28	0.48
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.48	0.48
2:D:28:HIS:NE2	2:D:241:ARG:HB3	2.28	0.48
4:F:292:ARG:HD3	4:F:379:HIS:O	2.13	0.48
2:B:309:ARG:NH1	2:B:339:SER:O	2.46	0.48
1:A:269:LEU:HD11	1:A:301:GLN:HB3	1.96	0.47
2:B:64:ILE:CD1	2:B:120:VAL:HG22	2.43	0.47
1:C:171:ILE:N	1:C:171:ILE:HD13	2.29	0.47
2:D:174:LYS:HD2	2:D:208:TYR:CD2	2.49	0.47
2:D:293:MET:O	2:D:299:MET:HE1	2.14	0.47
2:D:418:LEU:HG	2:D:418:LEU:O	2.12	0.47
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.96	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.48	0.47
1:A:339:ARG:HB2	1:A:341:ILE:HD12	1.94	0.47
2:D:103:LYS:HG3	2:D:401:GLU:OE2	2.14	0.47
4:F:247:LYS:HD3	4:F:247:LYS:N	2.29	0.47
2:B:131:GLN:OE1	2:B:249:ASP:HB2	2.15	0.47
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.44	0.47
2:D:105:HIS:ND1	2:D:150:LEU:HB2	2.30	0.47
4:F:130:VAL:HG12	4:F:130:VAL:O	2.13	0.47
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.49	0.47
1:A:298:PRO:HA	1:A:301:GLN:CG	2.43	0.47
1:A:402:ARG:HG2	1:A:405:VAL:HG21	1.96	0.47
2:B:73:MET:CE	2:B:92:PHE:CD1	2.98	0.47
4:F:135:TYR:HE1	4:F:145:ASN:HB3	1.79	0.47
4:F:138:ARG:HG3	4:F:145:ASN:OD1	2.15	0.47
2:B:320:ARG:HD3	2:B:320:ARG:HA	1.66	0.47
2:B:336:LYS:HE2	2:B:336:LYS:HB3	1.71	0.47
2:D:75:SER:HA	2:D:78:SER:OG	2.14	0.47
2:D:151:LEU:HD23	2:D:155:ILE:HD11	1.95	0.47
2:D:197:ASP:C	2:D:198:GLU:HG3	2.39	0.47
2:D:210:ILE:HG22	2:D:215:LEU:HD23	1.95	0.47
3:E:124:GLN:HG3	3:E:125:GLU:N	2.30	0.47
1:A:399:TYR:O	1:A:402:ARG:NH1	2.48	0.47
2:B:199:THR:OG1	2:B:265:PHE:CD1	2.67	0.47
1:C:255:PHE:CD1	1:C:352:LYS:HD3	2.50	0.47
2:D:105:HIS:O	2:D:150:LEU:HD22	2.15	0.47
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.50	0.47
4:F:148:ILE:CD1	4:F:161:LEU:HB2	2.45	0.47
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:202:ARG:HD3	4:F:204:TRP:NE1	2.28	0.47
2:D:121:ARG:HD3	2:D:158:GLU:OE2	2.13	0.47
2:B:203:ASP:O	2:B:207:LEU:HG	2.15	0.47
3:E:22:VAL:O	3:E:22:VAL:CG1	2.62	0.47
1:A:414:GLU:O	1:A:415:GLU:C	2.57	0.47
2:B:169:VAL:HA	2:B:202:ILE:O	2.15	0.47
1:C:3:GLU:O	1:C:132:LEU:HD12	2.15	0.47
1:C:48:SER:HB3	1:C:243:ARG:O	2.14	0.47
2:D:12:CYS:O	2:D:16:ILE:HG23	2.14	0.47
1:A:172:TYR:CG	1:A:173:PRO:HD2	2.50	0.46
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.96	0.46
2:B:294:PHE:HE1	2:B:330:MET:HE1	1.79	0.46
4:F:100:ILE:HG23	4:F:128:ARG:N	2.30	0.46
2:B:163:ILE:HA	2:B:197:ASP:OD2	2.15	0.46
1:A:250:VAL:HG22	1:A:254:GLU:OE1	2.16	0.46
2:B:135:LEU:HD23	2:B:152:ILE:HD11	1.97	0.46
1:C:71:GLU:HB2	1:C:72:PRO:HD2	1.97	0.46
2:D:16:ILE:HD11	2:D:136:THR:HG22	1.96	0.46
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.33	0.46
4:F:77:LEU:O	4:F:81:ILE:HG13	2.16	0.46
4:F:187:GLU:C	4:F:189:PRO:HD3	2.40	0.46
4:F:296:MET:HE3	4:F:380:HIS:HB2	1.95	0.46
3:E:47:LEU:HD12	3:E:47:LEU:C	2.40	0.46
4:F:135:TYR:O	4:F:138:ARG:HB2	2.14	0.46
1:A:9:VAL:HG22	1:A:68:VAL:HG11	1.94	0.46
2:B:409:THR:O	2:B:413:SER:HB2	2.15	0.46
2:D:32:PRO:HA	2:D:81:PHE:CD2	2.51	0.46
2:D:353:VAL:O	2:D:353:VAL:CG1	2.63	0.46
4:F:31:ARG:O	4:F:32:LYS:C	2.59	0.46
1:A:55:GLU:HA	1:A:60:LYS:O	2.16	0.46
2:B:272:PRO:HD2	2:B:361:LEU:HD13	1.98	0.46
4:F:49:PHE:CB	4:F:66:ARG:HD2	2.45	0.46
2:B:246:LEU:HA	2:B:246:LEU:HD23	1.66	0.46
2:D:102:ALA:HB2	2:D:403:MET:SD	2.56	0.46
2:D:218:THR:HG23	2:D:219:THR:N	2.31	0.46
4:F:247:LYS:HG2	4:F:247:LYS:O	2.16	0.46
2:D:353:VAL:O	2:D:353:VAL:HG13	2.16	0.46
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.50	0.46
4:F:128:ARG:O	4:F:129:GLU:C	2.59	0.46
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.45	0.46
1:A:319:TYR:HB2	1:A:355:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ALA:O	1:A:425:MET:HG2	2.16	0.46
2:D:47:ILE:O	2:D:51:TYR:HB2	2.16	0.46
2:D:221:THR:HG23	2:D:224:ASP:N	2.31	0.46
2:D:270:PHE:O	2:D:298:ASN:HB3	2.16	0.46
4:F:4:PHE:HB3	4:F:27:TRP:HZ3	1.79	0.46
2:B:386:THR:HG22	2:B:412:GLU:OE2	2.16	0.45
1:A:155:GLU:HA	1:A:197:HIS:CE1	2.52	0.45
2:B:144:GLY:O	2:B:148:GLY:HA3	2.17	0.45
2:B:301:ALA:O	2:B:303:CYS:N	2.47	0.45
1:C:105:ARG:HA	1:C:109:THR:HB	1.98	0.45
1:C:162:GLY:CA	3:E:94:ILE:HD11	2.47	0.45
1:C:221:ARG:NH2	2:D:323:MET:CB	2.78	0.45
4:F:146:VAL:HG23	4:F:187:GLU:OE2	2.16	0.45
1:A:291:ILE:HD13	1:A:373:ARG:HG3	1.99	0.45
1:A:414:GLU:C	1:A:416:GLY:H	2.24	0.45
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.97	0.45
4:F:146:VAL:HG21	4:F:233:PHE:CZ	2.52	0.45
4:F:188:LYS:HD3	4:F:323:GLU:OE1	2.16	0.45
1:A:1:MET:HB3	1:A:46:ASP:HB2	1.98	0.45
1:C:97:GLU:HG3	2:D:2:ARG:NH1	2.31	0.45
2:D:320:ARG:HG2	2:D:320:ARG:HH11	1.82	0.45
1:A:88:HIS:CD2	1:A:90:GLU:HB2	2.48	0.45
2:D:246:LEU:HD13	2:D:248:ALA:HB2	1.96	0.45
2:D:285:THR:O	2:D:289:LEU:HD12	2.16	0.45
2:D:73:MET:HE2	2:D:77:ARG:CZ	2.46	0.45
2:D:323:MET:HE3	2:D:353:VAL:HG11	1.99	0.45
3:E:130:ALA:HA	3:E:133:VAL:CG1	2.47	0.45
2:D:5:VAL:CG1	2:D:133:PHE:HD1	2.29	0.45
1:A:27:GLU:HG2	1:A:361:THR:OG1	2.16	0.45
1:C:28:HIS:O	1:C:36:MET:HE3	2.16	0.45
1:C:75:ILE:HB	1:C:94:THR:CG2	2.46	0.45
2:D:69:GLU:HG2	2:D:96:GLY:CA	2.46	0.45
1:A:194:THR:O	1:A:194:THR:HG22	2.17	0.45
1:C:291:ILE:HD13	1:C:373:ARG:HG3	1.99	0.45
2:D:61:PRO:HD3	2:D:84:ILE:HG12	1.98	0.45
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.52	0.45
2:B:196:THR:OG1	2:B:199:THR:HG23	2.17	0.45
2:B:262:ARG:NH2	2:B:414:ASN:OD1	2.50	0.45
4:F:87:LEU:O	4:F:88:SER:OG	2.26	0.45
4:F:343:TYR:O	4:F:344:ALA:C	2.60	0.45
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HE2	1:C:130:THR:OG1	2.17	0.44
4:F:73:ARG:HG2	4:F:76:SER:H	1.81	0.44
4:F:74:LYS:NZ	4:F:331:GLU:HG3	2.31	0.44
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.99	0.44
1:A:423:GLU:O	1:A:426:ALA:HB3	2.16	0.44
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.98	0.44
1:C:230:LEU:O	1:C:234:ILE:HD12	2.16	0.44
2:D:141:GLY:O	2:D:143:THR:N	2.47	0.44
2:D:303:CYS:HA	2:D:376:GLU:OE1	2.17	0.44
3:E:46:SER:HB3	3:E:49:GLU:HG3	1.99	0.44
2:B:167:PHE:CE2	2:B:233:MET:HG2	2.53	0.44
2:B:267:MET:HE3	2:B:267:MET:HB3	1.86	0.44
1:C:214:ARG:O	1:C:218:ASP:HA	2.17	0.44
4:F:131:PHE:CD1	4:F:182:ILE:HD11	2.52	0.44
1:C:345:ASP:OD1	1:C:345:ASP:C	2.60	0.44
4:F:14:TYR:HA	4:F:17:VAL:HB	2.00	0.44
1:A:27:GLU:CD	1:A:320:ARG:HH22	2.25	0.44
2:B:213:ARG:O	2:B:216:LYS:HD3	2.18	0.44
1:C:46:ASP:N	1:C:46:ASP:OD1	2.51	0.44
2:D:221:THR:C	2:D:223:GLY:N	2.73	0.44
2:D:175:VAL:CG1	2:D:222:TYR:HE1	2.30	0.44
4:F:47:LEU:HD23	4:F:48:PRO:N	2.33	0.44
4:F:146:VAL:HG11	4:F:233:PHE:CE1	2.52	0.44
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.99	0.44
4:F:135:TYR:HE2	4:F:166:ALA:N	2.13	0.44
4:F:262:MET:HE3	4:F:262:MET:HB3	1.77	0.44
4:F:2:TYR:HB2	4:F:27:TRP:CE2	2.53	0.44
4:F:226:GLU:CD	4:F:252:ASN:HD22	2.18	0.44
1:A:16:ILE:CD1	1:A:171:ILE:HD11	2.48	0.44
1:A:233:GLN:HG3	1:A:368:LEU:CD2	2.48	0.44
1:A:390:ARG:HD2	4:F:54:HIS:CD2	2.52	0.44
2:D:225:LEU:N	2:D:225:LEU:HD23	2.33	0.44
1:A:287:SER:OG	1:A:290:GLU:HG3	2.18	0.43
2:B:23:VAL:O	2:B:27:GLU:HG3	2.18	0.43
2:B:64:ILE:HD13	2:B:120:VAL:CG2	2.47	0.43
2:D:218:THR:HG23	2:D:219:THR:H	1.82	0.43
2:D:47:ILE:CD1	2:D:51:TYR:HD2	2.31	0.43
3:E:24:LEU:O	3:E:25:LYS:HB2	2.18	0.43
2:D:193:VAL:HG22	2:D:265:PHE:HE2	1.82	0.43
2:D:286:VAL:HA	2:D:289:LEU:HD13	1.99	0.43
2:D:389:PHE:CE1	2:D:408:PHE:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:61:ARG:HG3	3:E:61:ARG:HH11	1.82	0.43
3:E:83:ILE:O	3:E:87:ILE:HG13	2.17	0.43
4:F:21:LEU:HD22	4:F:27:TRP:CG	2.53	0.43
4:F:214:TYR:CD2	4:F:353:VAL:HG11	2.52	0.43
2:D:292:GLN:O	2:D:295:ASP:HB3	2.18	0.43
2:D:295:ASP:OD1	2:D:297:LYS:HG3	2.19	0.43
3:E:50:ILE:O	3:E:54:LEU:HB2	2.18	0.43
1:A:98:ASP:OD1	1:A:100:ALA:N	2.42	0.43
1:A:395:PHE:CD1	1:A:395:PHE:C	2.96	0.43
2:B:44:LEU:HD12	2:B:44:LEU:HA	1.76	0.43
2:B:334:GLN:O	2:B:338:SER:N	2.52	0.43
2:D:237:THR:HG22	2:D:240:LEU:HD12	1.99	0.43
2:B:372:THR:OG1	2:B:426:GLN:HB2	2.18	0.43
1:C:180:ALA:HB3	1:C:183:GLU:HG3	2.00	0.43
1:A:183:GLU:N	1:A:184:PRO:CD	2.81	0.43
2:B:363:MET:HB3	2:B:363:MET:HE3	1.89	0.43
2:B:389:PHE:CE1	2:B:408:PHE:HB3	2.54	0.43
2:D:377:LEU:C	2:D:377:LEU:CD2	2.91	0.43
3:E:125:GLU:OE2	3:E:125:GLU:HA	2.17	0.43
1:A:98:ASP:OD1	1:A:98:ASP:C	2.62	0.43
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.58	0.43
2:D:62:ARG:HG3	2:D:123:GLU:OE1	2.19	0.43
3:E:58:GLU:HG2	3:E:62:LYS:HD2	1.99	0.43
3:E:80:ARG:HA	3:E:83:ILE:HG22	2.00	0.43
3:E:127:ASP:O	3:E:131:GLU:HG2	2.19	0.43
4:F:224:SER:OG	4:F:238:CYS:HA	2.19	0.43
1:A:112:LYS:O	1:A:112:LYS:HG2	2.18	0.43
2:B:106:TYR:OH	2:B:407:GLU:OE2	2.28	0.43
4:F:223:THR:HG21	4:F:257:GLU:OE1	2.18	0.43
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.54	0.43
2:B:104:GLY:O	2:B:109:GLY:HA3	2.19	0.43
2:D:94:GLN:O	2:D:95:SER:C	2.62	0.43
1:A:217:LEU:HD23	1:A:217:LEU:HA	1.83	0.42
1:A:424:ASP:O	1:A:427:ALA:HB3	2.19	0.42
2:B:273:LEU:HD11	2:B:298:ASN:HA	2.01	0.42
2:D:28:HIS:CE1	2:D:241:ARG:HB3	2.54	0.42
2:D:215:LEU:HD22	2:D:215:LEU:H	1.84	0.42
2:D:246:LEU:CD1	2:D:248:ALA:HB2	2.49	0.42
1:A:293:ASN:CA	1:A:335:ILE:HD11	2.49	0.42
2:B:31:ASP:OD1	2:B:33:THR:CG2	2.67	0.42
2:B:293:MET:HE3	2:B:365:ALA:CB	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.44	0.42
2:D:44:LEU:O	2:D:47:ILE:HG22	2.19	0.42
1:A:153:LEU:HD12	1:A:153:LEU:O	2.20	0.42
1:A:286:LEU:HD23	1:A:290:GLU:HB3	2.00	0.42
2:B:296:SER:HA	2:B:299:MET:HG2	2.00	0.42
1:C:48:SER:HB3	1:C:243:ARG:C	2.44	0.42
2:D:23:VAL:O	2:D:27:GLU:CG	2.65	0.42
4:F:192:LEU:HD12	4:F:192:LEU:N	2.30	0.42
1:A:293:ASN:HA	1:A:335:ILE:HD11	2.02	0.42
1:C:166:LYS:HE2	1:C:197:HIS:O	2.20	0.42
1:C:233:GLN:NE2	1:C:361:THR:O	2.53	0.42
1:C:293:ASN:OD1	1:C:339:ARG:NH1	2.52	0.42
4:F:99:VAL:O	4:F:100:ILE:HD13	2.19	0.42
4:F:131:PHE:CE1	4:F:182:ILE:HD12	2.55	0.42
4:F:149:ALA:CB	4:F:161:LEU:HD23	2.46	0.42
2:B:23:VAL:HG21	2:B:230:SER:CB	2.46	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.55	0.42
1:C:333:ALA:O	1:C:337:THR:HG23	2.19	0.42
4:F:147:TRP:HA	4:F:183:GLN:O	2.19	0.42
4:F:148:ILE:HD13	4:F:162:ILE:HG13	1.98	0.42
1:C:151:SER:O	1:C:155:GLU:HG3	2.20	0.42
2:D:395:LEU:HD23	2:D:395:LEU:HA	1.72	0.42
3:E:8:VAL:CG1	3:E:9:ILE:N	2.82	0.42
4:F:21:LEU:HD22	4:F:27:TRP:CD1	2.54	0.42
4:F:142:ARG:O	4:F:142:ARG:HG2	2.20	0.42
1:A:56:THR:O	1:A:59:GLY:N	2.36	0.42
1:A:101:ASN:ND2	1:A:101:ASN:N	2.68	0.42
1:A:258:ASN:O	1:A:314:ALA:HB1	2.20	0.42
3:E:24:LEU:N	3:E:24:LEU:HD12	2.34	0.42
4:F:8:ASP:HB2	4:F:43:GLU:HA	2.02	0.42
1:A:63:PRO:C	1:A:65:ALA:N	2.77	0.42
2:B:2:ARG:NE	2:B:131:GLN:HG2	2.34	0.42
3:E:113:GLU:O	3:E:114:ALA:C	2.63	0.42
1:A:56:THR:OG1	1:A:60:LYS:HB3	2.19	0.42
1:A:69:ASP:C	1:A:71:GLU:H	2.28	0.42
1:A:88:HIS:O	1:A:89:PRO:C	2.63	0.42
1:C:305:CYS:HA	1:C:386:GLU:OE1	2.20	0.42
2:D:139:LEU:O	2:D:185:ALA:N	2.52	0.42
3:E:69:LEU:HD23	3:E:69:LEU:HA	1.89	0.42
4:F:326:LYS:HD3	4:F:328:TRP:CZ2	2.55	0.42
2:B:274:THR:HG21	2:B:361:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.55	0.42
2:D:285:THR:O	2:D:288:GLU:N	2.52	0.42
2:B:203:ASP:HB2	2:B:301:ALA:HA	2.02	0.41
2:D:5:VAL:HG12	2:D:133:PHE:HD1	1.85	0.41
4:F:86:GLU:O	4:F:87:LEU:HD23	2.20	0.41
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.02	0.41
1:A:72:PRO:CB	1:A:94:THR:HG21	2.47	0.41
1:C:54:SER:O	1:C:61:HIS:HA	2.20	0.41
1:C:72:PRO:O	1:C:73:THR:C	2.63	0.41
2:D:293:MET:HG3	2:D:367:PHE:HB2	2.00	0.41
4:F:146:VAL:C	4:F:147:TRP:CD1	2.98	0.41
1:A:72:PRO:O	1:A:73:THR:C	2.61	0.41
2:B:68:LEU:HD23	2:B:68:LEU:HA	1.85	0.41
2:B:350:LYS:HG3	8:B:501:A1D6E:C21	2.50	0.41
1:C:161:TYR:O	1:C:162:GLY:C	2.62	0.41
2:D:210:ILE:HG22	2:D:215:LEU:HD21	2.02	0.41
4:F:278:THR:O	4:F:282:SER:OG	2.36	0.41
4:F:325:LEU:HD23	4:F:325:LEU:HA	1.83	0.41
3:E:116:LEU:HD23	3:E:116:LEU:HA	1.84	0.41
3:E:130:ALA:CA	3:E:133:VAL:HG12	2.50	0.41
4:F:131:PHE:CE1	4:F:182:ILE:CD1	3.03	0.41
1:A:84:ARG:HG2	1:A:84:ARG:H	1.62	0.41
1:A:221:ARG:CD	2:B:323:MET:HE2	2.50	0.41
2:B:267:MET:HE3	2:B:299:MET:SD	2.60	0.41
1:C:119:LEU:CD1	1:C:156:ARG:NH2	2.83	0.41
1:C:221:ARG:NH2	2:D:323:MET:HG2	2.35	0.41
2:D:206:ALA:HB2	2:D:302:ALA:N	2.35	0.41
3:E:11:LEU:C	3:E:11:LEU:HD12	2.45	0.41
3:E:135:LYS:HB3	3:E:135:LYS:HE2	1.85	0.41
4:F:330:ILE:N	4:F:330:ILE:HD13	2.35	0.41
1:A:33:ASP:OD1	1:A:35:GLN:HB2	2.20	0.41
2:B:7:ILE:O	2:B:135:LEU:HA	2.19	0.41
2:B:403:MET:HE2	2:B:403:MET:HB3	1.90	0.41
2:D:357:PRO:HB2	2:D:361:LEU:O	2.21	0.41
3:E:125:GLU:OE2	3:E:128:LYS:HE3	2.21	0.41
1:A:109:THR:OG1	1:A:411:GLU:OE1	2.32	0.41
1:C:124:LYS:HA	1:C:124:LYS:HD3	1.80	0.41
1:C:162:GLY:HA2	3:E:94:ILE:HD11	2.01	0.41
1:C:276:ILE:HG23	1:C:369:ALA:HB3	2.03	0.41
2:D:1:MET:SD	2:D:128:ASP:HB2	2.61	0.41
2:D:333:VAL:O	2:D:337:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:99:VAL:O	4:F:99:VAL:HG23	2.19	0.41
4:F:137:ARG:O	4:F:137:ARG:HD2	2.20	0.41
1:A:241:SER:HB2	1:A:249:ASN:O	2.21	0.41
2:B:64:ILE:HG12	2:B:119:VAL:HG12	2.02	0.41
1:C:180:ALA:HA	2:D:256:ASN:OD1	2.21	0.41
2:D:256:ASN:HB3	8:D:502:A1D6E:C21	2.51	0.41
2:B:116:VAL:HG11	2:B:151:LEU:HD21	2.03	0.41
2:B:313:VAL:HB	2:B:349:VAL:HG22	2.02	0.41
2:B:316:ILE:HG23	2:B:366:THR:HB	2.03	0.41
2:B:396:HIS:HA	2:B:399:THR:OG1	2.20	0.41
1:C:324:VAL:HG22	1:C:327:ASP:OD2	2.21	0.41
1:C:327:ASP:O	1:C:328:VAL:C	2.63	0.41
2:D:31:ASP:CG	2:D:33:THR:HG22	2.44	0.41
2:D:192:LEU:O	2:D:196:THR:OG1	2.38	0.41
2:D:211:CYS:O	2:D:215:LEU:HB2	2.20	0.41
4:F:138:ARG:HB3	4:F:145:ASN:CG	2.45	0.41
4:F:138:ARG:CB	4:F:145:ASN:HD21	2.34	0.41
4:F:232:ASN:OD1	4:F:232:ASN:N	2.54	0.41
1:A:68:VAL:CG1	1:A:68:VAL:O	2.68	0.41
2:B:185:ALA:O	2:B:189:VAL:HG23	2.21	0.41
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.84	0.41
2:D:1:MET:HG3	2:D:128:ASP:CB	2.48	0.41
2:D:345:ILE:HG22	2:D:348:ASN:HB3	2.03	0.41
3:E:125:GLU:O	3:E:125:GLU:CD	2.64	0.41
1:C:67:PHE:CD1	1:C:67:PHE:N	2.88	0.40
2:D:47:ILE:CD1	2:D:51:TYR:CD2	3.04	0.40
2:D:293:MET:HE1	2:D:317:PHE:CZ	2.56	0.40
4:F:28:LYS:HB2	4:F:28:LYS:NZ	2.36	0.40
4:F:138:ARG:HD2	4:F:143:GLU:HB2	2.03	0.40
2:D:65:LEU:HD21	2:D:85:PHE:CD2	2.56	0.40
4:F:39:LEU:HA	4:F:61:LEU:O	2.21	0.40
4:F:81:ILE:HA	4:F:87:LEU:HD12	2.02	0.40
4:F:272:MET:HA	4:F:277:THR:O	2.22	0.40
2:B:67:ASP:O	2:B:92:PHE:HA	2.21	0.40
2:B:285:THR:O	2:B:288:GLU:N	2.54	0.40
1:C:60:LYS:NZ	1:C:85:GLN:O	2.42	0.40
2:D:221:THR:O	2:D:224:ASP:N	2.53	0.40
4:F:191:LEU:HA	4:F:197:ARG:O	2.21	0.40
1:A:86:LEU:HD12	1:A:86:LEU:HA	1.94	0.40
1:A:166:LYS:HD2	1:A:197:HIS:O	2.21	0.40
2:B:328:GLU:O	2:B:332:ASN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLU:HB2	1:C:72:PRO:CD	2.52	0.40
2:D:109:GLY:HA3	2:D:147:MET:HG3	2.03	0.40
1:A:151:SER:HB2	1:A:193:THR:HG22	2.03	0.40
1:A:153:LEU:HD12	1:A:153:LEU:C	2.46	0.40
1:A:425:MET:HE3	1:A:425:MET:HB3	1.72	0.40
2:B:322:SER:O	2:B:326:VAL:HG23	2.21	0.40
1:C:63:PRO:HD3	1:C:86:LEU:HG	2.04	0.40
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.36	0.40
3:E:9:ILE:O	3:E:10:GLU:C	2.64	0.40
4:F:146:VAL:HG21	4:F:233:PHE:HZ	1.86	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	435/440 (99%)	400 (92%)	30 (7%)	5 (1%)	11	27
1	C	438/440 (100%)	414 (94%)	20 (5%)	4 (1%)	14	33
2	B	425/431 (99%)	410 (96%)	14 (3%)	1 (0%)	43	66
2	D	417/431 (97%)	389 (93%)	26 (6%)	2 (0%)	24	46
3	E	117/143 (82%)	103 (88%)	12 (10%)	2 (2%)	7	17
4	F	322/380 (85%)	296 (92%)	21 (6%)	5 (2%)	7	18
All	All	2154/2265 (95%)	2012 (93%)	123 (6%)	19 (1%)	14	33

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	218	ASP
1	A	109	THR

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Mol	Chain	Res	Type
2	B	71	GLY
1	C	109	THR
3	E	10	GLU
4	F	129	GLU
4	F	253	TYR
4	F	255	ARG
4	F	32	LYS
1	A	41	THR
1	A	265	ILE
2	D	142	GLY
1	A	315	CYS
1	C	328	VAL
2	D	302	ALA
1	C	72	PRO
3	E	27	PRO
4	F	102	PRO
1	A	261	PRO

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	366/371 (99%)	358 (98%)	8 (2%)	45	72
1	C	370/371 (100%)	361 (98%)	9 (2%)	43	70
2	B	367/372 (99%)	358 (98%)	9 (2%)	42	69
2	D	362/372 (97%)	348 (96%)	14 (4%)	28	56
3	E	109/127 (86%)	106 (97%)	3 (3%)	38	67
4	F	295/338 (87%)	291 (99%)	4 (1%)	59	80
All	All	1869/1951 (96%)	1822 (98%)	47 (2%)	42	69

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP

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Mol	Chain	Res	Type
1	A	41	THR
1	A	71	GLU
1	A	101	ASN
1	A	132	LEU
1	A	159	VAL
1	A	250	VAL
1	A	379	SER
2	B	15	GLN
2	B	78	SER
2	B	115	SER
2	B	151	LEU
2	B	179	VAL
2	B	276	ARG
2	B	296	SER
2	B	356	ILE
2	B	413	SER
1	C	71	GLU
1	C	96	LYS
1	C	101	ASN
1	C	165	SER
1	C	286	LEU
1	C	318	LEU
1	C	335	ILE
1	C	368	LEU
1	C	440	VAL
2	D	5	VAL
2	D	35	SER
2	D	57	ASN
2	D	78	SER
2	D	111	GLU
2	D	113	VAL
2	D	115	SER
2	D	136	THR
2	D	138	SER
2	D	178	THR
2	D	323	MET
2	D	339	SER
2	D	377	LEU
2	D	392	LYS
3	E	53	LYS
3	E	62	LYS
3	E	131	GLU

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Mol	Chain	Res	Type
4	F	12	SER
4	F	13	VAL
4	F	18	SER
4	F	190	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	35	GLN
1	A	61	HIS
1	A	88	HIS
1	A	233	GLN
1	A	256	GLN
1	A	301	GLN
1	A	309	HIS
2	B	134	GLN
2	B	337	ASN
1	C	283	HIS
1	C	285	GLN
1	C	393	HIS
2	D	37	HIS
2	D	48	ASN
2	D	94	GLN
3	E	92	ASN
3	E	103	GLN
3	E	108	ASN
4	F	242	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 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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
9	GDP	B	502	7	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
5	GTP	C	501	7	33,34,34	0.98	2 (6%)	50,54,54	1.57	8 (16%)
11	ACP	F	401	-	31,33,33	0.52	1 (3%)	47,52,52	1.18	2 (4%)
8	A1D6E	B	501	-	28,28,28	3.00	9 (32%)	35,40,40	1.84	12 (34%)
10	MES	B	504	-	12,12,12	2.32	1 (8%)	15,16,16	1.87	2 (13%)
5	GTP	A	501	7	33,34,34	0.96	1 (3%)	50,54,54	1.57	8 (16%)
8	A1D6E	D	502	-	28,28,28	2.93	6 (21%)	35,40,40	1.99	8 (22%)
10	MES	B	503	-	12,12,12	2.33	1 (8%)	15,16,16	1.83	3 (20%)
9	GDP	D	501	-	29,30,30	1.17	2 (6%)	45,47,47	1.75	6 (13%)

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
9	GDP	B	502	7	-	5/16/32/32	0/3/3/3
5	GTP	C	501	7	-	10/22/38/38	0/3/3/3
11	ACP	F	401	-	-	5/19/38/38	0/3/3/3
8	A1D6E	B	501	-	-	5/8/18/18	0/4/4/4
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
5	GTP	A	501	7	-	9/22/38/38	0/3/3/3
8	A1D6E	D	502	-	-	5/8/18/18	0/4/4/4
10	MES	B	503	-	-	4/6/14/14	0/1/1/1
9	GDP	D	501	-	-	3/16/32/32	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	501	A1D6E	C09-N11	12.68	1.44	1.34
8	D	502	A1D6E	C09-N11	12.55	1.44	1.34
10	B	503	MES	C8-S	-7.82	1.66	1.77
10	B	504	MES	C8-S	-7.79	1.66	1.77
8	D	502	A1D6E	C18-N13	5.15	1.49	1.40
8	B	501	A1D6E	C18-N13	4.23	1.47	1.40
8	B	501	A1D6E	C07-N13	3.58	1.47	1.39
8	D	502	A1D6E	C05-C04	-3.50	1.37	1.42
8	D	502	A1D6E	C07-N13	3.44	1.46	1.39
8	B	501	A1D6E	C16-C17	3.41	1.56	1.51
8	D	502	A1D6E	C16-C17	3.22	1.56	1.51
8	B	501	A1D6E	C05-C04	-3.18	1.37	1.42
9	B	502	GDP	C5-C4	3.14	1.47	1.38
9	D	501	GDP	C5-C4	3.09	1.47	1.38
8	B	501	A1D6E	C14-N13	-2.95	1.42	1.46
11	F	401	ACP	PB-O3A	2.70	1.61	1.58
8	D	502	A1D6E	C14-N13	-2.66	1.42	1.46
8	B	501	A1D6E	C06-C01	2.61	1.40	1.36
9	D	501	GDP	C6-N1	-2.41	1.34	1.38
9	B	502	GDP	C6-N1	-2.35	1.34	1.38
5	A	501	GTP	C2-N3	2.22	1.38	1.33
5	C	501	GTP	C2-N3	2.21	1.38	1.33
5	C	501	GTP	PA-O3A	2.15	1.61	1.59
8	B	501	A1D6E	C20-C21	2.08	1.42	1.38
8	B	501	A1D6E	C07-N08	2.02	1.34	1.32
9	B	502	GDP	C5-N7	-2.01	1.35	1.39

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	PB-O3A-PA	-6.74	110.36	132.37
8	D	502	A1D6E	C07-C05-C04	6.30	119.65	115.47
9	B	502	GDP	C5-C4-N3	-6.07	118.73	128.39
9	D	501	GDP	C5-C4-N3	-5.82	119.12	128.39
5	C	501	GTP	C5-C4-N3	-5.02	120.41	128.39
9	B	502	GDP	C2-N3-C4	5.00	120.92	112.30
5	A	501	GTP	C5-C4-N3	-4.99	120.44	128.39
9	D	501	GDP	C2-N3-C4	4.93	120.79	112.30
5	C	501	GTP	C2-N3-C4	4.64	120.28	112.30
5	A	501	GTP	C2-N3-C4	4.62	120.27	112.30
10	B	504	MES	C5-N4-C3	4.52	118.58	108.84
9	B	502	GDP	N9-C4-N3	4.48	134.91	125.95
8	B	501	A1D6E	C07-C05-C04	4.45	118.43	115.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	502	A1D6E	C12-N11-C09	-4.41	118.28	123.59
9	D	501	GDP	N9-C4-N3	4.38	134.72	125.95
10	B	503	MES	C5-N4-C3	4.26	118.02	108.84
8	B	501	A1D6E	N11-C09-N08	4.20	120.99	116.96
8	D	502	A1D6E	C05-C04-N10	-4.01	118.56	122.80
8	D	502	A1D6E	C01-C06-C05	3.41	121.44	118.75
9	D	501	GDP	C6-C5-N7	3.34	136.37	130.29
9	B	502	GDP	C6-C5-N7	3.23	136.18	130.29
5	C	501	GTP	N9-C4-N3	3.21	132.38	125.95
5	A	501	GTP	N9-C4-N3	3.19	132.34	125.95
8	D	502	A1D6E	C09-N10-C04	2.89	120.12	115.54
8	B	501	A1D6E	C12-N11-C09	-2.89	120.11	123.59
5	C	501	GTP	C2-N1-C6	-2.86	119.92	125.11
5	A	501	GTP	C2-N1-C6	-2.85	119.94	125.11
8	B	501	A1D6E	C09-N10-C04	2.83	120.03	115.54
10	B	503	MES	C6-C5-N4	-2.82	105.83	110.12
8	B	501	A1D6E	C01-C06-C05	2.72	120.89	118.75
8	B	501	A1D6E	C02-C01-C06	-2.69	120.19	123.32
5	A	501	GTP	N9-C8-N7	-2.69	108.42	113.40
5	C	501	GTP	N9-C8-N7	-2.67	108.45	113.40
8	D	502	A1D6E	N11-C09-N10	2.58	119.44	116.96
9	B	502	GDP	C4-C5-N7	-2.56	106.61	110.67
8	B	501	A1D6E	N10-C09-N08	-2.56	122.06	126.25
10	B	504	MES	C6-C5-N4	-2.54	106.26	110.12
5	C	501	GTP	C8-N7-C5	2.53	108.77	104.26
5	A	501	GTP	C8-N7-C5	2.52	108.75	104.26
9	D	501	GDP	C4-C5-N7	-2.48	106.74	110.67
5	A	501	GTP	C5-C6-N1	2.48	119.57	113.25
5	C	501	GTP	C5-C6-N1	2.47	119.54	113.25
8	D	502	A1D6E	C02-C01-C06	-2.46	120.46	123.32
8	B	501	A1D6E	C05-C04-N10	-2.41	120.25	122.80
5	A	501	GTP	O6-C6-C5	-2.39	120.21	126.53
5	C	501	GTP	O6-C6-C5	-2.36	120.30	126.53
10	B	503	MES	O2S-S-C8	2.35	110.28	106.73
8	B	501	A1D6E	C05-C07-N08	-2.29	118.01	122.44
8	B	501	A1D6E	C09-N08-C07	2.25	121.22	113.99
8	B	501	A1D6E	C19-C20-C21	2.18	122.22	119.73
8	D	502	A1D6E	C05-C07-N08	-2.17	118.23	122.44
11	F	401	ACP	O3'-C3'-C4'	-2.17	104.85	111.08
9	D	501	GDP	O6-C6-C5	-2.11	120.96	126.53
9	B	502	GDP	O6-C6-C5	-2.10	120.98	126.53
8	B	501	A1D6E	C22-C17-C18	2.10	120.92	118.95

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	A1D6E	N08-C09-N11-C12
8	B	501	A1D6E	N10-C09-N11-C12
8	D	502	A1D6E	C05-C07-N13-C18
8	D	502	A1D6E	N08-C07-N13-C14
8	D	502	A1D6E	N08-C09-N11-C12
8	D	502	A1D6E	N10-C09-N11-C12
9	B	502	GDP	C5'-O5'-PA-O3A
9	B	502	GDP	C5'-O5'-PA-O1A
9	B	502	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C8-C7-N4-C5
10	B	504	MES	C7-C8-S-O2S
10	B	504	MES	C7-C8-S-O3S
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	C3'-C4'-C5'-O5'
8	B	501	A1D6E	N08-C07-N13-C14
10	B	504	MES	C8-C7-N4-C3
10	B	503	MES	C7-C8-S-O3S
10	B	503	MES	C7-C8-S-O1S
10	B	503	MES	C7-C8-S-O2S
10	B	504	MES	C7-C8-S-O1S
5	A	501	GTP	C5'-O5'-PA-O1A
8	B	501	A1D6E	N08-C07-N13-C18
8	D	502	A1D6E	N08-C07-N13-C18
11	F	401	ACP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O1A

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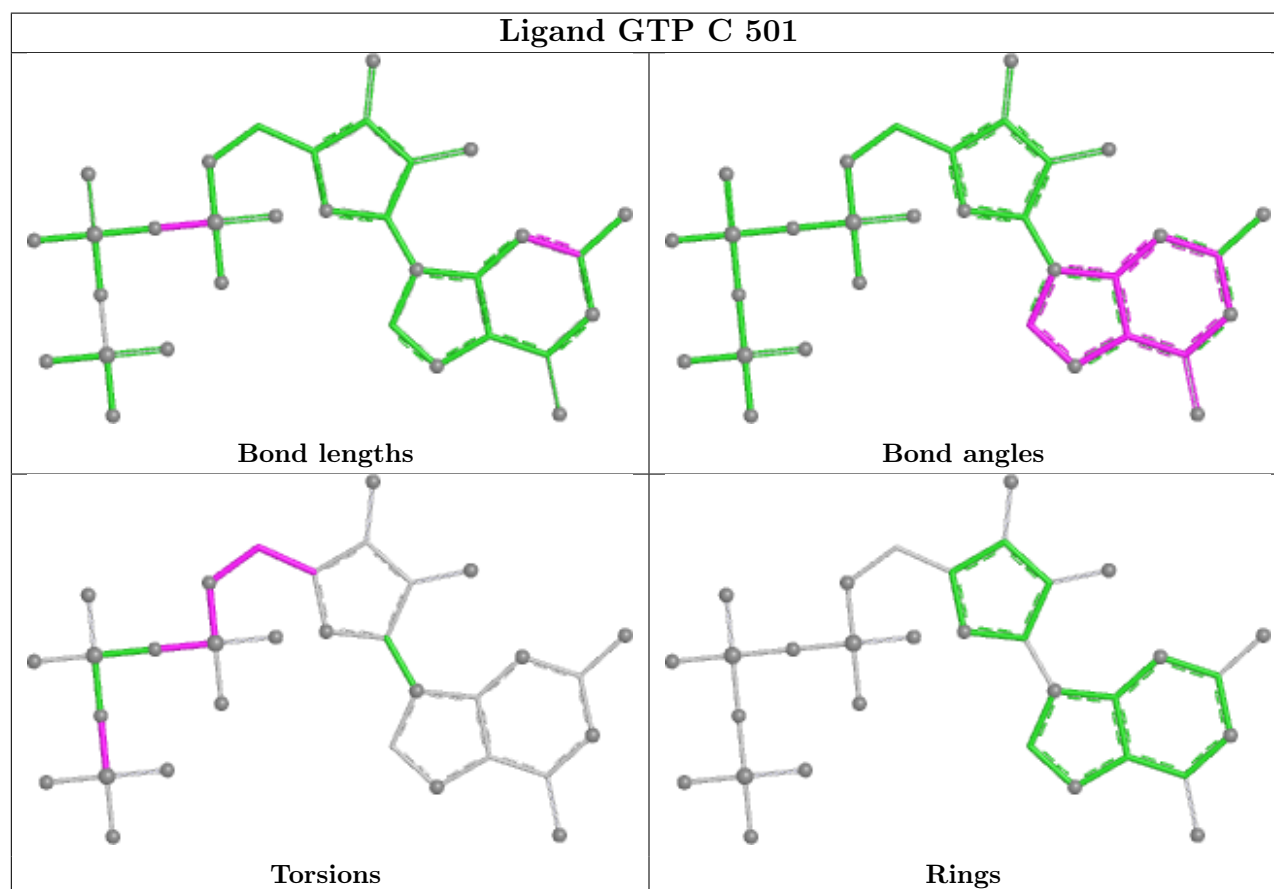
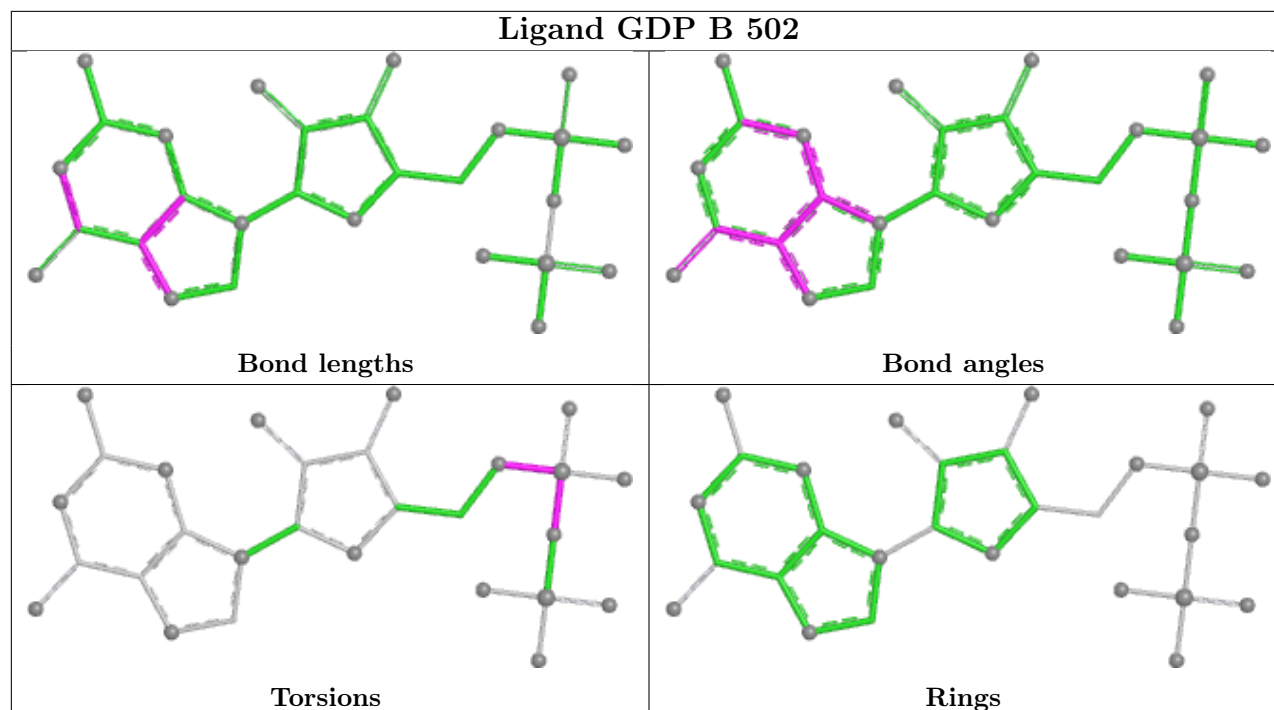
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C3'-C4'-C5'-O5'
9	B	502	GDP	PB-O3A-PA-O2A
11	F	401	ACP	C3'-C4'-C5'-O5'
8	B	501	A1D6E	C05-C07-N13-C14
5	C	501	GTP	PB-O3A-PA-O2A
9	B	502	GDP	PB-O3A-PA-O1A
11	F	401	ACP	O4'-C4'-C5'-O5'

There are no ring outliers.

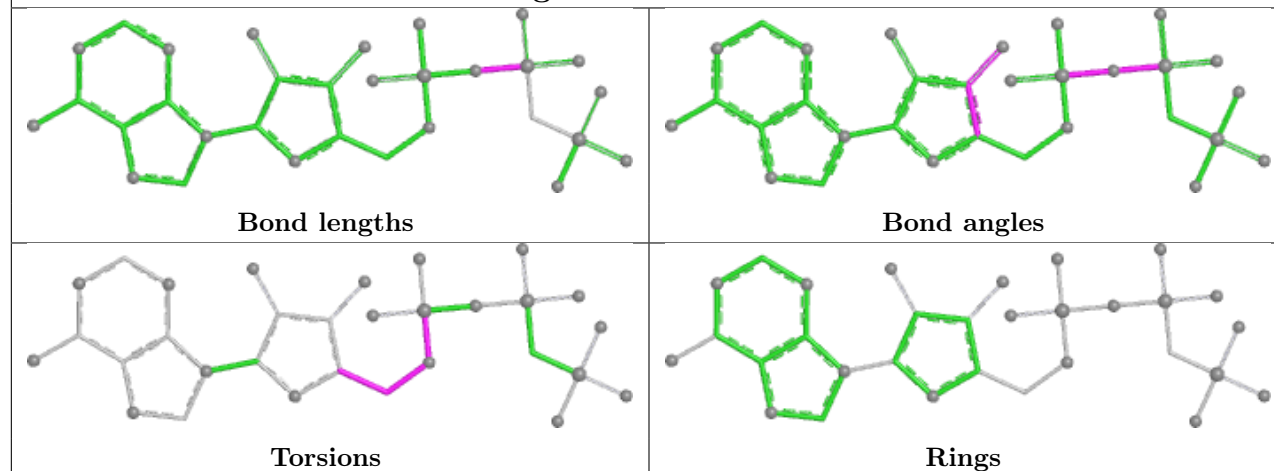
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	A1D6E	2	0
8	D	502	A1D6E	1	0

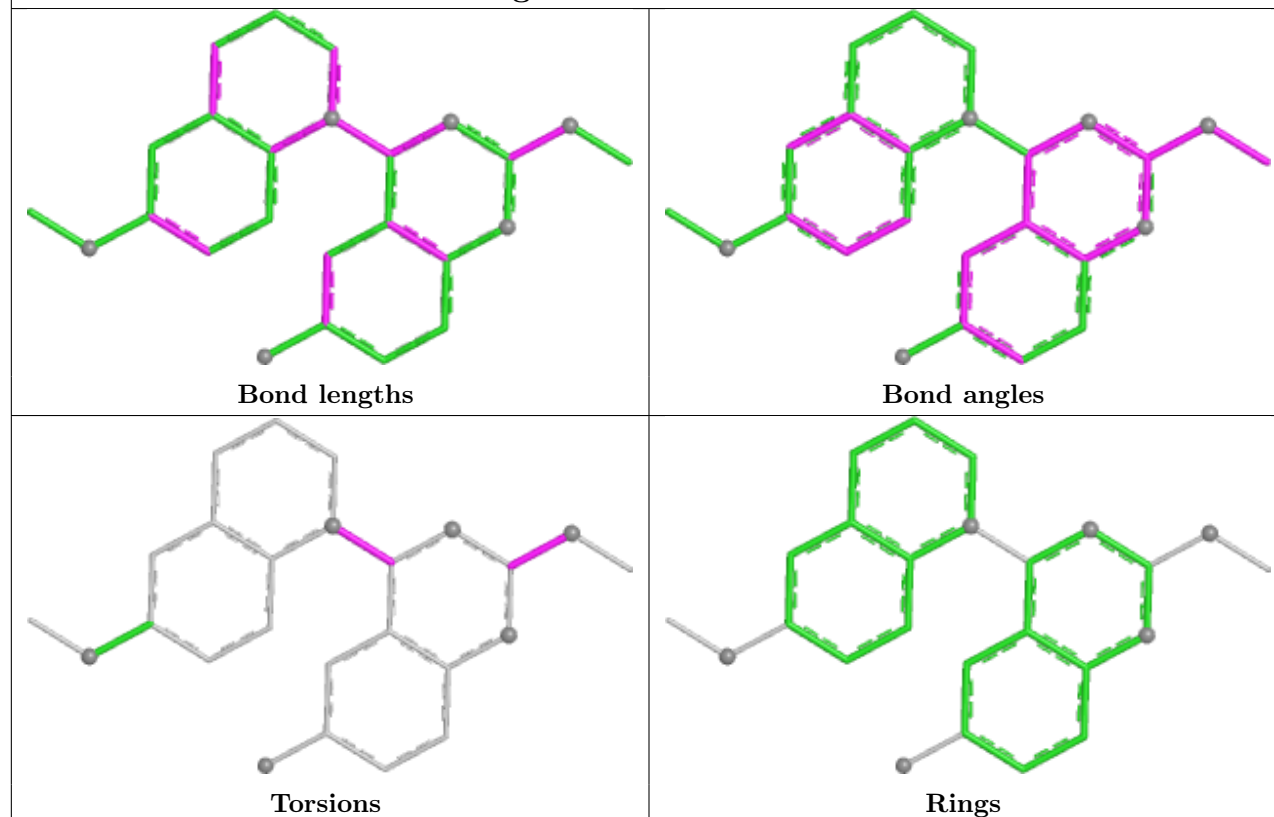
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

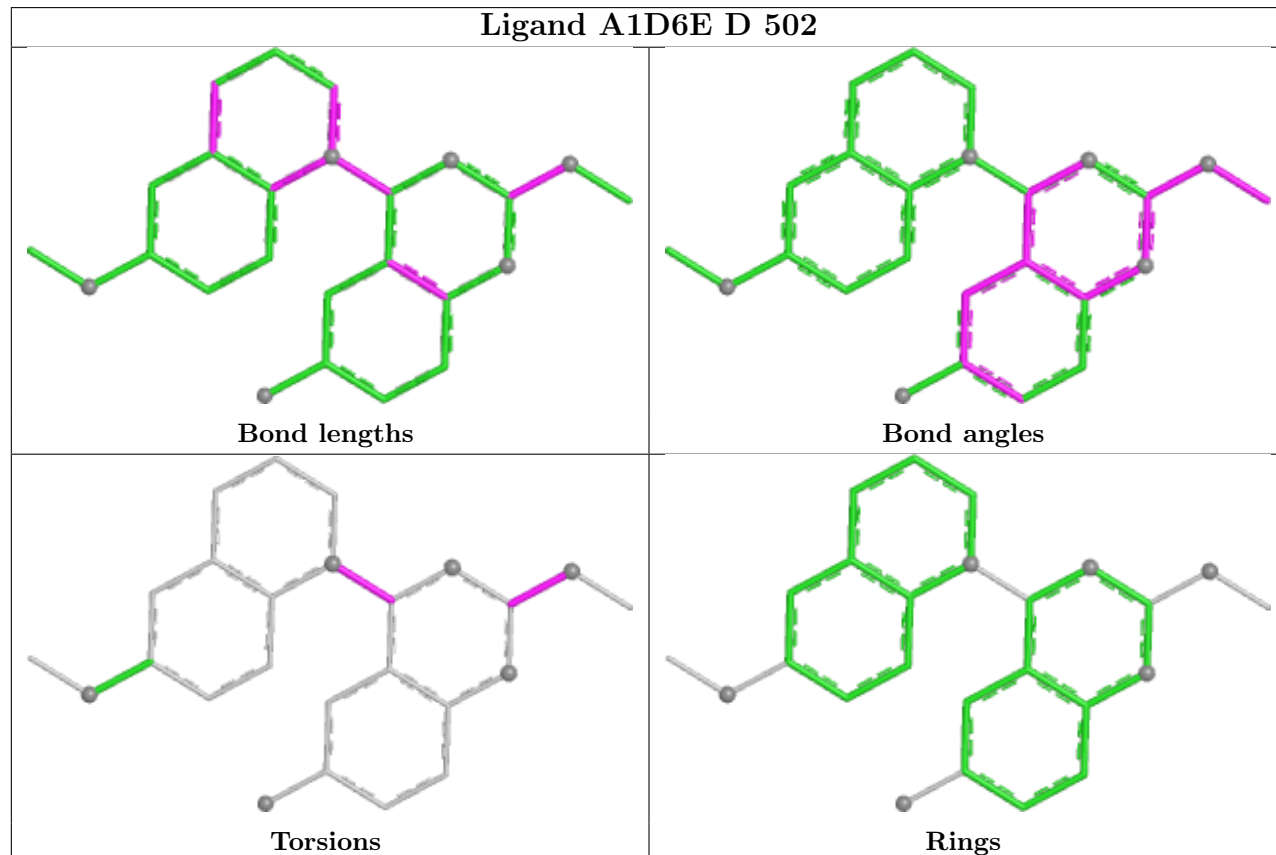
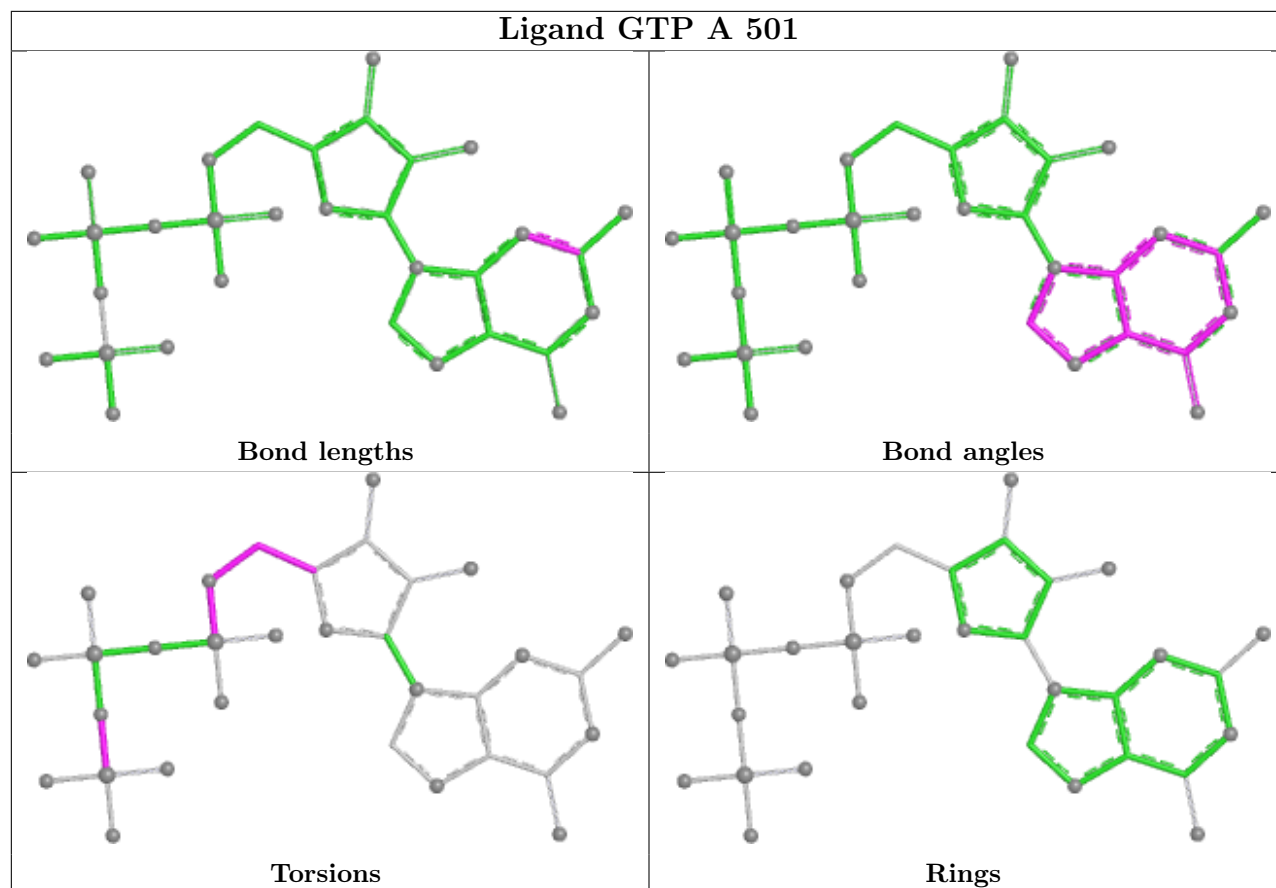


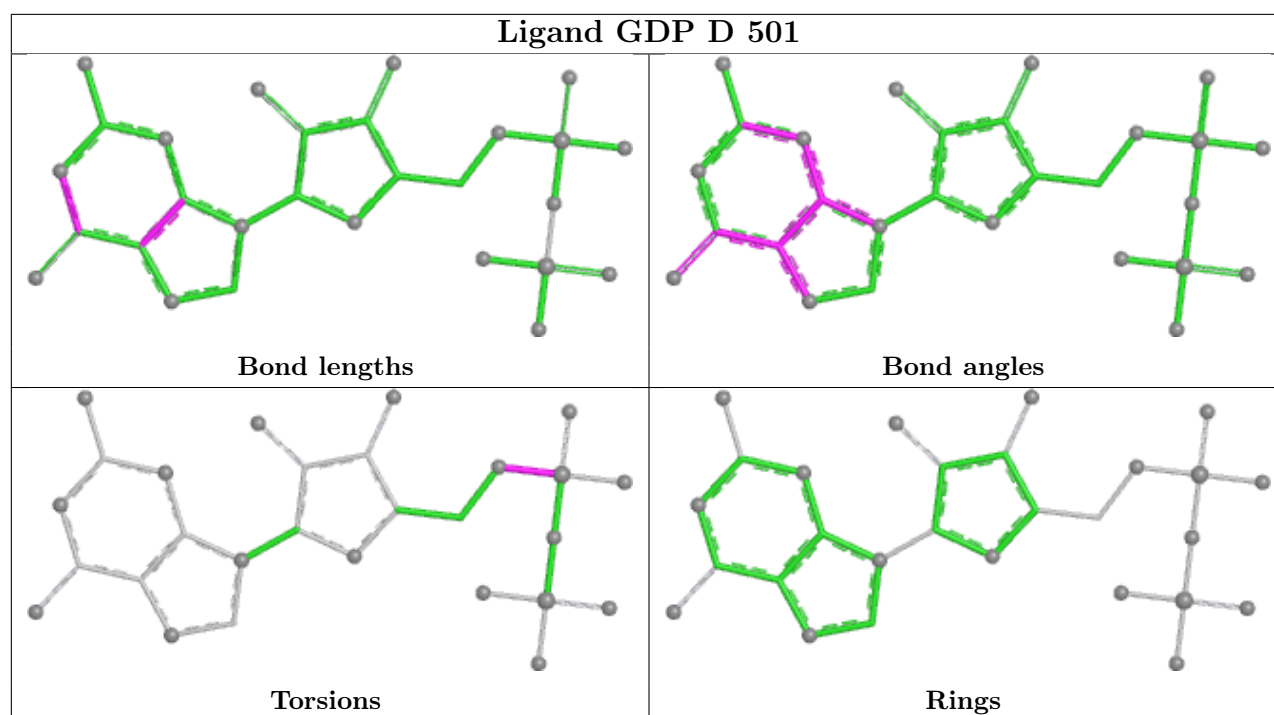
Ligand ACP F 401



Ligand A1D6E B 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/440 (99%)	0.11	6 (1%) 73 71	35, 52, 73, 112	0
1	C	440/440 (100%)	-0.22	4 (0%) 81 80	28, 41, 63, 76	0
2	B	427/431 (99%)	-0.01	6 (1%) 73 71	31, 49, 78, 125	0
2	D	421/431 (97%)	0.79	41 (9%) 13 11	39, 72, 103, 124	0
3	E	121/143 (84%)	0.49	6 (4%) 34 31	41, 62, 92, 114	0
4	F	332/380 (87%)	0.95	60 (18%) 3 3	45, 77, 141, 155	0
All	All	2178/2265 (96%)	0.30	123 (5%) 30 27	28, 56, 105, 155	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	141	GLY	6.5
4	F	173	ILE	4.6
2	D	73	MET	4.1
4	F	132	LEU	4.1
4	F	237	THR	4.1
4	F	245	ILE	4.1
1	A	437	VAL	4.1
4	F	130	VAL	3.9
2	D	397	TRP	3.9
2	D	431	ASP	3.8
4	F	362	ALA	3.8
3	E	28	SER	3.6
4	F	133	ALA	3.6
4	F	161	LEU	3.6
4	F	149	ALA	3.5
4	F	101	TYR	3.5
4	F	182	ILE	3.5
4	F	98	TYR	3.4
4	F	180	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
4	F	103	THR	3.3
2	D	11	GLN	3.3
2	D	140	GLY	3.3
4	F	99	VAL	3.2
1	A	179	THR	3.2
4	F	233	PHE	3.2
4	F	253	TYR	3.1
4	F	181	VAL	3.1
4	F	134	ALA	3.0
2	D	6	HIS	3.0
2	D	245	GLN	2.9
4	F	89	GLU	2.9
3	E	46	SER	2.9
2	D	54	ALA	2.9
4	F	247	LYS	2.9
2	D	171	PRO	2.9
4	F	166	ALA	2.9
4	F	242	ASN	2.8
2	D	39	ASP	2.8
2	D	394	PHE	2.8
2	D	170	MET	2.8
2	D	393	ALA	2.8
4	F	240	LEU	2.8
4	F	172	PHE	2.7
2	D	55	THR	2.7
4	F	372	THR	2.7
4	F	261	GLU	2.6
2	D	284	LEU	2.6
4	F	148	ILE	2.6
4	F	162	ILE	2.6
4	F	380	HIS	2.6
4	F	167	SER	2.5
3	E	59	GLU	2.5
2	D	180	VAL	2.5
2	B	279	GLN	2.5
4	F	169	LEU	2.5
1	A	282	TYR	2.5
2	D	321	MET	2.5
4	F	263	PHE	2.5
2	D	243	PRO	2.5
4	F	194	PRO	2.5
3	E	45	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	131	PHE	2.4
4	F	224	SER	2.4
2	D	97	ALA	2.4
4	F	186	LEU	2.4
2	D	323	MET	2.4
2	D	32	PRO	2.4
4	F	254	GLY	2.4
2	B	316	ILE	2.3
4	F	379	HIS	2.3
1	C	177	VAL	2.3
1	C	440	VAL	2.3
1	A	281	ALA	2.3
2	D	212	PHE	2.3
2	B	428	ALA	2.3
2	D	396	HIS	2.3
1	A	176	GLN	2.3
4	F	100	ILE	2.3
2	D	106	TYR	2.3
4	F	229	ASN	2.3
1	C	340	SER	2.3
2	D	80	PRO	2.3
4	F	90	SER	2.3
4	F	163	SER	2.3
2	D	101	TRP	2.3
2	D	220	PRO	2.2
2	D	216	LYS	2.2
2	D	362	LYS	2.2
4	F	231	ALA	2.2
4	F	129	GLU	2.2
2	D	391	ARG	2.2
2	D	71	GLY	2.2
2	D	273	LEU	2.2
3	E	139	LEU	2.2
4	F	179	VAL	2.2
2	D	178	THR	2.2
2	D	179	VAL	2.2
3	E	8	VAL	2.2
4	F	92	THR	2.2
4	F	164	SER	2.2
2	D	227	HIS	2.2
4	F	256	TYR	2.1
4	F	170	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	243	HIS	2.1
4	F	147	TRP	2.1
2	D	214	THR	2.1
2	B	280	GLN	2.1
2	D	335	ASN	2.1
4	F	191	LEU	2.1
4	F	168	GLU	2.1
1	A	44	GLY	2.1
2	B	281	TYR	2.1
4	F	230	SER	2.1
1	C	179	THR	2.1
2	D	218	THR	2.1
2	B	56	GLY	2.1
4	F	239	HIS	2.1
4	F	228	TYR	2.1
4	F	33	ASP	2.0
2	D	406	MET	2.0
2	D	72	THR	2.0
4	F	178	GLN	2.0
4	F	306	HIS	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.

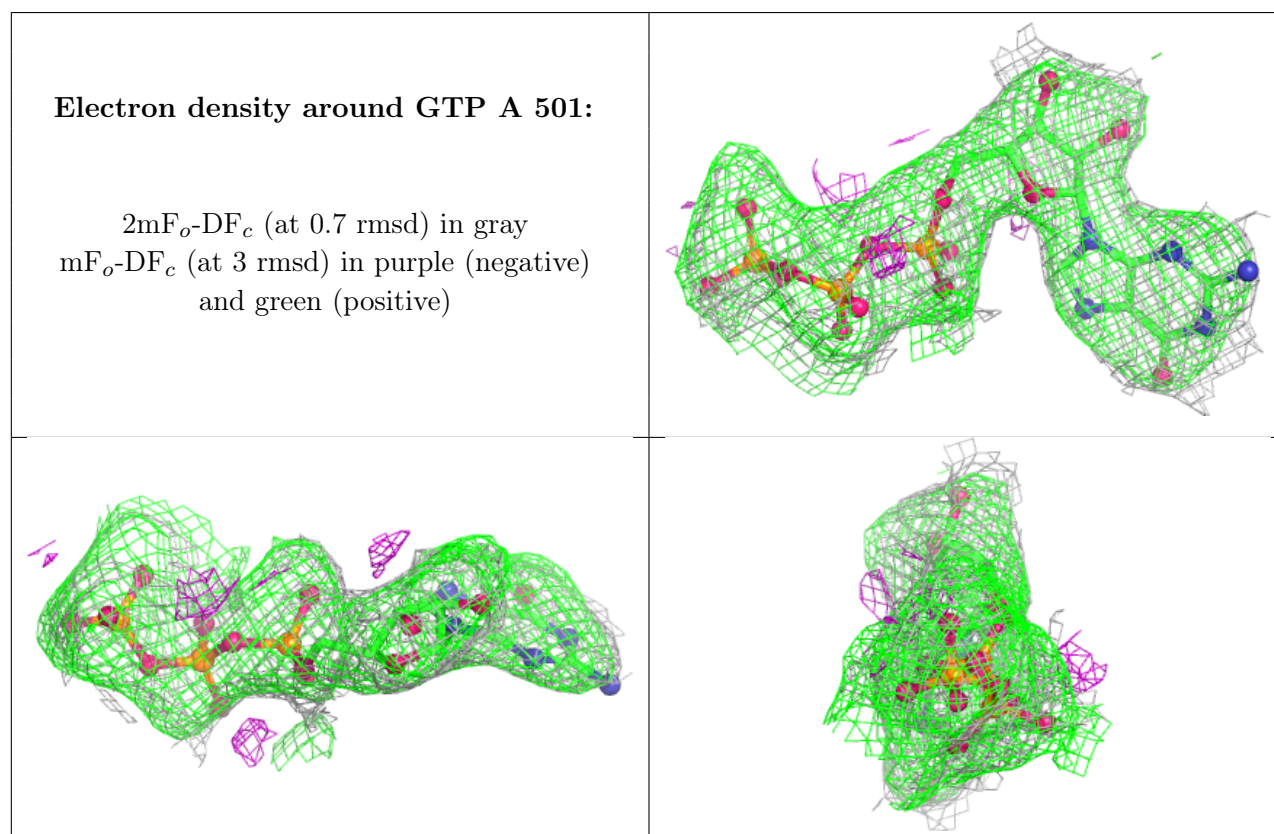
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GTP	A	501	32/32	-	-	40,42,47,48	32
5	GTP	C	501	32/32	-	-	32,35,39,40	32
6	CA	A	502	1/1	-	-	71,71,71,71	1

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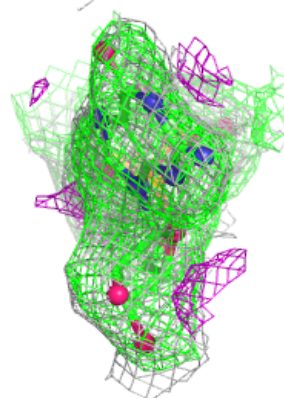
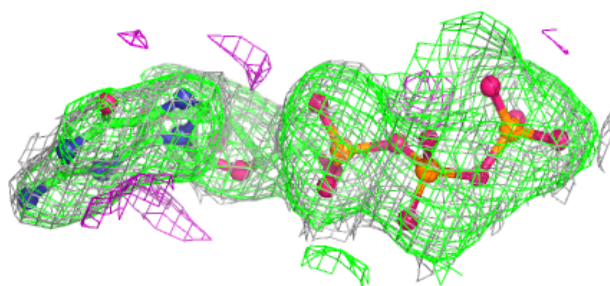
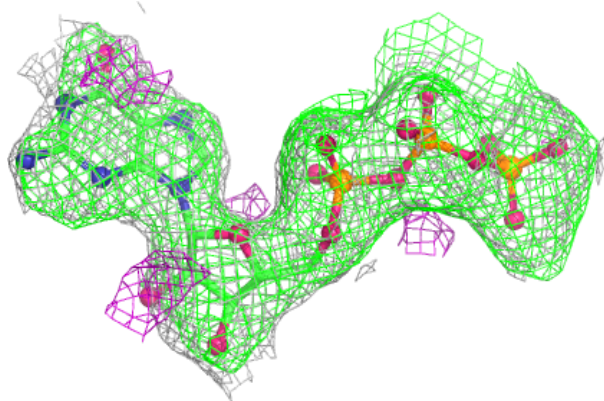
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CA	C	502	1/1	-	-	59,59,59,59	1
7	MG	A	503	1/1	-	-	46,46,46,46	1
7	MG	B	505	1/1	-	-	45,45,45,45	1
7	MG	C	503	1/1	-	-	39,39,39,39	1
8	A1D6E	B	501	25/25	0.93	0.10	36,50,63,65	0
8	A1D6E	D	502	25/25	0.93	0.10	42,56,69,70	0
9	GDP	B	502	28/28	-	-	35,38,40,41	28
9	GDP	D	501	28/28	-	-	71,79,86,87	28
10	MES	B	503	12/12	-	-	42,43,45,45	12
10	MES	B	504	12/12	-	-	57,62,63,64	12
11	ACP	F	401	31/31	-	-	99,107,130,130	45

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.

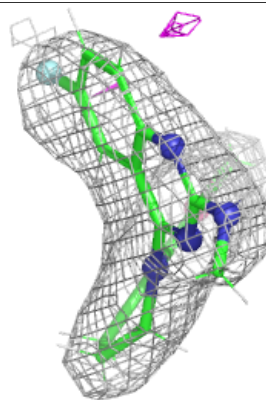
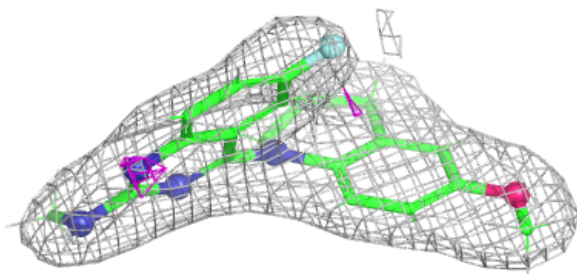
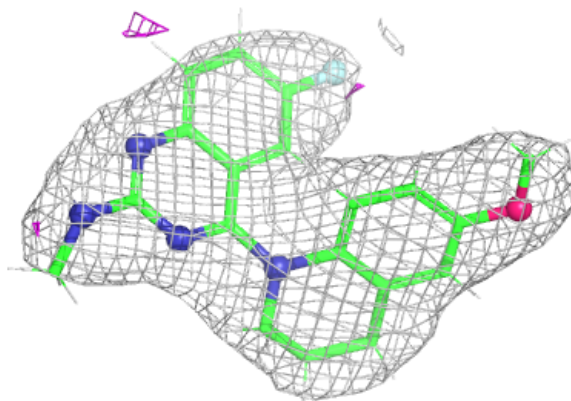


Electron density around GTP C 501:

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

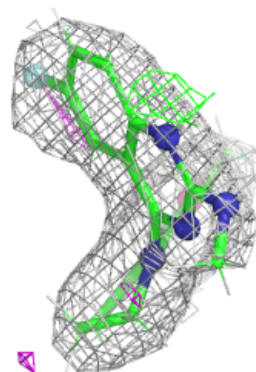
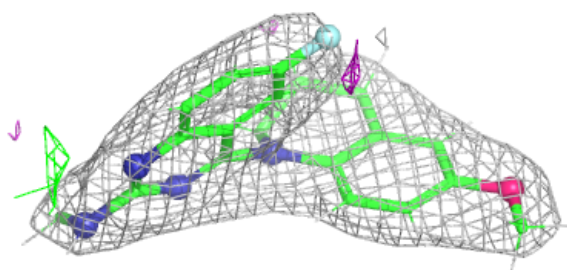
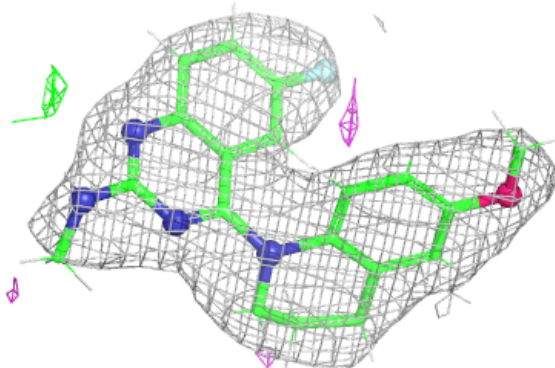
**Electron density around A1D6E B 501:**

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



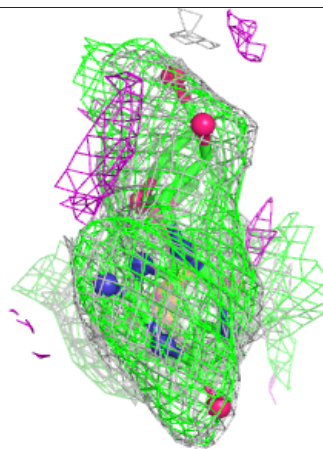
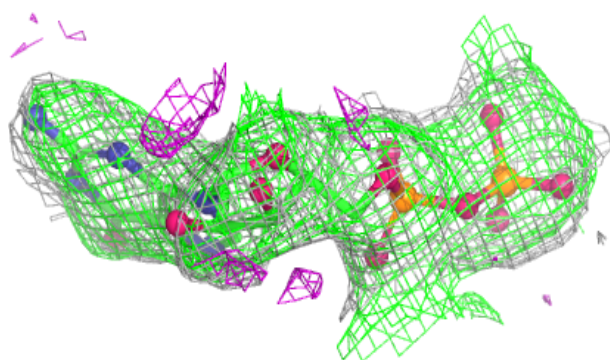
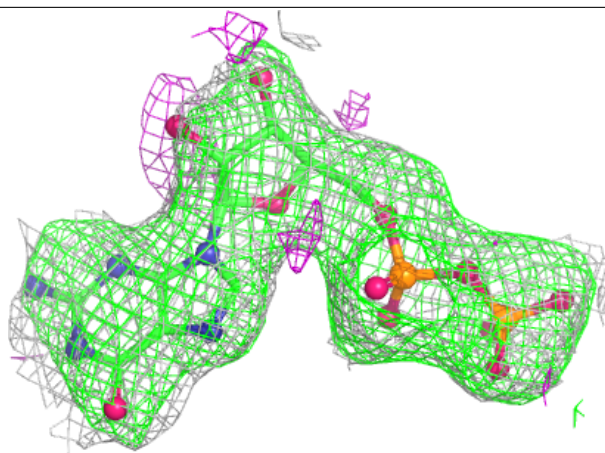
Electron density around A1D6E D 502:

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



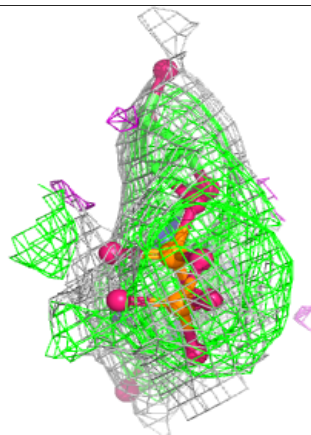
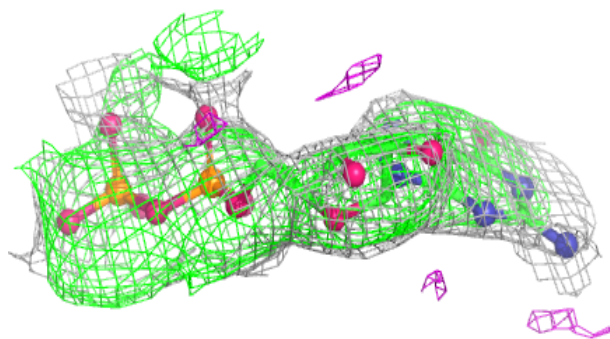
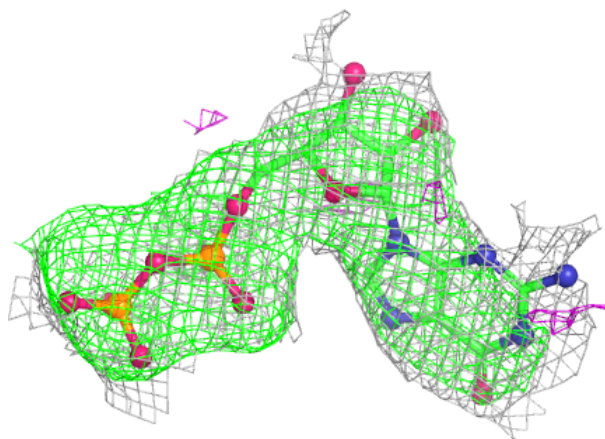
Electron density around GDP B 502:

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

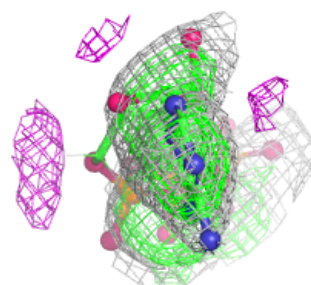
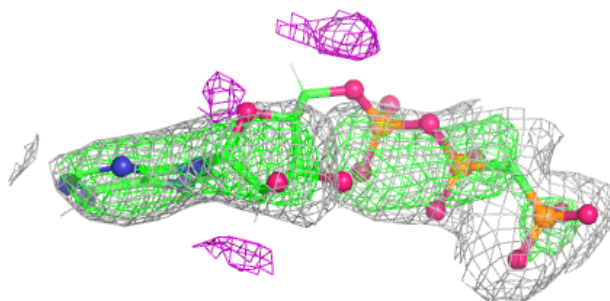
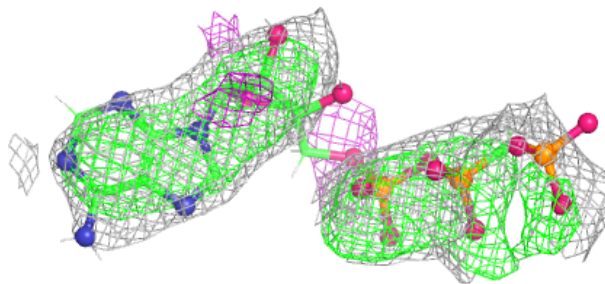


Electron density around GDP D 501:

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

**Electron density around ACP F 401:**

$2mF_o-DF_c$ (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.