



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:19 AM UTC

PDB ID : 5S5D / pdb_00005s5d
Title : Tubulin-Z32400357-complex
Authors : Muehlethaler, T.; Gioia, D.; Protá, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2020-11-08
Resolution : 1.90 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

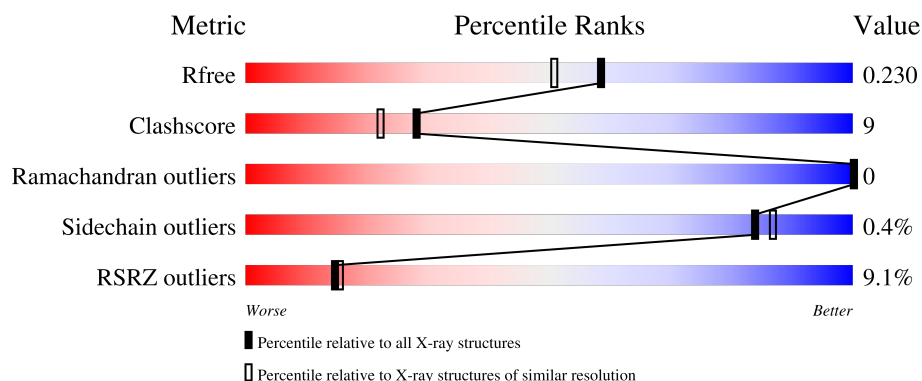
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	451	8% 78% 18% .
1	C	451	7% 83% 14% .
2	B	445	10% 75% 20% 5%
2	D	445	6% 81% 16% .
3	E	143	12% 72% 13% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18605 atoms, of which 36 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	1	1	0
			3349	2103	575	644	27			
2	D	431	Total	C	N	O	S	5	0	0
			3389	2126	580	656	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	122	Total	C	N	O	S	0	0	0
			1008	622	182	199	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	348	Total	C	N	O	S	0	0	0
			2859	1833	491	521	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	1	Total	Ca	0	0
			1	1		
7	C	2	Total	Ca	0	0
			2	2		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



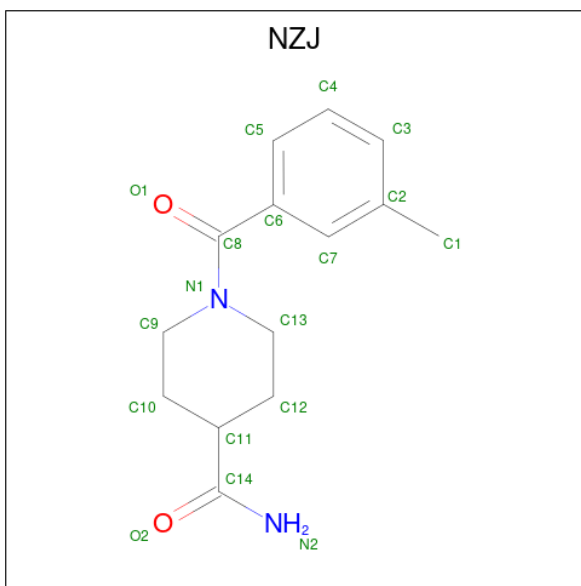
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



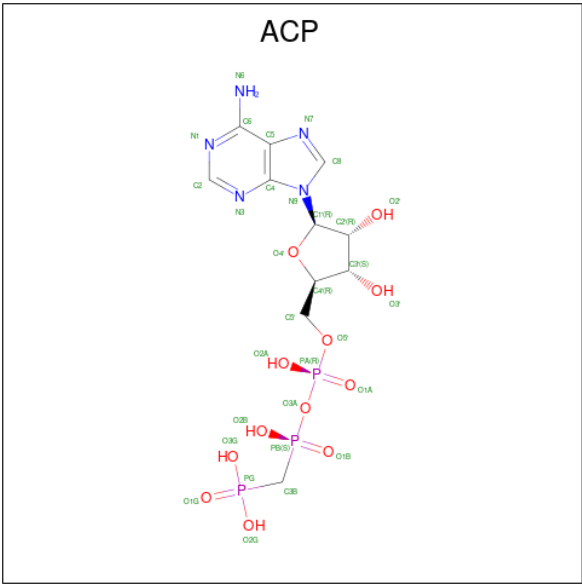
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 1-(3-methylbenzene-1-carbonyl)piperidine-4-carboxamide (CCD ID: NZJ) (formula: $C_{14}H_{18}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			36	14	18	2	2		
10	C	1	Total	C	H	N	O	0	0
			36	14	18	2	2		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

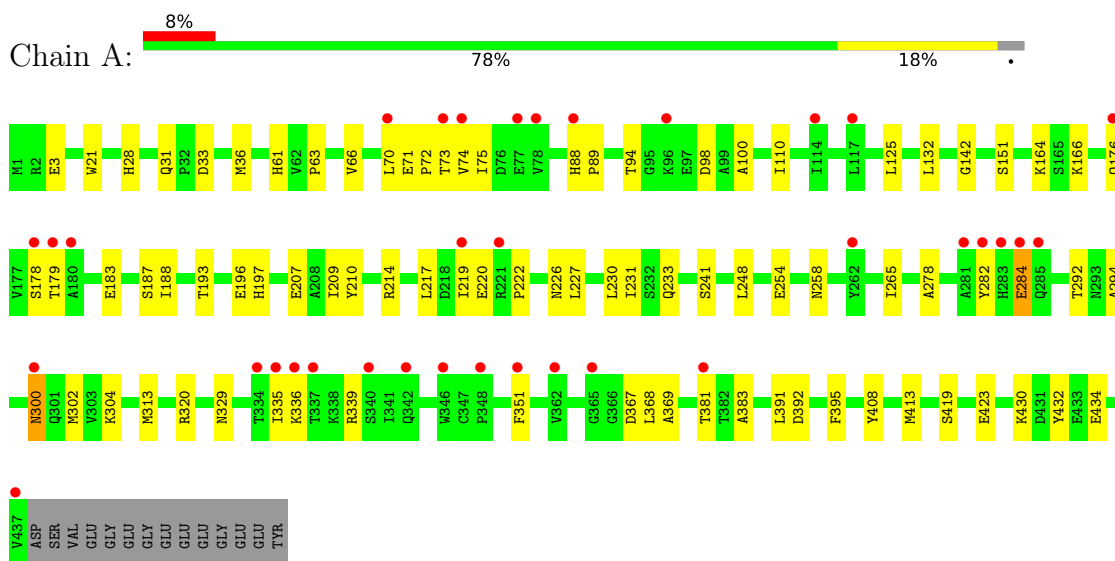
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	175	Total	O	0	0
			175	175		
12	B	165	Total	O	0	0
			165	165		
12	C	316	Total	O	0	0
			316	316		
12	D	128	Total	O	0	0
			128	128		
12	E	51	Total	O	0	0
			51	51		
12	F	61	Total	O	0	0
			61	61		

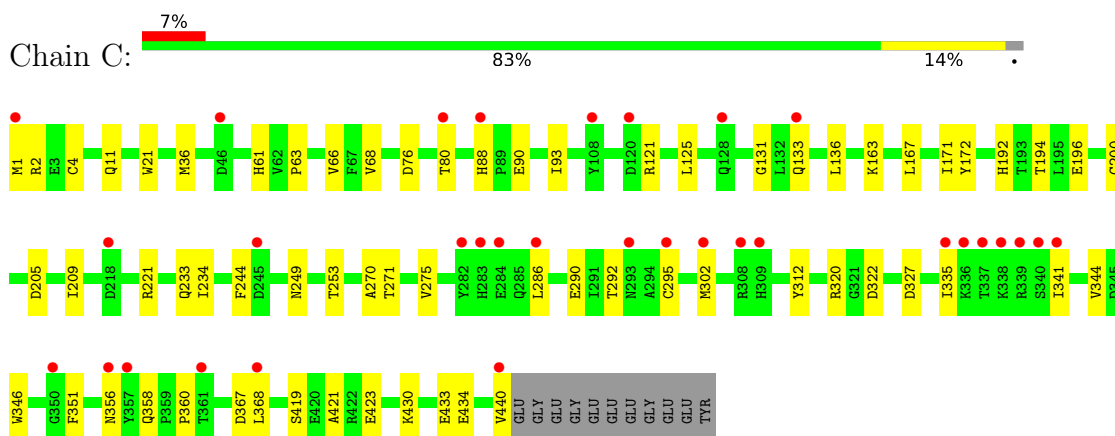
3 Residue-property plots [i](#)

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: Tubulin alpha-1B chain

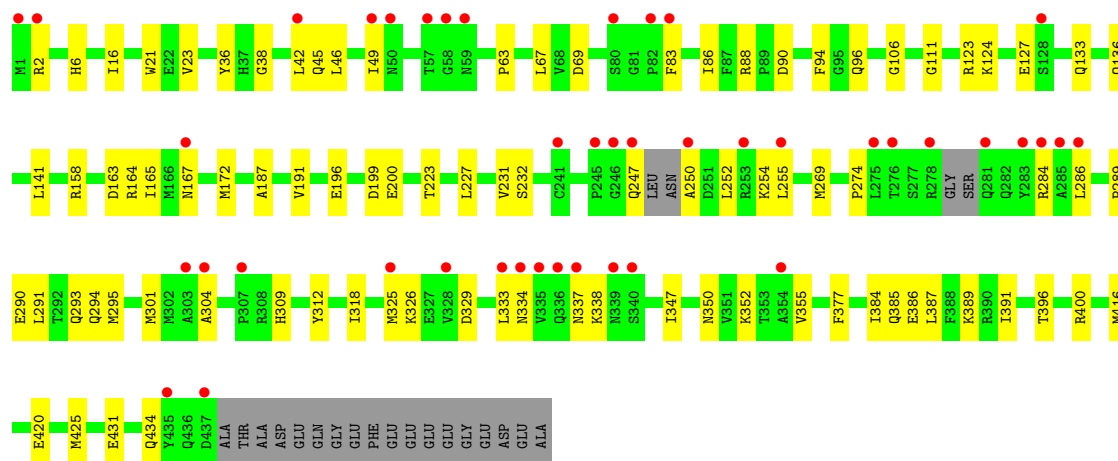


- Molecule 1: Tubulin alpha-1B chain

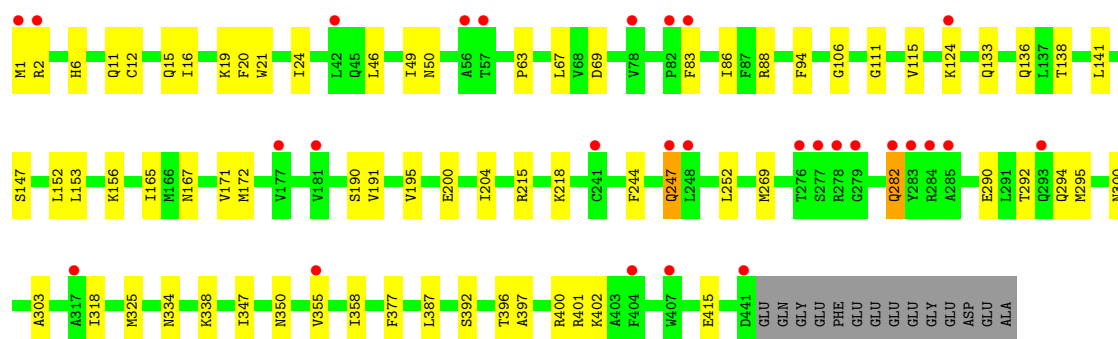
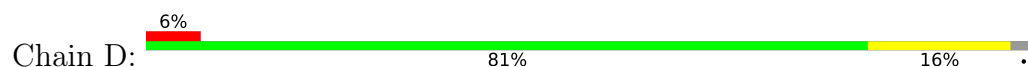


- Molecule 2: Tubulin beta-2B chain

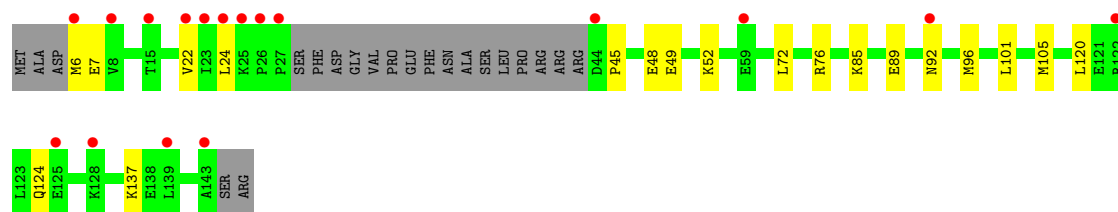




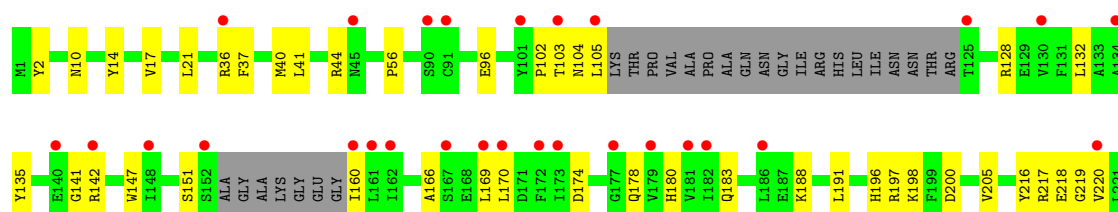
• Molecule 2: Tubulin beta-2B chain

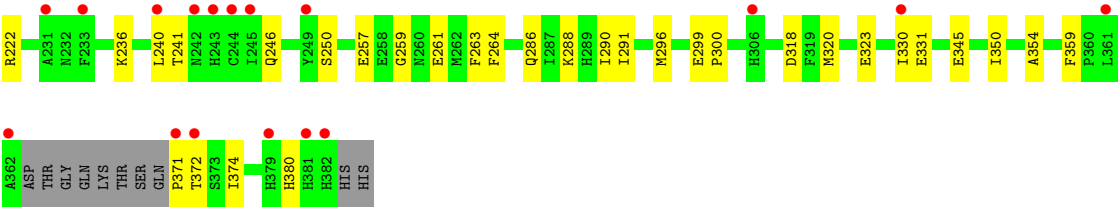


• Molecule 3: Stathmin-4



• 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	105.07Å 159.08Å 179.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.42 – 1.90 63.42 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.42-1.90) 99.9 (63.42-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.200 , 0.227 0.203 , 0.230	Depositor DCC
R_{free} test set	11889 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.7	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	0.96	EDS
Total number of atoms	18605	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: ACP, NZJ, GTP, GDP, CA, MES, 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	0.12	0/3494	0.31	0/4743
1	C	0.14	0/3521	0.36	2/4780 (0.0%)
2	B	0.12	0/3422	0.31	0/4630
2	D	0.10	0/3464	0.28	0/4692
3	E	0.10	0/1016	0.23	0/1348
4	F	0.09	0/2926	0.27	0/3954
All	All	0.12	0/17843	0.31	2/24147 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	ILE	CA-C-N	7.79	135.74	120.94
1	C	171	ILE	C-N-CA	7.79	135.74	120.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3416	0	3330	70	0
1	C	3443	0	3352	58	0
2	B	3349	0	3230	68	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3389	0	3266	57	0
3	E	1008	0	1024	14	0
4	F	2859	0	2823	57	0
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	2	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	1	0
9	B	12	0	12	3	0
10	B	18	18	0	0	0
10	C	18	18	0	0	0
11	F	31	0	14	4	0
12	A	175	0	0	5	0
12	B	165	0	0	3	0
12	C	316	0	0	8	0
12	D	128	0	0	4	0
12	E	51	0	0	1	0
12	F	61	0	0	2	0
All	All	18569	36	17099	308	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 9.

All (308) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:HG22	1:A:383:ALA:H	1.20	1.06
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.47	0.95
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.54	0.89
1:C:270:ALA:O	1:C:302:MET:HG2	1.74	0.87
4:F:241:THR:OG1	11:F:401:ACP:O3'	1.99	0.81
1:C:209:ILE:HD11	1:C:302:MET:CE	2.11	0.80
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.45	0.79
1:A:178:SER:OG	1:A:183:GLU:OE1	2.01	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.64	0.77
1:C:234:ILE:HD13	1:C:302:MET:CE	2.15	0.77
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.67	0.76
1:C:327:ASP:OD2	12:C:601:HOH:O	2.04	0.75
2:B:163:ASP:OD1	12:B:601:HOH:O	2.05	0.74
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.70	0.74
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.71	0.73
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.70	0.73
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.07	0.73
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.71	0.72
2:D:282:GLN:HA	2:D:282:GLN:HE21	1.56	0.71
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.21	0.70
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.10	0.70
2:B:83:PHE:O	2:B:86:ILE:HG22	1.92	0.69
2:B:96:GLN:HB3	1:C:1:MET:HE2	1.74	0.69
1:C:423:GLU:OE1	12:C:603:HOH:O	2.10	0.69
1:C:433:GLU:OE2	12:C:602:HOH:O	2.09	0.68
1:A:294:ALA:O	1:A:300:ASN:ND2	2.27	0.68
1:C:1:MET:O	12:C:604:HOH:O	2.11	0.68
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.27	0.68
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.58	0.67
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.07	0.67
1:C:423:GLU:OE2	12:C:605:HOH:O	2.12	0.67
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.27	0.67
3:E:48:GLU:HG2	3:E:52:LYS:HE3	1.77	0.66
1:C:367:ASP:OD1	12:C:606:HOH:O	2.12	0.66
4:F:371:PRO:HA	4:F:372:THR:O	1.95	0.66
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.77	0.66
4:F:371:PRO:HA	4:F:372:THR:HB	1.77	0.66
2:D:290:GLU:OE2	12:D:601:HOH:O	2.14	0.66
2:D:136:GLN:HA	2:D:167:ASN:O	1.96	0.65
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.31	0.65
1:A:179:THR:HA	2:B:352:LYS:HD2	1.78	0.65
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.79	0.64
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.37	0.64
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.80	0.64
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.28	0.64
2:B:141:LEU:HD12	2:B:172:MET:SD	2.39	0.63
1:C:234:ILE:HD13	1:C:302:MET:HE1	1.80	0.63
2:B:337:ASN:OD1	4:F:36:ARG:HD3	1.98	0.63
2:D:83:PHE:O	2:D:86:ILE:HG22	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.13	0.62
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.15	0.62
1:A:209:ILE:HD11	1:A:302:MET:SD	2.40	0.62
2:B:96:GLN:CB	1:C:1:MET:HE2	2.30	0.62
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.00	0.61
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.36	0.61
1:C:76:ASP:O	1:C:80:THR:HG22	2.01	0.61
4:F:246:GLN:O	4:F:250:SER:HB3	2.01	0.61
2:D:106:GLY:O	2:D:111:GLY:HA3	2.01	0.61
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.36	0.60
2:B:420:GLU:OE1	12:B:602:HOH:O	2.16	0.60
2:D:325:MET:HE2	2:D:355:VAL:HG21	1.82	0.60
1:C:322:ASP:OD1	12:C:607:HOH:O	2.16	0.60
3:E:48:GLU:CG	3:E:52:LYS:HE3	2.32	0.60
1:A:66:VAL:HG23	1:A:125:LEU:HD12	1.84	0.59
2:D:124:LYS:C	2:D:124:LYS:HD3	2.26	0.59
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.82	0.59
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.37	0.59
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.84	0.58
2:B:396:THR:O	2:B:400:ARG:HG3	2.02	0.58
4:F:371:PRO:CA	4:F:372:THR:HB	2.32	0.58
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.19	0.58
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.33	0.58
2:B:123:ARG:O	2:B:127:GLU:HG3	2.05	0.57
4:F:371:PRO:HA	4:F:372:THR:C	2.28	0.57
2:B:295:MET:CG	2:B:377:PHE:HB2	2.34	0.57
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.85	0.57
1:C:419:SER:O	1:C:423:GLU:HG3	2.05	0.57
2:B:69:ASP:O	2:B:94:PHE:HA	2.05	0.57
2:B:124:LYS:HD3	2:B:124:LYS:C	2.30	0.57
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.40	0.57
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.38	0.56
1:A:188:ILE:HD12	1:A:395:PHE:CD2	2.40	0.56
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.34	0.56
2:B:284:ARG:NH2	2:B:290:GLU:OE2	2.37	0.56
3:E:120:LEU:O	3:E:124:GLN:HG3	2.05	0.56
1:A:284:GLU:CD	1:A:284:GLU:H	2.14	0.56
2:B:304:ALA:N	12:B:610:HOH:O	2.39	0.56
2:D:215:ARG:O	2:D:218:LYS:HE3	2.04	0.56
2:B:164:ARG:O	9:B:504:MES:H31	2.06	0.56
2:D:2:ARG:NH1	12:D:604:HOH:O	2.31	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:PHE:HE1	3:E:24:LEU:HD11	1.71	0.56
2:D:152:LEU:O	2:D:156:LYS:HG2	2.05	0.56
3:E:92:ASN:O	3:E:96:MET:HG2	2.06	0.56
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.18	0.56
4:F:17:VAL:O	4:F:21:LEU:HG	2.06	0.56
3:E:85:LYS:O	3:E:89:GLU:HG3	2.06	0.56
2:D:69:ASP:O	2:D:94:PHE:HA	2.05	0.55
1:C:209:ILE:HD11	1:C:302:MET:HE1	1.88	0.55
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.37	0.55
1:A:176:GLN:CG	4:F:56:PRO:HB3	2.37	0.55
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.41	0.55
3:E:101:LEU:O	3:E:105:MET:HG2	2.07	0.55
4:F:151:SER:HB3	4:F:180:HIS:CG	2.42	0.55
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.07	0.55
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.42	0.54
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.06	0.54
2:D:397:ALA:O	2:D:401:ARG:NH1	2.40	0.54
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.43	0.54
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.43	0.54
1:A:430:LYS:O	1:A:434:GLU:HG3	2.07	0.54
2:B:136:GLN:HA	2:B:167:ASN:O	2.08	0.54
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.23	0.53
3:E:72:LEU:O	3:E:76:ARG:HG2	2.07	0.53
1:C:320:ARG:HA	1:C:356:ASN:O	2.08	0.53
1:A:329:ASN:HB3	3:E:6:MET:HE3	1.90	0.53
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.91	0.53
1:C:270:ALA:C	1:C:302:MET:HG2	2.33	0.53
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.90	0.53
1:A:187:SER:CB	1:A:391:LEU:HD21	2.38	0.53
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.45	0.52
2:D:282:GLN:HA	2:D:282:GLN:NE2	2.23	0.52
4:F:198:LYS:HE3	4:F:320:MET:HE1	1.90	0.52
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.89	0.52
2:B:290:GLU:O	2:B:294:GLN:HG3	2.10	0.52
2:D:115:VAL:HG23	2:D:153:LEU:HD23	1.90	0.52
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.45	0.52
1:A:28:HIS:O	1:A:36:MET:HE3	2.09	0.52
1:A:214:ARG:HG2	1:A:219:ILE:O	2.10	0.52
2:D:167:ASN:ND2	12:D:612:HOH:O	2.43	0.52
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.45	0.52
1:C:234:ILE:HD13	1:C:302:MET:HE2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:296:MET:SD	4:F:380:HIS:HB2	2.50	0.51
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.92	0.51
1:A:220:GLU:OE1	2:B:326:LYS:HD2	2.10	0.51
2:D:1:MET:HG3	2:D:50:ASN:CB	2.40	0.51
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.41	0.51
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.41	0.51
2:B:187:ALA:O	2:B:191:VAL:HG23	2.11	0.50
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.75	0.50
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.92	0.50
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.29	0.50
2:B:106:GLY:O	2:B:111:GLY:HA3	2.12	0.50
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.92	0.50
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.12	0.50
2:B:431:GLU:O	2:B:434:GLN:HG2	2.12	0.50
2:D:171:VAL:HA	2:D:204:ILE:O	2.12	0.50
2:B:334:ASN:OD1	2:B:338:LYS:HD3	2.11	0.50
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.92	0.50
2:D:387:LEU:HD23	2:D:387:LEU:C	2.37	0.49
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.48	0.49
2:B:2:ARG:HB2	2:B:133:GLN:NE2	2.27	0.49
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.46	0.49
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.47	0.49
2:B:199:ASP:OD1	9:B:504:MES:H62	2.12	0.49
2:D:141:LEU:HD12	2:D:172:MET:SD	2.52	0.49
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.95	0.49
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.95	0.49
2:B:158:ARG:NH1	2:B:196:GLU:O	2.45	0.49
2:B:42:LEU:H	2:B:42:LEU:HD12	1.78	0.49
2:B:325:MET:HE2	2:B:355:VAL:HG21	1.95	0.49
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.48	0.49
1:A:74:VAL:HB	12:A:610:HOH:O	2.13	0.49
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.95	0.49
1:C:271:THR:HG21	1:C:295:CYS:O	2.12	0.49
1:C:11:GLN:HE22	2:D:247:GLN:NE2	2.11	0.49
4:F:288:LYS:NZ	12:F:503:HOH:O	2.43	0.49
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.95	0.48
2:B:318:ILE:N	2:B:318:ILE:HD12	2.28	0.48
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.94	0.48
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.48	0.48
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.95	0.48
2:B:289:PRO:O	2:B:293:GLN:HG3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.14	0.48
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.95	0.48
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.14	0.48
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.78	0.47
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.96	0.47
2:D:402:LYS:HE2	2:D:415:GLU:OE1	2.14	0.47
3:E:45:PRO:HA	3:E:49:GLU:OE1	2.14	0.47
4:F:103:THR:HG23	4:F:128:ARG:NH2	2.29	0.47
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.49	0.47
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.96	0.47
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.31	0.47
2:D:2:ARG:HB3	2:D:133:GLN:HG2	1.95	0.47
4:F:141:GLY:O	4:F:142:ARG:HB2	2.13	0.47
4:F:102:PRO:HB2	4:F:104:ASN:OD1	2.14	0.47
2:D:396:THR:O	2:D:400:ARG:HG2	2.15	0.47
4:F:188:LYS:HD3	4:F:323:GLU:OE2	2.13	0.47
1:C:1:MET:HE3	1:C:131:GLY:HA3	1.96	0.47
4:F:350:ILE:O	4:F:354:ALA:HB3	2.15	0.47
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.48	0.47
2:D:15:GLN:O	2:D:19:LYS:HG2	2.15	0.47
2:D:318:ILE:N	2:D:318:ILE:HD12	2.30	0.46
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.96	0.46
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.98	0.46
9:B:504:MES:H51	9:B:504:MES:H81	1.55	0.46
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.98	0.46
2:D:67:LEU:N	2:D:67:LEU:HD12	2.30	0.46
4:F:286:GLN:O	4:F:290:ILE:HG13	2.15	0.46
1:A:66:VAL:HG23	1:A:125:LEU:CD1	2.45	0.46
1:C:11:GLN:HE22	2:D:247:GLN:CD	2.24	0.46
1:C:320:ARG:HG3	1:C:360:PRO:HG3	1.98	0.46
2:D:2:ARG:HB2	2:D:133:GLN:HE21	1.80	0.46
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.51	0.46
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.98	0.46
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.34	0.46
4:F:160:ILE:HD12	4:F:160:ILE:N	2.31	0.45
4:F:359:PHE:O	12:F:501:HOH:O	2.21	0.45
2:D:88:ARG:HD2	12:D:711:HOH:O	2.16	0.45
2:B:46:LEU:HA	2:B:49:ILE:HB	1.97	0.45
1:C:270:ALA:HB3	1:C:302:MET:CG	2.46	0.45
1:A:70:LEU:HB2	1:A:98:ASP:HA	1.97	0.45
1:A:176:GLN:HG3	4:F:56:PRO:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.52	0.45
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.47	0.45
2:D:191:VAL:O	2:D:195:VAL:HG23	2.17	0.45
1:A:193:THR:HG23	12:A:653:HOH:O	2.16	0.45
2:B:400:ARG:HH22	1:C:440:VAL:C	2.25	0.45
1:C:341:ILE:HD13	1:C:351:PHE:HZ	1.81	0.45
1:A:207:GLU:OE2	1:A:304:LYS:HD2	2.17	0.44
2:B:269:MET:HG2	2:B:384:ILE:HD13	1.99	0.44
2:B:325:MET:HE2	2:B:355:VAL:CG2	2.47	0.44
2:B:387:LEU:C	2:B:387:LEU:HD23	2.43	0.44
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.98	0.44
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.52	0.44
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.98	0.44
1:A:304:LYS:HB2	12:A:619:HOH:O	2.18	0.44
4:F:320:MET:CG	4:F:330:ILE:HD11	2.47	0.44
1:A:300:ASN:HB3	12:A:601:HOH:O	2.17	0.44
2:B:223:THR:O	2:B:227:LEU:HD13	2.18	0.44
1:A:151:SER:HB2	1:A:193:THR:OG1	2.18	0.43
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.53	0.43
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.99	0.43
1:C:430:LYS:HE2	1:C:434:GLU:OE2	2.18	0.43
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.18	0.43
2:B:42:LEU:HD12	2:B:42:LEU:N	2.33	0.43
2:B:200:GLU:OE2	2:B:255:LEU:HG	2.19	0.43
1:A:188:ILE:HD11	1:A:392:ASP:HA	1.99	0.43
2:B:23:VAL:HG21	2:B:232:SER:HB3	2.00	0.43
1:A:176:GLN:HG3	4:F:56:PRO:HG3	2.00	0.43
1:A:292:THR:HG22	1:A:335:ILE:HD12	2.01	0.43
3:E:7:GLU:O	3:E:22:VAL:HA	2.18	0.43
1:A:100:ALA:HA	2:B:254:LYS:CG	2.49	0.43
2:B:301:MET:HE1	2:B:312:TYR:OH	2.18	0.43
1:C:192:HIS:CG	1:C:421:ALA:HA	2.54	0.43
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.53	0.43
2:D:147:SER:HB2	2:D:190:SER:OG	2.19	0.43
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.19	0.43
4:F:135:TYR:CZ	4:F:166:ALA:HB2	2.54	0.43
1:A:188:ILE:HD12	1:A:395:PHE:CB	2.49	0.42
1:A:351:PHE:HE1	3:E:24:LEU:CD1	2.32	0.42
2:B:416:MET:O	2:B:420:GLU:HG3	2.18	0.42
1:C:194:THR:O	1:C:194:THR:HG22	2.18	0.42
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:GLN:O	2:D:15:GLN:HG2	2.19	0.42
4:F:216:TYR:OH	4:F:345:GLU:OE1	2.30	0.42
2:B:391:ILE:HG22	2:B:425:MET:HE1	2.00	0.42
4:F:96:GLU:O	4:F:183:GLN:HA	2.19	0.42
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.00	0.42
1:A:132:LEU:O	1:A:164:LYS:NZ	2.53	0.42
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.50	0.42
4:F:259:GLY:O	4:F:261:GLU:HG3	2.20	0.42
1:A:3:GLU:OE1	1:A:3:GLU:N	2.51	0.42
2:D:115:VAL:HG23	2:D:153:LEU:CD2	2.50	0.42
2:D:392:SER:O	2:D:396:THR:HG22	2.20	0.42
4:F:299:GLU:HB3	4:F:300:PRO:HD3	2.02	0.42
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.49	0.42
2:B:67:LEU:HD12	2:B:67:LEU:N	2.35	0.42
1:C:66:VAL:HG12	1:C:68:VAL:HG23	2.01	0.42
2:D:16:ILE:HD11	2:D:138:THR:HB	2.02	0.42
1:A:241:SER:HB2	1:A:248:LEU:O	2.20	0.41
1:A:408:TYR:HB3	1:A:413:MET:HE2	2.01	0.41
1:C:66:VAL:HG23	1:C:125:LEU:HD11	2.02	0.41
3:E:137:LYS:NZ	12:E:207:HOH:O	2.48	0.41
1:C:2:ARG:HD3	1:C:2:ARG:HA	1.73	0.41
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.49	0.41
2:D:294:GLN:HG2	2:D:300:ASN:ND2	2.34	0.41
4:F:178:GLN:N	4:F:178:GLN:OE1	2.52	0.41
2:B:333:LEU:O	2:B:337:ASN:ND2	2.53	0.41
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.55	0.41
1:A:166:LYS:HE2	1:A:197:HIS:O	2.20	0.41
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.50	0.41
4:F:217:ARG:NH2	4:F:374:ILE:HA	2.35	0.41
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.01	0.41
1:C:234:ILE:CD1	1:C:302:MET:HE1	2.50	0.41
2:B:247:GLN:O	2:B:250:ALA:HB2	2.21	0.41
1:A:320:ARG:HG3	12:A:681:HOH:O	2.20	0.41
1:C:133:GLN:NE2	1:C:253:THR:HG21	2.35	0.41
2:B:291:LEU:HD23	2:B:291:LEU:HA	1.92	0.41
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.51	0.41
1:A:75:ILE:HB	1:A:94:THR:CG2	2.51	0.41
2:B:309:HIS:ND1	2:B:386:GLU:OE2	2.37	0.41
2:D:1:MET:CE	2:D:50:ASN:HB2	2.47	0.41
4:F:151:SER:HB3	4:F:180:HIS:CE1	2.56	0.41
1:C:196:GLU:HG2	12:C:702:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:VAL:HG23	1:C:125:LEU:HD12	2.03	0.40
2:D:46:LEU:HA	2:D:49:ILE:HB	2.03	0.40
2:B:329:ASP:O	2:B:333:LEU:HG	2.20	0.40
1:A:31:GLN:HB2	1:A:33:ASP:OD1	2.22	0.40
1:A:187:SER:HB2	1:A:391:LEU:HD21	2.03	0.40
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.02	0.40
1:C:275:VAL:HG13	1:C:368:LEU:HD21	2.04	0.40
2:D:292:THR:O	2:D:295:MET:HG2	2.21	0.40
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.56	0.40
1:A:188:ILE:HD12	1:A:395:PHE:CG	2.57	0.40
1:A:227:LEU:O	1:A:231:ILE:HG13	2.21	0.40
1:A:419:SER:O	1:A:423:GLU:HG3	2.21	0.40
4:F:320:MET:HG2	4:F:330:ILE:HG13	2.02	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	435/451 (96%)	427 (98%)	8 (2%)	0	100	100
1	C	439/451 (97%)	430 (98%)	9 (2%)	0	100	100
2	B	418/445 (94%)	410 (98%)	8 (2%)	0	100	100
2	D	429/445 (96%)	421 (98%)	8 (2%)	0	100	100
3	E	118/143 (82%)	118 (100%)	0	0	100	100
4	F	340/384 (88%)	331 (97%)	9 (3%)	0	100	100
All	All	2179/2319 (94%)	2137 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	368/379 (97%)	365 (99%)	3 (1%)	73	75
1	C	372/379 (98%)	371 (100%)	1 (0%)	86	88
2	B	368/383 (96%)	368 (100%)	0	100	100
2	D	372/383 (97%)	369 (99%)	3 (1%)	73	75
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	315/342 (92%)	315 (100%)	0	100	100
All	All	1904/1993 (96%)	1897 (100%)	7 (0%)	84	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	TYR
1	A	284	GLU
1	A	300	ASN
1	C	163	LYS
2	D	200	GLU
2	D	247	GLN
2	D	282	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	300	ASN
1	A	301	GLN
1	A	393	HIS
2	B	15	GLN
2	B	192	HIS
2	B	282	GLN
2	B	294	GLN
1	C	11	GLN
1	C	85	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	133	GLN
1	C	393	HIS
2	D	133	GLN
2	D	167	ASN
2	D	281	GLN
2	D	282	GLN
2	D	294	GLN
2	D	300	ASN
2	D	349	ASN
3	E	92	ASN
3	E	103	GLN
3	E	115	HIS
3	E	136	ASN
4	F	269	GLN
4	F	306	HIS
4	F	348	GLN
4	F	380	HIS

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 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	A	501	6	33,34,34	0.85	1 (3%)	50,54,54	1.53	8 (16%)
8	GDP	B	501	6	29,30,30	1.12	2 (6%)	45,47,47	1.67	7 (15%)
10	NZJ	C	505	-	19,19,19	1.03	2 (10%)	26,26,26	1.24	4 (15%)
10	NZJ	B	505	-	19,19,19	1.04	2 (10%)	26,26,26	0.99	3 (11%)
11	ACP	F	401	6	31,33,33	1.68	8 (25%)	47,52,52	1.87	10 (21%)
9	MES	B	504	-	12,12,12	2.28	1 (8%)	15,16,16	1.88	5 (33%)
8	GDP	D	501	6	29,30,30	1.16	2 (6%)	45,47,47	1.69	6 (13%)
5	GTP	C	501	6	33,34,34	1.00	3 (9%)	50,54,54	1.51	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	9/22/38/38	0/3/3/3
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
10	NZJ	C	505	-	-	2/12/22/22	0/2/2/2
10	NZJ	B	505	-	-	2/12/22/22	0/2/2/2
11	ACP	F	401	6	-	9/19/38/38	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
8	GDP	D	501	6	-	3/16/32/32	0/3/3/3
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.62	1.66	1.77
11	F	401	ACP	C5-C4	4.80	1.47	1.39
8	D	501	GDP	C5-C4	3.10	1.47	1.38
8	B	501	GDP	C5-C4	3.00	1.47	1.38
11	F	401	ACP	PG-O2G	2.99	1.61	1.55
11	F	401	ACP	PG-O3G	2.95	1.61	1.55
11	F	401	ACP	C5-C6	2.73	1.48	1.41
11	F	401	ACP	PB-O3A	2.71	1.61	1.58
10	C	505	NZJ	C8-N1	2.56	1.40	1.34
10	B	505	NZJ	C8-N1	2.53	1.40	1.34
5	C	501	GTP	PA-O3A	2.51	1.62	1.59
11	F	401	ACP	C8-N7	2.35	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	501	GDP	C6-N1	-2.33	1.34	1.38
10	B	505	NZJ	C14-N2	2.33	1.38	1.32
10	C	505	NZJ	C14-N2	2.32	1.38	1.32
11	F	401	ACP	C5-N7	-2.27	1.34	1.39
5	C	501	GTP	C2-N3	2.25	1.38	1.33
8	B	501	GDP	C6-N1	-2.24	1.34	1.38
11	F	401	ACP	PB-O2B	2.15	1.61	1.56
5	A	501	GTP	C2-N3	2.09	1.38	1.33
5	C	501	GTP	PB-O3B	2.07	1.61	1.59

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	C5-C4-N3	-5.83	118.69	126.72
8	D	501	GDP	C5-C4-N3	-5.80	119.15	128.39
8	B	501	GDP	C5-C4-N3	-5.51	119.62	128.39
8	D	501	GDP	C2-N3-C4	4.98	120.87	112.30
8	B	501	GDP	C2-N3-C4	4.77	120.51	112.30
5	C	501	GTP	C5-C4-N3	-4.76	120.82	128.39
11	F	401	ACP	N3-C4-N9	4.68	135.12	127.17
5	A	501	GTP	C2-N3-C4	4.64	120.30	112.30
5	A	501	GTP	C5-C4-N3	-4.59	121.08	128.39
5	C	501	GTP	C2-N3-C4	4.37	119.83	112.30
8	B	501	GDP	N9-C4-N3	4.26	134.48	125.95
8	D	501	GDP	N9-C4-N3	4.25	134.45	125.95
11	F	401	ACP	PB-O3A-PA	-3.88	119.70	132.37
9	B	504	MES	C5-N4-C3	3.79	117.00	108.84
11	F	401	ACP	C2-N3-C4	3.65	120.75	111.83
8	D	501	GDP	C6-C5-N7	3.46	136.58	130.29
11	F	401	ACP	C4-C5-N7	-3.44	106.64	110.58
8	B	501	GDP	C6-C5-N7	3.22	136.15	130.29
11	F	401	ACP	N3-C2-N1	-3.16	123.80	128.58
5	C	501	GTP	N9-C4-N3	3.08	132.12	125.95
10	B	505	NZJ	O2-C14-N2	-2.94	117.85	123.04
10	C	505	NZJ	O2-C14-N2	-2.87	117.97	123.04
5	A	501	GTP	N9-C8-N7	-2.78	108.25	113.40
5	C	501	GTP	N9-C8-N7	-2.75	108.30	113.40
5	A	501	GTP	C2-N1-C6	-2.75	120.13	125.11
5	A	501	GTP	N9-C4-N3	2.75	131.45	125.95
9	B	504	MES	C6-C5-N4	-2.73	105.97	110.12
5	C	501	GTP	C2-N1-C6	-2.71	120.20	125.11
11	F	401	ACP	C4-N9-C8	2.70	108.57	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	C5-N7-C8	2.55	107.46	103.45
8	D	501	GDP	C4-C5-N7	-2.55	106.63	110.67
5	A	501	GTP	C8-N7-C5	2.53	108.76	104.26
9	B	504	MES	O1S-S-C8	2.51	110.52	106.73
8	B	501	GDP	O6-C6-C5	-2.51	119.92	126.53
5	C	501	GTP	O2A-PA-O3A	2.50	114.04	107.27
11	F	401	ACP	C3'-C2'-C1'	2.50	106.19	101.46
5	C	501	GTP	C8-N7-C5	2.50	108.71	104.26
5	A	501	GTP	C5-C6-N1	2.50	119.61	113.25
10	B	505	NZJ	O1-C8-N1	-2.45	118.49	122.35
9	B	504	MES	O2S-S-C8	2.39	110.34	106.73
5	C	501	GTP	C5-C6-N1	2.38	119.30	113.25
5	C	501	GTP	O6-C6-C5	-2.32	120.40	126.53
10	C	505	NZJ	O1-C8-N1	-2.28	118.76	122.35
5	A	501	GTP	O6-C6-C5	-2.25	120.58	126.53
8	B	501	GDP	C4-C5-N7	-2.22	107.15	110.67
9	B	504	MES	C7-N4-C5	2.17	117.01	111.24
10	B	505	NZJ	C11-C14-N2	2.13	119.98	116.45
8	B	501	GDP	O2A-PA-O3A	2.11	112.98	107.27
10	C	505	NZJ	C6-C8-N1	2.10	121.28	118.66
8	D	501	GDP	O6-C6-C5	-2.05	121.13	126.53
10	C	505	NZJ	C9-C10-C11	2.04	113.77	110.54
11	F	401	ACP	C6-C5-N7	2.03	136.00	132.09

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
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	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O2S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B	504	MES	C7-C8-S-O3S
10	B	505	NZJ	C10-C11-C14-N2
10	B	505	NZJ	C10-C11-C14-O2
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	O4'-C4'-C5'-O5'
11	F	401	ACP	C3'-C4'-C5'-O5'
9	B	504	MES	C7-C8-S-O1S
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
10	C	505	NZJ	C10-C11-C14-N2
10	C	505	NZJ	C10-C11-C14-O2
5	A	501	GTP	C4'-C5'-O5'-PA
11	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A

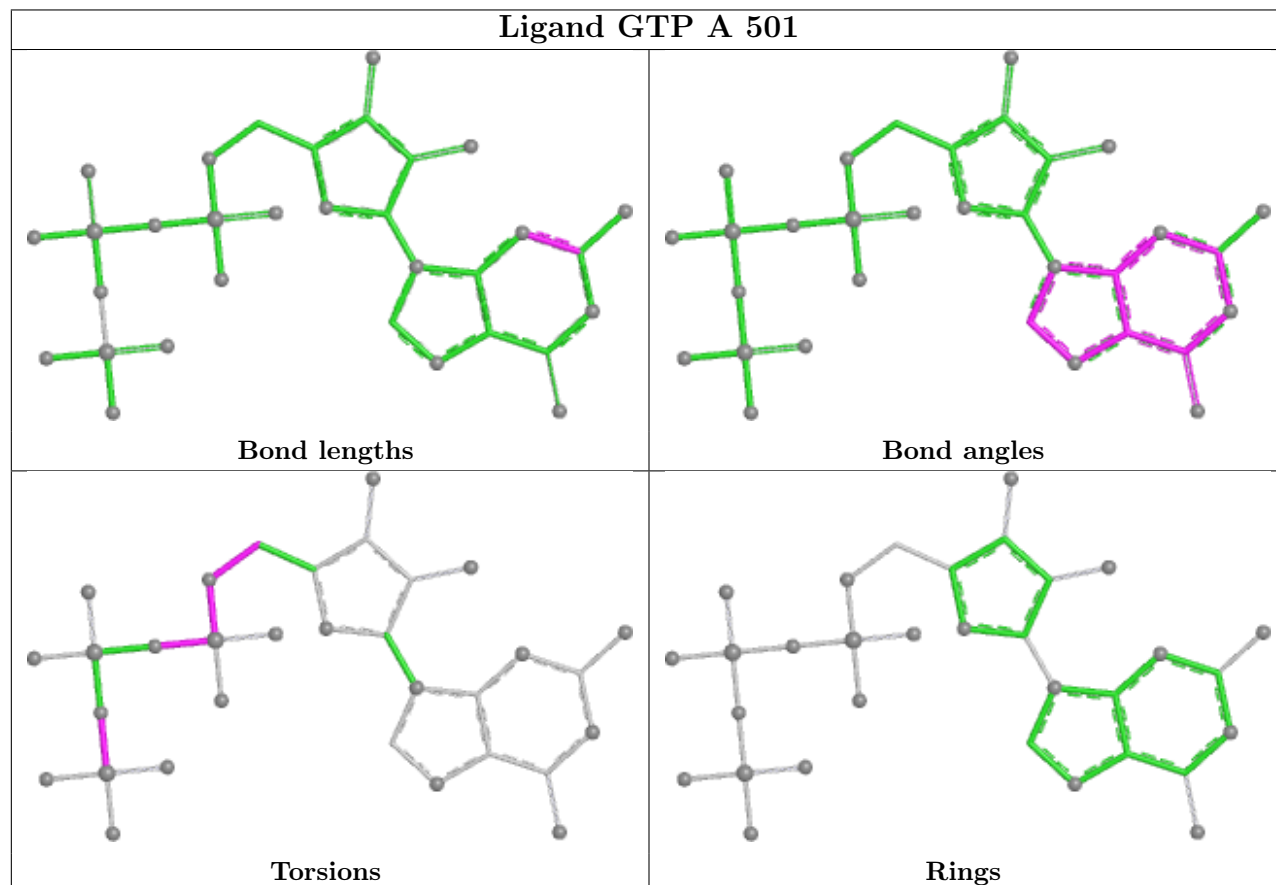
There are no ring outliers.

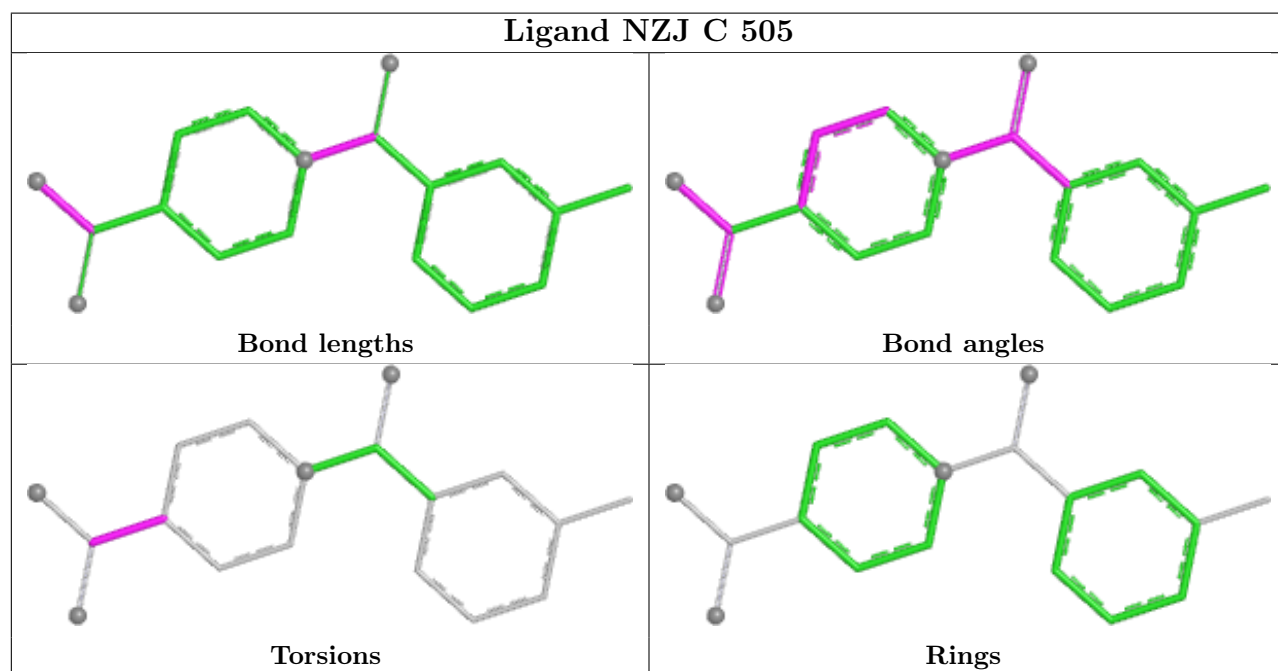
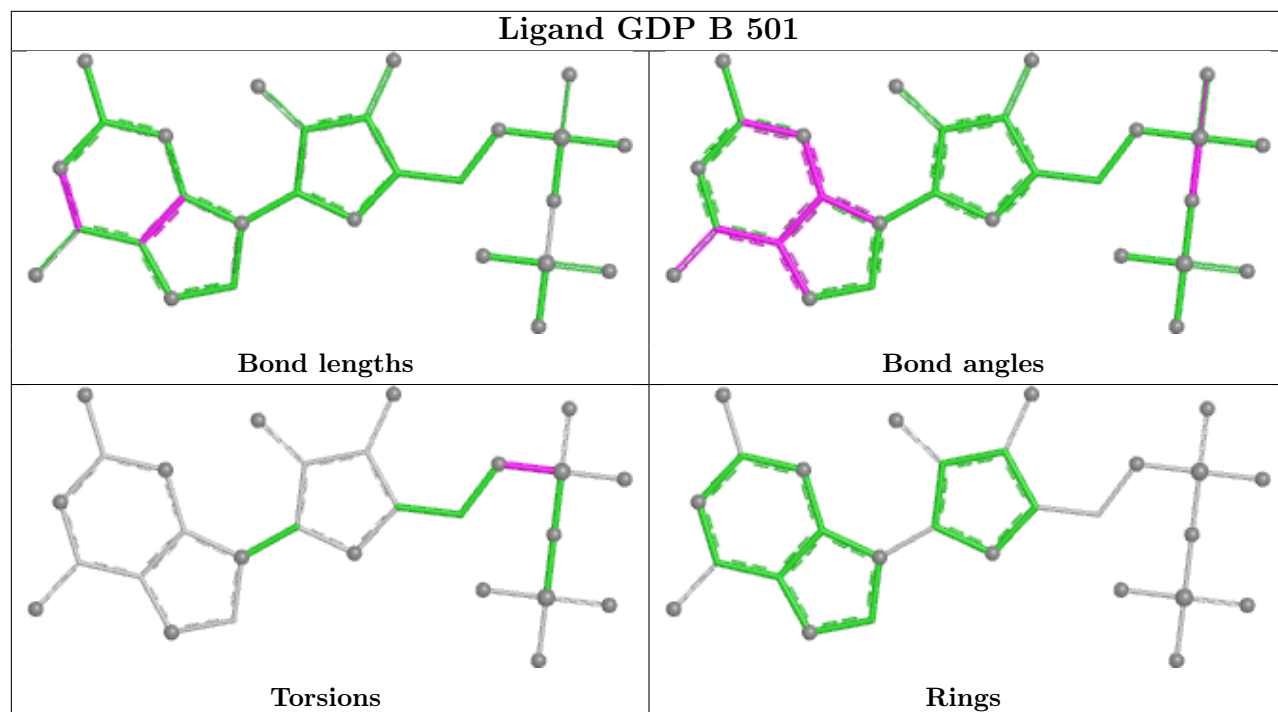
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
11	F	401	ACP	4	0
9	B	504	MES	3	0
8	D	501	GDP	1	0

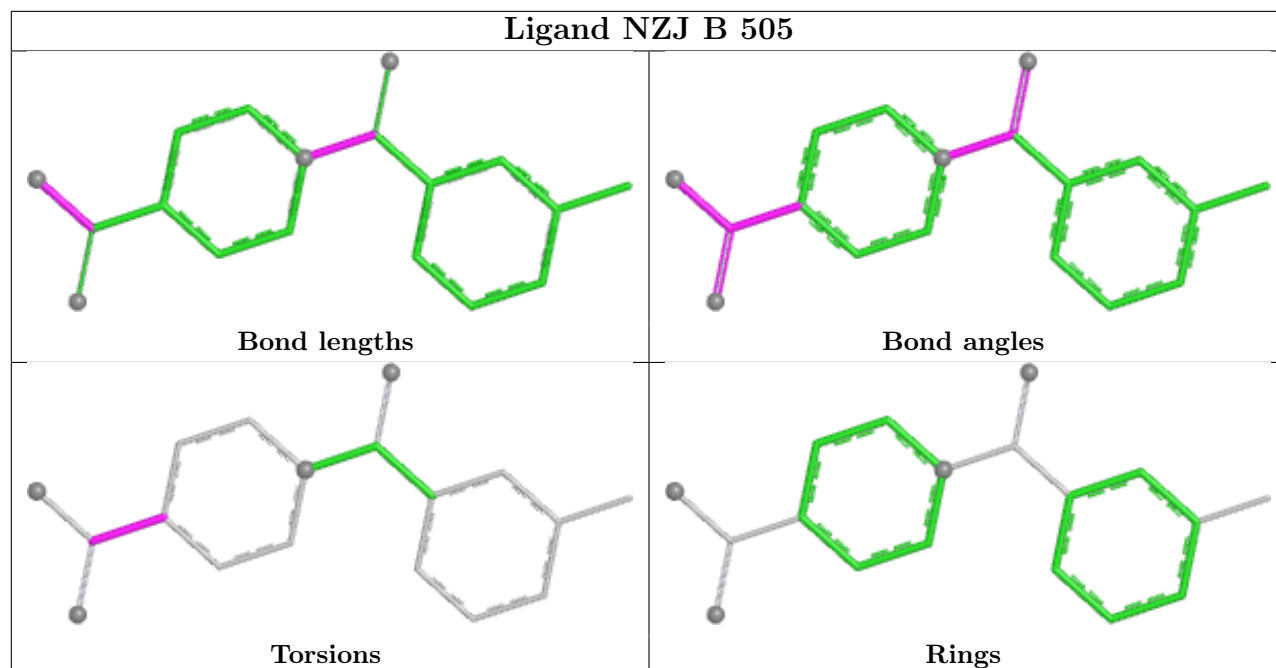
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

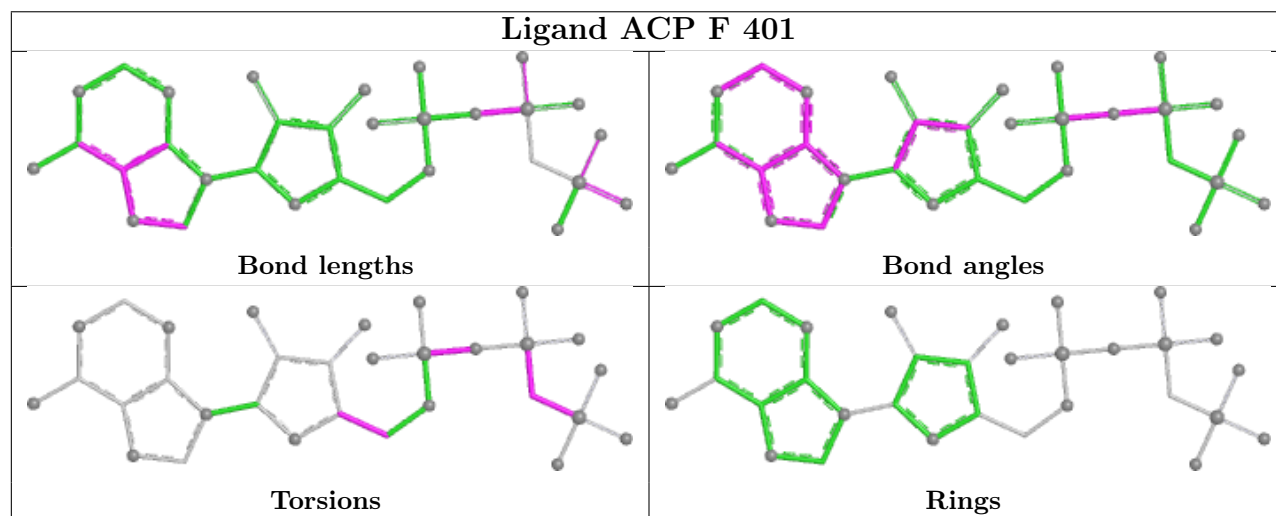


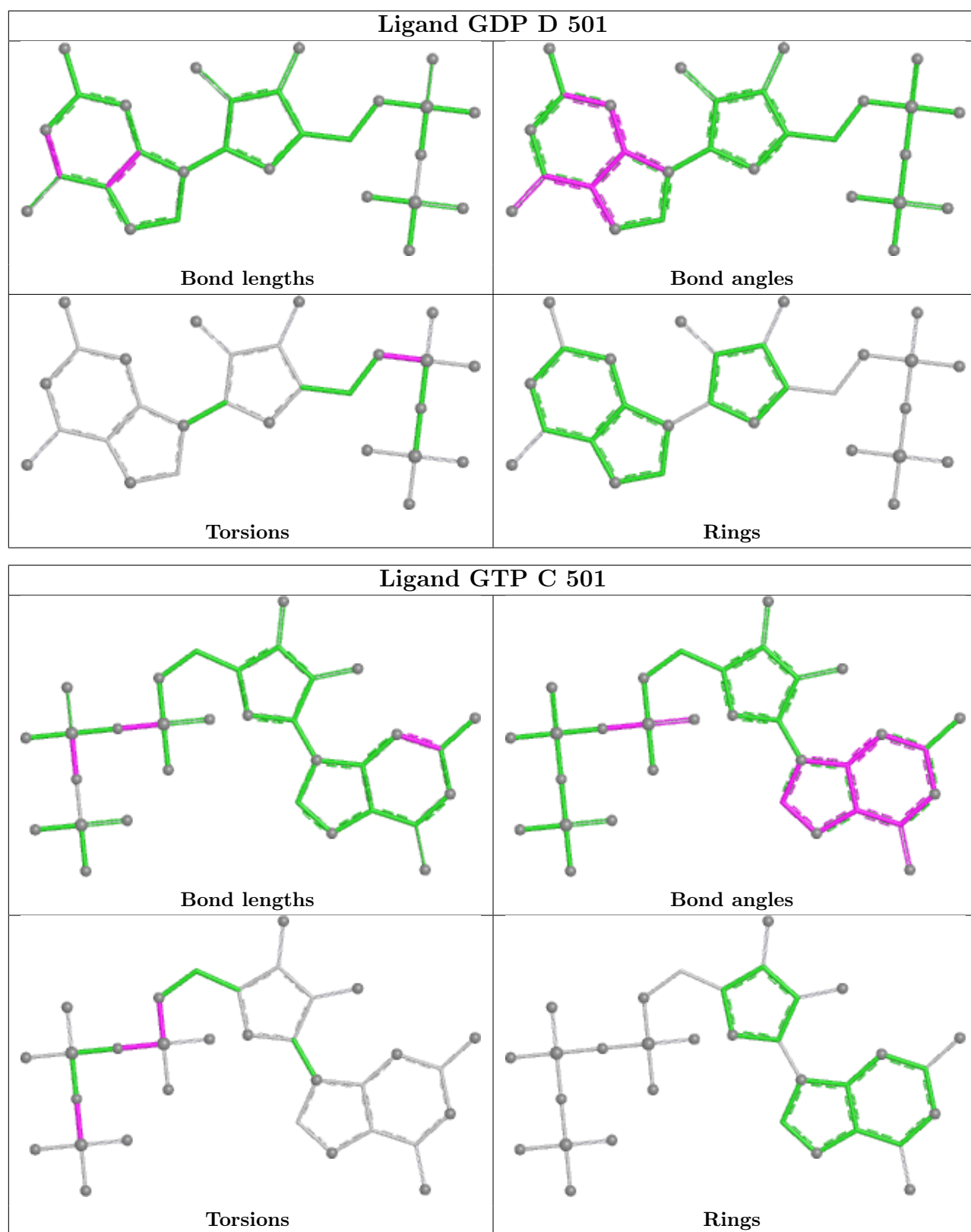


Ligand NZJ B 505



Ligand ACP F 401





5.7 Other polymers [i](#)

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	437/451 (96%)	0.58	35 (8%) 18 19	34, 50, 83, 140	0
1	C	440/451 (97%)	0.27	32 (7%) 21 22	17, 40, 59, 103	1 (0%)
2	B	423/445 (95%)	0.74	43 (10%) 12 12	24, 50, 90, 130	3 (0%)
2	D	431/445 (96%)	0.63	28 (6%) 25 26	34, 54, 83, 113	4 (0%)
3	E	122/143 (85%)	1.02	17 (13%) 6 6	38, 57, 102, 135	0
4	F	348/384 (90%)	1.08	45 (12%) 7 7	45, 76, 136, 166	0
All	All	2201/2319 (94%)	0.66	200 (9%) 15 15	17, 51, 102, 166	8 (0%)

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	253[A]	ARG	10.0
2	B	333	LEU	7.3
2	B	1	MET	5.7
3	E	143	ALA	5.6
1	A	179	THR	5.5
1	C	340	SER	5.1
2	B	250	ALA	4.9
4	F	240	LEU	4.9
2	D	407	TRP	4.9
1	A	437	VAL	4.8
2	B	276	THR	4.7
1	C	440	VAL	4.7
4	F	160	ILE	4.6
2	D	1	MET	4.4
3	E	26	PRO	4.4
4	F	152	SER	4.4
2	B	340	SER	4.4
1	A	282	TYR	4.2
2	B	57	THR	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	339	ASN	4.0
1	A	346	TRP	3.9
2	B	335	VAL	3.9
1	A	365	GLY	3.9
1	C	350	GLY	3.8
1	A	114	ILE	3.8
2	B	247	GLN	3.8
4	F	371	PRO	3.7
4	F	125	THR	3.7
4	F	105	LEU	3.7
1	C	357	TYR	3.7
2	B	325	MET	3.7
2	D	276	THR	3.7
1	C	286	LEU	3.6
2	B	255	LEU	3.6
4	F	330	ILE	3.6
2	D	285	ALA	3.6
4	F	179	VAL	3.6
1	A	281	ALA	3.5
2	B	285	ALA	3.5
1	A	262	TYR	3.5
4	F	130	VAL	3.5
4	F	362	ALA	3.5
2	D	277	SER	3.4
1	A	381	THR	3.4
1	A	180	ALA	3.4
3	E	24	LEU	3.4
2	B	275	LEU	3.4
2	D	82	PRO	3.4
2	B	246	GLY	3.4
1	A	340	SER	3.3
4	F	186	LEU	3.3
2	B	245	PRO	3.3
1	C	309	HIS	3.3
2	B	286	LEU	3.3
1	C	128	GLN	3.2
1	A	362	VAL	3.2
4	F	161	LEU	3.2
1	C	80	THR	3.2
2	D	247	GLN	3.2
3	E	23	ILE	3.2
2	B	83	PHE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	233	PHE	3.2
2	B	284	ARG	3.1
1	C	1	MET	3.1
1	C	283	HIS	3.1
1	C	308	ARG	3.0
2	B	328	VAL	3.0
2	D	283	TYR	3.0
4	F	90	SER	3.0
4	F	231	ALA	3.0
1	C	284	GLU	3.0
1	A	74	VAL	2.9
2	D	279	GLY	2.9
3	E	25	LYS	2.9
1	C	339	ARG	2.9
3	E	27	PRO	2.9
4	F	382	HIS	2.9
2	D	404	PHE	2.9
1	C	245	ASP	2.9
2	B	128	SER	2.9
4	F	173	ILE	2.9
2	D	83	PHE	2.8
3	E	6	MET	2.8
1	A	70	LEU	2.8
2	D	241	CYS	2.8
1	C	337	THR	2.8
4	F	181	VAL	2.8
2	D	278	ARG	2.7
4	F	134	ALA	2.7
4	F	361	LEU	2.7
2	B	58	GLY	2.7
4	F	244	CYS	2.7
1	C	120	ASP	2.7
2	B	337	ASN	2.7
2	D	181	VAL	2.7
1	A	337	THR	2.7
1	C	341	ILE	2.7
4	F	381	HIS	2.7
3	E	8	VAL	2.7
1	A	351	PHE	2.6
2	D	57	THR	2.6
2	B	42	LEU	2.6
1	A	283	HIS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	78	VAL	2.6
2	B	303	ALA	2.6
1	A	285	GLN	2.6
2	B	281	GLN	2.6
4	F	172	PHE	2.6
2	D	355	VAL	2.6
2	B	283	TYR	2.6
4	F	243	HIS	2.6
4	F	177	GLY	2.6
1	C	282	TYR	2.5
4	F	170	LEU	2.5
4	F	103	THR	2.5
2	D	282	GLN	2.5
2	B	435	TYR	2.5
4	F	249	TYR	2.5
1	A	335	ILE	2.5
1	A	300	ASN	2.5
4	F	142	ARG	2.5
4	F	140	GLU	2.5
2	B	241	CYS	2.5
1	A	117	LEU	2.5
1	C	88	HIS	2.4
2	D	42	LEU	2.4
2	B	336	GLN	2.4
2	B	304	ALA	2.4
3	E	22	VAL	2.4
3	E	92	ASN	2.4
4	F	91	CYS	2.4
1	C	293	ASN	2.4
1	C	302	MET	2.4
1	A	178	SER	2.4
1	C	295	CYS	2.4
1	A	221	ARG	2.3
4	F	169	LEU	2.3
1	C	361	THR	2.3
1	C	133	GLN	2.3
1	C	335	ILE	2.3
4	F	220	VAL	2.3
1	A	77	GLU	2.3
4	F	306	HIS	2.3
4	F	162	ILE	2.3
4	F	372	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	82	PRO	2.3
2	B	307	PRO	2.3
1	A	219	ILE	2.3
4	F	245	ILE	2.3
1	C	218	ASP	2.3
1	A	88	HIS	2.3
1	A	73	THR	2.3
1	C	368	LEU	2.3
2	D	56	ALA	2.2
4	F	101	TYR	2.2
4	F	167	SER	2.2
2	B	437	ASP	2.2
3	E	44	ASP	2.2
1	A	176	GLN	2.2
2	D	293	GLN	2.2
2	D	78	VAL	2.2
2	B	50	ASN	2.2
4	F	242	ASN	2.2
1	A	336	LYS	2.2
1	C	336	LYS	2.2
1	C	338	LYS	2.2
1	A	284	GLU	2.2
3	E	139	LEU	2.2
1	A	342	GLN	2.2
4	F	148	ILE	2.2
2	B	59	ASN	2.2
2	D	248	LEU	2.2
3	E	128	LYS	2.2
4	F	379	HIS	2.2
2	B	278	ARG	2.2
2	D	317	ALA	2.2
2	D	2	ARG	2.2
2	D	124	LYS	2.2
3	E	122	ARG	2.2
4	F	36	ARG	2.2
2	B	167	ASN	2.1
1	C	108	TYR	2.1
1	C	46	ASP	2.1
2	B	2	ARG	2.1
3	E	125	GLU	2.1
2	B	334	ASN	2.1
4	F	182	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	354	ALA	2.1
2	B	49	ILE	2.1
2	D	284	ARG	2.1
1	A	334	THR	2.1
3	E	59	GLU	2.1
2	B	80	SER	2.0
4	F	45	ASN	2.0
1	A	348	PRO	2.0
2	D	177	VAL	2.0
2	D	441	ASP	2.0
1	A	96	LYS	2.0
3	E	15	THR	2.0
1	C	356	ASN	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
9	MES	B	504	12/12	0.76	0.18	62,69,88,93	0
7	CA	B	503	1/1	0.81	0.12	87,87,87,87	0
11	ACP	F	401	31/31	0.85	0.13	75,87,95,99	0
6	MG	F	402	1/1	0.86	0.14	77,77,77,77	0
7	CA	A	504	1/1	0.87	0.12	98,98,98,98	0
10	NZJ	B	505	18/18	0.92	0.11	39,48,62,62	36
8	GDP	D	501	28/28	0.93	0.10	45,50,58,60	0
6	MG	D	502	1/1	0.93	0.07	51,51,51,51	0
10	NZJ	C	505	18/18	0.95	0.08	32,43,56,56	0
6	MG	C	502	1/1	0.98	0.03	32,32,32,32	0

Continued on next page...

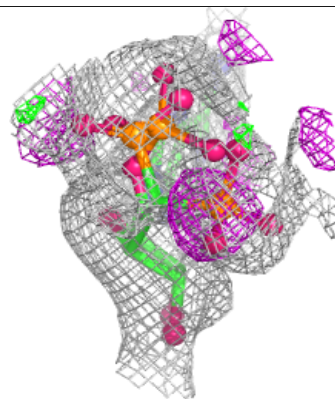
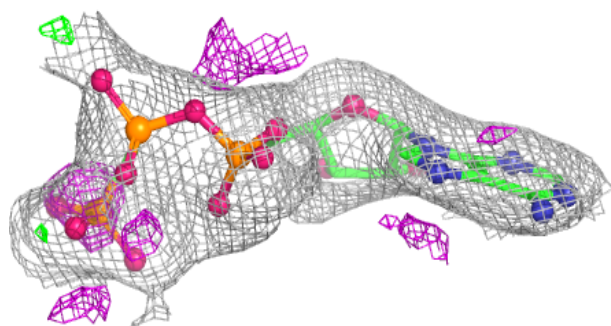
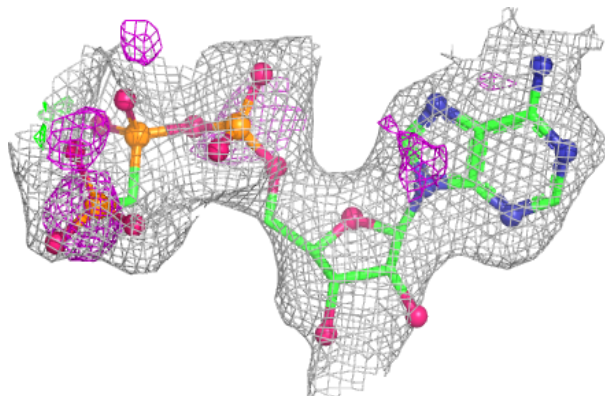
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GTP	A	501	32/32	0.98	0.05	31,35,38,40	0
8	GDP	B	501	28/28	0.98	0.05	30,33,38,41	0
5	GTP	C	501	32/32	0.98	0.05	28,32,34,35	0
6	MG	B	502	1/1	0.99	0.15	28,28,28,28	0
6	MG	A	502	1/1	0.99	0.03	37,37,37,37	0
7	CA	C	503	1/1	0.99	0.05	46,46,46,46	0
7	CA	C	504	1/1	0.99	0.05	45,45,45,45	0
7	CA	A	503	1/1	0.99	0.03	70,70,70,70	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.

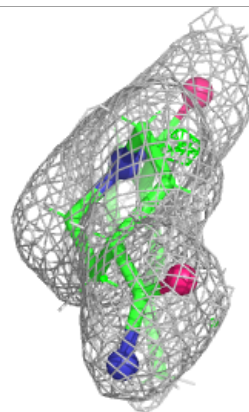
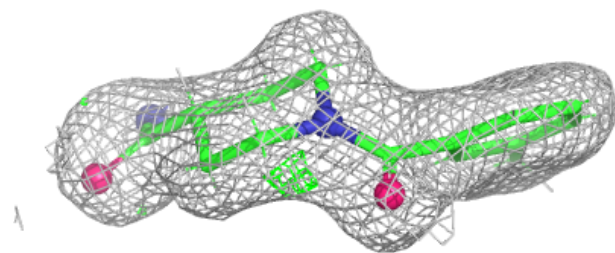
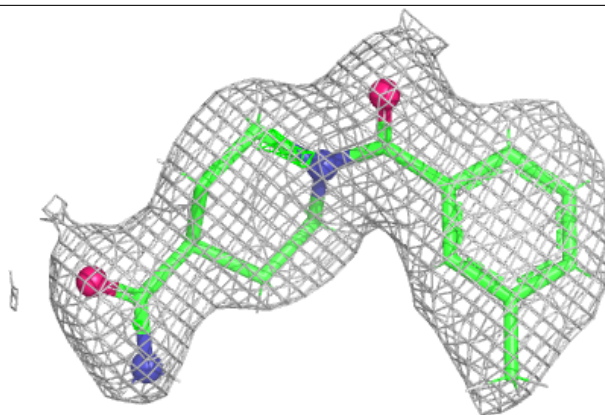
Electron density around ACP F 401:

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



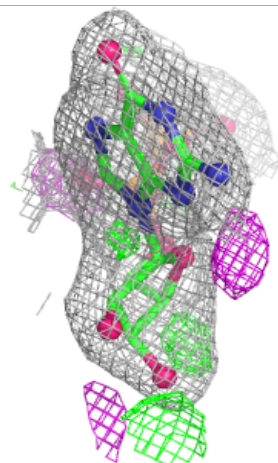
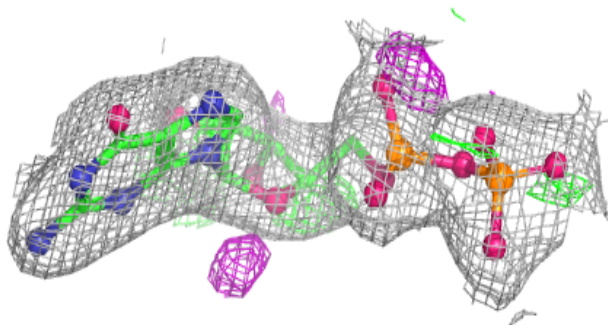
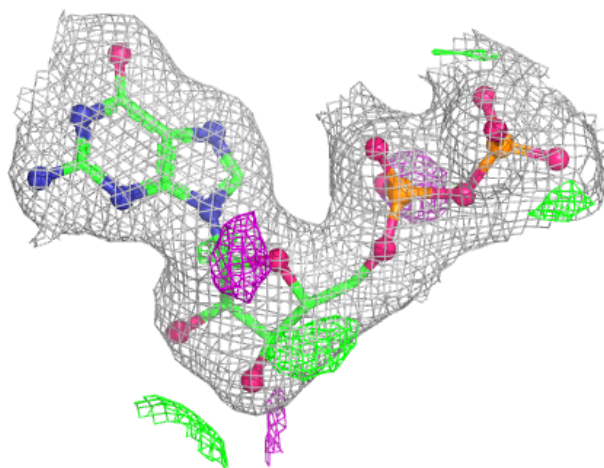
Electron density around NZJ B 505:

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



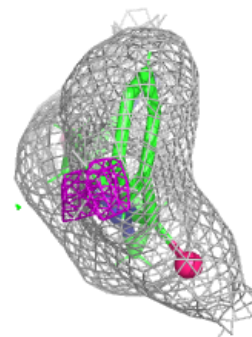
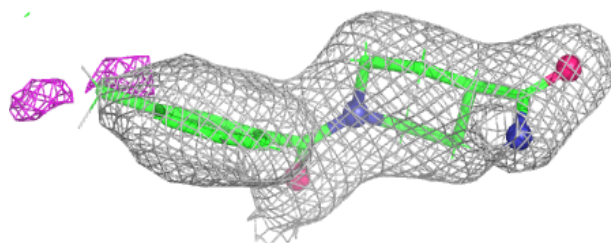
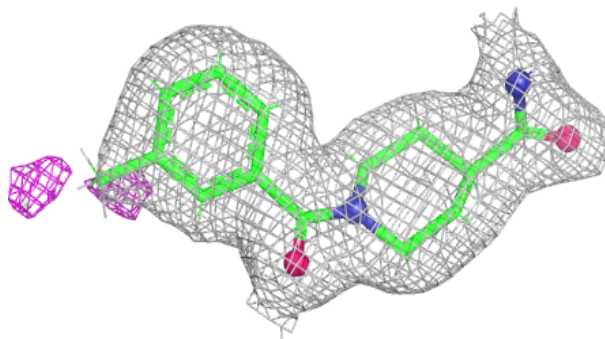
Electron density around GDP D 501:

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

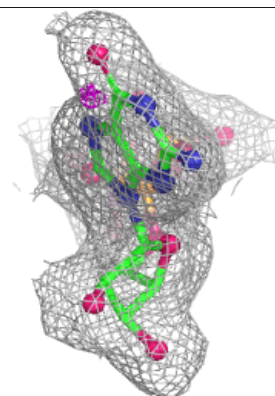
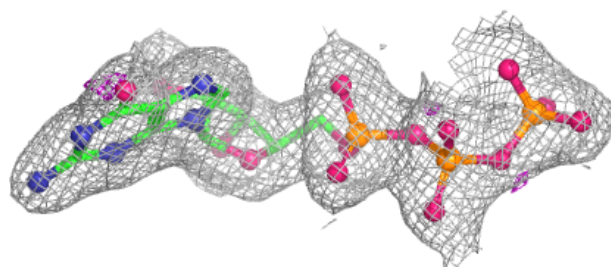
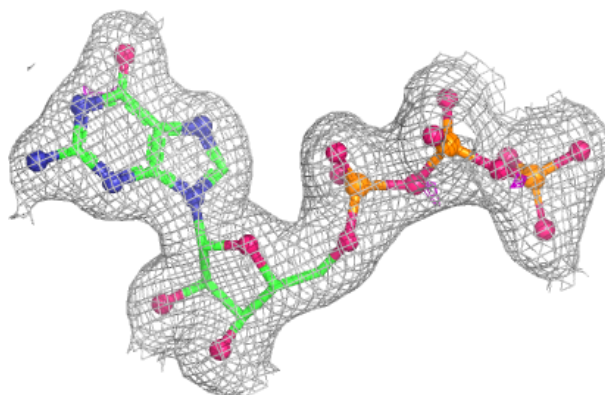


Electron density around NZJ C 505:

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

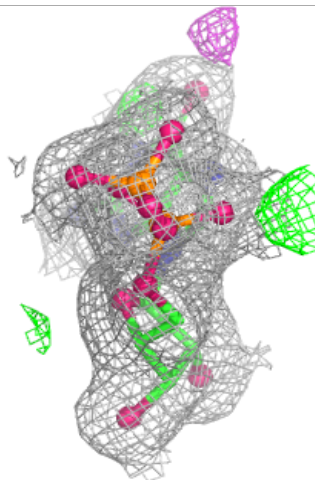
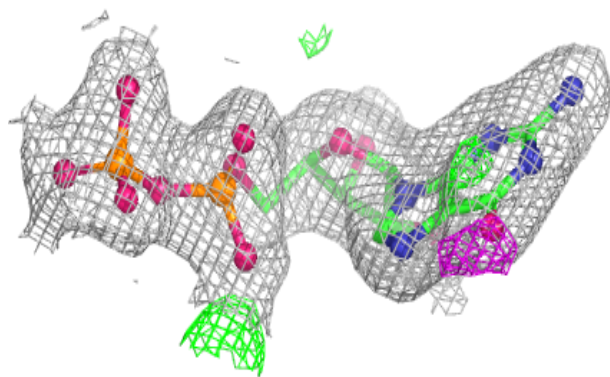
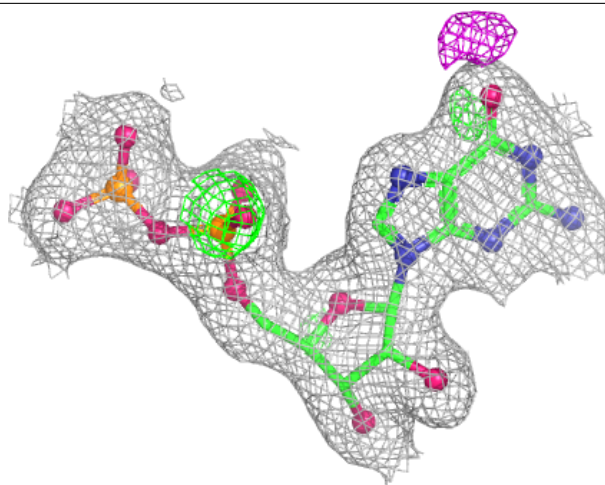
**Electron density around GTP A 501:**

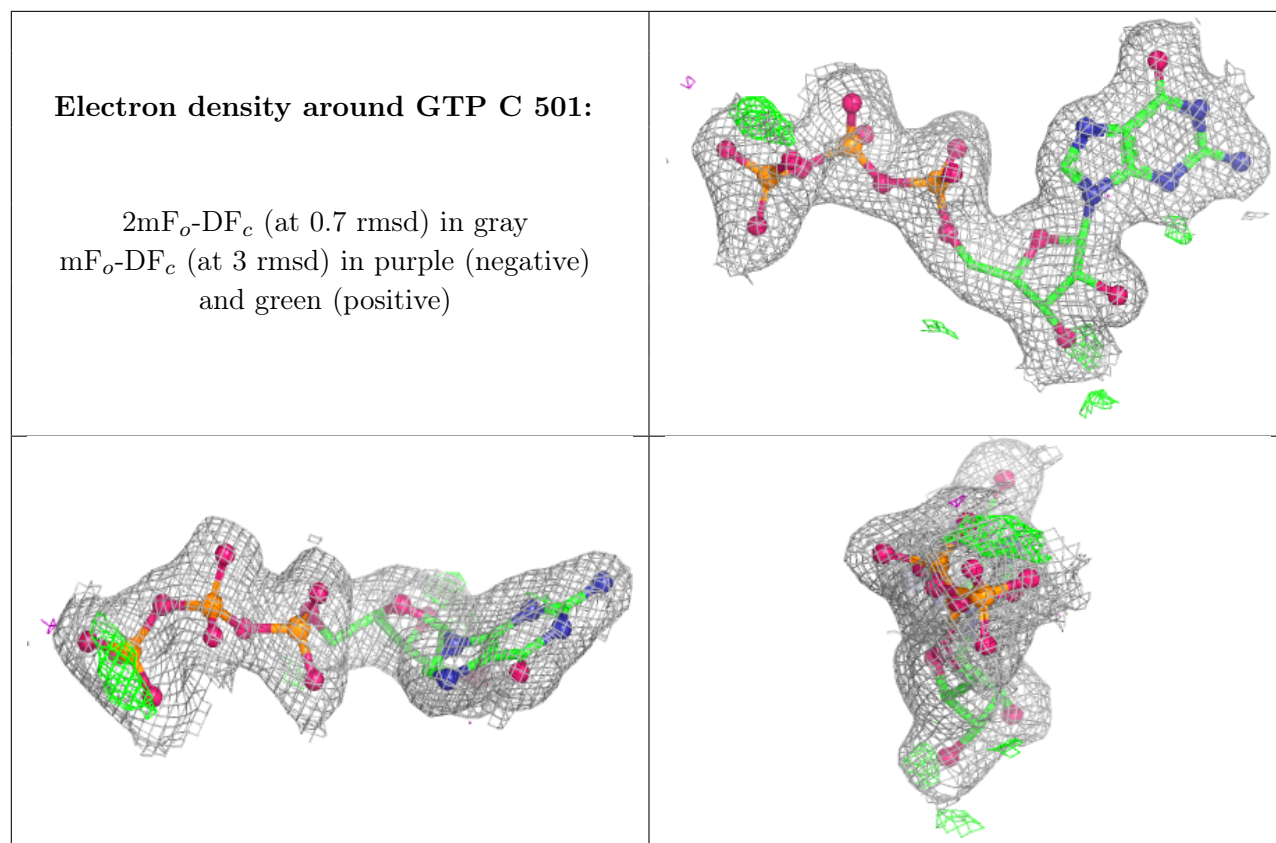
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.