



# Full wwPDB X-ray Structure Validation Report ⓘ

May 1, 2025 – 04:10 PM JST

PDB ID : 9LNV / pdb\_00009lnv  
Title : Crystal structure of T2R-TTL-YQVB6 Complex  
Authors : Wu, C.Y.; Wang, Y.X.; Chen, Q.F.  
Deposited on : 2025-01-22  
Resolution : 2.67 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](mailto: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 Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

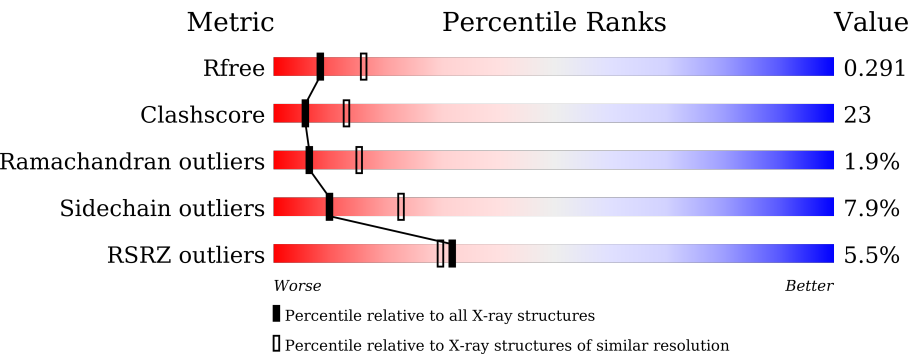
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 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))
$R_{free}$	164625	4708 (2.70-2.66)
Clashscore	180529	5138 (2.70-2.66)
Ramachandran outliers	177936	5071 (2.70-2.66)
Sidechain outliers	177891	5071 (2.70-2.66)
RSRZ outliers	164620	4708 (2.70-2.66)

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  $\geq 3$ , 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	450	<div><div>3%</div><div>56%</div><div>36%</div><div>6%</div><div></div></div>
1	C	450	<div><div>2%</div><div>62%</div><div>34%</div><div></div><div></div></div>
2	B	445	<div><div>2%</div><div>61%</div><div>33%</div><div></div><div></div></div>
2	D	445	<div><div>9%</div><div>43%</div><div>45%</div><div>7%</div><div>5%</div></div>
3	E	143	<div><div>6%</div><div>48%</div><div>30%</div><div>5%</div><div>16%</div></div>
4	F	384	<div><div>11%</div><div>45%</div><div>36%</div><div>6%</div><div>14%</div></div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	A1EPR	C	504	X	-	-	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17621 atoms, of which 58 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	439	Total	C	N	O	S	5	9	0
			3465	2200	584	657	24			
1	C	440	Total	C	N	O	S	8	7	0
			3466	2197	584	662	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	424	Total	C	N	O	S	14	4	0
			3343	2102	567	646	28			
2	B	428	Total	C	N	O	S	6	2	0
			3370	2118	576	649	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	0	0
			991	612	180	194	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63042
E	4	ALA	-	expression tag	UNP P63042

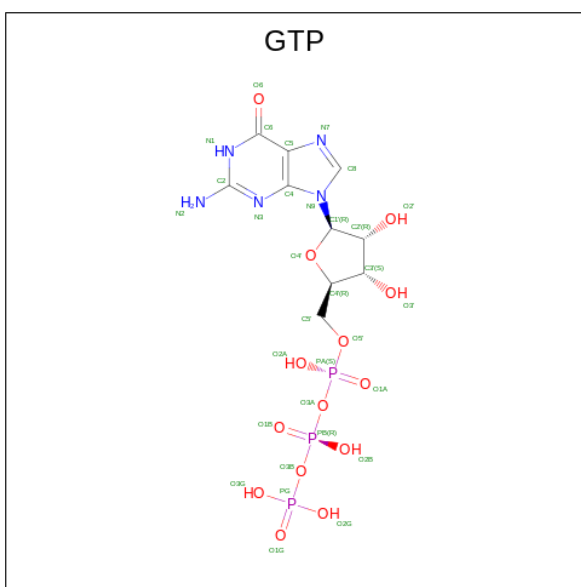
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	9	4	0
			2729	1762	457	496	14			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

- 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		

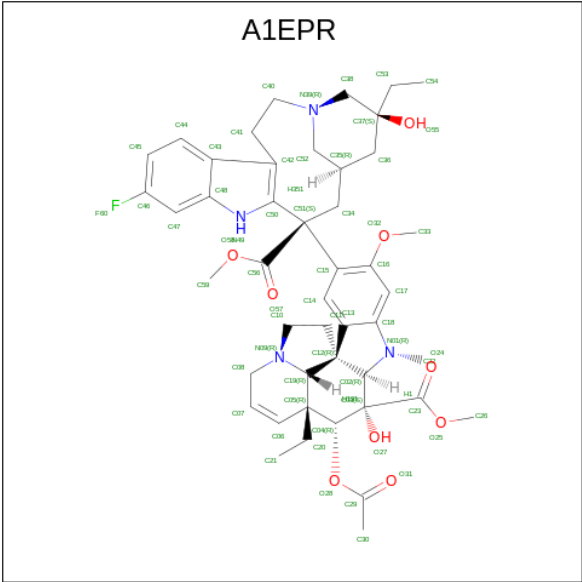
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

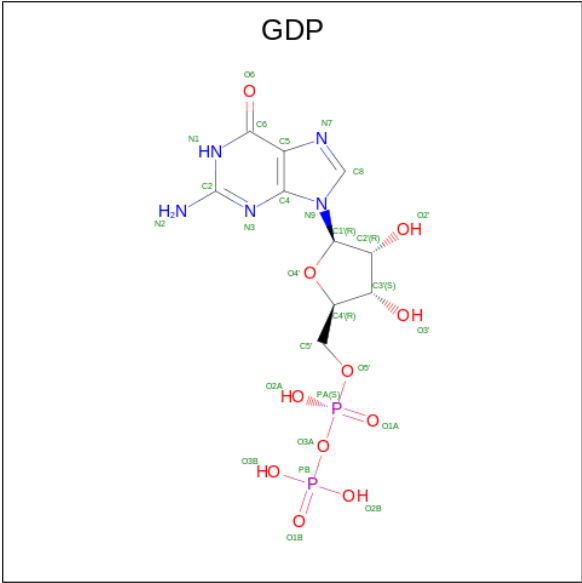
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	1	0
			1	1		
7	C	1	Total	Ca	1	0
			1	1		

- Molecule 8 is 10'-fluorovinblastine (CCD ID: A1EPR) (formula: C<sub>46</sub>H<sub>57</sub>FN<sub>4</sub>O<sub>9</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	C	1	Total	C	F	H	N	O	0	0
			118	46	1	58	4	9		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



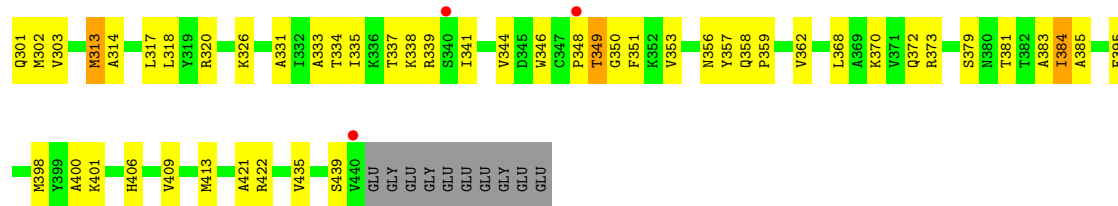
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	D	1	Total	C	N	O	P	28	0
			28	10	5	11	2		
9	B	1	Total	C	N	O	P	28	0
			28	10	5	11	2		

- Molecule 10 is water.

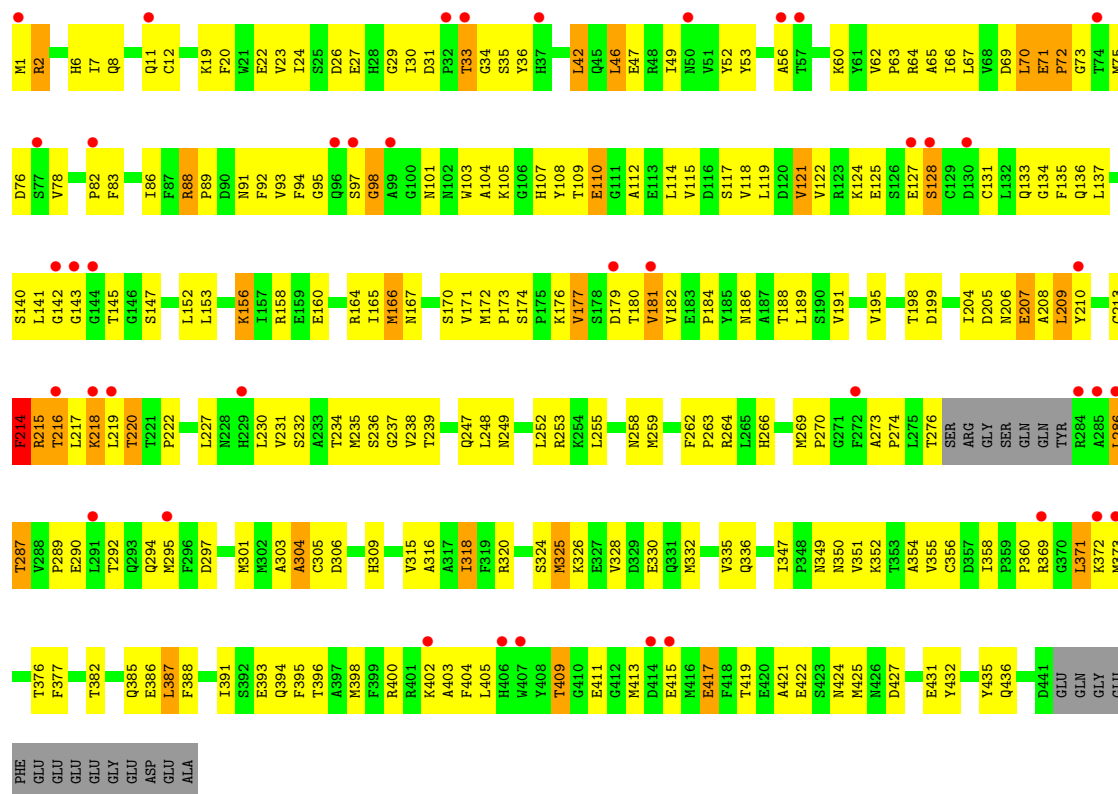
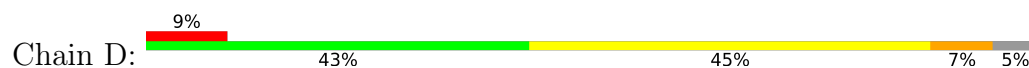
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	6	Total 6	O 6	0	0
10	B	9	Total 9	O 9	0	0



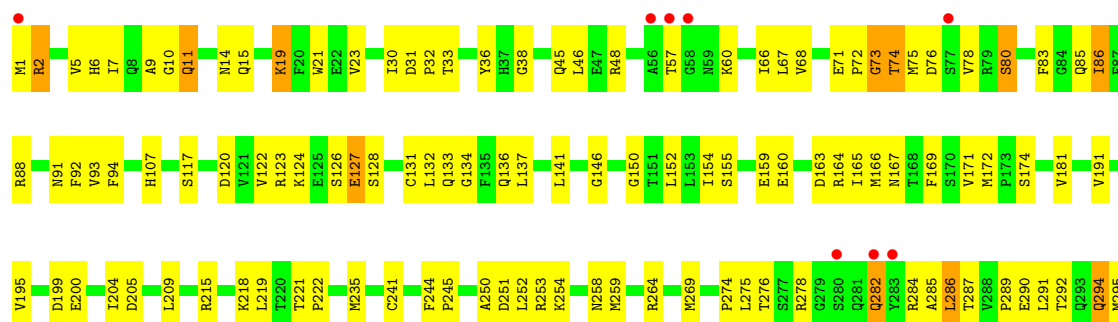


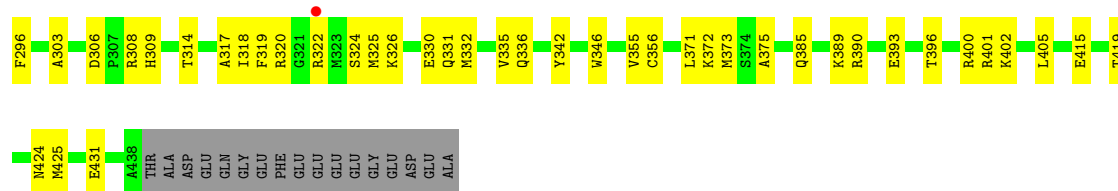


● Molecule 2: Tubulin beta chain

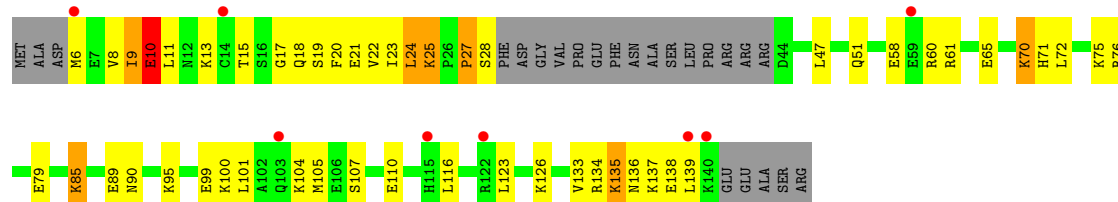


● Molecule 2: Tubulin beta chain

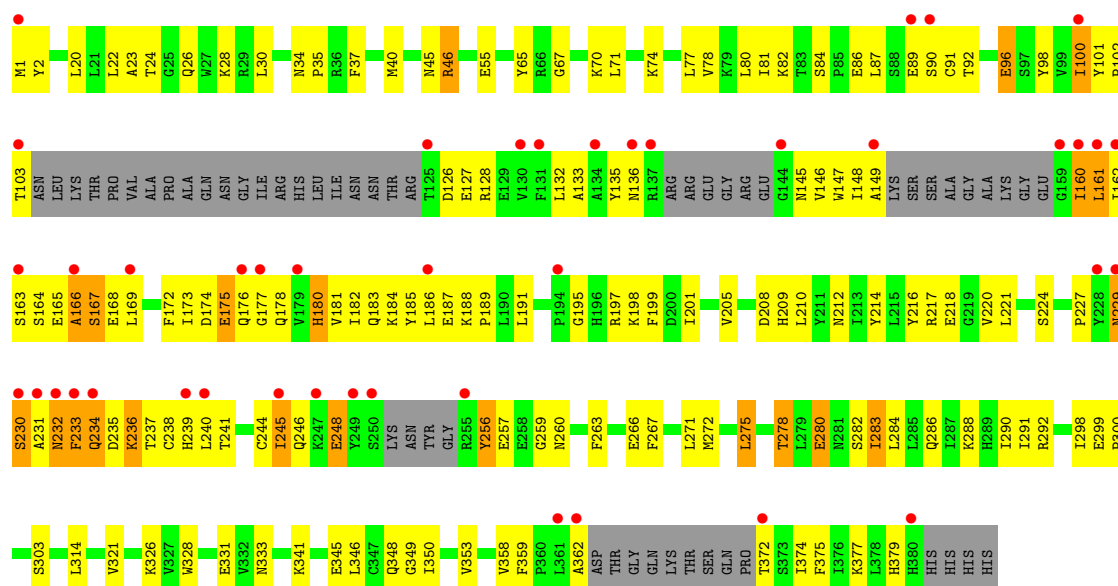
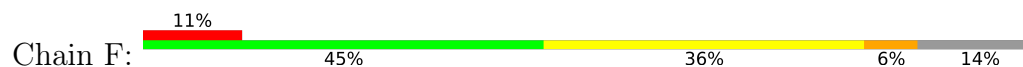




### • Molecule 3: Stathmin-4



### • 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, $\alpha$ , $\beta$ , $\gamma$	105.21Å 156.47Å 184.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.42 – 2.67 91.42 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.7 (91.42-2.67) 99.7 (91.42-2.67)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.65Å)	Xtriage
Refinement program	PHENIX (???)	Depositor
R, $R_{free}$	0.218 , 0.288 0.223 , 0.291	Depositor DCC
$R_{free}$ test set	4488 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	17621	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: A1EPR, GTP, CA, MG, GDP

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	0.36	0/3571	0.55	0/4849
1	C	0.40	0/3565	0.58	0/4842
2	B	0.40	0/3451	0.58	0/4675
2	D	0.31	0/3428	0.50	0/4645
3	E	0.37	0/999	0.54	0/1325
4	F	0.30	0/2802	0.47	0/3789
All	All	0.36	0/17816	0.54	0/24125

There are no bond length outliers.

There are no bond angle outliers.

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	3465	0	3402	156	0
1	C	3466	0	3393	144	0
2	B	3370	0	3250	126	0
2	D	3343	0	3230	218	0
3	E	991	0	1012	42	0
4	F	2729	0	2715	131	0
5	A	32	0	12	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	C	1	0	0	0	0
8	C	60	58	0	3	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	9	0	0	2	0
10	C	6	0	0	5	0
All	All	17563	58	17050	788	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 23.

All (788) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ILE:HG12	2:B:166:MET:HE2	1.30	1.12
2:D:135:PHE:HB2	2:D:166:MET:HE1	1.12	1.09
2:D:360:PRO:HG2	2:D:371:LEU:HD12	1.35	1.07
2:D:135:PHE:HB2	2:D:166:MET:CE	1.92	0.99
2:D:166:MET:HE3	2:D:166:MET:HA	1.41	0.99
4:F:1:MET:HE3	4:F:28:LYS:HB2	1.46	0.95
1:C:221:ARG:HG2	2:D:325:MET:HE3	1.50	0.93
2:D:259:MET:HE3	2:D:316:ALA:HB2	1.49	0.92
1:C:349:THR:O	10:C:601:HOH:O	1.88	0.92
1:A:137:VAL:HG21	1:A:154:MET:CE	2.02	0.90
2:B:284:ARG:NH1	2:B:285:ALA:O	2.04	0.90
1:C:181:VAL:HG12	1:C:398:MET:HE1	1.52	0.88
2:D:6:HIS:HE2	2:D:8:GLN:HB3	1.39	0.88
2:B:2:ARG:HD3	2:B:133:GLN:HG2	1.55	0.88
4:F:233:PHE:HB3	4:F:239:HIS:NE2	1.89	0.86
2:D:20:PHE:HB2	2:D:235:MET:CE	2.04	0.85
4:F:135:TYR:OH	4:F:165:GLU:HA	1.77	0.85
1:C:285:GLN:NE2	1:C:372:GLN:OE1	2.10	0.85
1:A:96:LYS:H	1:A:96:LYS:HD2	1.40	0.84
3:E:138:GLU:O	3:E:139:LEU:HD12	1.78	0.84
4:F:283:ILE:HD12	4:F:321:VAL:HG21	1.61	0.83
4:F:103:THR:HG22	4:F:174:ASP:OD1	1.78	0.82
2:B:73:GLY:O	2:B:75:MET:N	2.12	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:215:ARG:O	2:D:217:LEU:N	2.12	0.82
2:D:218:LYS:O	2:D:219:LEU:HD23	1.80	0.82
2:D:393:GLU:HA	2:D:396:THR:HG22	1.62	0.82
4:F:30:LEU:HD13	4:F:34:ASN:ND2	1.93	0.82
1:C:117:LEU:HD11	1:C:121:ARG:NH2	1.94	0.82
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.13	0.81
1:C:313:MET:HE3	1:C:435:VAL:HB	1.63	0.81
2:B:331:GLN:O	2:B:335:VAL:HG23	1.80	0.81
1:A:137:VAL:HG21	1:A:154:MET:HE1	1.61	0.81
1:C:248:LEU:HD12	1:C:357:TYR:OH	1.81	0.81
4:F:101:TYR:CD2	4:F:126:ASP:HB3	2.16	0.81
1:A:68[A]:VAL:HG22	1:A:93:ILE:HB	1.63	0.80
2:D:320:ARG:HA	2:D:356:CYS:O	1.81	0.80
3:E:75:LYS:O	3:E:79:GLU:HG3	1.81	0.80
4:F:102:PRO:HB3	4:F:173:ILE:O	1.82	0.80
2:D:71:GLU:HB2	2:D:98:GLY:HA2	1.64	0.80
2:D:7:ILE:O	2:D:137:LEU:HD12	1.83	0.79
2:B:264:ARG:NH1	2:B:431:GLU:OE1	2.13	0.79
2:D:181:VAL:O	2:D:398:MET:HE1	1.82	0.79
1:A:209:ILE:CD1	1:A:302:MET:HE2	2.13	0.79
4:F:162:ILE:HD11	4:F:234:GLN:HA	1.64	0.78
2:D:66:ILE:HD11	2:D:125:GLU:HG3	1.64	0.78
1:A:180:ALA:O	1:A:183:GLU:HG3	1.84	0.78
2:D:20:PHE:HB2	2:D:235:MET:HE2	1.64	0.78
2:D:191:VAL:O	2:D:195:VAL:HG23	1.82	0.78
1:A:155:GLU:HG2	1:A:197:HIS:NE2	1.99	0.78
4:F:271:LEU:HD23	4:F:275[A]:LEU:HD23	1.64	0.77
1:A:88:HIS:O	1:A:91:GLN:HG2	1.84	0.77
1:A:88:HIS:N	1:A:91:GLN:OE1	2.17	0.77
1:C:302:MET:N	1:C:302:MET:HE2	2.00	0.77
1:A:60:LYS:NZ	1:A:85:GLN:O	2.15	0.76
1:C:301:GLN:C	1:C:302:MET:HE2	2.10	0.76
2:D:274:PRO:HG2	2:D:371:LEU:HD22	1.68	0.76
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.66	0.76
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.26	0.75
2:B:75:MET:HE2	2:B:94:PHE:HD2	1.51	0.75
2:B:123:ARG:O	2:B:127:GLU:HG2	1.86	0.75
2:D:104:ALA:HB2	2:D:413:MET:HE3	1.67	0.75
2:B:285:ALA:HB2	2:B:372:LYS:HE3	1.69	0.75
1:A:155:GLU:HA	1:A:197:HIS:CD2	2.22	0.74
1:A:285:GLN:HG2	1:A:372[B]:GLN:OE1	1.88	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ILE:HG22	1:C:341:ILE:HD11	1.69	0.74
2:B:1:MET:HE2	2:B:1:MET:HA	1.69	0.74
1:A:155:GLU:HA	1:A:197:HIS:HD2	1.52	0.74
1:C:210:TYR:OH	1:C:221:ARG:HD2	1.87	0.74
1:A:317:LEU:HD21	1:A:377:MET:CE	2.18	0.74
4:F:71:LEU:HD22	4:F:298:ILE:HD13	1.70	0.74
2:B:2:ARG:HA	2:B:131:CYS:O	1.88	0.73
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.03	0.73
2:D:141:LEU:HD11	2:D:170:SER:HB3	1.70	0.73
3:E:126:LYS:HE2	3:E:126:LYS:HA	1.70	0.73
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.24	0.72
2:D:259:MET:CE	2:D:316:ALA:HB2	2.20	0.72
2:D:217:LEU:HD21	2:D:276:THR:HA	1.72	0.72
1:A:103:TYR:CD1	1:A:189:LEU:HD13	2.25	0.72
2:B:326:LYS:O	2:B:330:GLU:HG3	1.90	0.72
2:D:31:ASP:OD2	2:D:35:SER:HB2	1.90	0.71
2:B:278:ARG:NH1	10:B:601:HOH:O	2.04	0.71
4:F:326:LYS:HE2	4:F:328:TRP:CZ2	2.26	0.71
1:A:3:GLU:HG2	1:A:64:ARG:NH2	2.05	0.71
1:A:56:THR:HB	1:A:60:LYS:HB3	1.71	0.70
1:C:181:VAL:HG12	1:C:398:MET:CE	2.20	0.70
1:C:1:MET:HG3	1:C:131:GLY:HA3	1.72	0.70
1:A:2:ARG:O	1:A:51[B]:THR:HG23	1.92	0.70
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.24	0.70
2:D:402:LYS:O	2:D:402:LYS:HG2	1.91	0.69
2:D:101:ASN:OD1	2:D:180:THR:HG21	1.92	0.69
2:D:83:PHE:O	2:D:86:ILE:HG22	1.92	0.69
2:D:286:LEU:H	2:D:286:LEU:HD23	1.56	0.69
2:D:93:VAL:HG21	2:D:121:VAL:HG21	1.75	0.69
2:D:191:VAL:CB	2:D:425:MET:HE3	2.22	0.69
1:A:426:ALA:O	1:A:430:LYS:HG3	1.92	0.69
2:D:34:GLY:O	2:D:60:LYS:HA	1.93	0.69
4:F:199:PHE:CD1	4:F:221:LEU:HD23	2.28	0.69
2:D:360:PRO:HG2	2:D:371:LEU:CD1	2.20	0.69
1:A:285:GLN:OE1	1:A:372[B]:GLN:HG2	1.93	0.69
1:A:317:LEU:HD21	1:A:377:MET:HE3	1.74	0.69
4:F:101:TYR:CE2	4:F:126:ASP:HB3	2.28	0.68
4:F:237:THR:O	4:F:246:GLN:NE2	2.26	0.68
2:B:123:ARG:NH1	2:B:160:GLU:OE2	2.27	0.68
1:A:90:GLU:O	1:A:121:ARG:HD2	1.93	0.68
2:D:7:ILE:O	2:D:137:LEU:HA	1.93	0.68

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68[A]:VAL:HG21	1:A:118:VAL:HG22	1.75	0.68
2:D:135:PHE:CB	2:D:166:MET:HE1	2.08	0.67
1:C:1:MET:CE	1:C:1:MET:H1	2.07	0.67
2:D:104:ALA:HB2	2:D:413:MET:CE	2.25	0.67
4:F:146:VAL:O	4:F:184:LYS:HD2	1.95	0.67
1:A:209:ILE:HD11	1:A:302:MET:HE2	1.75	0.67
2:D:65:ALA:C	2:D:66:ILE:HD12	2.19	0.67
2:D:191:VAL:HB	2:D:425:MET:HE3	1.77	0.67
2:D:19:LYS:O	2:D:23:VAL:HG23	1.95	0.67
2:B:326:LYS:HE2	2:B:330:GLU:OE2	1.94	0.67
2:D:141:LEU:CD1	2:D:170:SER:HB3	2.25	0.66
1:C:1:MET:H1	1:C:1:MET:HE3	1.60	0.66
3:E:47:LEU:O	3:E:51:GLN:HG2	1.94	0.66
1:C:163:LYS:HG2	3:E:90:ASN:OD1	1.95	0.66
2:D:332:MET:O	2:D:336:GLN:HG3	1.95	0.66
3:E:72:LEU:HD13	2:B:159:GLU:HB2	1.76	0.66
4:F:166:ALA:O	4:F:168:GLU:N	2.29	0.66
2:B:191:VAL:HB	2:B:425:MET:HE3	1.78	0.66
1:C:349:THR:N	10:C:602:HOH:O	2.29	0.66
4:F:209:HIS:CE1	4:F:358:VAL:HG23	2.31	0.66
3:E:70:LYS:HE2	3:E:71:HIS:N	2.11	0.66
1:A:68[A]:VAL:HG21	1:A:118:VAL:CG2	2.27	0.65
4:F:71:LEU:HD22	4:F:298:ILE:CD1	2.26	0.65
3:E:126:LYS:HE2	3:E:126:LYS:CA	2.26	0.65
1:A:163:LYS:HA	1:A:163:LYS:HE3	1.79	0.65
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.77	0.65
4:F:78:VAL:CG1	4:F:82:LYS:HE3	2.26	0.65
4:F:245:ILE:HG22	4:F:245:ILE:O	1.97	0.65
1:A:285:GLN:HG2	1:A:372[B]:GLN:CD	2.21	0.65
2:D:23:VAL:HG21	2:D:232:SER:OG	1.97	0.65
2:B:83:PHE:O	2:B:86:ILE:HG12	1.97	0.65
2:D:209:LEU:HB3	2:D:227:LEU:HD22	1.78	0.64
2:D:295:MET:CE	2:D:377:PHE:HB2	2.26	0.64
4:F:172:PHE:O	4:F:175:GLU:HB2	1.97	0.64
2:B:154:ILE:CG1	2:B:166:MET:HE2	2.18	0.64
2:D:166:MET:CE	2:D:166:MET:HA	2.23	0.64
1:A:210:TYR:OH	1:A:221:ARG:HD2	1.98	0.64
2:D:107:HIS:O	2:D:152:LEU:HD22	1.97	0.64
2:D:209:LEU:CD1	2:D:230:LEU:HB2	2.28	0.63
1:C:337:THR:OG1	1:C:338:LYS:HG3	1.97	0.63
2:D:12:CYS:SG	2:D:140:SER:HB2	2.39	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HD21	1:A:428:LEU:HD13	1.80	0.63
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.29	0.63
2:D:387:LEU:HD23	2:D:387:LEU:C	2.23	0.63
2:B:284:ARG:HH22	2:B:290:GLU:CD	2.06	0.63
2:D:23:VAL:O	2:D:26:ASP:HB3	1.99	0.63
4:F:20:LEU:O	4:F:24:THR:HG23	1.99	0.63
1:A:434:GLU:O	1:A:437:VAL:HG12	1.99	0.63
2:D:158:ARG:HB3	3:E:123:LEU:HD11	1.80	0.63
2:D:180:THR:O	2:D:182:VAL:N	2.31	0.63
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.79	0.63
4:F:217:ARG:HG2	4:F:374:ILE:O	1.99	0.63
2:B:264:ARG:NH2	2:B:424:ASN:OD1	2.32	0.63
4:F:162:ILE:HD12	4:F:162:ILE:O	1.98	0.62
1:A:335:ILE:C	1:A:335:ILE:HD12	2.25	0.62
2:D:191:VAL:HG11	2:D:425:MET:HE3	1.81	0.62
2:D:208:ALA:HB2	2:D:304:ALA:N	2.15	0.62
4:F:184:LYS:HE2	4:F:185:TYR:O	1.99	0.62
1:C:180:ALA:O	1:C:183:GLU:HG3	2.00	0.62
4:F:236:LYS:O	4:F:237:THR:OG1	2.12	0.62
4:F:173:ILE:HD13	4:F:180:HIS:HB3	1.81	0.62
1:C:41:THR:O	1:C:41:THR:OG1	2.18	0.62
2:B:30:ILE:HD12	2:B:30:ILE:N	2.15	0.62
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.82	0.61
1:C:151[A]:SER:HB2	1:C:193:THR:HG22	1.81	0.61
1:A:302:MET:HE3	1:A:302:MET:HA	1.82	0.61
2:D:184:PRO:HG3	2:D:394:GLN:HB3	1.80	0.61
2:D:191:VAL:CG1	2:D:425:MET:HE3	2.31	0.61
1:C:335:ILE:CG2	1:C:341:ILE:HD11	2.30	0.61
2:D:6:HIS:NE2	2:D:8:GLN:HB3	2.13	0.61
4:F:77:LEU:O	4:F:81:ILE:HG13	2.01	0.61
2:D:306:ASP:HB3	2:D:309:HIS:ND1	2.15	0.61
1:C:233:GLN:HG3	1:C:368:LEU:HD23	1.83	0.60
2:D:292:THR:HG22	2:D:335:VAL:HG21	1.82	0.60
1:A:338:LYS:HD2	1:A:338:LYS:N	2.16	0.60
1:A:91:GLN:C	1:A:92:LEU:HD23	2.26	0.60
1:C:333:ALA:O	1:C:337:THR:HG23	2.02	0.60
1:C:335:ILE:HG22	1:C:341:ILE:CD1	2.31	0.60
1:C:227:LEU:O	1:C:231:ILE:HG13	2.02	0.60
4:F:163:SER:OG	4:F:164:SER:N	2.34	0.60
4:F:286:GLN:O	4:F:290:ILE:HG13	2.02	0.60
2:D:19:LYS:HD3	2:D:22:GLU:OE1	2.02	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:177:VAL:HG11	2:D:206:ASN:HD22	1.65	0.60
2:D:89:PRO:HA	2:D:92:PHE:HD1	1.67	0.59
2:D:209:LEU:HD13	2:D:230:LEU:HB2	1.85	0.59
2:D:112:ALA:O	2:D:115:VAL:HG12	2.03	0.59
1:C:1:MET:CG	1:C:131:GLY:HA3	2.32	0.59
2:D:105:LYS:HG3	2:D:411:GLU:HG3	1.84	0.59
2:D:210:TYR:HE1	2:D:222:PRO:CD	2.16	0.59
2:D:209:LEU:HD13	2:D:230:LEU:HD12	1.84	0.58
2:B:154:ILE:HG12	2:B:166:MET:CE	2.20	0.58
1:A:296:PHE:CZ	1:A:377:MET:HE1	2.38	0.58
2:D:274:PRO:HG2	2:D:371:LEU:CD2	2.33	0.58
2:D:382:THR:OG1	2:D:436:GLN:OE1	2.17	0.58
3:E:24:LEU:O	3:E:25:LYS:HB2	2.02	0.58
4:F:198:LYS:HD3	4:F:239:HIS:O	2.02	0.58
2:B:282:GLN:HA	2:B:282:GLN:OE1	2.03	0.58
2:D:142:GLY:O	2:D:186:ASN:ND2	2.31	0.58
4:F:100:ILE:HG22	4:F:173:ILE:HG21	1.86	0.58
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.39	0.58
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.33	0.58
4:F:100:ILE:CD1	4:F:182:ILE:HD12	2.34	0.58
4:F:102:PRO:HG3	4:F:177:GLY:C	2.28	0.58
4:F:178:GLN:N	4:F:178:GLN:OE1	2.35	0.58
1:A:238:ILE:HG23	1:A:378:LEU:HD11	1.85	0.58
4:F:189:PRO:HG2	4:F:191:LEU:HD21	1.85	0.58
1:C:152:LEU:HD13	3:E:105:MET:HE3	1.86	0.58
2:B:75:MET:HE2	2:B:94:PHE:CD2	2.37	0.58
1:A:36:MET:HE1	1:A:49:PHE:CE2	2.39	0.57
2:D:290:GLU:O	2:D:294:GLN:HB2	2.04	0.57
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.22	0.57
1:A:230:LEU:O	1:A:234:ILE:HD13	2.04	0.57
2:D:217:LEU:HD11	2:D:276:THR:O	2.03	0.57
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.39	0.57
2:D:118:VAL:HG11	2:D:153:LEU:HD11	1.86	0.57
2:D:213:CYS:SG	2:D:227:LEU:HD23	2.44	0.57
2:D:234:THR:O	2:D:237:GLY:N	2.36	0.57
2:D:274:PRO:HB3	2:D:286:LEU:HD21	1.86	0.57
3:E:100:LYS:O	3:E:104:LYS:HB2	2.04	0.57
2:B:36:TYR:CD2	2:B:46:LEU:HD11	2.39	0.57
1:A:163:LYS:HE3	1:A:163:LYS:CA	2.34	0.57
1:C:313:MET:HG2	1:C:346:TRP:CH2	2.38	0.57
1:C:151[A]:SER:HB2	1:C:193:THR:CG2	2.35	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:VAL:HA	1:A:413:MET:O	2.05	0.57
2:B:9:ALA:HA	2:B:68:VAL:O	2.05	0.57
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.86	0.56
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.38	0.56
2:B:332:MET:O	2:B:336:GLN:HG3	2.04	0.56
1:A:227:LEU:O	1:A:231:ILE:HG13	2.06	0.56
1:C:152:LEU:HD13	3:E:105:MET:CE	2.34	0.56
2:D:301:MET:HE1	2:D:377:PHE:CD2	2.39	0.56
4:F:1:MET:CE	4:F:28:LYS:HB2	2.28	0.56
2:B:74:THR:O	2:B:78:VAL:HG23	2.05	0.56
1:A:2:ARG:O	1:A:133:GLN:NE2	2.34	0.56
1:A:92:LEU:HD23	1:A:92:LEU:N	2.21	0.56
1:C:313:MET:HE1	1:C:435:VAL:HG21	1.88	0.56
1:C:317:LEU:C	1:C:318:LEU:HD12	2.30	0.56
2:D:118:VAL:O	2:D:122:VAL:HG23	2.05	0.56
2:D:180:THR:O	2:D:180:THR:HG22	2.06	0.56
1:C:275:VAL:HG13	1:C:368:LEU:HD11	1.86	0.56
2:D:125:GLU:HA	2:D:125:GLU:OE1	2.04	0.56
4:F:233:PHE:O	4:F:235:ASP:N	2.36	0.56
1:A:88:HIS:CE1	1:A:90:GLU:HB2	2.40	0.56
3:E:137:LYS:HG2	3:E:137:LYS:O	2.05	0.56
2:D:174:SER:HB2	2:D:207:GLU:HB2	1.87	0.56
4:F:87:LEU:O	4:F:90:SER:HB3	2.06	0.56
2:B:290:GLU:O	2:B:294:GLN:HB2	2.06	0.56
2:B:390:ARG:O	2:B:393:GLU:HG2	2.06	0.56
1:C:211:ASP:HB3	1:C:215:ARG:NH1	2.21	0.56
2:D:88:ARG:HD3	2:D:91:ASN:OD1	2.06	0.56
1:A:355:ILE:O	3:E:17:GLY:HA3	2.06	0.56
2:D:214:PHE:HE1	2:D:220:THR:HG23	1.72	0.55
4:F:149:ALA:HB3	4:F:161:LEU:H	1.71	0.55
2:B:48:ARG:NH2	2:B:250:ALA:HB1	2.21	0.55
2:D:176:LYS:HB3	2:D:210:TYR:CD2	2.41	0.55
1:C:335:ILE:HG23	1:C:339:ARG:HD2	1.87	0.55
1:C:241:SER:HA	1:C:249:ASN:HD21	1.71	0.55
1:C:400:ALA:C	1:C:401:LYS:HD2	2.32	0.55
3:E:85:LYS:HE3	3:E:89:GLU:OE2	2.07	0.55
3:E:135:LYS:O	3:E:135:LYS:HG2	2.06	0.55
2:B:284:ARG:NH2	2:B:290:GLU:OE2	2.38	0.55
1:A:23:LEU:HD23	1:A:236:SER:HB2	1.89	0.55
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.87	0.55
2:D:71:GLU:HB2	2:D:98:GLY:CA	2.35	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:GLN:HG3	2:B:136:GLN:O	2.06	0.55
1:A:3:GLU:O	1:A:133:GLN:HG2	2.07	0.55
1:A:141:PHE:HB3	1:A:187:SER:OG	2.07	0.55
2:B:48:ARG:NH2	2:B:241:CYS:O	2.40	0.55
1:C:233:GLN:HG3	1:C:368:LEU:CD2	2.36	0.54
1:C:313:MET:HG2	1:C:346:TRP:CZ2	2.43	0.54
2:D:119:LEU:HD11	2:D:156:LYS:HB3	1.89	0.54
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.43	0.54
2:B:32:PRO:O	2:B:86:ILE:HG23	2.08	0.54
2:D:292:THR:CG2	2:D:335:VAL:HG21	2.37	0.54
4:F:86:GLU:O	4:F:87:LEU:HD23	2.07	0.54
2:D:73:GLY:O	2:D:76:ASP:N	2.40	0.54
2:D:63:PRO:HD3	2:D:86:ILE:HG12	1.90	0.54
2:B:385:GLN:O	2:B:389:LYS:HG3	2.08	0.54
1:C:192:HIS:CG	1:C:421:ALA:HA	2.43	0.54
2:D:286:LEU:HD23	2:D:286:LEU:N	2.23	0.54
4:F:163:SER:HB3	4:F:169:LEU:HG	1.89	0.54
4:F:220:VAL:HG12	4:F:263:PHE:CD1	2.43	0.54
1:A:313:MET:HE3	1:A:380:ASN:OD1	2.08	0.53
3:E:134:ARG:C	3:E:136:ASN:H	2.16	0.53
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.72	0.53
4:F:283:ILE:CD1	4:F:321:VAL:HG11	2.39	0.53
2:B:5:VAL:HG23	2:B:132:LEU:HD11	1.91	0.53
1:C:107:HIS:CD2	1:C:152:LEU:HB2	2.43	0.53
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.90	0.53
1:A:103:TYR:CE2	1:A:148:GLY:HA2	2.44	0.53
2:D:128:SER:O	2:D:128:SER:OG	2.16	0.53
2:D:184:PRO:HB3	2:D:395:PHE:N	2.23	0.53
1:C:348:PRO:HA	10:C:604:HOH:O	2.07	0.53
2:D:177:VAL:HG11	2:D:206:ASN:ND2	2.23	0.53
4:F:235:ASP:O	4:F:236:LYS:HB2	2.07	0.53
1:C:48:SER:O	1:C:51:THR:HG23	2.09	0.53
4:F:278:THR:O	4:F:282:SER:OG	2.19	0.53
2:B:2:ARG:HG2	2:B:131:CYS:SG	2.49	0.53
1:A:75:ILE:HB	1:A:94:THR:CG2	2.39	0.53
2:D:382:THR:O	2:D:385:GLN:HG2	2.09	0.53
2:D:403:ALA:HB1	2:D:404:PHE:CD1	2.44	0.53
2:B:402:LYS:HE2	2:B:415:GLU:OE1	2.09	0.53
1:A:296:PHE:CE1	1:A:377:MET:HE1	2.43	0.53
1:C:209:ILE:HD11	1:C:302:MET:SD	2.49	0.53
1:C:362:VAL:HG21	1:C:370:LYS:HB2	1.91	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:126:LYS:HA	3:E:126:LYS:CE	2.38	0.53
2:B:136:GLN:HA	2:B:167:ASN:O	2.09	0.53
1:A:113:GLU:O	1:A:113:GLU:HG3	2.09	0.52
1:A:234:ILE:H	1:A:234:ILE:CD1	2.22	0.52
1:A:285:GLN:HG2	1:A:372[B]:GLN:CG	2.38	0.52
1:C:142:GLY:HA3	1:C:183:GLU:OE1	2.09	0.52
1:A:234:ILE:CD1	1:A:234:ILE:N	2.72	0.52
1:A:132:LEU:O	1:A:164:LYS:HE3	2.08	0.52
1:C:11:GLN:O	1:C:15:GLN:HG3	2.09	0.52
2:D:409:THR:HG23	2:D:413:MET:O	2.09	0.52
2:D:56:ALA:CB	2:D:62:VAL:HG23	2.40	0.52
2:D:292:THR:HG22	2:D:335:VAL:CG2	2.39	0.52
2:B:32:PRO:O	2:B:85:GLN:HG3	2.09	0.52
1:C:296:PHE:HB3	1:C:339:ARG:HD3	1.90	0.52
2:D:388:PHE:CD1	2:D:425:MET:HE2	2.45	0.52
4:F:96:GLU:O	4:F:183:GLN:HA	2.10	0.52
2:D:274:PRO:CG	2:D:371:LEU:HD22	2.39	0.52
2:D:388:PHE:HD1	2:D:425:MET:HE2	1.75	0.52
2:B:295:MET:HE2	2:B:296:PHE:HE1	1.75	0.52
1:A:285:GLN:HG2	1:A:372[B]:GLN:HG2	1.91	0.52
1:C:233:GLN:HA	1:C:233:GLN:OE1	2.08	0.52
2:B:75:MET:CE	2:B:94:PHE:HD2	2.22	0.52
1:A:287:SER:OG	1:A:290:GLU:HG3	2.10	0.52
4:F:67:GLY:O	4:F:70:LYS:HG3	2.10	0.52
2:B:372:LYS:O	2:B:373:MET:HG3	2.09	0.52
1:A:285:GLN:CG	1:A:372[B]:GLN:HG2	2.40	0.51
2:D:207:GLU:HG2	2:D:304:ALA:CB	2.41	0.51
1:A:212:ILE:HG21	1:A:230:LEU:HD21	1.92	0.51
3:E:9:ILE:HG22	3:E:10:GLU:H	1.75	0.51
2:B:76:ASP:O	2:B:80:SER:OG	2.29	0.51
1:A:229:ARG:NE	1:A:363:VAL:HG11	2.24	0.51
1:C:179:THR:HG21	2:D:247:GLN:HB3	1.93	0.51
2:D:315:VAL:HB	2:D:351:VAL:HG22	1.91	0.51
2:B:285:ALA:HB1	2:B:373:MET:HE3	1.92	0.51
1:A:116:ASP:OD1	1:A:156:ARG:NH2	2.43	0.51
1:A:180:ALA:HA	2:B:258:ASN:OD1	2.11	0.51
4:F:162:ILE:HD12	4:F:234:GLN:HG2	1.92	0.51
1:A:88:HIS:HE1	1:A:124:LYS:NZ	2.08	0.51
1:A:172:TYR:CD1	1:A:173:PRO:HD2	2.46	0.51
1:C:192:HIS:CD2	1:C:421:ALA:HA	2.46	0.51
2:D:20:PHE:CD1	2:D:235:MET:HE3	2.46	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:303:ALA:O	2:D:305:CYS:N	2.43	0.51
2:D:382:THR:HA	2:D:432:TYR:CD1	2.45	0.51
1:A:234:ILE:N	1:A:234:ILE:HD12	2.25	0.51
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.39	0.51
1:C:178:SER:HB2	1:C:183:GLU:OE2	2.11	0.51
2:D:26:ASP:OD2	2:D:369:ARG:HB2	2.11	0.51
2:D:171:VAL:HA	2:D:204:ILE:O	2.11	0.51
2:B:1:MET:HE2	2:B:1:MET:CA	2.40	0.51
2:B:67:LEU:N	2:B:67:LEU:HD12	2.26	0.51
1:C:70:LEU:HD13	1:C:110:ILE:HG22	1.93	0.50
4:F:146:VAL:HG23	4:F:187:GLU:OE2	2.11	0.50
4:F:80:LEU:O	4:F:84:SER:HB3	2.11	0.50
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.94	0.50
2:B:126:SER:C	2:B:128:SER:H	2.19	0.50
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.47	0.50
1:C:165:SER:HA	1:C:199:ASP:OD2	2.12	0.50
2:D:191:VAL:HG11	2:D:425:MET:CE	2.41	0.50
2:D:411:GLU:OE1	2:D:411:GLU:HA	2.10	0.50
4:F:346:LEU:O	4:F:350:ILE:HG13	2.11	0.50
2:D:231:VAL:O	2:D:235:MET:HG3	2.11	0.50
2:D:249:ASN:HB3	2:D:255:LEU:HD13	1.94	0.50
4:F:263:PHE:CE2	4:F:341:LYS:HD2	2.46	0.50
4:F:102:PRO:CG	4:F:177:GLY:HA2	2.42	0.50
4:F:248:GLU:O	4:F:248:GLU:HG2	2.11	0.50
2:D:355:VAL:HG23	2:D:355:VAL:O	2.11	0.50
2:B:141:LEU:HD12	2:B:172:MET:SD	2.51	0.50
2:B:396:THR:CG2	2:B:400:ARG:HH21	2.25	0.50
1:A:317:LEU:HD21	1:A:377:MET:HE2	1.93	0.50
1:C:409:VAL:HA	1:C:413:MET:O	2.12	0.50
2:D:2:ARG:HA	2:D:131:CYS:O	2.11	0.50
2:D:31:ASP:OD1	2:D:33:THR:HG23	2.11	0.50
2:D:191:VAL:HG21	2:D:425:MET:CE	2.42	0.50
3:E:8:VAL:C	3:E:9:ILE:HD13	2.37	0.50
3:E:9:ILE:HD13	3:E:9:ILE:N	2.26	0.50
4:F:353[A]:VAL:HG21	4:F:375:PHE:CD2	2.47	0.50
2:D:205:ASP:HB3	2:D:303:ALA:HA	1.93	0.50
3:E:13:LYS:HG2	3:E:18:GLN:HG2	1.94	0.50
4:F:233:PHE:HB3	4:F:239:HIS:CD2	2.47	0.50
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.47	0.49
4:F:231:ALA:O	4:F:232:ASN:HB3	2.10	0.49
1:C:66:VAL:HG12	1:C:68[A]:VAL:HG23	1.94	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:GLY:C	1:A:311:LYS:HE3	2.37	0.49
2:B:7:ILE:O	2:B:137:LEU:HA	2.12	0.49
4:F:100:ILE:HD12	4:F:182:ILE:HD12	1.95	0.49
4:F:148:ILE:HB	4:F:162:ILE:HG22	1.93	0.49
2:D:93:VAL:CG2	2:D:121:VAL:HG21	2.40	0.49
2:D:320:ARG:O	2:D:373:MET:HA	2.13	0.49
1:C:166:LYS:HE2	1:C:197:HIS:O	2.12	0.49
2:D:56:ALA:HB3	2:D:62:VAL:HG23	1.93	0.49
2:D:114:LEU:HD12	2:D:117:SER:HB2	1.95	0.49
3:E:6:MET:N	3:E:24:LEU:HD12	2.27	0.49
4:F:1:MET:HE3	4:F:28:LYS:CB	2.32	0.49
1:A:28:HIS:CE1	1:A:243:ARG:HB3	2.48	0.48
1:A:44:GLY:HA2	1:A:55:GLU:HB2	1.94	0.48
2:B:146:GLY:O	2:B:150:GLY:HA3	2.13	0.48
2:B:295:MET:HE1	2:B:317:ALA:HB1	1.95	0.48
4:F:46:ARG:NH1	4:F:46:ARG:HB3	2.28	0.48
4:F:244:CYS:C	4:F:246:GLN:H	2.21	0.48
4:F:314:LEU:HD22	4:F:350:ILE:HD11	1.95	0.48
2:B:292:THR:CG2	2:B:335:VAL:HG21	2.43	0.48
1:A:352:LYS:HZ2	3:E:21:GLU:CD	2.21	0.48
1:C:205:ASP:HB2	1:C:303:VAL:HA	1.96	0.48
2:D:264:ARG:O	2:D:266:HIS:N	2.44	0.48
2:D:287:THR:HB	2:D:289:PRO:HD2	1.95	0.48
1:C:395:PHE:CD1	1:C:422:ARG:HD3	2.48	0.48
1:A:1:MET:HE2	1:A:50:ASN:HB2	1.95	0.48
3:E:27:PRO:O	3:E:28:SER:CB	2.61	0.48
4:F:185:TYR:OH	4:F:239:HIS:HB3	2.13	0.48
1:A:258:ASN:OD1	1:A:352:LYS:HE2	2.14	0.48
4:F:98:TYR:HB3	4:F:127:GLU:HB2	1.96	0.48
1:A:115:ILE:HG23	1:A:116:ASP:N	2.28	0.48
1:C:271:THR:HG23	1:C:300:ASN:O	2.14	0.48
1:C:348:PRO:O	1:C:349:THR:OG1	2.21	0.48
2:D:12:CYS:HB3	2:D:140:SER:CB	2.43	0.48
2:D:97:SER:CB	2:D:110:GLU:HG2	2.44	0.48
2:D:269:MET:CE	2:D:305:CYS:HB2	2.43	0.48
4:F:55:GLU:HA	4:F:55:GLU:OE1	2.14	0.48
1:A:166:LYS:HE2	1:A:197:HIS:O	2.13	0.48
1:C:155:GLU:OE1	3:E:101:LEU:HD13	2.14	0.48
2:D:67:LEU:CD2	2:D:78:VAL:HG11	2.44	0.48
2:D:273:ALA:HA	2:D:274:PRO:C	2.39	0.48
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.96	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:VAL:CG1	8:C:504:A1EPR:C46	2.92	0.48
4:F:89:GLU:C	4:F:91:CYS:H	2.21	0.48
2:D:70:LEU:H	2:D:145:THR:HG21	1.78	0.47
4:F:132:LEU:O	4:F:135:TYR:HB3	2.13	0.47
2:B:1:MET:O	2:B:2:ARG:C	2.57	0.47
1:A:223:THR:O	1:A:227:LEU:HG	2.14	0.47
1:C:236:SER:O	1:C:240:ALA:HB2	2.14	0.47
1:C:244:PHE:HB2	1:C:356:ASN:HD21	1.79	0.47
1:C:439:SER:OG	2:B:401:ARG:HD3	2.14	0.47
1:A:100:ALA:HA	2:B:254:LYS:CD	2.44	0.47
1:A:276:ILE:HD12	1:A:283:HIS:CE1	2.50	0.47
1:C:285:GLN:HE21	1:C:373:ARG:HH22	1.63	0.47
2:D:103:TRP:HD1	2:D:147:SER:OG	1.96	0.47
4:F:22:LEU:C	4:F:24:THR:H	2.22	0.47
4:F:102:PRO:HG3	4:F:177:GLY:CA	2.44	0.47
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.96	0.47
1:A:195:LEU:HD12	1:A:266:HIS:CE1	2.49	0.47
2:D:97:SER:HB3	2:D:110:GLU:HG2	1.96	0.47
1:A:30:ILE:HD12	1:A:53:PHE:CE2	2.49	0.47
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.50	0.47
2:D:179:ASP:O	2:D:181:VAL:N	2.43	0.47
4:F:259:GLY:O	4:F:260:ASN:HB2	2.14	0.47
2:B:275:LEU:C	2:B:276:THR:HG23	2.39	0.47
1:A:141:PHE:O	1:A:147:SER:HB3	2.15	0.47
1:C:152:LEU:O	1:C:156:ARG:HG2	2.14	0.47
2:D:69:ASP:C	2:D:71:GLU:H	2.23	0.47
2:D:269:MET:HE2	2:D:305:CYS:HB2	1.96	0.47
4:F:160:ILE:HG13	4:F:240:LEU:CD2	2.44	0.47
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.50	0.47
1:A:360:PRO:HG3	1:A:374:ALA:HB3	1.97	0.47
1:C:151[B]:SER:HB3	1:C:193:THR:CG2	2.44	0.47
1:C:349:THR:O	1:C:351:PHE:N	2.46	0.47
2:D:29:GLY:O	2:D:36:TYR:HA	2.15	0.47
2:D:89:PRO:HA	2:D:92:PHE:CD1	2.48	0.47
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.13	0.47
2:B:287:THR:OG1	2:B:290:GLU:HG3	2.14	0.47
1:A:414:GLU:HG2	3:E:60:ARG:NE	2.30	0.47
4:F:173:ILE:CD1	4:F:180:HIS:HB3	2.45	0.47
1:A:307:PRO:HA	1:A:383:ALA:HB2	1.97	0.47
8:C:504:A1EPR:C59	2:B:221:THR:HG22	2.45	0.47
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.45	0.47
1:A:74:VAL:O	1:A:77:GLU:HB2	2.14	0.46
1:C:27:GLU:CD	1:C:320:ARG:HH22	2.23	0.46
4:F:26:GLN:HE22	4:F:362:ALA:H	1.62	0.46
2:B:322:ARG:NH1	2:B:322:ARG:HB2	2.30	0.46
1:A:137:VAL:HG21	1:A:154:MET:HE3	1.92	0.46
1:A:259:LEU:HD11	1:A:316[A]:CYS:SG	2.56	0.46
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.96	0.46
2:B:36:TYR:CZ	2:B:38:GLY:HA3	2.51	0.46
1:A:155:GLU:HG2	1:A:197:HIS:CD2	2.51	0.46
1:A:285:GLN:CD	1:A:372[B]:GLN:HG2	2.40	0.46
1:A:329:ASN:N	1:A:329:ASN:OD1	2.48	0.46
2:D:326:LYS:O	2:D:330:GLU:HG3	2.15	0.46
2:D:387:LEU:HD23	2:D:388:PHE:N	2.30	0.46
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.96	0.46
2:B:72:PRO:C	2:B:73:GLY:O	2.58	0.46
1:A:77:GLU:O	1:A:81:GLY:N	2.41	0.46
1:C:298:PRO:O	1:C:301:GLN:HG3	2.15	0.46
2:D:49:ILE:HD11	2:D:53:TYR:CD2	2.51	0.46
2:D:393:GLU:O	2:D:396:THR:N	2.48	0.46
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.98	0.46
4:F:135:TYR:HE2	4:F:166:ALA:HB2	1.81	0.46
2:B:120:ASP:OD1	2:B:123:ARG:NH2	2.46	0.46
1:A:158:SER:OG	1:A:166:LYS:NZ	2.38	0.46
1:C:10:GLY:HA2	1:C:69:ASP:OD1	2.16	0.46
2:D:124:LYS:O	2:D:127:GLU:HG2	2.16	0.46
2:D:237:GLY:HA3	2:D:376:THR:OG1	2.15	0.46
4:F:173:ILE:HG23	4:F:180:HIS:HB2	1.98	0.46
4:F:221:LEU:HD11	4:F:267:PHE:CD2	2.51	0.46
4:F:229:ASN:HB2	4:F:238:CYS:SG	2.56	0.46
2:B:11:GLN:HA	2:B:74:THR:HG21	1.97	0.46
2:B:308:ARG:HA	2:B:342:TYR:CE1	2.50	0.46
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.98	0.46
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.15	0.46
1:C:66:VAL:HG23	1:C:125:LEU:HD11	1.98	0.46
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.51	0.46
2:B:71:GLU:HB2	2:B:72:PRO:CD	2.46	0.46
1:A:1:MET:HG2	1:A:51[A]:THR:HG22	1.97	0.46
1:C:205:ASP:CB	1:C:303:VAL:HA	2.46	0.46
1:C:318:LEU:HD12	1:C:318:LEU:N	2.31	0.46
1:C:368:LEU:HD12	1:C:368:LEU:HA	1.79	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:LEU:CD1	3:E:105:MET:HE3	2.46	0.45
2:D:235:MET:O	2:D:239:THR:HG23	2.16	0.45
2:B:72:PRO:O	2:B:73:GLY:O	2.33	0.45
2:B:274:PRO:HG2	2:B:371:LEU:HD21	1.99	0.45
1:A:335:ILE:HD12	1:A:336:LYS:N	2.31	0.45
1:C:313:MET:HE3	1:C:346:TRP:HZ2	1.80	0.45
2:D:105:LYS:HE3	2:D:110:GLU:OE2	2.16	0.45
2:D:358:ILE:HG22	2:D:358:ILE:O	2.14	0.45
3:E:126:LYS:HE2	3:E:126:LYS:N	2.31	0.45
4:F:160:ILE:HD13	4:F:160:ILE:N	2.31	0.45
2:B:107:HIS:O	2:B:152:LEU:HD22	2.16	0.45
1:C:66:VAL:HG23	1:C:125:LEU:HD12	1.97	0.45
2:D:214:PHE:HA	2:D:219:LEU:O	2.17	0.45
3:E:15:THR:O	3:E:15:THR:HG22	2.16	0.45
1:C:41:THR:OG1	1:C:44:GLY:O	2.34	0.45
1:C:123:ARG:HA	1:C:123:ARG:HD3	1.80	0.45
1:C:242:LEU:N	1:C:242:LEU:HD23	2.31	0.45
1:C:401:LYS:HD2	1:C:401:LYS:N	2.31	0.45
3:E:95:LYS:HE3	3:E:99:GLU:OE2	2.16	0.45
4:F:353[B]:VAL:HG21	4:F:375:PHE:CD2	2.50	0.45
1:A:73:THR:H	1:A:73:THR:HG1	1.54	0.45
1:C:252:LEU:HD12	1:C:252:LEU:O	2.17	0.45
2:D:72:PRO:HD3	2:D:95:GLY:O	2.17	0.45
2:B:169:PHE:CE2	2:B:235:MET:HG2	2.51	0.45
1:A:363:VAL:O	1:A:363:VAL:HG12	2.17	0.45
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.51	0.45
1:C:349:THR:HA	10:C:602:HOH:O	2.16	0.45
2:D:30:ILE:HA	2:D:35:SER:O	2.17	0.45
2:D:309:HIS:ND1	2:D:386:GLU:OE2	2.49	0.45
1:A:100:ALA:HA	2:B:254:LYS:HD2	1.98	0.45
1:C:117:LEU:HD11	1:C:121:ARG:CZ	2.46	0.45
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.51	0.45
2:B:219:LEU:O	2:B:222:PRO:HD3	2.17	0.45
1:A:70:LEU:HD23	1:A:70:LEU:HA	1.78	0.45
1:C:285:GLN:HG3	1:C:373:ARG:HH12	1.81	0.45
2:D:274:PRO:HB3	2:D:286:LEU:CD2	2.46	0.45
1:A:372[B]:GLN:HG3	1:A:373:ARG:CZ	2.47	0.45
1:C:41:THR:O	1:C:55:GLU:OE1	2.35	0.45
4:F:166:ALA:O	4:F:167:SER:C	2.60	0.45
2:B:83:PHE:HB3	2:B:86:ILE:HD11	1.98	0.45
2:B:284:ARG:O	2:B:284:ARG:HG3	2.15	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:O	1:A:221:ARG:HG3	2.16	0.44
1:A:10:GLY:O	1:A:14:VAL:HG23	2.17	0.44
1:C:313:MET:CE	1:C:435:VAL:HB	2.41	0.44
2:D:184:PRO:HG3	2:D:394:GLN:CB	2.47	0.44
2:B:291:LEU:HA	2:B:291:LEU:HD23	1.38	0.44
1:A:3:GLU:HB3	1:A:64:ARG:NE	2.32	0.44
1:C:19:ALA:HB1	1:C:232:SER:OG	2.17	0.44
1:C:100:ALA:CB	2:D:253:ARG:HD2	2.47	0.44
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.51	0.44
1:C:266:HIS:CD2	1:C:266:HIS:O	2.70	0.44
2:D:103:TRP:O	2:D:104:ALA:C	2.59	0.44
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.98	0.44
4:F:102:PRO:HG3	4:F:177:GLY:HA2	1.98	0.44
1:A:143:GLY:O	1:A:147:SER:OG	2.23	0.44
1:A:311:LYS:HG2	1:A:436:GLY:HA2	1.99	0.44
1:C:8:HIS:CE1	1:C:17:GLY:HA2	2.53	0.44
1:C:362:VAL:CG2	1:C:370:LYS:HB2	2.47	0.44
2:D:165:ILE:HA	2:D:199:ASP:OD2	2.17	0.44
1:A:137:VAL:CG2	1:A:154:MET:HE1	2.42	0.44
1:A:201:ALA:HB3	1:A:267:PHE:CD2	2.52	0.44
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.99	0.44
1:C:234:ILE:HD13	1:C:302:MET:SD	2.57	0.44
1:C:334:THR:HG23	1:C:338:LYS:HE2	1.99	0.44
2:D:82:PRO:O	2:D:83:PHE:HB2	2.17	0.44
2:D:402:LYS:HG2	2:D:405:LEU:HB3	1.99	0.44
4:F:146:VAL:HG12	4:F:185:TYR:HB3	1.99	0.44
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.98	0.44
2:B:48:ARG:HH22	2:B:250:ALA:HB1	1.82	0.44
2:B:134:GLY:HA2	2:B:164:ARG:HB3	2.00	0.44
1:A:126:ALA:O	1:A:129:CYS:HB2	2.17	0.44
2:B:169:PHE:CD2	2:B:235:MET:HG2	2.52	0.44
1:A:386:GLU:O	1:A:390:ARG:HG2	2.17	0.44
4:F:197:ARG:HD2	4:F:224:SER:O	2.18	0.44
1:A:393:HIS:NE2	1:A:397:LEU:HD11	2.32	0.44
2:D:52:TYR:OH	2:D:136:GLN:OE1	2.17	0.44
4:F:82:LYS:HZ2	4:F:127:GLU:CD	2.25	0.44
2:B:372:LYS:HE3	2:B:372:LYS:HB2	1.79	0.44
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.00	0.44
1:A:192:HIS:CG	1:A:421:ALA:HA	2.53	0.44
1:C:253:THR:O	1:C:256:GLN:HB3	2.18	0.44
1:C:269:LEU:HD13	1:C:384:ILE:HD12	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:71:GLU:HG3	2:D:98:GLY:HA3	1.99	0.44
1:C:349:THR:OG1	2:B:181:VAL:HG23	2.18	0.43
1:C:5:ILE:O	1:C:135:PHE:HA	2.18	0.43
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.53	0.43
2:D:172:MET:HE2	2:D:387:LEU:HD21	2.01	0.43
2:D:215:ARG:O	2:D:216:THR:C	2.61	0.43
1:A:71:GLU:OE1	1:A:73:THR:OG1	2.23	0.43
1:C:1:MET:N	1:C:2:ARG:NH1	2.66	0.43
2:D:156:LYS:HD2	2:D:156:LYS:HA	1.74	0.43
2:D:294:GLN:O	2:D:297:ASP:HB3	2.18	0.43
2:D:382:THR:HA	2:D:432:TYR:HD1	1.84	0.43
1:C:180:ALA:HA	2:D:258:ASN:OD1	2.17	0.43
2:D:371:LEU:H	2:D:371:LEU:HG	1.55	0.43
1:A:155:GLU:HG2	1:A:197:HIS:HE2	1.80	0.43
1:C:230:LEU:O	1:C:234:ILE:HD12	2.18	0.43
2:D:172:MET:HA	2:D:173:PRO:HD3	1.89	0.43
2:D:199:ASP:O	2:D:266:HIS:HB2	2.19	0.43
2:D:306:ASP:HB3	2:D:309:HIS:HD1	1.82	0.43
2:D:424:ASN:O	2:D:427:ASP:HB2	2.18	0.43
4:F:377:LYS:HD3	4:F:379:HIS:CD2	2.54	0.43
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.01	0.43
2:B:205:ASP:CB	2:B:303:ALA:HA	2.48	0.43
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.49	0.43
3:E:76:ARG:NH2	2:B:155:SER:O	2.51	0.43
4:F:299:GLU:O	4:F:303:SER:HB2	2.18	0.43
2:B:286:LEU:HD23	2:B:286:LEU:N	2.34	0.43
1:C:3:GLU:HG2	1:C:64:ARG:CZ	2.49	0.43
2:D:349:ASN:O	2:D:352:LYS:NZ	2.48	0.43
2:D:372:LYS:O	2:D:373:MET:HB3	2.19	0.43
4:F:299:GLU:N	4:F:300:PRO:HD2	2.33	0.43
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.19	0.43
2:B:244:PHE:HB3	2:B:245:PRO:CD	2.49	0.43
1:A:110:ILE:O	1:A:110:ILE:HG22	2.18	0.43
1:A:221:ARG:HG2	2:B:325:MET:HB3	2.01	0.43
1:A:401:LYS:HE2	2:B:346:TRP:CD1	2.53	0.43
1:C:1:MET:O	1:C:2:ARG:CZ	2.67	0.43
1:C:349:THR:CA	10:C:602:HOH:O	2.67	0.43
2:D:210:TYR:O	2:D:213:CYS:N	2.51	0.43
2:D:295:MET:HE1	2:D:376:THR:O	2.19	0.43
4:F:100:ILE:HD13	4:F:182:ILE:HD12	2.01	0.43
2:B:319:PHE:HB2	2:B:355:VAL:HG22	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ALA:HB1	1:C:207:GLU:HB2	2.01	0.43
2:D:134:GLY:HA3	2:D:165:ILE:O	2.19	0.43
4:F:145:ASN:HB3	4:F:147:TRP:HE1	1.84	0.43
4:F:160:ILE:HG13	4:F:240:LEU:HD22	2.01	0.43
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.34	0.43
1:C:36:MET:HE1	1:C:49:PHE:CE2	2.53	0.42
1:C:320:ARG:O	1:C:373:ARG:HA	2.18	0.42
4:F:195:GLY:O	4:F:227:PRO:HB3	2.19	0.42
2:B:19:LYS:HE2	10:B:601:HOH:O	2.18	0.42
2:B:295:MET:HE2	2:B:296:PHE:CE1	2.52	0.42
2:B:295:MET:SD	2:B:375:ALA:HB1	2.59	0.42
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.01	0.42
1:C:151[B]:SER:HB3	1:C:193:THR:HG21	2.00	0.42
2:D:206:ASN:HA	2:D:209:LEU:HB2	2.01	0.42
2:D:217:LEU:HD23	2:D:217:LEU:HA	1.55	0.42
2:D:324:SER:O	2:D:328:VAL:HG23	2.18	0.42
2:B:124:LYS:HB2	2:B:124:LYS:HE3	1.79	0.42
2:B:199:ASP:C	2:B:200:GLU:HG3	2.45	0.42
1:A:344:VAL:O	1:A:345:ASP:C	2.62	0.42
1:A:437:VAL:O	1:A:438:ASP:O	2.37	0.42
1:C:190:THR:O	1:C:194[A]:THR:HB	2.19	0.42
2:D:209:LEU:HD11	2:D:230:LEU:HB2	1.97	0.42
2:D:264:ARG:HE	2:D:431:GLU:CD	2.26	0.42
3:E:11:LEU:HD12	3:E:20:PHE:HB3	2.00	0.42
4:F:102:PRO:O	4:F:103:THR:C	2.62	0.42
4:F:214:TYR:CD2	4:F:353[B]:VAL:HG11	2.54	0.42
4:F:238:CYS:SG	4:F:239:HIS:ND1	2.93	0.42
2:B:19:LYS:O	2:B:23:VAL:HG23	2.20	0.42
2:B:251:ASP:OD1	2:B:253:ARG:N	2.52	0.42
1:A:28:HIS:O	1:A:36:MET:HE3	2.19	0.42
1:C:313:MET:O	1:C:314:ALA:HB2	2.19	0.42
2:D:136:GLN:HA	2:D:167:ASN:HB3	2.01	0.42
4:F:162:ILE:HD12	4:F:162:ILE:C	2.44	0.42
2:B:320:ARG:HA	2:B:356:CYS:O	2.19	0.42
1:A:414:GLU:O	1:A:415:GLU:C	2.62	0.42
1:C:181:VAL:CG1	1:C:398:MET:CE	2.96	0.42
1:C:326:LYS:HE2	1:C:326:LYS:HB3	1.89	0.42
2:D:46:LEU:O	2:D:47:GLU:C	2.63	0.42
2:D:184:PRO:HB3	2:D:394:GLN:C	2.44	0.42
2:B:191:VAL:HB	2:B:425:MET:CE	2.48	0.42
1:A:100:ALA:HA	2:B:254:LYS:HE3	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ASP:OD2	1:A:429:GLU:OE2	2.37	0.42
1:C:331:ALA:O	1:C:335:ILE:HG12	2.20	0.42
2:D:165:ILE:HG21	2:D:252:LEU:HB3	2.01	0.42
2:D:393:GLU:O	2:D:396:THR:HG22	2.19	0.42
4:F:89:GLU:O	4:F:89:GLU:CG	2.68	0.42
4:F:224:SER:HA	4:F:246:GLN:OE1	2.20	0.42
2:B:402:LYS:HE2	2:B:415:GLU:CD	2.45	0.42
1:A:281:ALA:O	1:A:282:TYR:O	2.37	0.42
2:D:109:THR:HG21	3:E:137:LYS:CD	2.50	0.42
2:D:411:GLU:HA	3:E:137:LYS:HD2	2.02	0.42
2:B:33:THR:O	2:B:60:LYS:HD3	2.20	0.42
1:C:337:THR:OG1	1:C:338:LYS:N	2.52	0.42
2:D:270:PRO:HA	2:D:377:PHE:O	2.19	0.42
2:D:292:THR:CG2	2:D:335:VAL:CG2	2.97	0.42
4:F:100:ILE:HG21	4:F:173:ILE:HD12	2.02	0.42
1:A:182:VAL:O	1:A:185:TYR:HB2	2.19	0.42
2:D:318:ILE:HA	2:D:354:ALA:O	2.19	0.42
4:F:217:ARG:HG3	4:F:217:ARG:HH11	1.84	0.42
2:B:88:ARG:NH1	2:B:91:ASN:OD1	2.48	0.42
1:A:19:ALA:C	1:A:232:SER:OG	2.63	0.42
1:A:75:ILE:HB	1:A:94:THR:HG21	2.00	0.42
2:D:75:MET:HG3	2:D:94:PHE:HB3	2.01	0.42
3:E:27:PRO:O	3:E:28:SER:HB3	2.20	0.42
2:B:10:GLY:O	2:B:14:ASN:HB2	2.20	0.42
2:B:36:TYR:CE1	2:B:38:GLY:HA3	2.55	0.42
2:B:172:MET:HE3	2:B:172:MET:HB3	1.92	0.42
1:C:139:HIS:CG	1:C:150:THR:HG21	2.55	0.41
1:C:383:ALA:C	1:C:385:ALA:N	2.74	0.41
2:D:27:GLU:OE2	2:D:236:SER:OG	2.32	0.41
4:F:20:LEU:HD22	4:F:348:GLN:OE1	2.19	0.41
2:B:325:MET:HB3	2:B:325:MET:HE3	1.64	0.41
1:A:336:LYS:HD2	1:A:336:LYS:O	2.20	0.41
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.56	0.41
1:C:36:MET:O	1:C:37:PRO:C	2.63	0.41
2:D:31:ASP:C	2:D:33:THR:H	2.29	0.41
2:D:172:MET:HB2	2:D:205:ASP:HA	2.03	0.41
1:C:181:VAL:CG1	1:C:398:MET:HE1	2.36	0.41
4:F:135:TYR:O	4:F:145:ASN:ND2	2.53	0.41
4:F:256:TYR:HB2	4:F:257:GLU:OE2	2.19	0.41
2:B:66:ILE:HD12	2:B:122:VAL:HG22	2.01	0.41
2:B:68:VAL:HA	2:B:93:VAL:O	2.20	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.85	0.41
1:A:172:TYR:CG	1:A:173:PRO:HD2	2.55	0.41
1:C:67:PHE:CD1	1:C:67:PHE:N	2.89	0.41
2:D:2:ARG:HB3	2:D:133:GLN:HG2	2.01	0.41
2:D:153:LEU:HA	2:D:153:LEU:HD23	1.75	0.41
2:D:205:ASP:CB	2:D:303:ALA:HA	2.50	0.41
2:D:411:GLU:OE1	3:E:137:LYS:HE2	2.21	0.41
4:F:214:TYR:CD2	4:F:353[A]:VAL:HG11	2.55	0.41
2:B:134:GLY:HA3	2:B:165:ILE:O	2.21	0.41
2:B:163:ASP:OD1	2:B:163:ASP:C	2.63	0.41
1:A:1:MET:HE2	1:A:50:ASN:CB	2.49	0.41
1:A:63:PRO:CD	1:A:86:LEU:HG	2.50	0.41
1:A:321:GLY:O	1:A:357:TYR:HA	2.20	0.41
1:C:10:GLY:O	1:C:14:VAL:HG23	2.20	0.41
2:D:66:ILE:HD12	2:D:66:ILE:N	2.35	0.41
2:D:295:MET:HE3	2:D:377:PHE:HB2	1.99	0.41
2:B:30:ILE:N	2:B:30:ILE:CD1	2.83	0.41
1:C:241:SER:CA	1:C:249:ASN:HD21	2.31	0.41
1:C:271:THR:HG23	1:C:300:ASN:C	2.45	0.41
2:D:188:THR:HG22	2:D:421:ALA:HB1	2.03	0.41
2:D:315:VAL:O	2:D:351:VAL:HA	2.21	0.41
4:F:210:LEU:HD12	4:F:212:ASN:ND2	2.36	0.41
2:D:262:PHE:CZ	2:D:435:TYR:CE1	3.08	0.41
2:D:419:THR:O	2:D:422:GLU:HB3	2.20	0.41
1:A:118:VAL:HG11	1:A:153:LEU:HD22	2.03	0.41
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.55	0.41
1:C:155:GLU:OE2	1:C:193:THR:HG23	2.21	0.41
2:D:1:MET:O	2:D:2:ARG:C	2.63	0.41
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.50	0.41
2:D:108:TYR:CD2	3:E:133:VAL:HG11	2.56	0.41
2:D:172:MET:O	2:D:206:ASN:HB2	2.21	0.41
4:F:173:ILE:HD13	4:F:180:HIS:CB	2.47	0.41
2:B:171:VAL:HA	2:B:204:ILE:O	2.21	0.41
1:A:2:ARG:HB3	1:A:131:GLY:O	2.21	0.41
1:A:178:SER:HB2	1:A:183:GLU:OE2	2.21	0.41
1:A:298:PRO:HA	1:A:301:GLN:CD	2.46	0.41
1:C:358:GLN:CD	1:C:359:PRO:HD2	2.46	0.41
8:C:504:A1EPR:C56	8:C:504:A1EPR:O32	2.68	0.41
2:D:63:PRO:O	2:D:65:ALA:N	2.52	0.41
3:E:138:GLU:C	3:E:139:LEU:HD12	2.43	0.41
4:F:65:TYR:OH	4:F:208:ASP:O	2.38	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:146:VAL:HG13	4:F:163:SER:O	2.21	0.41
4:F:148:ILE:HG22	4:F:183:GLN:O	2.20	0.41
2:B:259:MET:HA	2:B:314:THR:OG1	2.20	0.41
2:B:287:THR:OG1	2:B:289:PRO:HD2	2.21	0.41
1:A:211:ASP:HB3	1:A:215:ARG:NH1	2.35	0.41
4:F:229:ASN:O	4:F:230:SER:C	2.64	0.41
4:F:245:ILE:O	4:F:245:ILE:CG2	2.66	0.41
1:A:202:PHE:CE1	1:A:268:PRO:HG2	2.56	0.40
2:D:2:ARG:HD2	2:D:131:CYS:SG	2.61	0.40
2:D:65:ALA:O	2:D:66:ILE:HD12	2.21	0.40
2:B:31:ASP:O	2:B:33:THR:N	2.54	0.40
2:B:204:ILE:CG2	2:B:209:LEU:HD11	2.51	0.40
4:F:235:ASP:O	4:F:236:LYS:CB	2.69	0.40
4:F:197:ARG:HH12	4:F:257:GLU:CD	2.29	0.40
2:B:269:MET:HE2	2:B:269:MET:HB3	1.65	0.40
1:C:242:LEU:HD21	1:C:252:LEU:HB3	2.03	0.40
2:D:42:LEU:HD12	2:D:42:LEU:HA	1.75	0.40
1:C:90:GLU:HB3	1:C:121:ARG:HD2	2.04	0.40
1:C:114:ILE:HG12	1:C:114:ILE:O	2.21	0.40
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.56	0.40
2:B:191:VAL:HG21	2:B:425:MET:HE2	2.04	0.40
2:B:274:PRO:CG	2:B:371:LEU:HD21	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/450 (99%)	403 (90%)	37 (8%)	6 (1%)	10	23
1	C	445/450 (99%)	422 (95%)	20 (4%)	3 (1%)	19	38
2	B	428/445 (96%)	401 (94%)	23 (5%)	4 (1%)	14	32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	424/445 (95%)	368 (87%)	44 (10%)	12 (3%)	4	9
3	E	116/143 (81%)	106 (91%)	6 (5%)	4 (3%)	3	6
4	F	323/384 (84%)	284 (88%)	28 (9%)	11 (3%)	3	6
All	All	2182/2317 (94%)	1984 (91%)	158 (7%)	40 (2%)	6	16

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	TYR
1	A	438	ASP
1	C	349	THR
2	D	215	ARG
2	D	216	THR
3	E	27	PRO
4	F	166	ALA
4	F	167	SER
4	F	248	GLU
2	B	74	THR
2	B	215	ARG
2	D	143	GLY
2	D	214	PHE
2	D	304	ALA
4	F	136	ASN
4	F	230	SER
2	B	73	GLY
1	A	366	GLY
1	C	41	THR
2	D	2	ARG
2	D	98	GLY
3	E	135	LYS
4	F	236	LYS
2	B	2	ARG
1	A	81	GLY
1	C	350	GLY
2	D	72	PRO
2	D	218	LYS
3	E	10	GLU
3	E	25	LYS
4	F	23	ALA
4	F	133	ALA
4	F	234	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	F	280	GLU
2	D	64	ARG
2	D	70	LEU
1	A	114	ILE
1	A	346	TRP
2	D	181	VAL
4	F	245	ILE

### 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	378/378 (100%)	337 (89%)	41 (11%)	5	11
1	C	378/378 (100%)	360 (95%)	18 (5%)	21	44
2	B	369/383 (96%)	351 (95%)	18 (5%)	21	44
2	D	369/383 (96%)	337 (91%)	32 (9%)	8	18
3	E	108/127 (85%)	94 (87%)	14 (13%)	3	7
4	F	303/342 (89%)	276 (91%)	27 (9%)	8	17
All	All	1905/1991 (96%)	1755 (92%)	150 (8%)	10	23

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	18	ASN
1	A	26	LEU
1	A	47	ASP
1	A	56	THR
1	A	60	LYS
1	A	62	VAL
1	A	71	GLU
1	A	73	THR
1	A	74	VAL
1	A	82	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	96	LYS
1	A	113	GLU
1	A	117	LEU
1	A	118	VAL
1	A	120	ASP
1	A	150	THR
1	A	163	LYS
1	A	176	GLN
1	A	181	VAL
1	A	188	ILE
1	A	219	ILE
1	A	232	SER
1	A	234	ILE
1	A	251	ASP
1	A	253	THR
1	A	257	THR
1	A	259	LEU
1	A	280	LYS
1	A	302	MET
1	A	311	LYS
1	A	326	LYS
1	A	329	ASN
1	A	334	THR
1	A	335	ILE
1	A	338	LYS
1	A	362	VAL
1	A	363	VAL
1	A	368	LEU
1	A	390	ARG
1	A	437	VAL
1	C	1	MET
1	C	7	ILE
1	C	46	ASP
1	C	77	GLU
1	C	130	THR
1	C	188	ILE
1	C	193	THR
1	C	237	SER
1	C	238	ILE
1	C	241	SER
1	C	251	ASP
1	C	276	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	284	GLU
1	C	286	LEU
1	C	313	MET
1	C	379	SER
1	C	381	THR
1	C	384	ILE
2	D	11	GLN
2	D	24	ILE
2	D	33	THR
2	D	42	LEU
2	D	46	LEU
2	D	71	GLU
2	D	88	ARG
2	D	110	GLU
2	D	121	VAL
2	D	128	SER
2	D	156	LYS
2	D	160	GLU
2	D	164	ARG
2	D	166	MET
2	D	177	VAL
2	D	198	THR
2	D	207	GLU
2	D	209	LEU
2	D	214	PHE
2	D	220	THR
2	D	238	VAL
2	D	286	LEU
2	D	287	THR
2	D	318	ILE
2	D	325	MET
2	D	371	LEU
2	D	387	LEU
2	D	391	ILE
2	D	400	ARG
2	D	409	THR
2	D	415	GLU
2	D	417	GLU
3	E	9	ILE
3	E	10	GLU
3	E	19	SER
3	E	22	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	E	23	ILE
3	E	24	LEU
3	E	58	GLU
3	E	61	ARG
3	E	65	GLU
3	E	70	LYS
3	E	85	LYS
3	E	107	SER
3	E	110	GLU
3	E	116	LEU
4	F	45	ASN
4	F	46	ARG
4	F	92	THR
4	F	96	GLU
4	F	100	ILE
4	F	128	ARG
4	F	160	ILE
4	F	161	LEU
4	F	175	GLU
4	F	176	GLN
4	F	180	HIS
4	F	186	LEU
4	F	188	LYS
4	F	229	ASN
4	F	232	ASN
4	F	233	PHE
4	F	241	THR
4	F	256	TYR
4	F	266	GLU
4	F	275[A]	LEU
4	F	275[B]	LEU
4	F	278	THR
4	F	283	ILE
4	F	292	ARG
4	F	333	ASN
4	F	345	GLU
4	F	372	THR
2	B	11	GLN
2	B	15	GLN
2	B	19	LYS
2	B	57	THR
2	B	80	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	86	ILE
2	B	117	SER
2	B	127	GLU
2	B	174	SER
2	B	195	VAL
2	B	218	LYS
2	B	282	GLN
2	B	286	LEU
2	B	294	GLN
2	B	318	ILE
2	B	324	SER
2	B	405	LEU
2	B	419	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	61	HIS
1	A	88	HIS
1	A	197	HIS
1	C	133	GLN
2	D	50	ASN
2	D	206	ASN
2	D	339	ASN
2	D	349	ASN
4	F	212	ASN
4	F	229	ASN
2	B	229	HIS
2	B	247	GLN
2	B	339	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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
8	A1EPR	C	504	-	64,68,68	5.09	30 (46%)	81,110,110	2.59	28 (34%)
9	GDP	D	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	4 (13%)
5	GTP	C	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.56	7 (21%)
5	GTP	A	501	6	26,34,34	1.11	2 (7%)	32,54,54	1.63	7 (21%)

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	501	-	-	0/12/32/32	0/3/3/3
8	A1EPR	C	504	-	1/1/17/17	8/38/131/131	0/7/9/9
9	GDP	D	501	-	-	0/12/32/32	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	504	A1EPR	C06-C07	12.68	1.56	1.32
8	C	504	A1EPR	C18-C13	12.20	1.54	1.39
8	C	504	A1EPR	C14-C13	11.44	1.56	1.39
8	C	504	A1EPR	C14-C15	10.54	1.55	1.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	504	A1EPR	C16-C15	10.06	1.57	1.39
8	C	504	A1EPR	C18-N01	9.95	1.57	1.39
8	C	504	A1EPR	C47-C48	9.81	1.57	1.41
8	C	504	A1EPR	C17-C16	9.55	1.56	1.38
8	C	504	A1EPR	C47-C46	9.18	1.51	1.36
8	C	504	A1EPR	C17-C18	9.08	1.54	1.39
8	C	504	A1EPR	C11-C10	8.87	1.69	1.52
8	C	504	A1EPR	C44-C43	7.20	1.57	1.42
8	C	504	A1EPR	C44-C45	6.62	1.50	1.36
8	C	504	A1EPR	C05-C06	5.85	1.62	1.51
8	C	504	A1EPR	O58-C56	5.71	1.44	1.33
8	C	504	A1EPR	C45-C46	5.69	1.48	1.37
8	C	504	A1EPR	C19-N09	5.24	1.56	1.47
8	C	504	A1EPR	O25-C23	5.12	1.43	1.33
8	C	504	A1EPR	C03-C23	5.10	1.65	1.52
8	C	504	A1EPR	O28-C04	5.08	1.55	1.44
8	C	504	A1EPR	C03-C04	-4.90	1.40	1.53
8	C	504	A1EPR	C05-C19	-4.66	1.42	1.53
8	C	504	A1EPR	C08-C07	4.44	1.60	1.49
8	C	504	A1EPR	C12-C02	4.39	1.71	1.55
8	C	504	A1EPR	C42-C50	4.17	1.45	1.39
5	C	501	GTP	C5-C6	-3.99	1.39	1.47
5	A	501	GTP	C5-C6	-3.96	1.39	1.47
8	C	504	A1EPR	O32-C16	3.74	1.43	1.37
8	C	504	A1EPR	C02-N01	-3.52	1.39	1.47
8	C	504	A1EPR	C12-C13	-2.75	1.47	1.51
9	D	501	GDP	C6-N1	-2.45	1.34	1.37
9	B	501	GDP	C6-N1	-2.34	1.34	1.37
5	C	501	GTP	C2-N3	2.26	1.38	1.33
8	C	504	A1EPR	C36-C35	2.24	1.60	1.54
5	A	501	GTP	C2-N3	2.24	1.38	1.33
8	C	504	A1EPR	O28-C29	2.23	1.40	1.35

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	504	A1EPR	C11-C12-C13	-10.00	94.12	112.35
8	C	504	A1EPR	C11-C12-C02	7.34	126.17	112.34
8	C	504	A1EPR	O28-C29-C30	6.49	123.03	111.09
8	C	504	A1EPR	C14-C13-C18	-5.67	115.55	120.31
8	C	504	A1EPR	C12-C19-C05	-5.13	114.40	118.20
8	C	504	A1EPR	O32-C16-C15	4.92	121.62	116.58

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	504	A1EPR	C14-C13-C12	4.60	136.94	129.00
8	C	504	A1EPR	C17-C16-C15	-4.50	118.06	122.20
8	C	504	A1EPR	C19-C05-C06	4.48	112.86	108.28
8	C	504	A1EPR	C05-C06-C07	-4.20	114.69	124.02
5	A	501	GTP	PA-O3A-PB	-3.93	119.33	132.83
8	C	504	A1EPR	C36-C35-C52	3.80	113.15	108.72
8	C	504	A1EPR	O28-C29-O31	-3.73	115.55	122.96
5	A	501	GTP	PB-O3B-PG	-3.73	120.04	132.83
9	B	501	GDP	PA-O3A-PB	-3.62	120.40	132.83
8	C	504	A1EPR	O25-C23-C03	3.60	118.27	112.22
5	C	501	GTP	PB-O3B-PG	-3.57	120.57	132.83
9	D	501	GDP	PA-O3A-PB	-3.46	120.95	132.83
9	B	501	GDP	C3'-C2'-C1'	3.39	106.08	100.98
9	D	501	GDP	C3'-C2'-C1'	3.34	106.01	100.98
8	C	504	A1EPR	O25-C23-O24	-3.31	118.14	123.93
5	C	501	GTP	PA-O3A-PB	-3.28	121.58	132.83
5	C	501	GTP	C5-C6-N1	3.19	119.58	113.95
5	A	501	GTP	C5-C6-N1	3.17	119.54	113.95
8	C	504	A1EPR	C05-C19-N09	3.15	118.36	111.72
8	C	504	A1EPR	C53-C37-C38	-3.07	104.65	111.80
5	A	501	GTP	C3'-C2'-C1'	3.06	105.58	100.98
8	C	504	A1EPR	C44-C43-C42	-3.01	128.97	134.17
5	A	501	GTP	C8-N7-C5	3.00	108.70	102.99
5	C	501	GTP	C3'-C2'-C1'	2.98	105.47	100.98
5	C	501	GTP	C8-N7-C5	2.93	108.57	102.99
5	C	501	GTP	C2-N1-C6	-2.86	119.83	125.10
5	A	501	GTP	C2-N1-C6	-2.84	119.86	125.10
8	C	504	A1EPR	C08-C07-C06	-2.84	118.37	123.02
8	C	504	A1EPR	C03-C02-C12	-2.82	108.37	114.18
8	C	504	A1EPR	C20-C05-C06	-2.72	104.76	107.99
8	C	504	A1EPR	C14-C15-C16	2.42	120.24	116.78
8	C	504	A1EPR	C13-C12-C02	2.39	105.93	102.21
8	C	504	A1EPR	C33-O32-C16	-2.38	113.94	117.53
9	B	501	GDP	C8-N7-C5	2.34	107.45	102.99
9	D	501	GDP	C8-N7-C5	2.30	107.36	102.99
9	B	501	GDP	C5-C6-N1	2.26	117.95	113.95
8	C	504	A1EPR	C45-C46-C47	-2.22	120.78	123.23
8	C	504	A1EPR	O32-C16-C17	-2.21	120.32	124.12
8	C	504	A1EPR	C36-C37-C38	-2.21	106.59	109.29
9	D	501	GDP	C5-C6-N1	2.18	117.80	113.95
5	C	501	GTP	O6-C6-C5	-2.16	120.16	124.37
8	C	504	A1EPR	O58-C56-C51	2.16	114.56	111.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	O6-C6-C5	-2.15	120.17	124.37
8	C	504	A1EPR	C04-C03-C23	2.02	115.99	110.85

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	C	504	A1EPR	N39

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
8	C	504	A1EPR	C03-C23-O25-C26
8	C	504	A1EPR	O24-C23-O25-C26
8	C	504	A1EPR	C30-C29-O28-C04
8	C	504	A1EPR	O31-C29-O28-C04
8	C	504	A1EPR	C04-C03-C23-O24
8	C	504	A1EPR	C04-C03-C23-O25
5	C	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O5'
8	C	504	A1EPR	C36-C37-C53-C54
5	C	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	O4'-C4'-C5'-O5'
8	C	504	A1EPR	O55-C37-C53-C54
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3B-PG-O1G

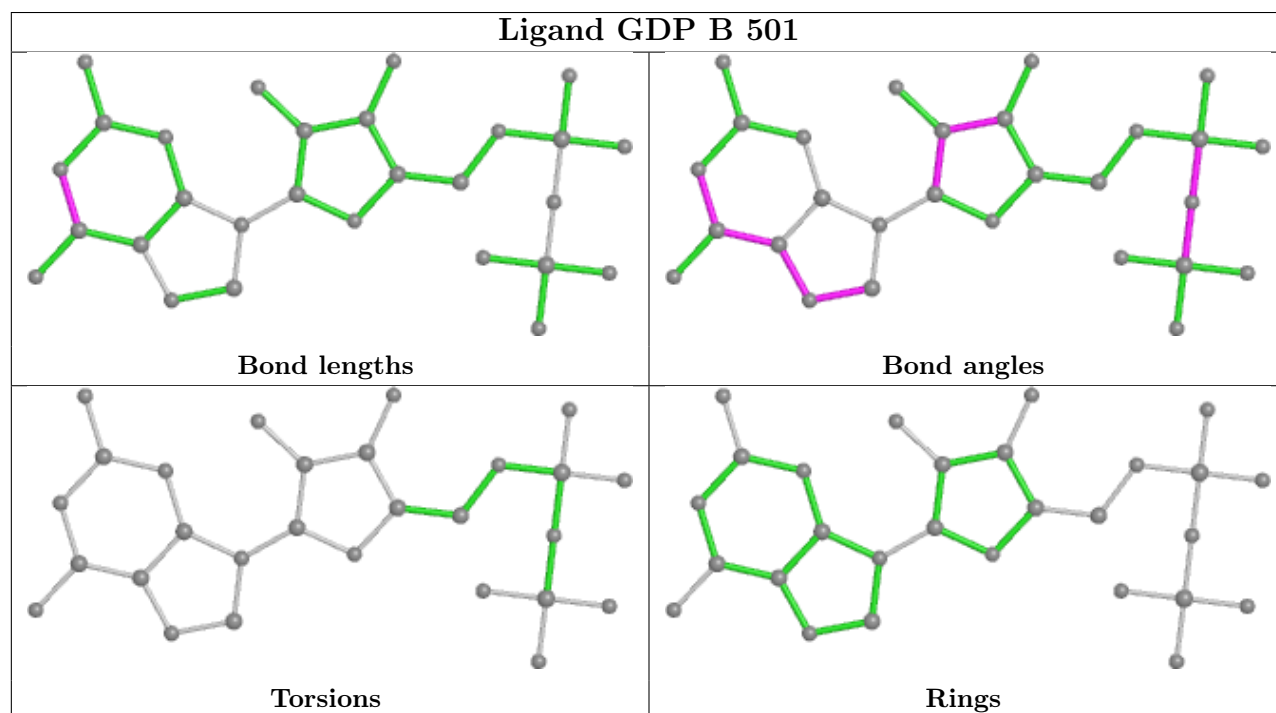
There are no ring outliers.

1 monomer is involved in 3 short contacts:

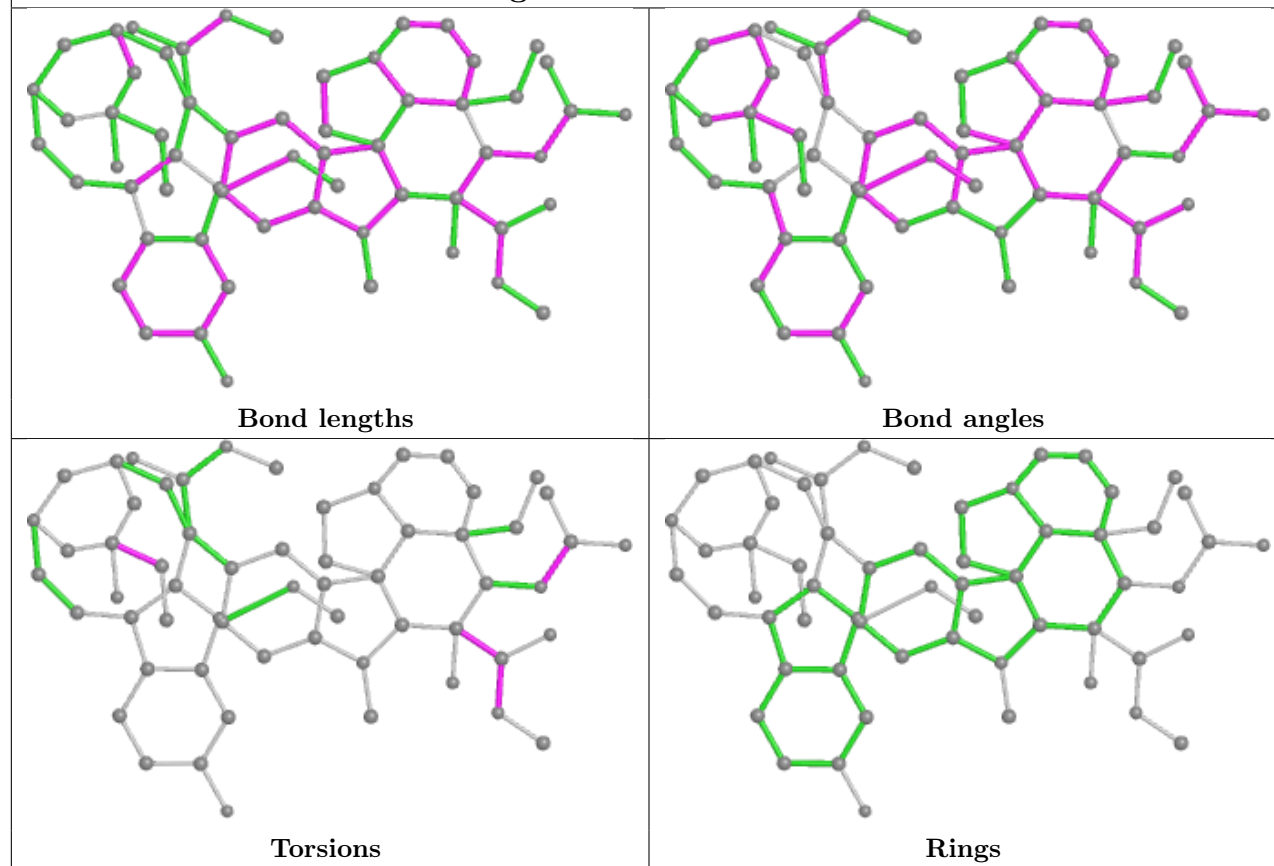
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	504	A1EPR	3	0

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

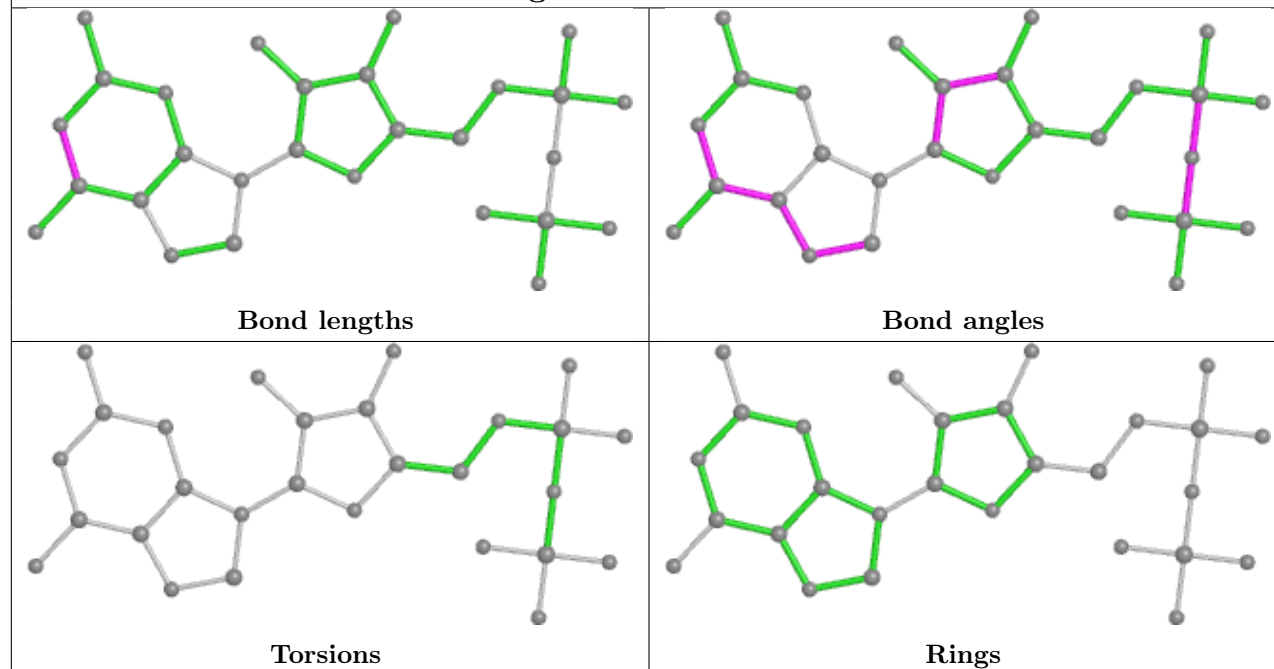
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



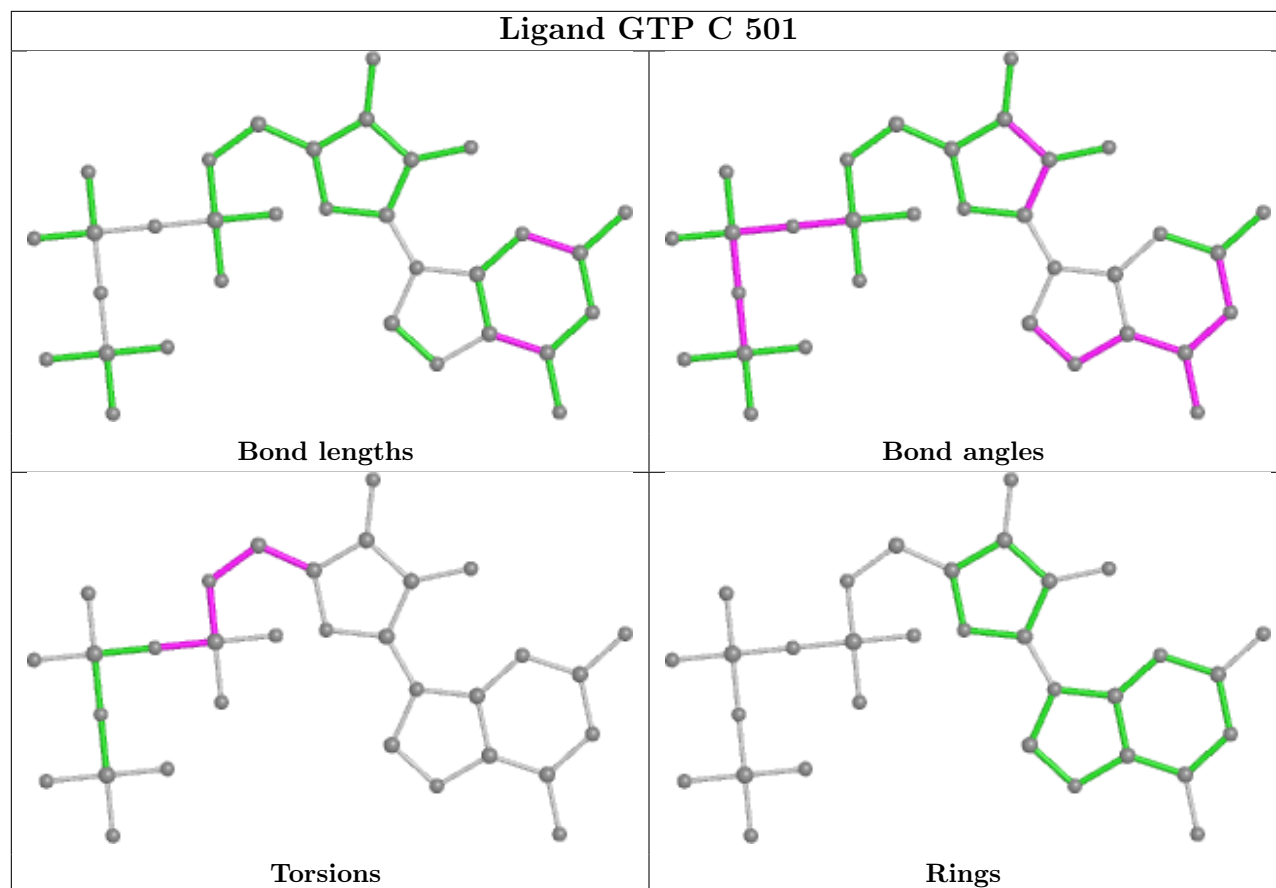
## Ligand A1EPR C 504



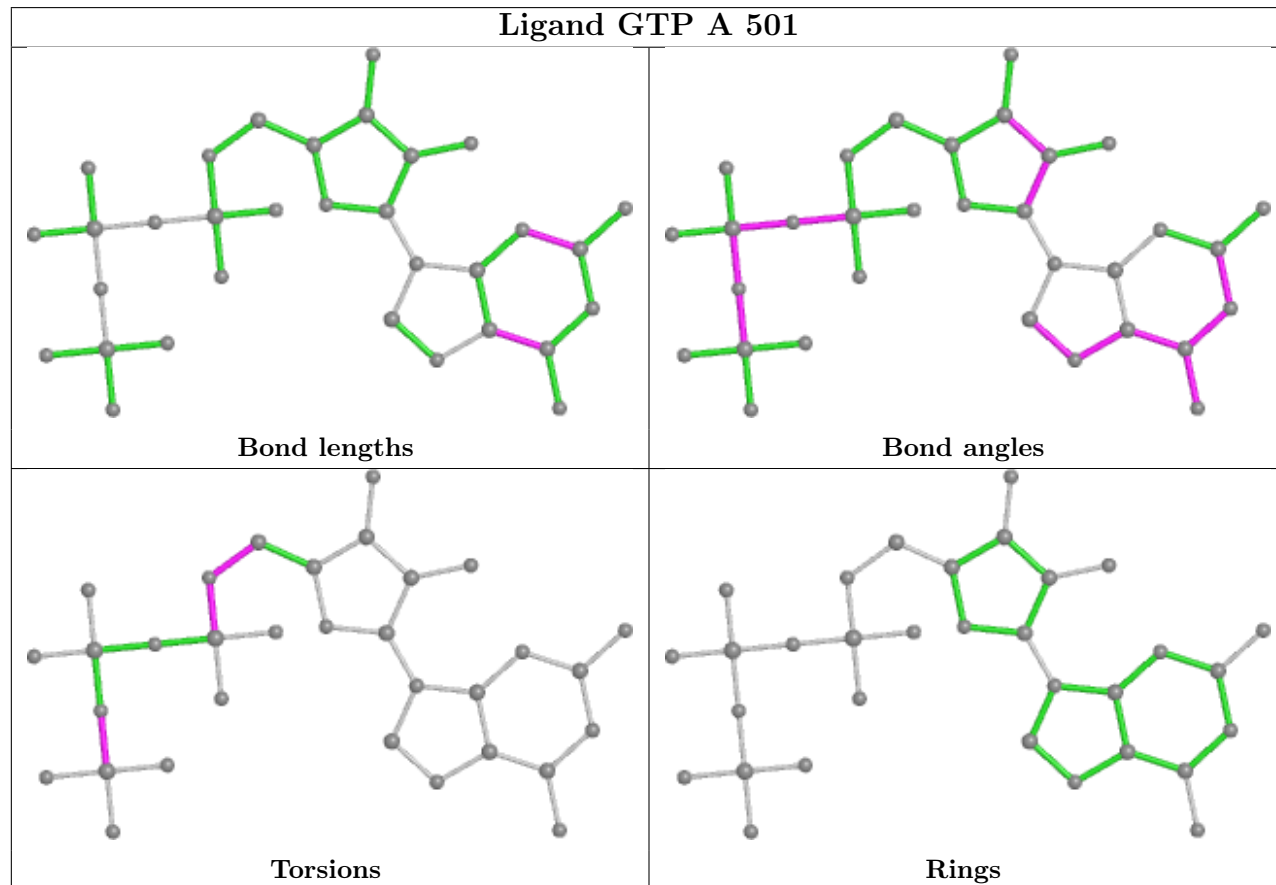
## Ligand GDP D 501



## Ligand GTP C 501



## Ligand GTP A 501



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	439/450 (97%)	-0.07	12 (2%) 56 55	20, 41, 68, 116	9 (2%)
1	C	440/450 (97%)	-0.27	7 (1%) 70 70	16, 35, 56, 72	7 (1%)
2	B	428/445 (96%)	-0.31	9 (2%) 63 62	20, 34, 65, 105	5 (1%)
2	D	424/445 (95%)	0.65	41 (9%) 15 14	28, 58, 90, 124	6 (1%)
3	E	120/143 (83%)	0.54	8 (6%) 25 23	28, 55, 82, 93	0
4	F	331/384 (86%)	0.63	43 (12%) 9 8	29, 59, 110, 128	4 (1%)
All	All	2182/2317 (94%)	0.12	120 (5%) 32 30	16, 45, 87, 128	31 (1%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	233	PHE	6.6
2	D	1	MET	5.6
4	F	231	ALA	5.5
2	B	1	MET	5.4
4	F	234	GLN	5.1
4	F	245	ILE	4.9
4	F	162	ILE	4.8
1	A	439	SER	4.7
3	E	140	LYS	4.7
4	F	250	SER	4.6
2	B	283	TYR	4.5
4	F	160	ILE	4.4
2	D	284	ARG	4.4
1	A	282	TYR	4.2
4	F	169	LEU	4.1
2	D	130	ASP	4.0
3	E	139	LEU	4.0
4	F	125	THR	3.9
2	B	57	THR	3.9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	369	ARG	3.7
2	D	37	HIS	3.7
3	E	6	MET	3.7
4	F	372	THR	3.7
4	F	1	MET	3.6
4	F	159	GLY	3.6
2	D	285	ALA	3.6
4	F	249	TYR	3.6
2	D	56	ALA	3.5
1	A	262	TYR	3.5
1	C	440	VAL	3.4
4	F	362	ALA	3.4
4	F	239	HIS	3.3
4	F	232	ASN	3.3
2	D	82	PRO	3.2
4	F	103	THR	3.2
4	F	240	LEU	3.2
2	D	415	GLU	3.1
2	B	280	SER	3.1
4	F	144	GLY	3.1
4	F	89	GLU	3.1
1	A	437	VAL	3.1
2	D	57	THR	3.0
3	E	59	GLU	3.0
4	F	179	VAL	3.0
2	D	216	THR	2.8
4	F	90	SER	2.8
1	A	281	ALA	2.8
1	A	283	HIS	2.8
4	F	130	VAL	2.7
2	D	218	LYS	2.7
2	D	127	GLU	2.7
4	F	161	LEU	2.7
1	C	348	PRO	2.7
2	D	99	ALA	2.7
2	D	414	ASP	2.6
4	F	163	SER	2.6
2	D	50	ASN	2.6
4	F	186	LEU	2.6
2	D	181	VAL	2.6
2	D	96	GLN	2.5
4	F	137	ARG	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	97	SER	2.5
4	F	247	LYS	2.5
1	A	438	ASP	2.5
1	C	247	ALA	2.5
4	F	230	SER	2.5
2	D	372	LYS	2.5
2	D	74	THR	2.5
2	D	272	PHE	2.4
3	E	14	CYS	2.4
1	A	94	THR	2.4
1	A	96	LYS	2.4
2	D	77	SER	2.4
4	F	134	ALA	2.4
2	D	142	GLY	2.4
1	C	340	SER	2.4
4	F	177	GLY	2.3
3	E	103	GLN	2.3
2	D	295	MET	2.3
2	D	373	MET	2.3
2	B	322	ARG	2.3
1	A	346	TRP	2.3
4	F	380	HIS	2.2
4	F	149	ALA	2.2
2	B	58	GLY	2.2
1	C	284	GLU	2.2
2	D	406	HIS	2.2
2	D	11	GLN	2.2
4	F	131	PHE	2.2
2	B	77	SER	2.2
2	D	33	THR	2.2
2	D	210	TYR	2.2
4	F	229	ASN	2.2
4	F	100	ILE	2.2
4	F	255	ARG	2.2
4	F	228	TYR	2.2
2	D	402	LYS	2.2
4	F	166	ALA	2.2
2	D	144	GLY	2.2
2	D	32	PRO	2.1
2	B	282	GLN	2.1
2	D	286	LEU	2.1
1	C	283	HIS	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	229	HIS	2.1
3	E	115	HIS	2.1
2	B	56	ALA	2.1
4	F	194	PRO	2.1
1	A	48	SER	2.1
2	D	143	GLY	2.1
2	D	407	TRP	2.1
2	D	128	SER	2.1
1	C	285	GLN	2.1
4	F	136	ASN	2.1
4	F	176	GLN	2.0
2	D	219	LEU	2.0
1	A	95	GLY	2.0
2	D	291	LEU	2.0
4	F	361	LEU	2.0
3	E	122	ARG	2.0
2	D	179	ASP	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

## 6.5 Other polymers [i](#)

There are no such residues in this entry.