Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2023 – 07:41 AM EDT

PDB ID	:	3RYI
Title	:	GDP-Tubulin: rb3 stathmin-like domain complex
Authors	:	Nawrotek, A.; Knossow, M.; Gigant, B.
Deposited on	:	2011-05-11
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

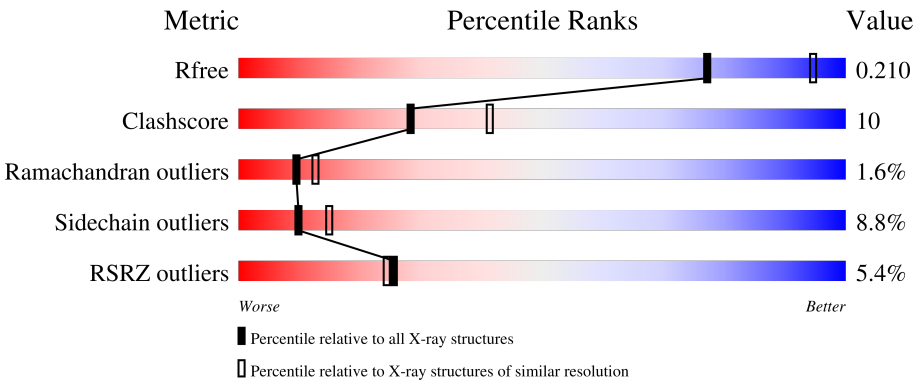
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	2%, 80%, 13%, • •
1	C	451	4%, 77%, 14%, • 5%
2	B	445	8%, 73%, 20%, • •
2	D	445	3%, 76%, 18%, • •
3	E	143	17%, 69%, 24%, • 5%

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
6	SO4	C	454	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15541 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	433	3389	2144	575	647	23	0	1	0
1	C	429	3333	2112	565	633	23	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
A	340	SER	THR	SEE REMARK 999	UNP D0VWZ0
C	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
C	340	SER	THR	SEE REMARK 999	UNP D0VWZ0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	431	3428	2155	582	664	27	0	7	0
2	D	431	3449	2163	588	672	26	0	10	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	317	THR	ALA	SEE REMARK 999	UNP D0VWY9
B	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	335	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	375	SER	ALA	SEE REMARK 999	UNP D0VWY9
D	317	THR	ALA	SEE REMARK 999	UNP D0VWY9
D	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	335	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	375	SER	ALA	SEE REMARK 999	UNP D0VWY9

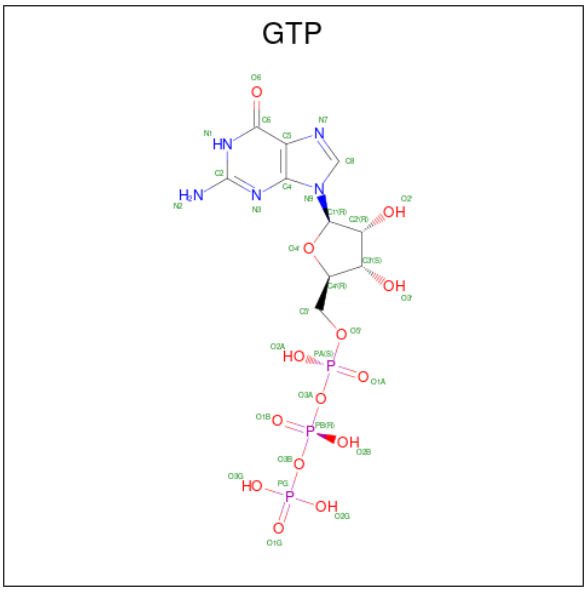
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	136	1101	680	199	218	4	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	ACE	-	SEE REMARK 999	UNP P63043
E	4	ALA	-	SEE REMARK 999	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

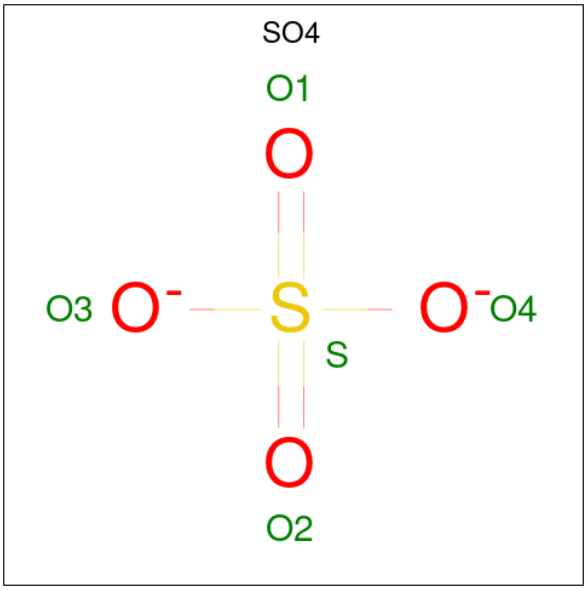
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



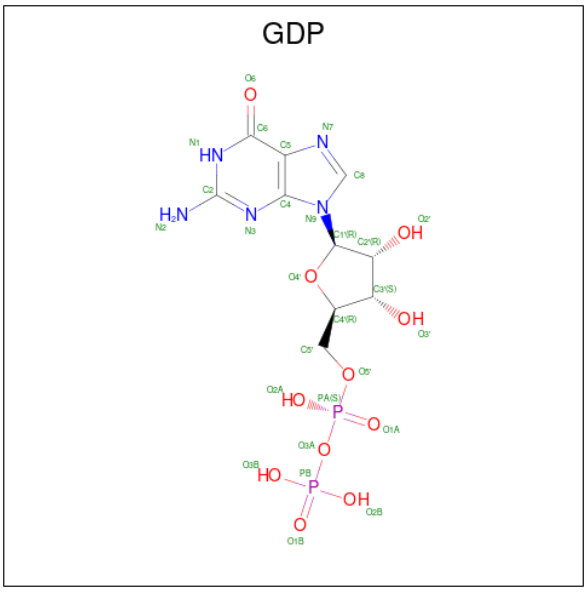
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	B	1	5	4	1	0	0
			Total	O	S		
6	C	1	5	4	1	0	0
			Total	O	S		
6	C	1	5	4	1	0	0
			Total	O	S		
6	C	1	5	4	1	0	0
			Total	O	S		
6	D	1	5	4	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	D	1	5	4	1	0	0
			Total	O	S		
6	E	1	5	4	1	0	0

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 8 is water.

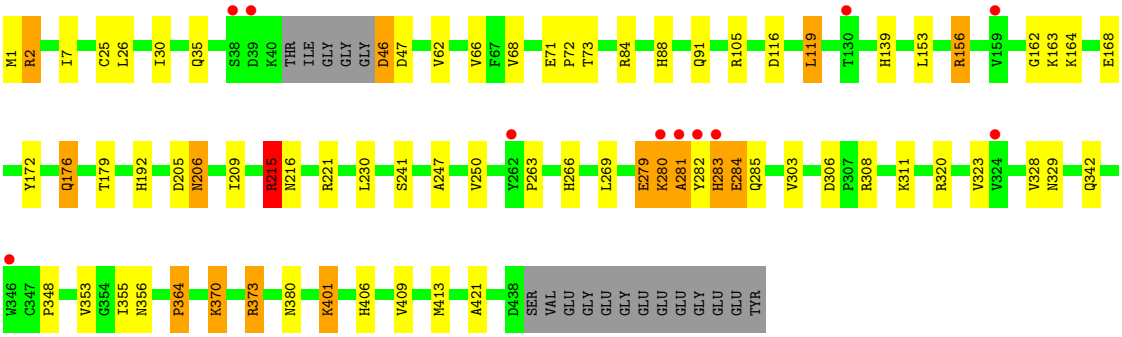
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	192	192	192	0	0
			Total	O		
8	B	128	128	128	0	0
			Total	O		
8	C	143	143	143	0	0
			Total	O		
8	D	161	161	161	0	0
			Total	O		
8	E	35	35	35	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

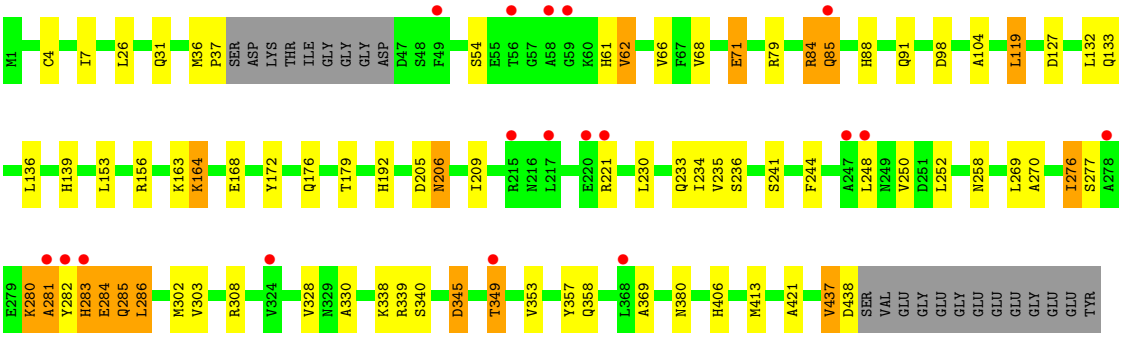
• Molecule 1: Tubulin alpha chain

Chain A:



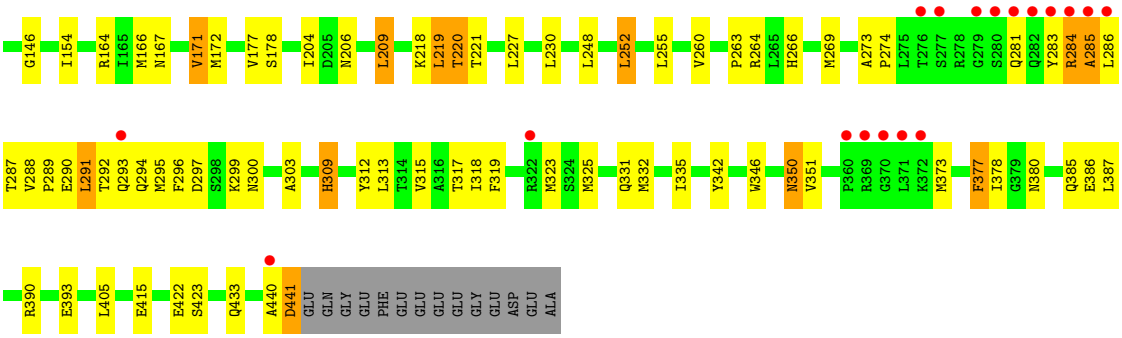
• Molecule 1: Tubulin alpha chain

Chain C:



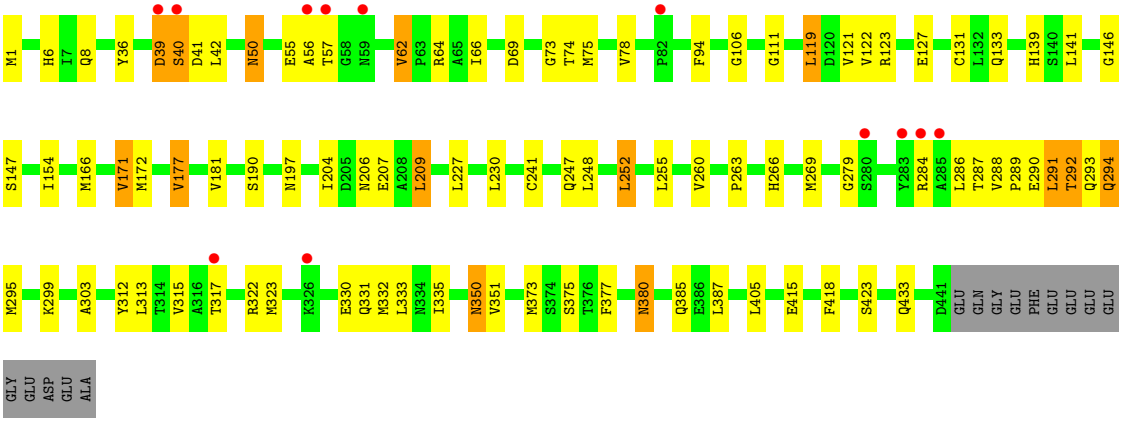
• Molecule 2: Tubulin beta chain

Chain B:



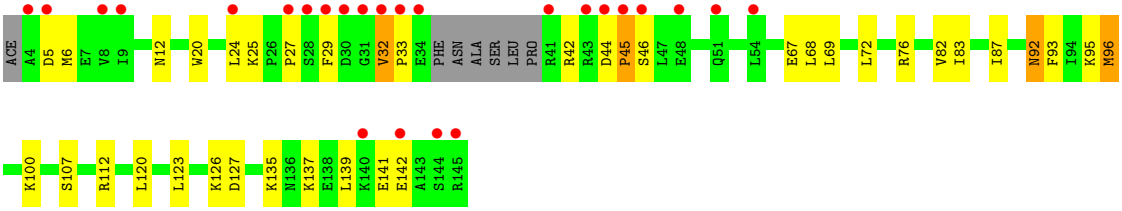
- Molecule 2: Tubulin beta chain

Chain D:



- Molecule 3: Stathmin-4

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.72Å 127.60Å 250.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.59 – 2.40 46.59 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (46.59-2.40) 97.6 (46.59-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.167 , 0.201 0.177 , 0.210	Depositor DCC
R_{free} test set	4075 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	47.6	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15541	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GTP, GDP, SO4, 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	0.46	0/3464	0.68	0/4702
1	C	0.48	0/3413	0.69	0/4636
2	B	0.48	0/3515	0.72	0/4761
2	D	0.47	0/3531	0.72	1/4782 (0.0%)
3	E	0.49	0/1116	0.71	0/1488
All	All	0.47	0/15039	0.70	1/20369 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	177	VAL	C-N-CA	5.50	135.46	121.70

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	3389	0	3292	71	0
1	C	3333	0	3236	61	0
2	B	3428	0	3279	91	0
2	D	3449	0	3304	58	0
3	E	1101	0	1083	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	32	0	12	1	0
4	C	32	0	12	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	25	0	0	0	0
6	B	5	0	0	0	0
6	C	15	0	0	0	0
6	D	10	0	0	0	0
6	E	5	0	0	0	0
7	B	28	0	12	2	0
7	D	28	0	12	2	0
8	A	192	0	0	3	0
8	B	128	0	0	5	0
8	C	143	0	0	4	0
8	D	161	0	0	2	0
8	E	35	0	0	2	0
All	All	15541	0	14242	285	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 10.

All (285) 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:C:340:SER:HB2	8:C:609:HOH:O	1.42	1.18
1:A:46:ASP:N	1:A:47:ASP:HA	1.52	1.18
1:C:281:ALA:HB1	1:C:282:TYR:C	1.68	1.13
1:C:281:ALA:HB1	1:C:282:TYR:CB	1.82	1.09
1:A:283:HIS:CB	1:A:284:GLU:OE2	2.02	1.08
1:A:119:LEU:HD21	1:A:156:ARG:HG2	1.38	1.05
2:D:241:CYS:HB2	8:D:647:HOH:O	1.53	1.04
1:A:71:GLU:OE2	1:A:73:THR:HB	1.60	1.01
1:C:281:ALA:HB1	1:C:282:TYR:CA	1.91	1.00
2:B:294[B]:GLN:HE21	2:B:294[B]:GLN:N	1.60	0.99
1:A:215:ARG:HD3	1:A:216:ASN:OD1	1.65	0.96
2:D:295[A]:MET:HG3	2:D:377[A]:PHE:HB2	1.45	0.96
8:A:461:HOH:O	2:B:440:ALA:HB1	1.67	0.94
2:B:219:LEU:O	2:B:220:THR:HG23	1.65	0.94
1:C:281:ALA:CB	1:C:282:TYR:CB	2.48	0.91
1:A:206:ASN:HD21	4:A:600:GTP:HN22	1.19	0.90
1:A:284:GLU:CB	1:A:285:GLN:HA	2.01	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:TRP:HB3	2:B:440:ALA:HB3	1.55	0.89
1:C:206:ASN:HD21	4:C:600:GTP:HN22	1.21	0.87
1:C:286:LEU:H	1:C:286:LEU:HD12	1.38	0.87
2:D:206:ASN:HD21	7:D:600:GDP:HN22	1.18	0.87
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.56	0.87
1:C:234:ILE:HD13	1:C:302:MET:HE2	1.56	0.87
2:B:206:ASN:HD21	7:B:600:GDP:HN22	1.16	0.86
1:A:71:GLU:OE2	1:A:73:THR:CB	2.25	0.85
1:C:281:ALA:CB	1:C:282:TYR:C	2.45	0.85
1:C:234:ILE:HD13	1:C:302:MET:CE	2.07	0.83
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.25	0.82
2:D:295[A]:MET:CG	2:D:377[A]:PHE:HB2	2.09	0.81
1:C:281:ALA:CA	1:C:282:TYR:CB	2.58	0.81
1:A:284:GLU:HB2	1:A:285:GLN:HA	1.63	0.80
2:B:292:THR:HB	2:B:335:ILE:HD11	1.62	0.79
3:E:92:ASN:O	3:E:96:MET:HE3	1.82	0.79
2:D:317:THR:HG21	2:D:332:MET:HE1	1.63	0.79
1:A:46:ASP:N	1:A:47:ASP:CA	2.34	0.79
1:A:280:LYS:O	1:A:281:ALA:HB2	1.84	0.77
1:C:308:ARG:HD2	8:C:609:HOH:O	1.86	0.76
3:E:92:ASN:OD1	3:E:96:MET:CE	2.34	0.75
3:E:92:ASN:OD1	3:E:96:MET:HE1	1.85	0.75
2:B:294[A]:GLN:O	2:B:296[A]:PHE:N	2.20	0.74
1:A:119:LEU:CD2	1:A:156:ARG:HG2	2.14	0.74
2:B:219:LEU:O	2:B:220:THR:CG2	2.35	0.74
2:B:317:THR:HG21	2:B:332:MET:HE1	1.70	0.74
1:A:401:LYS:NZ	2:B:440:ALA:HB2	2.03	0.74
1:C:281:ALA:CB	1:C:282:TYR:CA	2.66	0.73
1:A:280:LYS:O	1:A:281:ALA:CB	2.34	0.73
1:A:284:GLU:HB3	1:A:285:GLN:CA	2.18	0.73
2:B:440:ALA:HA	2:B:441:ASP:C	2.09	0.72
2:B:292:THR:HB	2:B:335:ILE:CD1	2.19	0.72
1:A:284:GLU:CB	1:A:285:GLN:CA	2.65	0.72
2:B:56:ALA:HB3	2:B:60:LYS:HG3	1.72	0.72
1:A:329:ASN:HD21	3:E:20:TRP:HE1	1.38	0.72
2:B:317:THR:HG21	2:B:332:MET:CE	2.20	0.70
2:B:292:THR:CB	2:B:335:ILE:HD11	2.21	0.70
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.22	0.70
1:C:281:ALA:HA	1:C:282:TYR:CB	2.22	0.69
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.23	0.69
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:291:LEU:HG	2:D:375:SER:HB2	1.75	0.69
2:D:263:PRO:O	2:D:266:HIS:HD2	1.75	0.69
2:D:75:MET:HE1	2:D:94:PHE:HB3	1.74	0.68
2:D:295[A]:MET:HG3	2:D:377[A]:PHE:CB	2.23	0.68
1:C:276:ILE:HG13	1:C:369:ALA:HB3	1.76	0.67
2:B:309:HIS:HD2	2:B:386:GLU:OE1	1.78	0.67
3:E:112:ARG:HD2	8:E:638:HOH:O	1.94	0.67
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.77	0.66
1:A:215:ARG:CD	1:A:216:ASN:OD1	2.41	0.66
2:B:294[B]:GLN:N	2:B:294[B]:GLN:NE2	2.39	0.66
2:B:30:ILE:HD11	2:B:49:ILE:HD11	1.78	0.65
1:A:46:ASP:C	1:A:46:ASP:OD1	2.34	0.65
1:A:279:GLU:CG	1:A:279:GLU:O	2.44	0.65
2:B:263:PRO:O	2:B:266:HIS:HD2	1.79	0.65
2:D:75:MET:CE	2:D:94:PHE:HB3	2.26	0.65
2:D:312:TYR:CE2	2:D:377[A]:PHE:HZ	2.14	0.65
2:D:332:MET:O	2:D:335:ILE:HG22	1.98	0.63
3:E:92:ASN:O	3:E:96:MET:CE	2.47	0.63
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.47	0.63
1:A:1:MET:O	1:A:2:ARG:HB2	1.99	0.62
2:D:1:MET:N	2:D:131:CYS:SG	2.66	0.62
2:B:312:TYR:CE2	2:B:377[A]:PHE:HZ	2.17	0.62
2:B:6:HIS:HE1	2:B:8:GLN:HG3	1.65	0.61
2:B:167:ASN:ND2	8:B:590:HOH:O	2.33	0.61
1:C:282:TYR:O	1:C:284:GLU:N	2.34	0.61
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.13	0.61
1:C:132:LEU:O	1:C:164:LYS:NZ	2.28	0.61
1:A:263:PRO:O	1:A:266:HIS:HD2	1.85	0.60
2:B:6:HIS:CE1	2:B:8:GLN:HG3	2.35	0.60
1:A:26:LEU:HD21	1:A:364:PRO:HD3	1.84	0.60
1:C:284:GLU:O	1:C:285:GLN:C	2.40	0.60
1:A:279:GLU:O	1:A:279:GLU:HG3	2.00	0.60
2:B:209:LEU:HB3	2:B:227:LEU:HG	1.82	0.60
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.82	0.60
2:B:66:ILE:HG12	2:B:121:VAL:HG12	1.84	0.60
2:B:219:LEU:O	2:B:220:THR:CB	2.50	0.60
1:A:119:LEU:HD21	1:A:156:ARG:CG	2.25	0.59
2:B:1:MET:N	2:B:131:CYS:SG	2.65	0.59
2:B:286:LEU:HA	2:B:290:GLU:OE1	2.02	0.59
2:D:147[A]:SER:HB2	2:D:190:SER:HG	1.67	0.59
2:B:106:GLY:O	2:B:111:GLY:HA3	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:SER:OG	1:C:62:VAL:HG13	2.02	0.58
2:D:317:THR:HG22	2:D:377[B]:PHE:HD1	1.68	0.58
3:E:32:VAL:HB	3:E:33:PRO:CD	2.33	0.58
2:B:294[B]:GLN:HE21	2:B:294[B]:GLN:CA	2.17	0.58
2:D:66:ILE:HG12	2:D:121:VAL:HG12	1.86	0.57
2:B:133:GLN:NE2	2:B:252:LEU:H	2.03	0.57
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.45	0.57
2:D:56:ALA:HB2	2:D:62:VAL:HG12	1.85	0.57
2:B:293[B]:GLN:C	2:B:294[B]:GLN:HE21	2.08	0.57
1:C:281:ALA:CB	1:C:283:HIS:N	2.67	0.57
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.70	0.57
2:D:286:LEU:HD11	2:D:294[A]:GLN:HE22	1.69	0.57
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.70	0.56
2:D:106:GLY:O	2:D:111:GLY:HA3	2.05	0.56
1:A:283:HIS:CB	1:A:284:GLU:CD	2.74	0.56
2:D:133:GLN:NE2	2:D:252:LEU:H	2.04	0.56
3:E:32:VAL:HB	3:E:33:PRO:HD2	1.88	0.56
1:C:84:ARG:O	1:C:85:GLN:HB2	2.06	0.55
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.88	0.55
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.87	0.55
2:B:50:ASN:O	2:B:64:ARG:NH2	2.31	0.55
1:A:156:ARG:CG	1:A:156:ARG:HH11	2.20	0.54
2:B:288:VAL:HG12	2:B:331:GLN:HG3	1.89	0.54
2:B:294[B]:GLN:NE2	2:B:294[B]:GLN:CA	2.70	0.54
1:C:244:PHE:HD2	1:C:357:TYR:HH	1.56	0.54
1:C:281:ALA:HB3	1:C:283:HIS:N	2.22	0.54
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.90	0.54
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.89	0.54
2:D:209:LEU:HB3	2:D:227:LEU:HG	1.90	0.54
1:C:36:MET:HG3	1:C:61:HIS:CD2	2.42	0.54
2:D:380:ASN:ND2	8:D:526:HOH:O	2.41	0.54
8:A:461:HOH:O	2:B:440:ALA:CB	2.38	0.53
1:A:116:ASP:OD1	1:A:156:ARG:NH2	2.41	0.53
1:C:282:TYR:C	1:C:284:GLU:H	2.11	0.53
2:B:346:TRP:HB3	2:B:440:ALA:CB	2.36	0.53
3:E:44:ASP:N	3:E:45:PRO:HA	2.22	0.53
2:B:296[B]:PHE:CE1	2:B:342:TYR:HB2	2.44	0.53
2:B:297[A]:ASP:HB3	2:B:300:ASN:HD22	1.74	0.53
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.90	0.52
2:B:101:ASN:HD22	1:C:258:ASN:HD21	1.57	0.52
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:ARG:NH1	8:B:650:HOH:O	2.41	0.52
1:C:282:TYR:C	1:C:284:GLU:N	2.62	0.52
2:B:101:ASN:HA	8:B:603:HOH:O	2.09	0.52
2:B:56:ALA:HB3	2:B:60:LYS:CG	2.38	0.52
1:A:88:HIS:H	1:A:91:GLN:NE2	2.08	0.52
2:B:178:SER:OG	1:C:349:THR:HG21	2.10	0.52
2:D:350:ASN:HD22	2:D:350:ASN:H	1.58	0.51
2:B:315:VAL:HB	2:B:351:VAL:HB	1.93	0.51
1:C:88:HIS:H	1:C:91:GLN:NE2	2.09	0.51
2:D:287:THR:N	2:D:290:GLU:OE1	2.24	0.51
2:D:288:VAL:N	2:D:289:PRO:HD2	2.25	0.51
1:A:47:ASP:OD1	1:A:47:ASP:C	2.49	0.51
2:D:50:ASN:O	2:D:64:ARG:NH2	2.33	0.51
2:B:350:ASN:H	2:B:350:ASN:HD22	1.59	0.51
1:A:311:LYS:HG2	1:A:342:GLN:HG2	1.93	0.50
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.28	0.50
1:A:215:ARG:HD3	1:A:216:ASN:N	2.25	0.50
2:B:284:ARG:O	2:B:285:ALA:HB2	2.11	0.50
2:D:119:LEU:O	2:D:123:ARG:HG3	2.11	0.50
2:D:315:VAL:HB	2:D:351:VAL:HB	1.93	0.50
2:B:335:ILE:HG13	8:B:618:HOH:O	2.10	0.50
1:C:209:ILE:HD11	1:C:302:MET:CE	2.40	0.50
1:A:401:LYS:HZ1	2:B:440:ALA:HB2	1.76	0.50
2:B:206:ASN:HD21	7:B:600:GDP:N2	1.98	0.49
2:D:197:ASN:HD21	3:E:126:LYS:HE3	1.76	0.49
2:B:264:ARG:HH11	2:B:264:ARG:HB3	1.78	0.49
2:D:139:HIS:HD2	2:D:146:GLY:O	1.96	0.49
2:D:288:VAL:O	2:D:292:THR:CG2	2.60	0.49
3:E:92:ASN:OD1	3:E:96:MET:HE2	2.10	0.49
2:B:139:HIS:HD2	2:B:146:GLY:O	1.96	0.49
2:B:164:ARG:HD2	8:B:650:HOH:O	2.13	0.49
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.95	0.48
1:A:279:GLU:O	1:A:279:GLU:OE2	2.31	0.48
1:C:345:ASP:OD2	1:C:438:ASP:HB3	2.13	0.48
1:A:241:SER:HB2	8:A:560:HOH:O	2.12	0.48
2:B:287:THR:CG2	2:B:289:PRO:HD2	2.43	0.48
2:D:36:TYR:OH	2:D:39:ASP:O	2.31	0.48
1:A:323:VAL:CG2	1:A:373:ARG:HG3	2.43	0.48
1:A:323:VAL:HG22	1:A:373:ARG:HG3	1.96	0.48
1:A:156:ARG:HH11	1:A:156:ARG:HG3	1.78	0.48
2:B:171:VAL:HA	2:B:204:ILE:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:PRO:HB3	2:B:286:LEU:HD21	1.94	0.48
1:A:401:LYS:HZ3	2:B:440:ALA:HB2	1.77	0.48
2:D:171:VAL:HA	2:D:204:ILE:O	2.14	0.47
2:B:133:GLN:HE22	2:B:252:LEU:H	1.62	0.47
1:C:88:HIS:H	1:C:91:GLN:HE21	1.63	0.47
1:A:282:TYR:O	1:A:283:HIS:O	2.31	0.47
2:D:292:THR:HG21	2:D:331:GLN:HB3	1.97	0.47
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.96	0.47
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.31	0.47
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.97	0.47
1:A:88:HIS:H	1:A:91:GLN:HE21	1.63	0.47
1:C:79:ARG:HD3	8:C:525:HOH:O	2.15	0.47
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.50	0.47
1:A:176:GLN:H	1:A:176:GLN:NE2	2.13	0.47
2:D:206:ASN:HD21	7:D:600:GDP:N2	2.00	0.47
2:D:286:LEU:HD11	2:D:294[A]:GLN:NE2	2.29	0.46
2:D:312:TYR:CE2	2:D:377[A]:PHE:CZ	3.00	0.46
1:C:233:GLN:NE2	8:C:575:HOH:O	2.48	0.46
3:E:27:PRO:HB2	3:E:29:PHE:O	2.15	0.46
1:A:284:GLU:HB3	1:A:285:GLN:C	2.35	0.46
2:B:390:ARG:O	2:B:393:GLU:HG2	2.15	0.46
2:D:39:ASP:O	2:D:40:SER:C	2.53	0.46
2:D:74:THR:O	2:D:78:VAL:HG23	2.15	0.46
1:A:62:VAL:HG11	1:A:88:HIS:HD2	1.80	0.46
1:C:31:GLN:NE2	1:C:37:PRO:HG3	2.30	0.46
1:A:247:ALA:HB1	3:E:12:ASN:HB2	1.96	0.46
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.97	0.46
2:D:405:LEU:HD21	2:D:415:GLU:HG2	1.98	0.45
2:B:56:ALA:CB	2:B:60:LYS:HE2	2.46	0.45
1:C:119:LEU:HD21	1:C:156:ARG:HB3	1.98	0.45
1:A:156:ARG:CG	1:A:156:ARG:NH1	2.78	0.45
2:B:219:LEU:O	2:B:220:THR:OG1	2.32	0.45
2:B:264:ARG:HH11	2:B:264:ARG:CB	2.29	0.45
1:C:284:GLU:O	1:C:286:LEU:N	2.50	0.45
3:E:96:MET:HE3	3:E:96:MET:HB2	1.68	0.45
1:C:283:HIS:O	1:C:284:GLU:CB	2.65	0.45
2:D:288:VAL:O	2:D:292:THR:HG22	2.17	0.45
1:A:139:HIS:HE1	1:A:168:GLU:OE1	1.99	0.44
1:A:176:GLN:H	1:A:176:GLN:HE21	1.65	0.44
2:B:385:GLN:HE22	2:B:433:GLN:HE21	1.65	0.44
2:D:133:GLN:HE22	2:D:252:LEU:H	1.63	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:THR:HG22	2:B:319:PHE:HZ	1.82	0.44
1:C:192:HIS:CG	1:C:421:ALA:HA	2.53	0.44
1:A:47:ASP:OD1	1:A:47:ASP:O	2.34	0.44
2:B:285:ALA:O	2:B:286:LEU:HB2	2.17	0.44
2:D:69:ASP:O	2:D:94:PHE:HA	2.18	0.44
2:B:293[A]:GLN:O	2:B:294[A]:GLN:C	2.53	0.44
1:C:139:HIS:HE1	1:C:168:GLU:OE1	1.99	0.44
1:A:355:ILE:HD11	3:E:20:TRP:HH2	1.82	0.44
1:C:205:ASP:HB3	1:C:303:VAL:HA	2.00	0.44
2:D:69:ASP:HB2	2:D:75:MET:HE2	1.98	0.44
2:B:221:THR:HG21	1:C:330:ALA:HB2	2.00	0.44
2:B:295[A]:MET:CG	2:B:377[A]:PHE:HB2	2.48	0.44
2:D:415:GLU:O	2:D:418:PHE:HB2	2.17	0.44
2:B:36:TYR:OH	2:B:40:SER:O	2.35	0.43
2:B:273:ALA:CB	2:B:294[B]:GLN:HG3	2.48	0.43
2:D:385:GLN:HE22	2:D:433:GLN:HE21	1.64	0.43
3:E:112:ARG:CD	8:E:638:HOH:O	2.62	0.43
2:B:318:ILE:HD11	2:B:378:ILE:HD12	2.00	0.43
2:B:295[A]:MET:HG3	2:B:377[A]:PHE:HB2	1.99	0.43
2:D:286:LEU:HD22	2:D:290:GLU:HB3	2.00	0.43
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.00	0.43
1:A:370:LYS:H	1:A:370:LYS:HD3	1.84	0.43
2:B:292:THR:HG22	2:B:319:PHE:CZ	2.54	0.43
2:B:30:ILE:CD1	2:B:49:ILE:HD11	2.48	0.43
1:C:163:LYS:NZ	3:E:93:PHE:HB2	2.33	0.43
1:A:71:GLU:HG2	1:A:72:PRO:N	2.34	0.42
2:B:69:ASP:O	2:B:94:PHE:HA	2.19	0.42
2:D:295[B]:MET:HE2	2:D:295[B]:MET:HB2	1.64	0.42
2:B:317:THR:HG21	2:B:332:MET:HE2	2.01	0.42
1:A:281:ALA:O	1:A:282:TYR:C	2.58	0.42
2:D:75:MET:HE3	2:D:94:PHE:HB3	2.01	0.42
1:C:328:VAL:HG11	1:C:353:VAL:HG11	2.01	0.42
1:A:323:VAL:HG22	1:A:373:ARG:CG	2.50	0.42
2:B:154:ILE:HG23	2:B:166:MET:HG2	2.02	0.42
2:B:294[A]:GLN:O	2:B:295[A]:MET:C	2.58	0.42
2:D:123:ARG:O	2:D:127:GLU:HG2	2.19	0.42
1:A:215:ARG:HD3	1:A:216:ASN:CG	2.34	0.42
1:C:209:ILE:CD1	1:C:302:MET:CE	2.98	0.42
2:D:40:SER:O	2:D:42:LEU:N	2.52	0.42
1:C:104:ALA:HB2	1:C:413:MET:SD	2.60	0.42
1:A:25:CYS:HB3	1:A:30:ILE: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:7:ILE:HG23	1:C:66:VAL:HG13	2.03	0.41
1:A:221:ARG:HG2	2:B:325:MET:HB3	2.02	0.41
1:C:280:LYS:O	1:C:281:ALA:O	2.39	0.41
2:B:291:LEU:O	2:B:295[A]:MET:HB3	2.21	0.41
1:C:286:LEU:H	1:C:286:LEU:CD1	2.17	0.41
2:B:405:LEU:HD21	2:B:415:GLU:HG2	2.02	0.41
1:A:192:HIS:CG	1:A:421:ALA:HA	2.56	0.41
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.41
2:B:288:VAL:HB	2:B:289:PRO:HD3	2.02	0.41
1:C:62:VAL:HG21	1:C:88:HIS:HD2	1.86	0.41
1:C:437:VAL:HG23	1:C:438:ASP:N	2.35	0.41
2:D:39:ASP:HB2	2:D:40:SER:H	1.75	0.41
1:C:71:GLU:HB2	1:C:98:ASP:HB3	2.02	0.41
1:C:133:GLN:HE22	1:C:252:LEU:H	1.68	0.41
3:E:83:ILE:O	3:E:87:ILE:HG12	2.21	0.41
1:A:205:ASP:HB3	1:A:303:VAL:HA	2.03	0.40
1:C:270:ALA:O	1:C:302:MET:HG2	2.21	0.40
1:C:281:ALA:HB1	1:C:282:TYR:O	2.16	0.40
1:A:7:ILE:HG23	1:A:66:VAL:HG13	2.04	0.40
1:A:306:ASP:OD1	1:A:308:ARG:HB2	2.20	0.40
2:B:293[A]:GLN:O	2:B:294[A]:GLN:O	2.40	0.40
1:A:406:HIS:CG	2:B:263:PRO:HD3	2.56	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	430/451 (95%)	404 (94%)	19 (4%)	7 (2%)	9 13
1	C	427/451 (95%)	407 (95%)	14 (3%)	6 (1%)	11 15
2	B	436/445 (98%)	415 (95%)	14 (3%)	7 (2%)	9 13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	439/445 (99%)	420 (96%)	14 (3%)	5 (1%)	14 20
3	E	133/143 (93%)	121 (91%)	8 (6%)	4 (3%)	4 3
All	All	1865/1935 (96%)	1767 (95%)	69 (4%)	29 (2%)	9 13

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	281	ALA
2	B	60	LYS
2	B	220	THR
2	B	284	ARG
1	C	280	LYS
1	C	281	ALA
1	C	285	GLN
2	D	41	ASP
3	E	32	VAL
1	A	162	GLY
1	A	164	LYS
1	A	283	HIS
2	B	58	GLY
2	B	281	GLN
2	B	285	ALA
1	C	283	HIS
1	C	284	GLU
2	D	40	SER
3	E	6	MET
1	A	215	ARG
1	C	85	GLN
3	E	42	ARG
2	B	57	THR
2	D	57	THR
2	D	73	GLY
2	D	279	GLY
1	A	364	PRO
3	E	45	PRO

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	365/379 (96%)	341 (93%)	24 (7%)	16 26
1	C	357/379 (94%)	328 (92%)	29 (8%)	11 18
2	B	375/385 (97%)	345 (92%)	30 (8%)	12 18
2	D	379/385 (98%)	344 (91%)	35 (9%)	9 13
3	E	114/125 (91%)	91 (80%)	23 (20%)	1 1
All	All	1590/1653 (96%)	1449 (91%)	141 (9%)	10 14

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	46	ASP
1	A	68	VAL
1	A	84	ARG
1	A	105	ARG
1	A	119	LEU
1	A	153	LEU
1	A	156	ARG
1	A	163	LYS
1	A	176	GLN
1	A	179	THR
1	A	206	ASN
1	A	215	ARG
1	A	250	VAL
1	A	269	LEU
1	A	279	GLU
1	A	280	LYS
1	A	284	GLU
1	A	320	ARG
1	A	356	ASN
1	A	370	LYS
1	A	373	ARG
1	A	380	ASN
1	A	401	LYS
2	B	57	THR
2	B	62	VAL
2	B	119	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	122	VAL
2	B	139	HIS
2	B	141	LEU
2	B	171	VAL
2	B	177	VAL
2	B	209	LEU
2	B	218	LYS
2	B	219	LEU
2	B	230	LEU
2	B	248	LEU
2	B	252	LEU
2	B	255	LEU
2	B	260	VAL
2	B	283	TYR
2	B	291	LEU
2	B	299	LYS
2	B	309	HIS
2	B	313	LEU
2	B	323	MET
2	B	350	ASN
2	B	373	MET
2	B	377[A]	PHE
2	B	377[B]	PHE
2	B	380	ASN
2	B	422	GLU
2	B	423	SER
2	B	441	ASP
1	C	26	LEU
1	C	62	VAL
1	C	68	VAL
1	C	71	GLU
1	C	84	ARG
1	C	119	LEU
1	C	127	ASP
1	C	153	LEU
1	C	164	LYS
1	C	176	GLN
1	C	179	THR
1	C	206	ASN
1	C	221	ARG
1	C	235	VAL
1	C	236	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	241	SER
1	C	248	LEU
1	C	250	VAL
1	C	269	LEU
1	C	276	ILE
1	C	277	SER
1	C	286	LEU
1	C	338	LYS
1	C	339	ARG
1	C	345	ASP
1	C	349	THR
1	C	358	GLN
1	C	380	ASN
1	C	437	VAL
2	D	39	ASP
2	D	50	ASN
2	D	55	GLU
2	D	62	VAL
2	D	119	LEU
2	D	122	VAL
2	D	141	LEU
2	D	171	VAL
2	D	177	VAL
2	D	181	VAL
2	D	207	GLU
2	D	209	LEU
2	D	230	LEU
2	D	247	GLN
2	D	248	LEU
2	D	252	LEU
2	D	255	LEU
2	D	260	VAL
2	D	284	ARG
2	D	291	LEU
2	D	292	THR
2	D	293[A]	GLN
2	D	293[B]	GLN
2	D	294[A]	GLN
2	D	294[B]	GLN
2	D	299	LYS
2	D	313	LEU
2	D	322	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	323	MET
2	D	330	GLU
2	D	333	LEU
2	D	350	ASN
2	D	373	MET
2	D	380	ASN
2	D	423	SER
3	E	5	ASP
3	E	24	LEU
3	E	25	LYS
3	E	46	SER
3	E	67	GLU
3	E	68	LEU
3	E	69	LEU
3	E	72	LEU
3	E	76	ARG
3	E	82	VAL
3	E	92	ASN
3	E	95	LYS
3	E	96	MET
3	E	100	LYS
3	E	107	SER
3	E	120	LEU
3	E	123	LEU
3	E	127	ASP
3	E	135	LYS
3	E	137	LYS
3	E	139	LEU
3	E	141	GLU
3	E	142	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	35	GLN
1	A	88	HIS
1	A	91	GLN
1	A	139	HIS
1	A	176	GLN
1	A	197	HIS
1	A	206	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	249	ASN
1	A	258	ASN
1	A	266	HIS
1	A	301	GLN
1	A	329	ASN
1	A	356	ASN
1	A	358	GLN
1	A	380	ASN
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	101	ASN
2	B	133	GLN
2	B	136	GLN
2	B	139	HIS
2	B	206	ASN
2	B	229	HIS
2	B	266	HIS
2	B	300	ASN
2	B	309	HIS
2	B	350	ASN
2	B	380	ASN
2	B	385	GLN
2	B	433	GLN
1	C	8	HIS
1	C	31	GLN
1	C	88	HIS
1	C	91	GLN
1	C	107	HIS
1	C	133	GLN
1	C	139	HIS
1	C	197	HIS
1	C	206	ASN
1	C	233	GLN
1	C	256	GLN
1	C	301	GLN
1	C	380	ASN
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	133	GLN
2	D	136	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	139	HIS
2	D	197	ASN
2	D	206	ASN
2	D	266	HIS
2	D	300	ASN
2	D	350	ASN
2	D	380	ASN
2	D	385	GLN
2	D	433	GLN
2	D	436	GLN
3	E	111	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
6	SO4	D	456	-	4,4,4	0.21	0	6,6,6	0.17	0
6	SO4	C	454	-	4,4,4	0.15	0	6,6,6	0.08	0
7	GDP	D	600	-	24,30,30	1.19	3 (12%)	30,47,47	1.55	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	GDP	B	600	-	24,30,30	1.01	1 (4%)	30,47,47	1.43	5 (16%)
6	SO4	A	452	-	4,4,4	0.16	0	6,6,6	0.13	0
6	SO4	A	455	-	4,4,4	0.16	0	6,6,6	0.07	0
6	SO4	E	146	-	4,4,4	0.12	0	6,6,6	0.08	0
6	SO4	A	453	-	4,4,4	0.18	0	6,6,6	0.08	0
6	SO4	A	456	-	4,4,4	0.12	0	6,6,6	0.08	0
6	SO4	A	454	-	4,4,4	0.19	0	6,6,6	0.17	0
4	GTP	C	600	5	26,34,34	1.33	4 (15%)	32,54,54	1.24	3 (9%)
4	GTP	A	600	5	26,34,34	1.13	3 (11%)	32,54,54	1.18	3 (9%)
6	SO4	D	457	-	4,4,4	0.22	0	6,6,6	0.13	0
6	SO4	C	452	-	4,4,4	0.16	0	6,6,6	0.12	0
6	SO4	C	453	-	4,4,4	0.17	0	6,6,6	0.10	0
6	SO4	B	456	-	4,4,4	0.14	0	6,6,6	0.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	C	600	5	-	6/18/38/38	0/3/3/3
4	GTP	A	600	5	-	6/18/38/38	0/3/3/3
7	GDP	B	600	-	-	5/12/32/32	0/3/3/3
7	GDP	D	600	-	-	5/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	600	GDP	C8-N7	-3.01	1.29	1.35
4	C	600	GTP	C2'-C1'	2.93	1.58	1.53
4	A	600	GTP	O4'-C1'	2.75	1.44	1.41
4	A	600	GTP	C8-N7	-2.44	1.30	1.35
4	C	600	GTP	C8-N7	-2.40	1.30	1.35
7	D	600	GDP	C8-N7	-2.36	1.31	1.35
4	C	600	GTP	O4'-C1'	2.33	1.44	1.41
4	A	600	GTP	PA-O5'	2.19	1.68	1.59
7	D	600	GDP	PB-O2B	2.16	1.63	1.54
4	C	600	GTP	PA-O2A	2.14	1.65	1.55
7	D	600	GDP	C6-N1	-2.02	1.34	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	600	GDP	PA-O3A-PB	-4.00	119.09	132.83
7	B	600	GDP	PA-O3A-PB	-3.75	119.97	132.83
7	D	600	GDP	O4'-C1'-C2'	-3.43	101.91	106.93
4	C	600	GTP	PB-O3B-PG	-2.90	122.88	132.83
4	A	600	GTP	PB-O3B-PG	-2.85	123.06	132.83
4	C	600	GTP	PA-O3A-PB	-2.77	123.33	132.83
4	A	600	GTP	PA-O3A-PB	-2.73	123.44	132.83
4	C	600	GTP	C8-N7-C5	2.67	108.08	102.99
7	B	600	GDP	O4'-C1'-C2'	-2.57	103.17	106.93
4	A	600	GTP	C8-N7-C5	2.48	107.71	102.99
7	D	600	GDP	O2B-PB-O3A	2.43	112.78	104.64
7	B	600	GDP	C8-N7-C5	2.41	107.58	102.99
7	D	600	GDP	O3B-PB-O2B	-2.32	98.78	107.64
7	B	600	GDP	C5-C6-N1	2.26	117.95	113.95
7	D	600	GDP	C5-C6-N1	2.25	117.92	113.95
7	B	600	GDP	O3B-PB-O2B	2.18	115.98	107.64
7	D	600	GDP	C2-N1-C6	-2.01	121.40	125.10

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	GTP	C5'-O5'-PA-O1A
4	A	600	GTP	C5'-O5'-PA-O2A
4	C	600	GTP	C5'-O5'-PA-O1A
4	C	600	GTP	C5'-O5'-PA-O2A
7	B	600	GDP	C5'-O5'-PA-O1A
7	D	600	GDP	C5'-O5'-PA-O1A
4	C	600	GTP	PB-O3B-PG-O3G
7	B	600	GDP	C5'-O5'-PA-O3A
7	D	600	GDP	C5'-O5'-PA-O3A
7	B	600	GDP	C5'-O5'-PA-O2A
7	D	600	GDP	C5'-O5'-PA-O2A
4	A	600	GTP	PB-O3A-PA-O2A
4	C	600	GTP	PB-O3A-PA-O2A
7	B	600	GDP	PB-O3A-PA-O2A
4	A	600	GTP	PB-O3B-PG-O1G
4	C	600	GTP	PB-O3B-PG-O1G
4	A	600	GTP	PB-O3B-PG-O3G
4	A	600	GTP	C5'-O5'-PA-O3A
4	C	600	GTP	C5'-O5'-PA-O3A
7	B	600	GDP	PB-O3A-PA-O1A
7	D	600	GDP	PB-O3A-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	D	600	GDP	PB-O3A-PA-O2A

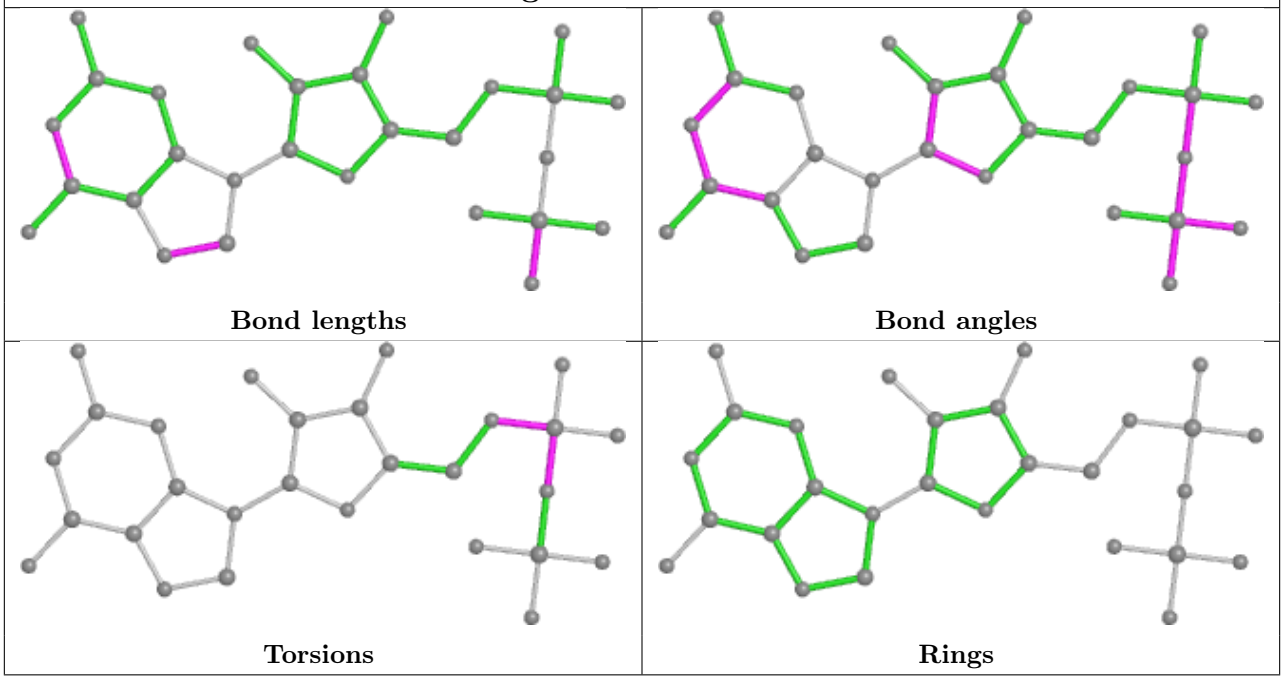
There are no ring outliers.

4 monomers are involved in 6 short contacts:

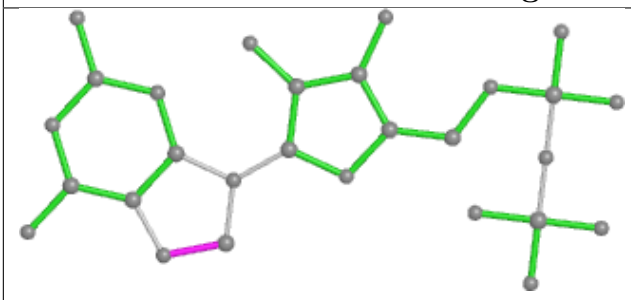
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	600	GDP	2	0
7	B	600	GDP	2	0
4	C	600	GTP	1	0
4	A	600	GTP	1	0

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 then 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.

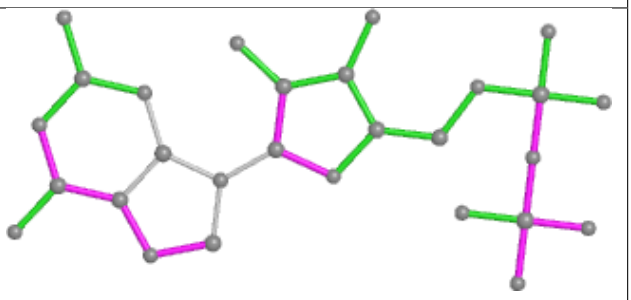
Ligand GDP D 600



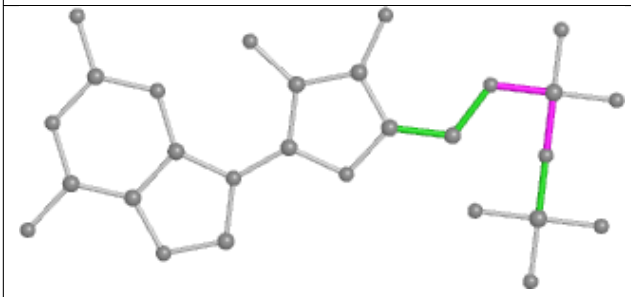
Ligand GDP B 600



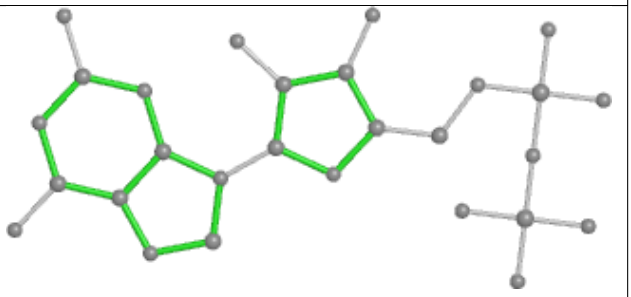
Bond lengths



Bond angles

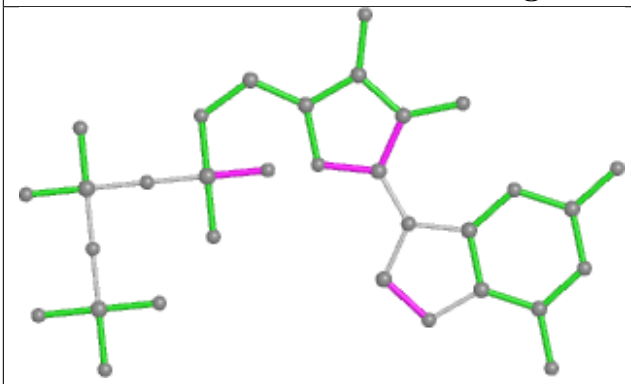


Torsions

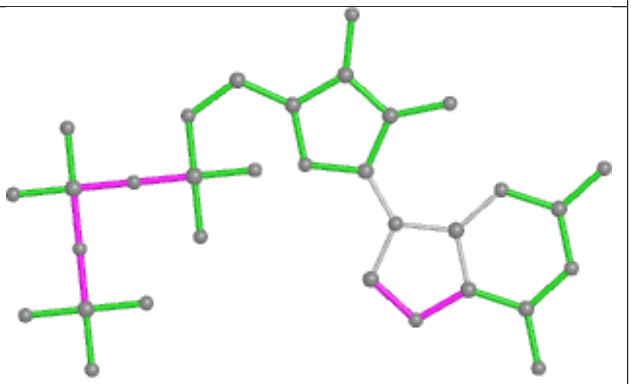


Rings

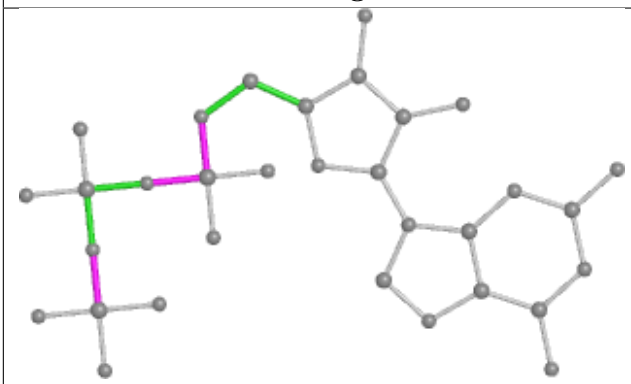
Ligand GTP C 600



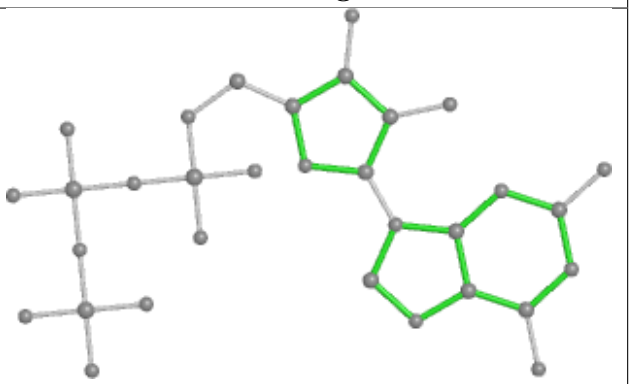
Bond lengths



Bond angles

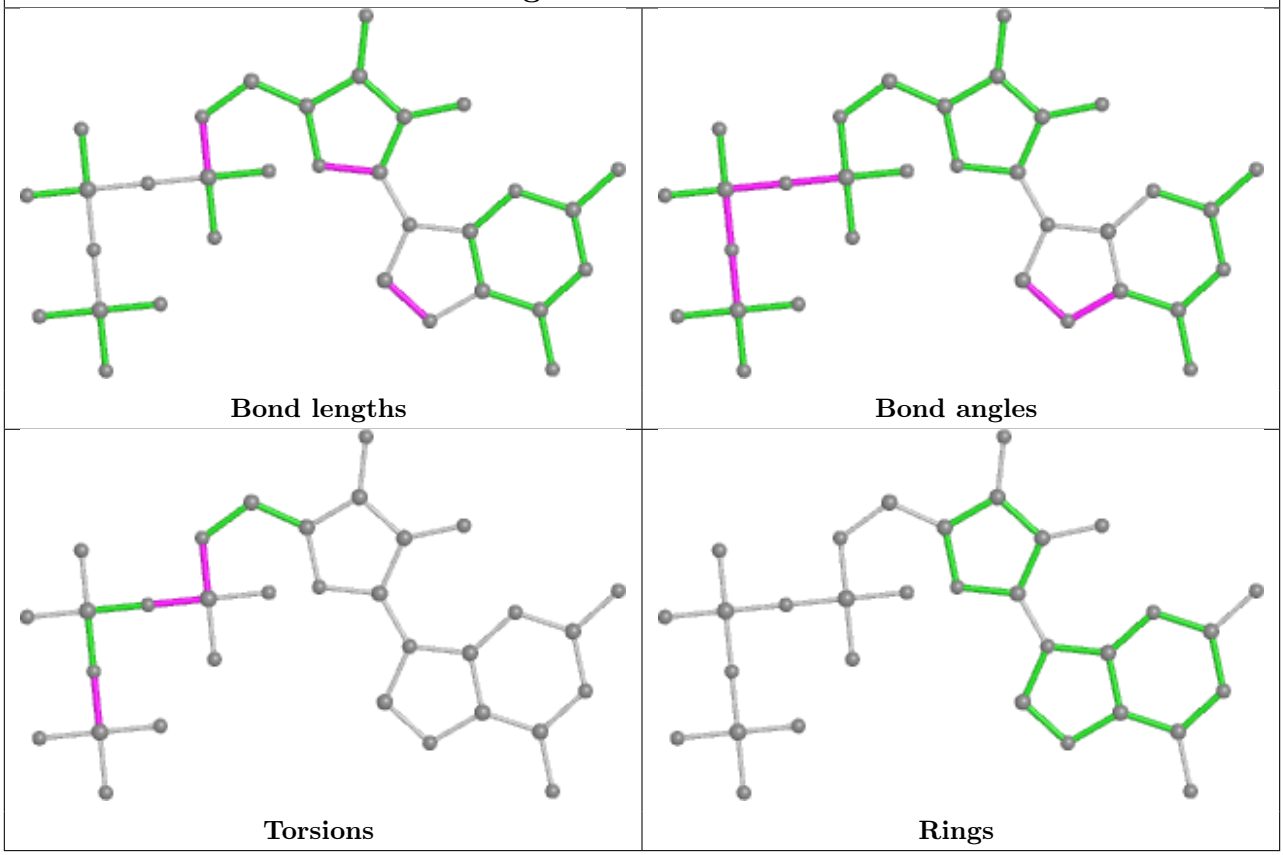


Torsions



Rings

Ligand GTP A 600



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	433/451 (96%)	-0.13	11 (2%)	57	55	41, 60, 91, 133	0
1	C	429/451 (95%)	0.12	18 (4%)	36	35	44, 68, 106, 145	0
2	B	431/445 (96%)	0.33	34 (7%)	12	11	39, 63, 115, 171	1 (0%)
2	D	431/445 (96%)	-0.07	12 (2%)	53	51	38, 55, 99, 138	1 (0%)
3	E	136/143 (95%)	0.90	25 (18%)	1	1	60, 80, 128, 155	0
All	All	1860/1935 (96%)	0.13	100 (5%)	25	24	38, 63, 107, 171	2 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	283	TYR	10.8
3	E	33	PRO	9.0
3	E	32	VAL	8.9
3	E	31	GLY	8.4
2	B	371	LEU	7.6
2	B	283	TYR	7.5
2	D	284	ARG	6.1
2	B	282	GLN	5.6
1	C	281	ALA	5.3
1	C	56	THR	5.3
3	E	45	PRO	5.3
2	B	285	ALA	5.2
3	E	144	SER	5.1
1	C	217	LEU	5.0
2	B	280	SER	5.0
3	E	41	ARG	5.0
3	E	43	ARG	4.9
3	E	30	ASP	4.9
3	E	4	ALA	4.9
2	B	57	THR	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	440	ALA	4.8
1	A	282	TYR	4.8
2	B	279	GLY	4.4
2	B	37	HIS	3.9
1	A	281	ALA	3.8
2	B	38	GLY	3.8
2	B	36	TYR	3.7
3	E	145	ARG	3.7
2	D	285	ALA	3.7
1	C	58	ALA	3.6
2	B	59	ASN	3.6
2	B	49	ILE	3.5
3	E	8	VAL	3.5
2	B	284	ARG	3.5
2	B	369	ARG	3.4
3	E	51	GLN	3.3
2	B	277	SER	3.3
3	E	142	GLU	3.2
2	B	39	ASP	3.2
1	A	130	THR	3.2
2	B	42	LEU	3.1
1	C	283	HIS	3.1
2	B	281	GLN	3.1
2	D	82	PRO	3.0
3	E	5	ASP	3.0
1	C	282	TYR	3.0
1	C	324	VAL	3.0
2	B	372	LYS	2.9
3	E	34	GLU	2.9
3	E	140	LYS	2.8
1	C	278	ALA	2.7
3	E	48	GLU	2.7
2	B	98	GLY	2.7
3	E	24	LEU	2.7
2	D	56	ALA	2.6
1	A	280	LYS	2.6
1	C	349	THR	2.6
2	D	59	ASN	2.6
2	D	39	ASP	2.6
3	E	29	PHE	2.6
2	B	111	GLY	2.6
1	C	247	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	54	LEU	2.5
1	A	38	SER	2.5
3	E	44	ASP	2.5
1	C	221	ARG	2.5
2	B	322	ARG	2.5
1	A	262	TYR	2.5
1	C	248	LEU	2.4
2	D	280	SER	2.4
1	C	59	GLY	2.4
1	A	346	TRP	2.4
2	B	56	ALA	2.4
2	B	112	ALA	2.4
1	A	283	HIS	2.4
1	C	49	PHE	2.4
2	B	61	TYR	2.4
1	C	368	LEU	2.4
2	B	360	PRO	2.3
2	B	370	GLY	2.3
1	A	159	VAL	2.3
3	E	28	SER	2.3
2	B	99	ALA	2.3
2	B	276	THR	2.2
2	D	57	THR	2.2
3	E	27	PRO	2.2
1	C	85	GLN	2.2
2	B	293[A]	GLN	2.2
2	D	326	LYS	2.2
2	B	93	VAL	2.2
3	E	46	SER	2.2
2	B	115	VAL	2.1
2	D	40	SER	2.1
1	A	39	ASP	2.1
3	E	9	ILE	2.1
2	D	317	THR	2.0
1	C	215	ARG	2.0
1	A	324	VAL	2.0
2	B	286	LEU	2.0
1	C	220	GLU	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)

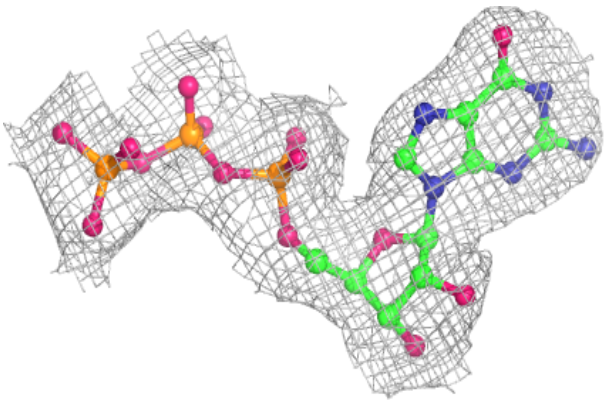
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

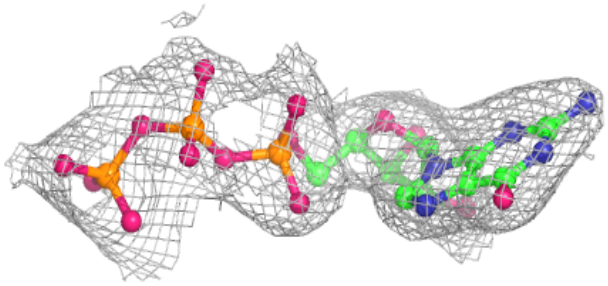
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	A	456	5/5	0.48	0.33	191,196,197,197	0
6	SO4	C	454	5/5	0.64	0.57	208,213,213,214	0
6	SO4	A	455	5/5	0.86	0.21	148,152,154,154	0
6	SO4	D	457	5/5	0.86	0.13	136,140,141,141	0
6	SO4	B	456	5/5	0.89	0.14	115,119,119,120	0
6	SO4	C	453	5/5	0.89	0.35	142,146,146,147	0
6	SO4	A	453	5/5	0.90	0.15	131,135,136,137	0
6	SO4	E	146	5/5	0.93	0.15	129,133,134,135	0
6	SO4	A	454	5/5	0.96	0.13	99,103,104,104	0
5	MG	C	601	1/1	0.97	0.13	61,61,61,61	0
6	SO4	C	452	5/5	0.97	0.10	96,100,101,101	0
6	SO4	A	452	5/5	0.97	0.18	90,94,95,96	0
4	GTP	C	600	32/32	0.98	0.14	49,55,58,60	0
5	MG	A	601	1/1	0.98	0.17	54,54,54,54	0
7	GDP	B	600	28/28	0.98	0.15	51,53,55,57	0
6	SO4	D	456	5/5	0.99	0.12	73,79,79,79	0
4	GTP	A	600	32/32	0.99	0.16	43,46,49,51	0
7	GDP	D	600	28/28	0.99	0.10	39,41,46,47	0

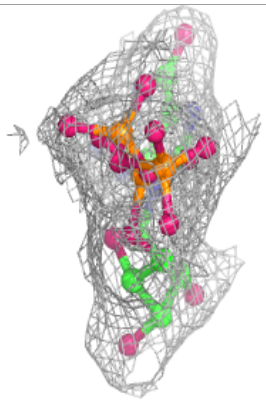
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP C 600:

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

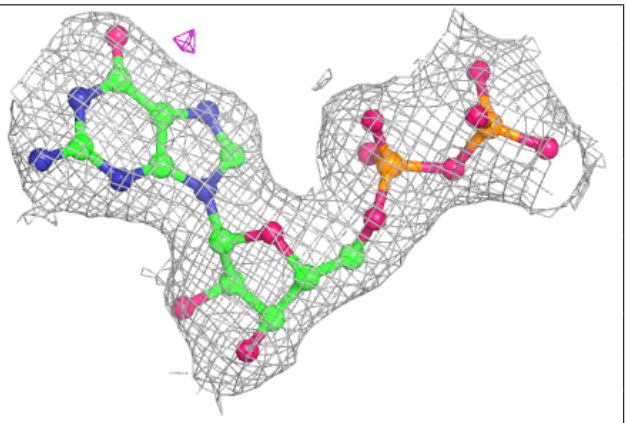


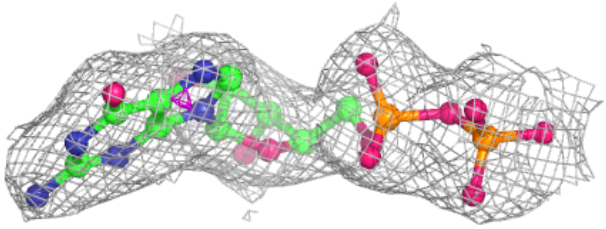


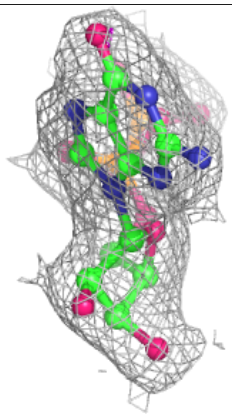


Electron density around GDP B 600:

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

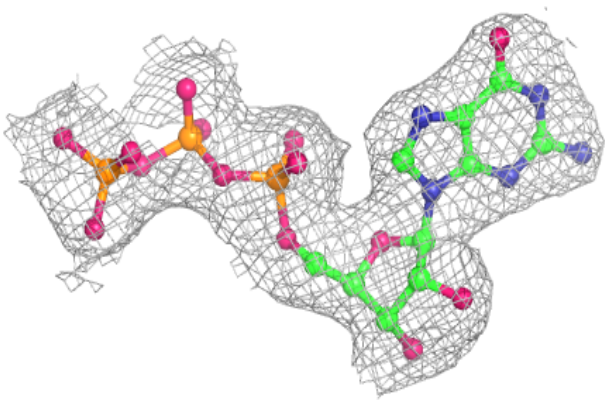


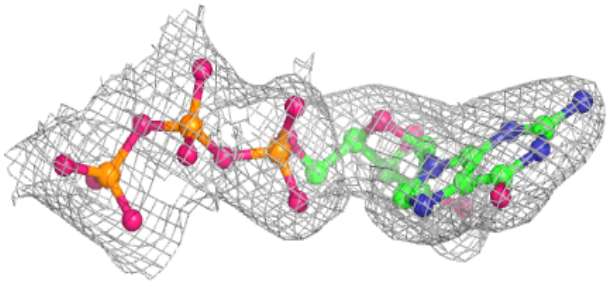


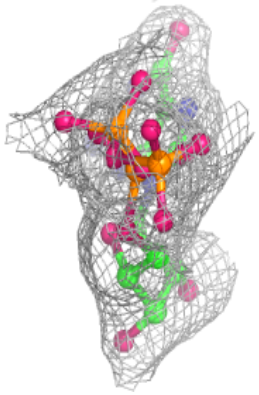


Electron density around GTP A 600:

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

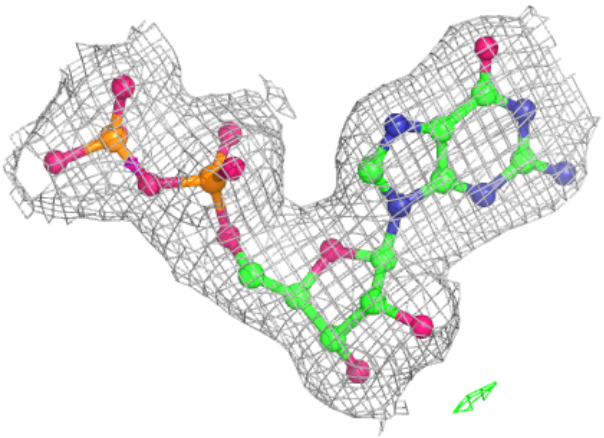


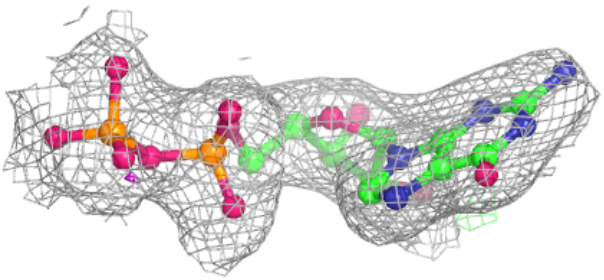


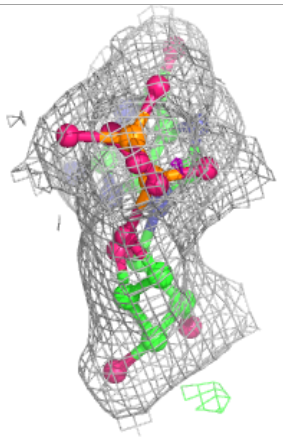


Electron density around GDP D 600:

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







6.5 Other polymers (i)

There are no such residues in this entry.