



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 02:30 pm GMT

PDB ID : 2QAG
Title : Crystal structure of human septin trimer 2/6/7
Authors : Sirajuddin, M.
Deposited on : 2007-06-15
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

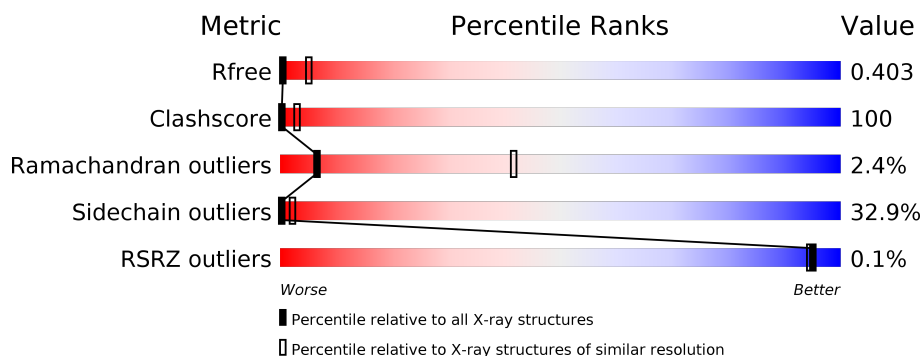
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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}	111664	1008 (4.38-3.62)
Clashscore	122126	1012 (4.34-3.66)
Ramachandran outliers	120053	1000 (4.36-3.64)
Sidechain outliers	120020	1023 (4.38-3.62)
RSRZ outliers	108989	1107 (4.40-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	361	
2	B	427	
3	C	418	

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
4	GDP	A	362	-	-	X	-
4	GDP	C	419	-	-	X	-
5	GTP	B	428	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4495 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 Septin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1765	1129	302	328	6			

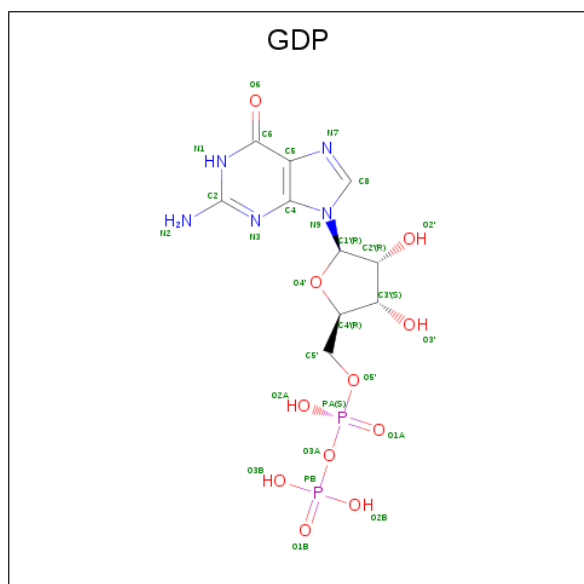
- Molecule 2 is a protein called Septin-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	246	Total	C	N	O	S	0	0	0
			1369	837	254	269	9			

- Molecule 3 is a protein called Septin-7.

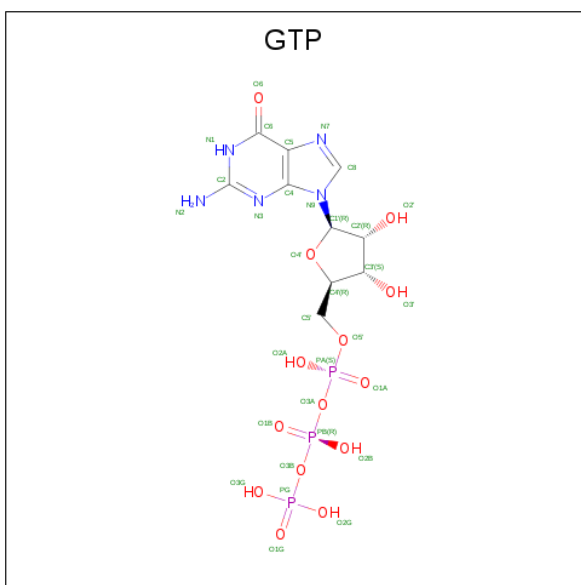
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	224	Total	C	N	O	S	0	0	0
			1273	788	230	247	8			

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
4	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



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

ARG GLN MET PHE VAL GLN ARG VAL LYS LYS LYS ALA LEU LYS HIS GLU LYS PHE ASP ARG LEU LYS LYS HIS GLN ASP GLU LYS LYS LYS LEU LEU SER SER LEU ASP ASP VAL ASN PHE GLN LYS ARG LYS THR

ALA	GLU	LEU	LEU	GLN	SER	GLN	GLY	SER	GLN	ALA	GLY	GLY	SER	GLN	THR	LEU	LYS	ARG	ASP	LYS	GLU	LYS	LYS	ASN
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- Molecule 3: Septin-7



MET	VAL	ALA	ALA	GLN	GLN	LYS	ASN	LEU	GLY	GLY	TYR	VAL	VAL	GLY	PHE
R23	R23	K24	S26	V26	K27	ARG	G29	F30	E31	F32	T33	L34	M35	V36	V37
G38	E39	S40	G41	G42	L44	G43	K44	S45	T46	L47	I48	N49	S50	L51	F52
F53	L54	T55	L56	S58	P59	E60									

[illegible]

R128	R130	R132	R133	R134	R135	R136	R137	ARG	V139	Q140	C141	C142	L143	L144	L145	L146	A147	P148	SER	G150	K154	D157	I158	M161	R162	R163	L164	H165	E166	K167	V168	M169	L173	L174	L175	A176	K177	A177	D178	T179	L180	T181	P182	E183	E184	C185	F188	I192	M193	K194	E195	L196
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I203	I204	P207	GUU	THR	ASP	ASP	GLU	GLU	GLU	ASN	LYS	LYS	LEU	VAL	LYS	L225	P226	L227	A228	V229	V230	G231	SER	ASN	THR	ILE	ILE	ILE	GLU	VAL	ASN	GLY	LYS	ARG	VAL	ARG	G245	E246	V248	P249	V250	G251	V252	A253	E254	V255	GLU	ASN	G258	E259	H260	L266
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R267	L270	I271	R272		Q276	K279	N283	H286	E287	Z288	N289	L296	A ALA	V VAL	T THR	T TRP	A ASN	S ASP	A ASN	A ASN	A ASN	L LYS	L LYS	G GLY	L LEU	L LEU	G GLN	L LYS	T THR	S SER	P PRO	L LEU	A ALA	G ARG	A ARG	C CYS	G GLU	H HIS	V VAL	A ALA	L LYS	M MET	L LYS	M MET	M MET	G GLU	F PHE
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GLU GLN VAL VAL PHE GLU MET LYS VAL VAL GLN LYS LYS GLU GLU LYS VAL VAL GLN LYS LYS LEU LEU ASP ASP SER SER GLU GLU ALA ALA GLU GLU LEU LEU GLN GLN ARG ARG HIS HIS LYS LYS GLU GLU LEU LEU GLU GLU GLU GLU LYS LYS ASN ASN LEU LEU ALA ALA GLN GLN HIS HIS LYS LYS GLU GLU LEU LEU GLU GLU GLU GLU ASP ASP ARG ARG GLN GLN PHE PHE GLU GLU ASP ASP LYS LYS GLU GLU TRP TRP ALA ALA GLN GLN LYS LYS ARG ARG TRP TRP

LEU
GLU
GLN
GLN
ASN
SER
SER
ARG
THR
LEU
GLU
LYS
ASN
LYS
LYS
LYS
GLY
LYS
ILE
PHE

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	252.51 Å 252.51 Å 156.49 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 4.00 49.13 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.15-4.00) 98.3 (49.13-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 4.00 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.376 , 0.392 0.401 , 0.403	Depositor DCC
R_{free} test set	2125 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	96.4	Xtriage
Anisotropy	1.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 217.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	4495	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP

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	0.54	2/1789 (0.1%)	0.86	7/2421 (0.3%)
2	B	0.40	0/1367	0.62	0/1865
3	C	0.62	2/1281 (0.2%)	0.85	3/1762 (0.2%)
All	All	0.53	4/4437 (0.1%)	0.79	10/6048 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	44
2	B	0	49
3	C	0	39
All	All	0	132

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	PHE	CD2-CE2	5.68	1.50	1.39
1	A	240	VAL	CA-CB	-5.67	1.42	1.54
3	C	231	GLY	N-CA	5.30	1.53	1.46
3	C	230	VAL	CA-CB	-5.03	1.44	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	VAL	CB-CA-C	-7.97	96.26	111.40
1	A	164	ASP	CB-CG-OD1	-6.38	112.56	118.30
3	C	96	PRO	N-CA-CB	5.92	110.41	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	LEU	CB-CA-C	-5.72	99.33	110.20
3	C	50	SER	N-CA-C	5.32	125.36	111.00
1	A	231	LEU	CB-CA-C	-5.30	100.12	110.20
1	A	230	LEU	N-CA-C	5.21	125.08	111.00
1	A	123	ASP	CB-CG-OD2	5.20	122.98	118.30
3	C	49	ASN	CB-CA-C	5.08	120.56	110.40
1	A	240	VAL	CB-CA-C	-5.01	101.89	111.40

There are no chirality outliers.

All (132) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ARG	Peptide
1	A	133	GLU	Peptide
1	A	134	SER	Peptide
1	A	142	ILE	Peptide
1	A	143	ASP	Peptide
1	A	147	HIS	Peptide
1	A	154	SER	Peptide
1	A	157	GLY	Peptide
1	A	160	LEU	Peptide
1	A	166	ALA	Peptide
1	A	171	ILE	Peptide
1	A	175	VAL	Peptide
1	A	177	ILE	Peptide
1	A	184	ALA	Peptide
1	A	185	ASP	Peptide
1	A	186	THR	Peptide
1	A	198	ARG	Peptide
1	A	209	LYS	Peptide
1	A	22	ASN	Peptide
1	A	238	SER	Peptide
1	A	241	GLY	Peptide
1	A	242	SER	Peptide
1	A	243	ASN	Peptide
1	A	256	ARG	Peptide
1	A	259	PRO	Peptide
1	A	260	TRP	Peptide
1	A	267	ASN	Peptide
1	A	281	ILE	Peptide
1	A	282	THR	Peptide
1	A	283	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	A	285	GLN	Peptide
1	A	286	ASP	Peptide
1	A	287	LEU	Peptide
1	A	300	ARG	Peptide
1	A	301	SER	Peptide
1	A	303	ARG	Peptide
1	A	33	LYS	Peptide
1	A	35	GLY	Peptide
1	A	38	PHE	Peptide
1	A	46	SER	Peptide
1	A	47	GLY	Peptide
1	A	56	SER	Peptide
1	A	60	THR	Peptide
1	A	99	VAL	Peptide
2	B	100	VAL	Peptide
2	B	105	PHE	Peptide
2	B	106	GLY	Peptide
2	B	111	LYS	Peptide
2	B	119	VAL	Peptide
2	B	122	ILE	Peptide
2	B	123	ASP	Peptide
2	B	127	GLU	Peptide
2	B	128	ALA	Peptide
2	B	130	LEU	Peptide
2	B	131	GLN	Peptide
2	B	132	GLU	Peptide
2	B	137	ARG	Peptide
2	B	142	THR	Peptide
2	B	143	TYR	Peptide
2	B	148	ILE	Peptide
2	B	150	VAL	Peptide
2	B	151	CYS	Peptide
2	B	155	ILE	Peptide
2	B	156	ALA	Peptide
2	B	157	PRO	Peptide
2	B	163	LYS	Peptide
2	B	175	SER	Peptide
2	B	176	LYS	Peptide
2	B	18	PRO	Peptide
2	B	180	ILE	Peptide
2	B	181	PRO	Peptide
2	B	183	ILE	Peptide

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Mol	Chain	Res	Type	Group
2	B	207	SER	Peptide
2	B	21	GLY	Peptide
2	B	212	ILE	Peptide
2	B	215	PHE	Peptide
2	B	222	VAL	Peptide
2	B	234	PRO	Peptide
2	B	236	ALA	Peptide
2	B	249	LYS	Peptide
2	B	258	TRP	Peptide
2	B	260	THR	Peptide
2	B	280	ARG	Peptide
2	B	282	ASN	Peptide
2	B	34	ASN	Peptide
2	B	37	VAL	Peptide
2	B	40	GLY	Peptide
2	B	51	THR	Peptide
2	B	76	GLN	Peptide
2	B	82	GLN	Peptide
2	B	89	GLN	Peptide
2	B	93	VAL	Peptide
2	B	99	ILE	Peptide
3	C	117	SER	Peptide
3	C	132	ARG	Peptide
3	C	139	VAL	Peptide
3	C	142	CYS	Peptide
3	C	145	PHE	Peptide
3	C	146	ILE	Peptide
3	C	150	GLY	Peptide
3	C	16	ASN	Peptide
3	C	166	GLU	Peptide
3	C	167	LYS	Peptide
3	C	17	LEU	Peptide
3	C	177	ALA	Peptide
3	C	180	LEU	Peptide
3	C	19	ASN	Peptide
3	C	20	GLN	Peptide
3	C	203	ILE	Peptide
3	C	204	TYR	Peptide
3	C	225	LEU	Peptide
3	C	228	ALA	Peptide
3	C	253	ALA	Peptide
3	C	254	GLU	Peptide

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Mol	Chain	Res	Type	Group
3	C	259	GLU	Peptide
3	C	26	VAL	Peptide
3	C	270	LEU	Peptide
3	C	272	ARG	Peptide
3	C	286	HIS	Peptide
3	C	288	GLU	Peptide
3	C	30	PHE	Peptide
3	C	31	GLU	Peptide
3	C	33	THR	Peptide
3	C	34	LEU	Peptide
3	C	40	SER	Peptide
3	C	41	GLY	Peptide
3	C	42	LEU	Peptide
3	C	74	VAL	Peptide
3	C	75	GLU	Peptide
3	C	76	GLN	Peptide
3	C	88	LEU	Peptide
3	C	91	THR	Peptide

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	1765	0	1694	481	0
2	B	1369	0	854	180	0
3	C	1273	0	822	149	0
4	A	28	0	12	14	0
4	C	28	0	12	15	0
5	B	32	0	12	18	0
All	All	4495	0	3406	791	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 100.

All (791) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:VAL:HG12	1:A:266:GLU:CG	1.46	1.43
1:A:183:LYS:HD2	4:A:362:GDP:C5	1.67	1.29
1:A:279:MET:O	1:A:282:THR:HG22	1.34	1.26
2:B:54:GLY:CA	2:B:57:THR:HG23	1.70	1.22
1:A:183:LYS:HD2	4:A:362:GDP:C4	1.73	1.21
1:A:265:VAL:CG1	1:A:266:GLU:HG2	1.69	1.21
1:A:22:ASN:C	1:A:24:PRO:HD2	1.62	1.20
1:A:258:TYR:HB3	1:A:260:TRP:O	1.35	1.19
1:A:282:THR:HG23	1:A:283:HIS:CD2	1.78	1.18
1:A:173:ASN:CA	1:A:294:LEU:HD22	1.73	1.18
2:B:257:PRO:HB2	2:B:258:TRP:CD1	1.79	1.17
3:C:148:PRO:HG2	3:C:150:GLY:CA	1.73	1.17
1:A:175:VAL:HG12	1:A:176:ASN:HB2	1.17	1.17
1:A:282:THR:HG23	1:A:283:HIS:H	1.05	1.16
1:A:267:ASN:HB3	1:A:270:HIS:CB	1.77	1.15
2:B:166:ASP:O	2:B:169:THR:HG22	1.47	1.15
3:C:43:GLY:HA2	3:C:46:THR:HG22	1.15	1.15
1:A:208:ILE:HD13	1:A:209:LYS:H	1.10	1.14
2:B:185:LYS:HG3	5:B:428:GTP:C6	1.81	1.14
1:A:173:ASN:HA	1:A:294:LEU:CD2	1.78	1.14
1:A:208:ILE:CD1	1:A:209:LYS:H	1.60	1.13
1:A:245:LEU:C	1:A:246:ILE:HD13	1.67	1.12
2:B:57:THR:HG22	5:B:428:GTP:O1A	1.48	1.11
2:B:116:LYS:N	2:B:117:PRO:HD2	1.57	1.11
1:A:139:ARG:H	1:A:141:ILE:HG23	0.96	1.11
2:B:185:LYS:HE3	5:B:428:GTP:C4	1.85	1.11
3:C:43:GLY:HA2	3:C:46:THR:CG2	1.79	1.10
3:C:45:SER:HA	3:C:48:ILE:HD12	1.21	1.10
1:A:173:ASN:HA	1:A:294:LEU:HD22	1.22	1.10
1:A:179:PRO:HG3	1:A:210:ILE:HD13	1.10	1.09
1:A:275:LYS:O	1:A:279:MET:HB3	1.53	1.08
1:A:23:LEU:N	1:A:24:PRO:HD2	1.67	1.08
1:A:211:TYR:OH	1:A:214:PRO:HD2	1.54	1.08
3:C:42:LEU:HA	4:C:419:GDP:H5''	1.16	1.08
3:C:43:GLY:O	3:C:46:THR:HG23	1.53	1.07
1:A:130:LEU:HB2	1:A:295:HIS:HE1	1.19	1.07
1:A:239:VAL:HG12	1:A:273:PHE:HA	1.24	1.07
1:A:224:PHE:CD2	1:A:224:PHE:C	2.27	1.06
3:C:46:THR:O	3:C:50:SER:HB2	1.55	1.06
1:A:122:ILE:HD12	1:A:126:PHE:HE1	1.20	1.06
1:A:179:PRO:CG	1:A:210:ILE:HD13	1.84	1.06
3:C:43:GLY:CA	3:C:46:THR:CG2	2.33	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ASP:OD2	1:A:145:ARG:HD3	1.53	1.05
3:C:148:PRO:HG2	3:C:150:GLY:HA3	1.07	1.05
1:A:283:HIS:HB3	1:A:285:GLN:HE21	1.15	1.05
1:A:282:THR:HG23	1:A:283:HIS:HD2	0.88	1.04
3:C:34:LEU:O	3:C:34:LEU:HD13	1.53	1.04
1:A:79:VAL:HG23	1:A:99:VAL:O	1.57	1.04
1:A:83:ALA:HA	1:A:95:LEU:O	1.57	1.04
2:B:116:LYS:H	2:B:117:PRO:HD2	1.15	1.04
2:B:185:LYS:HA	5:B:428:GTP:O6	1.56	1.03
2:B:54:GLY:CA	2:B:57:THR:CG2	2.36	1.03
1:A:265:VAL:CG1	1:A:266:GLU:CG	2.30	1.03
2:B:46:LEU:O	2:B:151:CYS:HA	1.58	1.03
1:A:282:THR:CG2	1:A:283:HIS:HD2	1.71	1.03
1:A:267:ASN:HB3	1:A:270:HIS:HB3	1.38	1.02
1:A:213:LEU:O	1:A:213:LEU:HD23	1.59	1.02
2:B:64:ASN:O	2:B:65:THR:HG23	1.59	1.02
1:A:54:ILE:HG13	1:A:58:PHE:CE2	1.95	1.02
1:A:201:ASP:O	1:A:204:GLU:HB2	1.59	1.01
1:A:55:ASN:HA	1:A:60:THR:O	1.61	1.01
1:A:125:GLN:OE1	1:A:144:ASN:HB2	1.61	1.00
2:B:54:GLY:HA2	2:B:57:THR:CG2	1.92	1.00
2:B:113:ASP:O	2:B:117:PRO:HG3	1.62	1.00
2:B:155:ILE:N	2:B:155:ILE:HD13	1.75	1.00
1:A:156:PHE:HE1	1:A:186:THR:HB	1.26	0.99
1:A:175:VAL:HG12	1:A:176:ASN:CB	1.92	0.99
1:A:239:VAL:CG1	1:A:273:PHE:HA	1.93	0.98
3:C:179:THR:HG23	3:C:180:LEU:CD2	1.93	0.98
3:C:42:LEU:CA	4:C:419:GDP:H5"	1.93	0.98
1:A:175:VAL:CG1	1:A:176:ASN:HB2	1.92	0.98
1:A:258:TYR:HB2	1:A:261:GLY:O	1.63	0.98
1:A:284:MET:O	1:A:287:LEU:HG	1.63	0.98
1:A:179:PRO:HG3	1:A:210:ILE:CD1	1.94	0.98
1:A:267:ASN:OD1	1:A:270:HIS:HB2	1.64	0.97
2:B:249:LYS:CB	2:B:250:MET:HA	1.93	0.97
1:A:156:PHE:CE1	1:A:186:THR:CG2	2.47	0.97
1:A:82:GLU:HG2	1:A:97:LEU:O	1.63	0.97
1:A:57:LEU:HD21	1:A:276:LEU:HD21	1.47	0.97
3:C:148:PRO:CG	3:C:150:GLY:HA3	1.93	0.97
1:A:285:GLN:HA	1:A:287:LEU:HB2	1.46	0.97
1:A:196:LYS:O	1:A:200:LEU:HD12	1.65	0.97
1:A:153:ILE:HG21	1:A:160:LEU:HG	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:THR:HG23	1:A:283:HIS:N	1.80	0.96
2:B:249:LYS:CB	2:B:250:MET:SD	2.54	0.96
3:C:42:LEU:HA	4:C:419:GDP:C5'	1.93	0.96
1:A:151:TYR:HD2	1:A:152:PHE:N	1.64	0.95
1:A:139:ARG:N	1:A:141:ILE:HG23	1.82	0.95
3:C:77:SER:HA	3:C:88:LEU:O	1.66	0.95
1:A:23:LEU:N	1:A:24:PRO:CD	2.30	0.95
1:A:271:ASN:ND2	1:A:273:PHE:HB2	1.82	0.94
2:B:58:LEU:O	2:B:61:THR:HG22	1.67	0.94
3:C:43:GLY:CA	3:C:46:THR:HG22	1.95	0.94
1:A:39:THR:O	1:A:147:HIS:HB2	1.66	0.94
1:A:177:ILE:HB	1:A:210:ILE:HG22	1.48	0.94
1:A:265:VAL:HG12	1:A:266:GLU:HG3	1.45	0.94
1:A:208:ILE:HD13	1:A:209:LYS:N	1.82	0.93
1:A:29:ARG:O	1:A:32:VAL:HB	1.65	0.93
2:B:54:GLY:HA3	2:B:57:THR:HG23	1.50	0.93
1:A:283:HIS:CD2	1:A:283:HIS:H	1.84	0.93
1:A:268:PRO:HD3	1:A:271:ASN:O	1.69	0.93
2:B:206:VAL:HA	2:B:209:GLY:HA2	1.48	0.93
1:A:237:PHE:HD2	1:A:237:PHE:H	0.99	0.92
1:A:237:PHE:N	1:A:237:PHE:CD2	2.36	0.92
1:A:265:VAL:HG12	1:A:266:GLU:HG2	0.92	0.92
1:A:173:ASN:C	1:A:175:VAL:N	2.23	0.91
2:B:114:SER:O	2:B:117:PRO:HG2	1.70	0.91
1:A:130:LEU:HB2	1:A:295:HIS:CE1	2.04	0.91
3:C:182:PRO:HA	3:C:185:CYS:CB	2.00	0.91
1:A:156:PHE:CE1	1:A:186:THR:HG21	2.05	0.91
3:C:286:HIS:HA	3:C:289:ASN:CB	2.00	0.91
3:C:33:THR:HB	3:C:139:VAL:O	1.70	0.91
1:A:160:LEU:HD12	1:A:199:ILE:HG12	1.52	0.91
2:B:155:ILE:HD13	2:B:155:ILE:H	1.31	0.90
1:A:173:ASN:C	1:A:294:LEU:HD22	1.91	0.90
1:A:39:THR:HB	1:A:96:ARG:O	1.71	0.90
3:C:49:ASN:HB3	3:C:54:THR:O	1.69	0.90
1:A:267:ASN:HB3	1:A:270:HIS:HB2	1.49	0.90
3:C:58:SER:N	3:C:59:PRO:HD3	1.87	0.90
1:A:224:PHE:HD2	1:A:224:PHE:C	1.73	0.90
3:C:40:SER:HA	3:C:44:LYS:NZ	1.87	0.90
1:A:175:VAL:HG12	1:A:176:ASN:N	1.85	0.90
1:A:240:VAL:HG22	4:A:362:GDP:O6	1.71	0.90
1:A:39:THR:HA	1:A:96:ARG:O	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:PHE:O	1:A:224:PHE:HD2	1.54	0.89
1:A:156:PHE:HE1	1:A:186:THR:CB	1.84	0.89
1:A:57:LEU:CD2	1:A:276:LEU:HD21	2.03	0.89
1:A:81:ILE:HD12	1:A:81:ILE:O	1.72	0.89
1:A:183:LYS:CD	4:A:362:GDP:C5	2.54	0.89
1:A:43:VAL:HG22	1:A:100:VAL:HG21	1.51	0.88
1:A:212:HIS:O	1:A:214:PRO:HD3	1.73	0.88
1:A:285:GLN:HB2	1:A:288:GLN:HG3	1.54	0.88
3:C:36:VAL:HA	3:C:143:LEU:O	1.73	0.88
1:A:257:LEU:C	1:A:257:LEU:HD23	1.94	0.87
1:A:36:PHE:O	1:A:93:VAL:HG22	1.75	0.87
2:B:169:THR:O	2:B:173:LEU:HB2	1.75	0.87
1:A:285:GLN:CB	1:A:288:GLN:HG3	2.04	0.87
1:A:179:PRO:CG	1:A:210:ILE:CD1	2.52	0.86
1:A:199:ILE:O	1:A:203:ILE:HD12	1.75	0.86
1:A:267:ASN:CB	1:A:270:HIS:CB	2.54	0.86
1:A:153:ILE:H	1:A:153:ILE:HD13	1.41	0.86
1:A:82:GLU:CG	1:A:97:LEU:O	2.23	0.85
3:C:49:ASN:OD1	3:C:56:LEU:HG	1.76	0.85
1:A:267:ASN:CB	1:A:270:HIS:HB2	2.06	0.85
2:B:116:LYS:N	2:B:117:PRO:CD	2.39	0.84
2:B:60:ASP:HB3	2:B:65:THR:O	1.75	0.84
3:C:179:THR:HG23	3:C:180:LEU:HD23	1.59	0.84
2:B:153:TYR:CE2	2:B:166:ASP:HB3	2.12	0.84
1:A:122:ILE:HD12	1:A:126:PHE:CE1	2.11	0.84
1:A:177:ILE:HB	1:A:210:ILE:CG2	2.07	0.83
2:B:54:GLY:HA3	2:B:57:THR:CG2	2.05	0.83
3:C:58:SER:N	3:C:59:PRO:CD	2.41	0.83
1:A:282:THR:CG2	1:A:283:HIS:H	1.90	0.83
1:A:199:ILE:O	1:A:203:ILE:CD1	2.27	0.83
1:A:283:HIS:HD2	1:A:283:HIS:H	1.26	0.82
1:A:211:TYR:CZ	1:A:214:PRO:HD2	2.15	0.82
2:B:294:HIS:O	2:B:298:TYR:CB	2.27	0.81
3:C:41:GLY:O	4:C:419:GDP:H5''	1.80	0.81
1:A:240:VAL:HG13	4:A:362:GDP:C6	2.14	0.81
1:A:143:ASP:OD2	1:A:145:ARG:HB2	1.81	0.81
3:C:179:THR:HG23	3:C:180:LEU:HD22	1.60	0.80
1:A:211:TYR:O	1:A:211:TYR:CD2	2.33	0.80
1:A:283:HIS:HB3	1:A:285:GLN:NE2	1.94	0.80
1:A:285:GLN:HB2	1:A:288:GLN:CG	2.11	0.80
1:A:268:PRO:CD	1:A:271:ASN:O	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASN:CA	1:A:60:THR:O	2.29	0.80
3:C:40:SER:HA	3:C:44:LYS:HZ3	1.45	0.80
2:B:166:ASP:HA	2:B:169:THR:CG2	2.12	0.80
2:B:276:GLU:O	2:B:280:ARG:CB	2.30	0.80
1:A:54:ILE:CG1	1:A:58:PHE:CE2	2.64	0.79
1:A:240:VAL:HG13	4:A:362:GDP:O6	1.82	0.79
3:C:188:PHE:O	3:C:192:ILE:CG1	2.30	0.79
1:A:29:ARG:O	1:A:32:VAL:CB	2.30	0.79
2:B:44:ASN:O	2:B:149:HIS:HB2	1.83	0.79
3:C:173:LEU:CB	3:C:227:LEU:O	2.31	0.79
2:B:115:TYR:O	2:B:118:ILE:CB	2.31	0.79
1:A:151:TYR:CD2	1:A:152:PHE:N	2.50	0.79
1:A:279:MET:HG3	1:A:280:LEU:N	1.98	0.79
3:C:248:TYR:HB2	3:C:251:GLY:O	1.81	0.79
2:B:171:LYS:O	2:B:174:ASP:HB3	1.80	0.79
1:A:175:VAL:HA	1:A:294:LEU:HD13	1.62	0.79
1:A:258:TYR:CB	1:A:261:GLY:O	2.30	0.79
3:C:188:PHE:O	3:C:192:ILE:HG12	1.82	0.79
3:C:179:THR:CG2	3:C:180:LEU:HD23	2.13	0.78
1:A:283:HIS:CB	1:A:285:GLN:HE21	1.95	0.78
1:A:122:ILE:CD1	1:A:126:PHE:HE1	1.96	0.77
2:B:182:ILE:HD12	2:B:183:ILE:H	1.47	0.77
1:A:153:ILE:HG22	1:A:164:ASP:OD2	1.84	0.77
2:B:153:TYR:CZ	2:B:169:THR:HG21	2.18	0.77
2:B:64:ASN:O	2:B:65:THR:CG2	2.32	0.77
1:A:267:ASN:CG	1:A:270:HIS:HB2	2.05	0.77
2:B:250:MET:O	2:B:251:MET:HG3	1.84	0.77
3:C:41:GLY:O	4:C:419:GDP:C5'	2.32	0.77
3:C:43:GLY:C	3:C:46:THR:HG23	2.03	0.77
2:B:168:VAL:O	2:B:172:LYS:HB2	1.85	0.77
1:A:125:GLN:HB3	1:A:144:ASN:O	1.84	0.77
3:C:122:TYR:O	3:C:125:ALA:HB3	1.85	0.77
1:A:151:TYR:HE1	1:A:167:PHE:HB3	1.48	0.76
1:A:258:TYR:CB	1:A:260:TRP:O	2.26	0.76
2:B:185:LYS:HG3	5:B:428:GTP:N1	2.00	0.76
1:A:274:LEU:HD22	1:A:278:THR:OG1	1.86	0.76
3:C:77:SER:CA	3:C:88:LEU:O	2.34	0.76
2:B:54:GLY:HA2	2:B:57:THR:HG23	1.52	0.76
2:B:153:TYR:CZ	2:B:166:ASP:HB3	2.22	0.75
2:B:153:TYR:OH	2:B:166:ASP:HB3	1.86	0.75
2:B:153:TYR:CE2	2:B:155:ILE:HG23	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:HD12	1:A:142:ILE:N	2.02	0.75
1:A:177:ILE:CB	1:A:210:ILE:HG22	2.16	0.75
3:C:34:LEU:C	3:C:34:LEU:HD22	2.06	0.75
3:C:43:GLY:C	3:C:46:THR:CG2	2.54	0.75
1:A:211:TYR:O	1:A:211:TYR:HD2	1.70	0.74
1:A:36:PHE:O	1:A:93:VAL:CG2	2.34	0.74
1:A:181:ILE:HD11	1:A:236:PRO:HG2	1.69	0.74
1:A:282:THR:CG2	1:A:283:HIS:CD2	2.57	0.74
1:A:285:GLN:C	1:A:288:GLN:H	1.91	0.74
3:C:258:GLY:C	3:C:260:HIS:CB	2.56	0.74
1:A:172:HIS:HD2	1:A:209:LYS:HB2	1.52	0.74
1:A:211:TYR:CE2	1:A:213:LEU:HA	2.22	0.74
3:C:109:GLN:N	3:C:110:PRO:CD	2.49	0.74
1:A:153:ILE:HD13	1:A:153:ILE:N	2.02	0.74
1:A:177:ILE:HG22	1:A:179:PRO:N	2.03	0.74
1:A:79:VAL:CG2	1:A:99:VAL:O	2.34	0.74
1:A:156:PHE:HE1	1:A:186:THR:CG2	1.94	0.74
1:A:258:TYR:CD2	1:A:260:TRP:CE3	2.76	0.74
3:C:148:PRO:HG2	3:C:150:GLY:N	2.03	0.74
1:A:146:VAL:O	1:A:175:VAL:HG11	1.88	0.74
1:A:224:PHE:CD2	1:A:225:LYS:N	2.55	0.74
1:A:156:PHE:CE1	1:A:186:THR:HB	2.17	0.73
1:A:99:VAL:HG12	1:A:100:VAL:O	1.88	0.73
1:A:47:GLY:HA2	2:B:158:THR:HG21	1.70	0.73
2:B:257:PRO:HB2	2:B:258:TRP:HD1	1.47	0.73
1:A:155:PRO:O	1:A:187:LEU:HD21	1.88	0.73
1:A:183:LYS:CD	4:A:362:GDP:C4	2.65	0.73
1:A:143:ASP:CG	1:A:145:ARG:HD3	2.08	0.73
1:A:246:ILE:HD13	1:A:246:ILE:N	2.04	0.73
1:A:282:THR:CG2	1:A:283:HIS:N	2.48	0.72
1:A:292:GLN:O	1:A:296:TYR:CB	2.38	0.72
2:B:166:ASP:C	2:B:169:THR:HG22	2.09	0.72
3:C:255:VAL:HA	3:C:258:GLY:HA2	1.72	0.72
1:A:271:ASN:HD21	1:A:273:PHE:HB2	1.52	0.72
1:A:49:GLY:CA	1:A:52:THR:HG22	2.19	0.72
3:C:109:GLN:N	3:C:110:PRO:HD2	2.05	0.72
1:A:39:THR:CB	1:A:96:ARG:O	2.38	0.72
1:A:39:THR:CA	1:A:96:ARG:O	2.38	0.71
1:A:173:ASN:CA	1:A:294:LEU:CD2	2.50	0.71
1:A:55:ASN:CG	1:A:61:ASP:HA	2.11	0.71
1:A:132:ASP:O	1:A:135:GLY:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ILE:CD1	1:A:209:LYS:N	2.44	0.71
1:A:34:LYS:O	1:A:34:LYS:HD2	1.90	0.71
1:A:121:TYR:O	1:A:125:GLN:HG2	1.89	0.71
2:B:292:THR:O	2:B:296:GLU:CB	2.39	0.71
1:A:156:PHE:CZ	2:B:185:LYS:HB3	2.26	0.70
1:A:164:ASP:OD1	1:A:164:ASP:N	2.16	0.70
3:C:44:LYS:O	3:C:48:ILE:HG13	1.92	0.70
3:C:174:ILE:N	3:C:174:ILE:HD12	2.05	0.70
3:C:181:THR:O	3:C:185:CYS:N	2.23	0.70
1:A:139:ARG:H	1:A:141:ILE:CG2	1.90	0.70
1:A:172:HIS:CD2	1:A:209:LYS:HB2	2.26	0.70
1:A:257:LEU:CD2	1:A:257:LEU:C	2.59	0.70
1:A:288:GLN:O	1:A:291:THR:HG22	1.92	0.70
2:B:153:TYR:CE1	2:B:169:THR:HG21	2.27	0.70
1:A:57:LEU:HD11	1:A:277:ARG:HA	1.74	0.70
1:A:279:MET:O	1:A:282:THR:CG2	2.27	0.70
1:A:239:VAL:HG12	1:A:273:PHE:CA	2.12	0.69
1:A:263:VAL:HG13	2:B:257:PRO:HG3	1.74	0.69
3:C:38:GLY:HA3	3:C:44:LYS:CE	2.23	0.69
2:B:155:ILE:CD1	2:B:155:ILE:N	2.49	0.69
3:C:45:SER:HA	3:C:48:ILE:CD1	2.12	0.69
1:A:198:ARG:O	1:A:202:GLU:HG2	1.92	0.69
2:B:185:LYS:CE	5:B:428:GTP:C4	2.73	0.69
1:A:151:TYR:HE1	1:A:167:PHE:CB	2.05	0.69
1:A:237:PHE:HB2	1:A:272:ASP:HB3	1.74	0.69
1:A:149:CYS:N	1:A:176:ASN:O	2.20	0.69
1:A:201:ASP:O	1:A:204:GLU:CB	2.40	0.69
2:B:119:VAL:O	2:B:123:ASP:N	2.21	0.69
1:A:208:ILE:HD12	1:A:209:LYS:H	1.57	0.68
2:B:185:LYS:HD2	5:B:428:GTP:C5	2.29	0.68
2:B:251:MET:SD	2:B:251:MET:N	2.65	0.68
2:B:57:THR:CG2	5:B:428:GTP:O1A	2.37	0.68
1:A:151:TYR:HD2	1:A:152:PHE:H	1.40	0.68
1:A:156:PHE:HZ	2:B:188:ALA:HB2	1.58	0.68
1:A:264:GLU:H	1:A:270:HIS:CE1	2.12	0.68
2:B:66:LYS:C	2:B:67:PHE:HD1	1.96	0.68
2:B:176:LYS:CB	2:B:177:VAL:O	2.42	0.68
2:B:171:LYS:HA	2:B:174:ASP:HB3	1.76	0.68
1:A:201:ASP:O	1:A:204:GLU:N	2.26	0.68
1:A:211:TYR:C	1:A:211:TYR:CD2	2.67	0.68
1:A:257:LEU:HD23	1:A:258:TYR:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:HD23	1:A:277:ARG:HG2	1.74	0.68
1:A:242:SER:OG	1:A:254:ARG:HB3	1.93	0.68
2:B:174:ASP:HB2	2:B:210:VAL:HG12	1.76	0.68
3:C:47:LEU:O	3:C:51:LEU:CB	2.41	0.68
3:C:283:ASN:O	3:C:287:TYR:CB	2.42	0.67
1:A:155:PRO:O	1:A:187:LEU:CD2	2.42	0.67
1:A:167:PHE:O	1:A:171:ILE:HG22	1.93	0.67
1:A:139:ARG:CB	1:A:141:ILE:N	2.58	0.67
1:A:258:TYR:HD2	1:A:260:TRP:CE3	2.12	0.67
1:A:198:ARG:O	1:A:202:GLU:CG	2.43	0.67
1:A:156:PHE:CE1	2:B:185:LYS:HG2	2.30	0.67
1:A:188:THR:O	1:A:192:ARG:HB2	1.95	0.67
1:A:153:ILE:CG2	1:A:164:ASP:OD2	2.43	0.67
2:B:125:GLN:O	2:B:128:ALA:HB3	1.95	0.66
1:A:43:VAL:HG22	1:A:100:VAL:CG2	2.25	0.66
3:C:45:SER:CA	3:C:48:ILE:HD12	2.11	0.66
2:B:46:LEU:HA	2:B:100:VAL:O	1.95	0.66
2:B:157:PRO:HG3	2:B:184:ALA:O	1.95	0.66
1:A:42:VAL:O	1:A:100:VAL:HG23	1.96	0.66
1:A:149:CYS:SG	1:A:150:PHE:O	2.53	0.66
1:A:271:ASN:ND2	1:A:273:PHE:CB	2.56	0.66
1:A:61:ASP:C	1:A:62:LEU:HD23	2.16	0.66
2:B:273:LYS:O	2:B:277:MET:HG2	1.96	0.66
1:A:240:VAL:CG2	4:A:362:GDP:O6	2.43	0.66
3:C:174:ILE:HD11	3:C:226:PRO:HG2	1.78	0.66
3:C:38:GLY:HA3	3:C:44:LYS:HD3	1.76	0.66
2:B:257:PRO:HB2	2:B:258:TRP:NE1	2.11	0.65
3:C:77:SER:CB	3:C:88:LEU:O	2.45	0.65
2:B:185:LYS:CG	5:B:428:GTP:C6	2.72	0.65
1:A:268:PRO:HG3	1:A:271:ASN:O	1.97	0.65
1:A:197:LYS:HA	1:A:200:LEU:HB2	1.78	0.65
1:A:59:LEU:HG	1:A:59:LEU:O	1.97	0.65
1:A:245:LEU:HB2	1:A:253:VAL:O	1.96	0.65
3:C:188:PHE:O	3:C:192:ILE:HG13	1.96	0.65
2:B:302:LYS:O	2:B:306:MET:SD	2.54	0.65
1:A:156:PHE:CE1	1:A:186:THR:CB	2.72	0.65
1:A:283:HIS:CD2	1:A:283:HIS:N	2.61	0.65
2:B:120:GLU:O	2:B:124:ALA:HB2	1.97	0.65
1:A:279:MET:CG	1:A:280:LEU:N	2.58	0.64
1:A:22:ASN:C	1:A:24:PRO:CD	2.54	0.64
1:A:23:LEU:O	1:A:27:VAL:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:154:LYS:O	3:C:157:ASP:N	2.30	0.64
1:A:122:ILE:CD1	1:A:126:PHE:CE1	2.77	0.64
1:A:148:CYS:SG	1:A:149:CYS:O	2.56	0.64
1:A:276:LEU:HD23	1:A:277:ARG:N	2.13	0.64
1:A:55:ASN:O	1:A:59:LEU:N	2.30	0.64
2:B:250:MET:C	2:B:251:MET:HG3	2.18	0.64
2:B:60:ASP:O	2:B:64:ASN:N	2.30	0.64
1:A:179:PRO:CD	1:A:210:ILE:CD1	2.76	0.64
1:A:147:HIS:O	1:A:286:ASP:HB2	1.98	0.64
2:B:153:TYR:HB3	2:B:170:MET:CE	2.28	0.64
2:B:250:MET:C	2:B:251:MET:CG	2.66	0.64
1:A:175:VAL:HG12	1:A:176:ASN:CA	2.28	0.63
1:A:29:ARG:O	1:A:32:VAL:CG2	2.46	0.63
2:B:257:PRO:CB	2:B:258:TRP:CD1	2.71	0.63
3:C:141:CYS:HB2	3:C:169:ASN:O	1.99	0.63
3:C:79:VAL:HA	3:C:87:GLN:HA	1.80	0.63
2:B:185:LYS:HA	5:B:428:GTP:C6	2.33	0.63
1:A:139:ARG:C	1:A:141:ILE:N	2.52	0.63
1:A:177:ILE:HD13	1:A:210:ILE:HG22	1.81	0.63
1:A:285:GLN:O	1:A:288:GLN:HB2	1.98	0.63
1:A:43:VAL:HG11	1:A:167:PHE:CZ	2.33	0.63
1:A:79:VAL:HG22	1:A:80:GLN:N	2.14	0.63
2:B:186:ALA:HB2	2:B:237:VAL:O	1.98	0.63
1:A:165:VAL:HG12	1:A:166:ALA:N	2.13	0.63
2:B:60:ASP:CB	2:B:65:THR:O	2.46	0.63
1:A:285:GLN:CA	1:A:288:GLN:HG3	2.28	0.63
1:A:81:ILE:C	1:A:81:ILE:HD12	2.19	0.63
1:A:122:ILE:HD12	1:A:175:VAL:HG23	1.81	0.62
1:A:179:PRO:HD3	1:A:210:ILE:HG21	1.80	0.62
1:A:54:ILE:CG2	1:A:55:ASN:N	2.63	0.62
2:B:54:GLY:C	2:B:57:THR:HG23	2.19	0.62
3:C:40:SER:HA	3:C:44:LYS:HZ1	1.63	0.62
2:B:236:ALA:O	2:B:270:ASP:CB	2.48	0.62
1:A:265:VAL:CG1	1:A:266:GLU:HG3	2.11	0.62
1:A:55:ASN:CB	1:A:60:THR:O	2.47	0.62
1:A:148:CYS:SG	1:A:149:CYS:N	2.71	0.62
1:A:161:LYS:O	1:A:164:ASP:N	2.33	0.62
1:A:119:ILE:HD11	1:A:170:ALA:O	1.98	0.62
1:A:211:TYR:CZ	1:A:214:PRO:CD	2.82	0.62
1:A:177:ILE:H	1:A:177:ILE:HD12	1.64	0.62
2:B:166:ASP:HA	2:B:169:THR:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLN:O	1:A:288:GLN:N	2.30	0.62
3:C:47:LEU:O	3:C:51:LEU:HB3	1.99	0.62
1:A:172:HIS:HD2	1:A:209:LYS:CB	2.13	0.61
1:A:258:TYR:HD2	1:A:260:TRP:HE3	1.47	0.61
2:B:166:ASP:CA	2:B:169:THR:HG22	2.30	0.61
3:C:154:LYS:O	3:C:157:ASP:CB	2.48	0.61
3:C:192:ILE:HA	3:C:195:GLU:CB	2.30	0.61
1:A:179:PRO:CD	1:A:210:ILE:HD13	2.31	0.61
1:A:151:TYR:O	1:A:179:PRO:HA	1.99	0.61
3:C:192:ILE:O	3:C:195:GLU:CB	2.49	0.61
3:C:30:PHE:O	3:C:88:LEU:HA	2.01	0.61
2:B:185:LYS:HE3	5:B:428:GTP:N9	2.14	0.61
2:B:19:LEU:CB	3:C:77:SER:O	2.48	0.61
3:C:148:PRO:CG	3:C:150:GLY:CA	2.65	0.61
1:A:177:ILE:HG22	1:A:179:PRO:CD	2.31	0.61
1:A:61:ASP:O	1:A:62:LEU:HD23	2.01	0.61
3:C:57:TYR:C	3:C:59:PRO:HD3	2.20	0.61
1:A:180:VAL:HG22	1:A:181:ILE:N	2.15	0.60
1:A:196:LYS:O	1:A:200:LEU:CD1	2.47	0.60
1:A:84:SER:O	1:A:95:LEU:HB2	2.01	0.60
1:A:160:LEU:HD23	1:A:164:ASP:HB2	1.82	0.60
1:A:213:LEU:CD2	1:A:213:LEU:O	2.44	0.60
1:A:279:MET:SD	1:A:279:MET:C	2.79	0.60
3:C:23:ARG:C	3:C:25:SER:H	2.05	0.60
3:C:267:ARG:O	3:C:271:ILE:CB	2.50	0.60
1:A:150:PHE:HB3	1:A:152:PHE:CE1	2.37	0.60
2:B:185:LYS:CD	5:B:428:GTP:C5	2.85	0.60
1:A:208:ILE:HG23	1:A:209:LYS:N	2.16	0.60
1:A:180:VAL:CG2	1:A:181:ILE:N	2.64	0.60
1:A:173:ASN:HA	1:A:294:LEU:HD21	1.79	0.60
1:A:265:VAL:HG12	1:A:266:GLU:N	2.15	0.60
3:C:43:GLY:O	3:C:46:THR:CG2	2.39	0.60
1:A:268:PRO:CG	1:A:271:ASN:O	2.50	0.60
2:B:185:LYS:HG3	5:B:428:GTP:C5	2.37	0.60
3:C:34:LEU:HB3	3:C:91:THR:O	2.01	0.60
1:A:189:LEU:HA	1:A:192:ARG:HB2	1.83	0.59
2:B:274:LEU:O	2:B:278:LEU:CB	2.50	0.59
2:B:166:ASP:N	2:B:166:ASP:OD1	2.34	0.59
3:C:108:TRP:C	3:C:110:PRO:HD2	2.23	0.59
1:A:279:MET:SD	1:A:280:LEU:HA	2.42	0.59
1:A:240:VAL:CG1	4:A:362:GDP:O6	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:TYR:HB3	2:B:170:MET:HE3	1.84	0.59
2:B:19:LEU:CB	3:C:77:SER:N	2.65	0.59
2:B:206:VAL:HA	2:B:209:GLY:CA	2.27	0.59
3:C:140:GLN:O	3:C:168:VAL:CB	2.51	0.59
3:C:259:GLU:N	3:C:260:HIS:CB	2.66	0.59
1:A:200:LEU:O	1:A:203:ILE:HB	2.03	0.59
2:B:154:PHE:HA	2:B:182:ILE:HG23	1.85	0.59
1:A:22:ASN:O	1:A:24:PRO:HD2	2.00	0.58
2:B:175:SER:N	2:B:176:LYS:HA	2.17	0.58
2:B:67:PHE:HD1	2:B:67:PHE:N	2.01	0.58
3:C:47:LEU:O	3:C:51:LEU:HB2	2.02	0.58
1:A:45:GLU:O	1:A:47:GLY:HA3	2.03	0.58
1:A:49:GLY:HA2	4:A:362:GDP:O1A	2.04	0.58
2:B:85:THR:CB	2:B:98:THR:HA	2.34	0.58
3:C:42:LEU:CA	4:C:419:GDP:C5'	2.69	0.58
1:A:263:VAL:HG13	2:B:257:PRO:CG	2.33	0.58
1:A:38:PHE:CE1	1:A:147:HIS:HB3	2.38	0.58
3:C:110:PRO:O	3:C:114:TYR:N	2.35	0.58
1:A:29:ARG:HA	1:A:32:VAL:HG23	1.85	0.58
2:B:165:LEU:O	2:B:169:THR:HB	2.03	0.58
3:C:132:ARG:H	3:C:134:MET:HE3	1.68	0.58
1:A:156:PHE:CZ	1:A:186:THR:CG2	2.86	0.57
2:B:185:LYS:HE3	5:B:428:GTP:N3	2.19	0.57
1:A:199:ILE:O	1:A:203:ILE:HD13	2.04	0.57
2:B:225:ILE:O	2:B:229:MET:HG2	2.04	0.57
2:B:277:MET:HG3	2:B:278:LEU:N	2.18	0.57
3:C:38:GLY:HA3	3:C:44:LYS:CD	2.34	0.57
3:C:48:ILE:O	3:C:52:PHE:HB2	2.04	0.57
1:A:229:ARG:NH2	1:A:230:LEU:CD1	2.67	0.57
2:B:171:LYS:O	2:B:174:ASP:CB	2.52	0.57
3:C:174:ILE:CD1	3:C:174:ILE:N	2.67	0.57
3:C:34:LEU:O	3:C:34:LEU:CD1	2.42	0.57
1:A:151:TYR:CE1	1:A:167:PHE:HB3	2.36	0.57
2:B:171:LYS:CA	2:B:174:ASP:HB3	2.35	0.57
1:A:265:VAL:CB	1:A:266:GLU:HG3	2.34	0.57
1:A:80:GLN:OE1	1:A:80:GLN:HA	2.04	0.57
1:A:41:MET:HA	1:A:98:THR:O	2.05	0.57
1:A:143:ASP:OD2	1:A:145:ARG:CD	2.42	0.56
1:A:47:GLY:HA2	2:B:158:THR:CG2	2.35	0.56
3:C:43:GLY:HA2	4:C:419:GDP:O1A	2.04	0.56
3:C:157:ASP:O	3:C:161:MET:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:PRO:C	2:B:258:TRP:CD1	2.79	0.56
3:C:43:GLY:CA	3:C:46:THR:HG21	2.29	0.56
3:C:35:MET:O	3:C:143:LEU:N	2.38	0.56
1:A:55:ASN:O	1:A:60:THR:N	2.38	0.56
1:A:143:ASP:CB	1:A:145:ARG:HD3	2.36	0.56
1:A:200:LEU:HA	1:A:203:ILE:HD13	1.88	0.56
2:B:120:GLU:O	2:B:124:ALA:CB	2.54	0.56
3:C:51:LEU:HD12	3:C:51:LEU:O	2.06	0.56
2:B:67:PHE:CD1	2:B:67:PHE:N	2.72	0.56
1:A:172:HIS:HD2	1:A:209:LYS:HG3	1.71	0.56
1:A:263:VAL:HG22	2:B:257:PRO:HG3	1.86	0.56
2:B:182:ILE:CD1	2:B:183:ILE:H	2.16	0.56
1:A:122:ILE:CG1	1:A:123:ASP:N	2.68	0.55
1:A:288:GLN:C	1:A:291:THR:HG22	2.26	0.55
2:B:54:GLY:HA3	2:B:57:THR:HG21	1.87	0.55
2:B:90:GLU:N	2:B:93:VAL:O	2.32	0.55
3:C:173:LEU:C	3:C:174:ILE:HD12	2.27	0.55
1:A:122:ILE:HG13	1:A:126:PHE:CD1	2.42	0.55
3:C:71:THR:CB	3:C:95:THR:CB	2.84	0.55
1:A:179:PRO:CD	1:A:210:ILE:HD12	2.37	0.55
3:C:141:CYS:HA	3:C:168:VAL:CB	2.37	0.55
3:C:34:LEU:O	3:C:92:ILE:HA	2.07	0.55
1:A:204:GLU:C	1:A:206:HIS:H	2.10	0.55
1:A:43:VAL:HG11	1:A:167:PHE:CE1	2.42	0.55
2:B:60:ASP:O	2:B:64:ASN:CA	2.55	0.55
1:A:206:HIS:CD2	1:A:208:ILE:HG13	2.42	0.55
1:A:38:PHE:CE2	1:A:40:LEU:HB3	2.41	0.55
2:B:153:TYR:HE2	2:B:155:ILE:HG23	1.69	0.55
1:A:177:ILE:HG22	1:A:179:PRO:HD3	1.89	0.54
2:B:60:ASP:O	2:B:64:ASN:HA	2.07	0.54
1:A:224:PHE:O	1:A:228:THR:HG22	2.07	0.54
1:A:203:ILE:H	1:A:203:ILE:HD12	1.73	0.54
1:A:201:ASP:C	1:A:204:GLU:HB2	2.25	0.54
3:C:192:ILE:HD11	3:C:226:PRO:CD	2.38	0.54
2:B:19:LEU:CB	3:C:77:SER:H	2.20	0.54
1:A:173:ASN:C	1:A:175:VAL:CA	2.76	0.54
2:B:171:LYS:C	2:B:174:ASP:HB3	2.28	0.54
2:B:249:LYS:CB	2:B:250:MET:CA	2.75	0.54
1:A:290:VAL:HA	1:A:294:LEU:HD12	1.89	0.53
1:A:274:LEU:CD2	1:A:277:ARG:HG2	2.37	0.53
1:A:87:GLU:C	1:A:92:GLY:HA2	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:GLY:C	4:C:419:GDP:H5''	2.28	0.53
1:A:298:ASN:O	1:A:302:GLU:CB	2.56	0.53
1:A:29:ARG:O	1:A:32:VAL:HG23	2.08	0.53
2:B:153:TYR:HE2	2:B:166:ASP:HB3	1.68	0.53
3:C:46:THR:O	3:C:50:SER:CB	2.45	0.53
1:A:263:VAL:HG22	2:B:257:PRO:CG	2.38	0.53
3:C:43:GLY:N	4:C:419:GDP:H5'	2.24	0.53
1:A:156:PHE:CZ	1:A:186:THR:HG22	2.43	0.53
2:B:205:LEU:O	2:B:209:GLY:HA2	2.09	0.53
2:B:205:LEU:O	2:B:210:VAL:HG23	2.09	0.53
3:C:176:LYS:O	3:C:179:THR:N	2.38	0.53
1:A:212:HIS:O	1:A:214:PRO:CD	2.54	0.53
2:B:166:ASP:HA	2:B:169:THR:HG21	1.88	0.53
1:A:44:GLY:O	1:A:50:LYS:HE2	2.09	0.53
3:C:39:GLU:O	3:C:44:LYS:NZ	2.41	0.53
1:A:285:GLN:O	1:A:288:GLN:CB	2.57	0.53
3:C:72:VAL:O	3:C:94:ASP:O	2.26	0.53
1:A:39:THR:CG2	1:A:145:ARG:O	2.57	0.52
1:A:178:VAL:HG12	1:A:179:PRO:O	2.10	0.52
1:A:189:LEU:HD12	1:A:190:LYS:N	2.24	0.52
1:A:242:SER:CB	1:A:255:GLY:O	2.56	0.52
1:A:242:SER:HB3	1:A:255:GLY:O	2.09	0.52
2:B:119:VAL:O	2:B:123:ASP:CB	2.57	0.52
3:C:116:ASP:O	3:C:120:GLU:N	2.37	0.52
1:A:196:LYS:HB2	1:A:197:LYS:HE3	1.91	0.52
1:A:288:GLN:O	1:A:291:THR:CG2	2.58	0.52
1:A:45:GLU:O	1:A:48:LEU:HG	2.09	0.52
1:A:201:ASP:HA	1:A:204:GLU:HB2	1.91	0.52
1:A:245:LEU:CA	1:A:246:ILE:HD13	2.39	0.52
3:C:60:GLU:HG2	4:C:419:GDP:O3B	2.10	0.52
2:B:299:ARG:O	2:B:303:LEU:N	2.30	0.52
1:A:28:HIS:CD2	1:A:28:HIS:C	2.83	0.52
1:A:151:TYR:CD2	1:A:151:TYR:C	2.82	0.52
2:B:56:SER:O	2:B:60:ASP:OD2	2.27	0.52
1:A:289:GLU:O	1:A:293:ASP:N	2.32	0.52
1:A:125:GLN:CB	1:A:144:ASN:O	2.58	0.52
1:A:175:VAL:CG1	1:A:176:ASN:N	2.56	0.52
1:A:265:VAL:C	1:A:266:GLU:HG3	2.29	0.52
1:A:131:HIS:HD2	1:A:132:ASP:OD1	1.93	0.51
1:A:285:GLN:HB3	1:A:288:GLN:NE2	2.25	0.51
3:C:34:LEU:HD22	3:C:35:MET:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:LEU:N	4:C:419:GDP:H5''	2.25	0.51
2:B:185:LYS:HD2	5:B:428:GTP:N7	2.25	0.51
1:A:265:VAL:CG1	1:A:266:GLU:N	2.73	0.51
1:A:189:LEU:HD12	1:A:190:LYS:H	1.75	0.51
1:A:61:ASP:OD2	1:A:62:LEU:N	2.44	0.51
1:A:151:TYR:C	1:A:151:TYR:HD2	2.14	0.51
1:A:28:HIS:CG	1:A:29:ARG:N	2.78	0.51
1:A:122:ILE:HB	1:A:146:VAL:HG21	1.93	0.51
1:A:276:LEU:HD23	1:A:276:LEU:C	2.31	0.51
2:B:113:ASP:O	2:B:117:PRO:CG	2.46	0.51
1:A:151:TYR:HE1	1:A:167:PHE:CG	2.29	0.51
1:A:186:THR:O	5:B:428:GTP:N2	2.44	0.50
1:A:54:ILE:HG13	1:A:58:PHE:CZ	2.45	0.50
1:A:153:ILE:HG21	1:A:160:LEU:CG	2.29	0.50
1:A:165:VAL:CG1	1:A:166:ALA:N	2.73	0.50
1:A:173:ASN:O	1:A:175:VAL:N	2.44	0.50
1:A:177:ILE:HG22	1:A:178:VAL:C	2.32	0.50
3:C:38:GLY:HA3	3:C:44:LYS:HE2	1.92	0.50
1:A:278:THR:O	1:A:282:THR:HB	2.12	0.50
1:A:285:GLN:HB3	1:A:288:GLN:HE21	1.77	0.50
2:B:166:ASP:O	2:B:170:MET:N	2.42	0.50
1:A:146:VAL:HB	1:A:175:VAL:HG21	1.93	0.50
1:A:156:PHE:CZ	2:B:185:LYS:CB	2.95	0.50
1:A:268:PRO:O	1:A:270:HIS:N	2.45	0.50
2:B:174:ASP:HB2	2:B:210:VAL:CG1	2.41	0.50
3:C:135:PRO:CB	3:C:136:ASP:HA	2.41	0.50
1:A:151:TYR:OH	1:A:164:ASP:HA	2.11	0.50
1:A:229:ARG:HH21	1:A:230:LEU:HD13	1.76	0.50
1:A:82:GLU:CB	1:A:97:LEU:O	2.59	0.50
2:B:153:TYR:HE2	2:B:155:ILE:CG2	2.25	0.50
3:C:147:ALA:HB2	3:C:175:ALA:H	1.77	0.50
1:A:173:ASN:C	1:A:175:VAL:HA	2.32	0.50
1:A:284:MET:O	1:A:287:LEU:CG	2.48	0.50
1:A:122:ILE:HG13	1:A:126:PHE:HD1	1.76	0.50
1:A:57:LEU:CD2	1:A:276:LEU:CD2	2.83	0.50
1:A:188:THR:O	1:A:192:ARG:N	2.45	0.49
1:A:258:TYR:CD2	1:A:260:TRP:CZ3	3.01	0.49
1:A:181:ILE:HB	1:A:238:SER:OG	2.13	0.49
1:A:172:HIS:HD2	1:A:209:LYS:CG	2.25	0.49
1:A:285:GLN:HB2	1:A:288:GLN:CD	2.32	0.49
1:A:206:HIS:CD2	1:A:208:ILE:CG1	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ILE:CG1	1:A:210:ILE:HG22	2.42	0.49
3:C:40:SER:HB3	4:C:419:GDP:O3B	2.13	0.49
1:A:54:ILE:HG13	1:A:58:PHE:CD2	2.45	0.49
2:B:114:SER:C	2:B:117:PRO:HG2	2.33	0.49
1:A:156:PHE:CE2	2:B:185:LYS:CB	2.96	0.49
1:A:139:ARG:CA	1:A:141:ILE:N	2.76	0.49
1:A:148:CYS:SG	1:A:149:CYS:C	2.91	0.49
1:A:258:TYR:CE2	1:A:260:TRP:CZ3	3.00	0.49
1:A:57:LEU:HD22	1:A:276:LEU:HD21	1.88	0.49
2:B:116:LYS:H	2:B:117:PRO:CD	2.04	0.49
1:A:156:PHE:CE2	2:B:185:LYS:HB3	2.48	0.48
1:A:263:VAL:HG13	2:B:257:PRO:HD3	1.94	0.48
3:C:49:ASN:CB	3:C:54:THR:O	2.53	0.48
1:A:153:ILE:H	1:A:153:ILE:CD1	2.05	0.48
1:A:183:LYS:HG3	4:A:362:GDP:C6	2.47	0.48
1:A:197:LYS:O	1:A:200:LEU:HB2	2.13	0.48
1:A:229:ARG:HE	1:A:229:ARG:HB3	1.36	0.48
3:C:154:LYS:O	3:C:157:ASP:CA	2.61	0.48
1:A:199:ILE:HG22	1:A:203:ILE:CD1	2.44	0.48
3:C:41:GLY:O	4:C:419:GDP:O5'	2.31	0.48
1:A:141:ILE:HD12	1:A:142:ILE:H	1.74	0.48
1:A:130:LEU:CD1	1:A:295:HIS:CE1	2.96	0.48
1:A:49:GLY:HA2	1:A:52:THR:HG22	1.95	0.48
2:B:155:ILE:HD13	2:B:182:ILE:O	2.14	0.48
3:C:147:ALA:CB	3:C:175:ALA:H	2.27	0.48
1:A:228:THR:HG23	1:A:229:ARG:N	2.29	0.48
2:B:272:VAL:O	2:B:275:ARG:N	2.46	0.48
3:C:266:LEU:O	3:C:270:LEU:CB	2.62	0.48
1:A:79:VAL:HG22	1:A:80:GLN:H	1.78	0.48
1:A:97:LEU:HD23	1:A:97:LEU:C	2.34	0.48
1:A:179:PRO:HD2	1:A:210:ILE:HD12	1.95	0.47
1:A:130:LEU:HD12	1:A:295:HIS:CE1	2.49	0.47
3:C:154:LYS:O	3:C:158:ILE:N	2.45	0.47
1:A:163:LEU:O	1:A:163:LEU:HD13	2.13	0.47
1:A:195:LEU:O	1:A:199:ILE:HG13	2.13	0.47
1:A:195:LEU:O	1:A:199:ILE:CG1	2.62	0.47
1:A:23:LEU:O	1:A:27:VAL:N	2.29	0.47
1:A:258:TYR:CE2	1:A:260:TRP:HZ3	2.33	0.47
1:A:83:ALA:CA	1:A:95:LEU:O	2.46	0.47
2:B:153:TYR:HB3	2:B:170:MET:HE2	1.97	0.47
2:B:257:PRO:C	2:B:258:TRP:CG	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ILE:O	1:A:126:PHE:CD1	2.68	0.47
1:A:177:ILE:CD1	1:A:210:ILE:HG22	2.43	0.47
1:A:49:GLY:O	1:A:53:LEU:HB3	2.15	0.47
2:B:153:TYR:OH	2:B:166:ASP:CB	2.59	0.47
2:B:75:THR:O	2:B:76:GLN:CB	2.61	0.47
1:A:121:TYR:HA	1:A:124:GLU:HB3	1.97	0.47
1:A:39:THR:O	1:A:147:HIS:CB	2.53	0.47
1:A:49:GLY:HA3	1:A:52:THR:HG22	1.94	0.47
3:C:26:VAL:O	3:C:27:LYS:O	2.31	0.47
2:B:169:THR:O	2:B:173:LEU:CB	2.56	0.47
2:B:170:MET:O	2:B:174:ASP:N	2.48	0.47
2:B:35:LYS:C	2:B:37:VAL:H	2.17	0.47
1:A:50:LYS:NZ	4:A:362:GDP:O2B	2.42	0.47
3:C:248:TYR:HB3	3:C:249:PRO:HD2	1.96	0.47
3:C:61:TYR:CD1	3:C:61:TYR:C	2.86	0.46
3:C:33:THR:O	3:C:139:VAL:O	2.31	0.46
3:C:33:THR:HG23	3:C:91:THR:CB	2.45	0.46
1:A:197:LYS:O	1:A:201:ASP:N	2.44	0.46
1:A:258:TYR:CD2	1:A:260:TRP:HE3	2.26	0.46
3:C:50:SER:O	3:C:53:LEU:HD23	2.15	0.46
1:A:40:LEU:HA	1:A:148:CYS:O	2.14	0.46
1:A:268:PRO:HA	1:A:270:HIS:N	2.30	0.46
3:C:132:ARG:N	3:C:134:MET:HE3	2.31	0.46
1:A:54:ILE:HG23	1:A:55:ASN:N	2.31	0.46
2:B:250:MET:O	2:B:251:MET:CG	2.59	0.46
1:A:240:VAL:CG1	4:A:362:GDP:C6	2.93	0.46
1:A:52:THR:HG23	1:A:53:LEU:N	2.31	0.46
1:A:176:ASN:HD22	1:A:176:ASN:HA	1.58	0.46
1:A:201:ASP:CA	1:A:204:GLU:HB2	2.46	0.46
3:C:176:LYS:O	3:C:179:THR:HB	2.16	0.46
1:A:79:VAL:CG2	1:A:80:GLN:N	2.79	0.46
2:B:155:ILE:O	2:B:183:ILE:HA	2.16	0.46
3:C:276:GLN:O	3:C:279:LYS:HG2	2.16	0.46
1:A:156:PHE:CZ	1:A:186:THR:HG21	2.50	0.45
1:A:163:LEU:C	1:A:163:LEU:HD13	2.36	0.45
1:A:167:PHE:O	1:A:171:ILE:CG2	2.61	0.45
1:A:245:LEU:O	1:A:246:ILE:HD13	2.12	0.45
1:A:29:ARG:C	1:A:32:VAL:HG23	2.36	0.45
1:A:286:ASP:OD1	1:A:286:ASP:N	2.31	0.45
1:A:46:SER:HB3	1:A:50:LYS:NZ	2.31	0.45
2:B:84:ASN:O	2:B:99:ILE:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:23:ARG:C	3:C:25:SER:N	2.68	0.45
1:A:54:ILE:O	1:A:58:PHE:CG	2.69	0.45
2:B:137:ARG:CB	2:B:138:ARG:CB	2.93	0.45
1:A:55:ASN:OD1	1:A:61:ASP:HA	2.16	0.45
1:A:172:HIS:CD2	1:A:209:LYS:HG3	2.50	0.45
1:A:34:LYS:C	1:A:34:LYS:HD2	2.35	0.45
1:A:231:LEU:HD12	1:A:231:LEU:HA	1.67	0.45
1:A:164:ASP:O	1:A:168:MET:HG3	2.16	0.45
1:A:82:GLU:O	1:A:97:LEU:N	2.49	0.45
2:B:169:THR:CG2	2:B:170:MET:N	2.79	0.45
1:A:143:ASP:HB2	1:A:145:ARG:HD3	1.97	0.45
3:C:148:PRO:CB	3:C:150:GLY:HA3	2.47	0.45
3:C:79:VAL:CB	3:C:87:GLN:CB	2.95	0.45
1:A:39:THR:HG21	1:A:145:ARG:O	2.17	0.45
1:A:155:PRO:O	1:A:187:LEU:HD22	2.17	0.45
1:A:158:HIS:HB3	1:A:159:GLY:H	1.55	0.45
1:A:160:LEU:CD1	1:A:199:ILE:HG12	2.35	0.45
2:B:25:PHE:O	2:B:26:ASP:O	2.35	0.45
2:B:60:ASP:HA	2:B:65:THR:O	2.17	0.45
3:C:46:THR:O	3:C:50:SER:N	2.44	0.45
2:B:180:ILE:HA	2:B:181:PRO:HD3	1.37	0.44
2:B:250:MET:C	2:B:251:MET:SD	2.96	0.44
3:C:178:ASP:OD2	3:C:248:TYR:OH	2.29	0.44
3:C:248:TYR:HB3	3:C:249:PRO:CD	2.47	0.44
3:C:258:GLY:HA3	3:C:259:GLU:HA	1.64	0.44
1:A:149:CYS:SG	1:A:150:PHE:N	2.90	0.44
1:A:153:ILE:CG2	1:A:160:LEU:HG	2.31	0.44
1:A:57:LEU:HD21	1:A:276:LEU:CD2	2.33	0.44
2:B:288:GLU:O	2:B:292:THR:CB	2.65	0.44
3:C:116:ASP:C	3:C:119:PHE:H	2.20	0.44
2:B:29:PRO:O	2:B:32:LEU:N	2.51	0.44
1:A:122:ILE:HG13	1:A:123:ASP:N	2.22	0.44
1:A:183:LYS:HD2	4:A:362:GDP:C8	2.52	0.44
3:C:179:THR:CG2	3:C:180:LEU:N	2.80	0.44
3:C:181:THR:HA	3:C:182:PRO:HD3	1.74	0.44
3:C:192:ILE:O	3:C:195:GLU:N	2.50	0.44
3:C:231:GLY:HA3	4:C:419:GDP:N7	2.32	0.44
1:A:150:PHE:N	1:A:150:PHE:CD1	2.86	0.44
1:A:161:LYS:HB2	1:A:164:ASP:OD1	2.18	0.44
1:A:29:ARG:CA	1:A:32:VAL:HG23	2.47	0.43
1:A:188:THR:OG1	1:A:191:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:CYS:SG	2:B:152:LEU:C	2.96	0.43
2:B:155:ILE:CD1	2:B:182:ILE:O	2.67	0.43
3:C:249:PRO:HB2	3:C:250:TRP:CE3	2.53	0.43
3:C:247:GLN:CB	3:C:252:VAL:CB	2.97	0.43
1:A:163:LEU:HA	1:A:163:LEU:HD22	1.64	0.43
1:A:54:ILE:HG22	1:A:55:ASN:N	2.34	0.43
2:B:64:ASN:C	2:B:65:THR:HG23	2.35	0.43
1:A:288:GLN:CA	1:A:291:THR:HG22	2.49	0.43
2:B:277:MET:HG3	2:B:278:LEU:H	1.83	0.43
2:B:57:THR:O	2:B:61:THR:HB	2.19	0.43
3:C:43:GLY:H	4:C:419:GDP:PA	2.41	0.43
3:C:39:GLU:O	3:C:44:LYS:CE	2.67	0.43
1:A:176:ASN:OD1	1:A:290:VAL:HG22	2.18	0.43
1:A:172:HIS:HB2	1:A:209:LYS:O	2.19	0.43
1:A:199:ILE:O	1:A:202:GLU:HB2	2.19	0.43
2:B:186:ALA:CB	2:B:237:VAL:O	2.65	0.43
2:B:82:GLN:O	2:B:101:SER:O	2.37	0.43
1:A:82:GLU:HB2	1:A:97:LEU:HB3	2.01	0.42
3:C:182:PRO:HA	3:C:185:CYS:H	1.84	0.42
1:A:189:LEU:O	1:A:193:GLU:HG2	2.19	0.42
1:A:119:ILE:O	1:A:119:ILE:CG2	2.64	0.42
1:A:150:PHE:CB	1:A:152:PHE:CE1	3.02	0.42
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.75	0.42
1:A:206:HIS:HB3	1:A:208:ILE:HB	2.00	0.42
1:A:263:VAL:HG13	2:B:257:PRO:CD	2.49	0.42
2:B:149:HIS:O	2:B:178:ASN:CB	2.67	0.42
3:C:179:THR:HG23	3:C:180:LEU:N	2.34	0.42
1:A:204:GLU:C	1:A:206:HIS:N	2.73	0.42
1:A:29:ARG:HA	1:A:32:VAL:CG2	2.49	0.42
2:B:182:ILE:HD12	2:B:183:ILE:N	2.24	0.42
2:B:57:THR:HG21	5:B:428:GTP:H5'	2.01	0.42
1:A:164:ASP:O	1:A:168:MET:N	2.46	0.42
1:A:156:PHE:CD1	2:B:185:LYS:HE2	2.55	0.42
2:B:289:GLN:O	2:B:293:ARG:N	2.52	0.42
2:B:185:LYS:CG	5:B:428:GTP:C5	3.01	0.42
2:B:55:LYS:O	2:B:59:MET:HG2	2.19	0.42
1:A:226:GLU:O	1:A:230:LEU:HB2	2.19	0.42
1:A:284:MET:HB3	1:A:284:MET:HE3	1.93	0.42
2:B:151:CYS:SG	2:B:153:TYR:N	2.92	0.42
3:C:192:ILE:O	3:C:196:ILE:N	2.53	0.42
1:A:43:VAL:O	1:A:152:PHE:CD1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:VAL:HG12	1:A:44:GLY:N	2.34	0.42
1:A:242:SER:HB2	1:A:255:GLY:O	2.19	0.42
1:A:288:GLN:HA	1:A:291:THR:HG22	2.01	0.42
3:C:116:ASP:O	3:C:119:PHE:N	2.52	0.42
3:C:193:MET:CE	3:C:225:LEU:O	2.67	0.42
1:A:149:CYS:O	1:A:177:ILE:HA	2.20	0.42
1:A:38:PHE:O	1:A:95:LEU:HD23	2.20	0.42
2:B:215:PHE:CB	2:B:216:PRO:CD	2.97	0.42
1:A:177:ILE:CG2	1:A:179:PRO:HD3	2.48	0.42
2:B:25:PHE:O	2:B:26:ASP:C	2.58	0.42
1:A:151:TYR:CE1	1:A:167:PHE:CG	3.09	0.41
1:A:134:SER:HA	1:A:135:GLY:HA3	1.79	0.41
1:A:193:GLU:HA	1:A:196:LYS:HE3	2.02	0.41
1:A:56:SER:OG	1:A:254:ARG:NH2	2.41	0.41
1:A:229:ARG:NH2	1:A:230:LEU:HD13	2.32	0.41
1:A:198:ARG:O	1:A:202:GLU:HG3	2.18	0.41
3:C:226:PRO:HB2	3:C:227:LEU:H	1.61	0.41
1:A:237:PHE:CB	1:A:272:ASP:HB3	2.47	0.41
2:B:182:ILE:HD11	2:B:237:VAL:CB	2.51	0.41
1:A:148:CYS:HA	1:A:176:ASN:HB3	2.03	0.41
2:B:85:THR:HA	2:B:98:THR:HA	2.02	0.41
3:C:163:ARG:C	3:C:165:HIS:H	2.24	0.41
1:A:197:LYS:HA	1:A:200:LEU:HD13	2.03	0.41
1:A:197:LYS:HB3	1:A:197:LYS:HE2	1.80	0.41
1:A:36:PHE:O	1:A:93:VAL:HG23	2.17	0.41
1:A:165:VAL:HG22	1:A:206:HIS:CE1	2.56	0.41
1:A:181:ILE:HD13	1:A:238:SER:OG	2.21	0.41
1:A:197:LYS:CA	1:A:200:LEU:HB2	2.48	0.41
1:A:289:GLU:C	1:A:291:THR:N	2.73	0.41
1:A:81:ILE:CD1	1:A:81:ILE:C	2.88	0.41
2:B:206:VAL:CA	2:B:209:GLY:HA2	2.33	0.41
1:A:119:ILE:O	1:A:119:ILE:HG23	2.21	0.41
1:A:150:PHE:CB	1:A:152:PHE:HE1	2.34	0.41
1:A:193:GLU:O	1:A:197:LYS:HD2	2.20	0.41
2:B:47:CYS:HA	2:B:152:LEU:O	2.20	0.41
1:A:254:ARG:O	1:A:265:VAL:HG23	2.21	0.41
1:A:26:GLN:HA	1:A:26:GLN:NE2	2.35	0.41
1:A:36:PHE:H	1:A:93:VAL:HG23	1.86	0.41
2:B:170:MET:O	2:B:173:LEU:C	2.59	0.41
1:A:173:ASN:HD22	1:A:294:LEU:CD2	2.34	0.40
1:A:43:VAL:HG21	1:A:167:PHE:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:PHE:CZ	1:A:175:VAL:HG22	2.56	0.40
1:A:271:ASN:C	1:A:273:PHE:H	2.24	0.40
2:B:54:GLY:CA	2:B:57:THR:HG21	2.39	0.40
1:A:165:VAL:O	1:A:169:LYS:N	2.53	0.40
1:A:224:PHE:O	1:A:224:PHE:CD2	2.42	0.40
1:A:258:TYR:O	1:A:261:GLY:O	2.40	0.40
1:A:156:PHE:CZ	2:B:185:LYS:HG2	2.56	0.40
1:A:150:PHE:N	1:A:150:PHE:HD1	2.20	0.40
1:A:165:VAL:HG22	1:A:206:HIS:HE1	1.87	0.40
1:A:285:GLN:CB	1:A:288:GLN:NE2	2.84	0.40
3:C:182:PRO:HD2	3:C:183:GLU:H	1.86	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	212/361 (59%)	189 (89%)	18 (8%)	5 (2%)	6	42
2	B	216/427 (51%)	190 (88%)	21 (10%)	5 (2%)	7	42
3	C	202/418 (48%)	172 (85%)	25 (12%)	5 (2%)	6	40
All	All	630/1206 (52%)	551 (88%)	64 (10%)	15 (2%)	6	42

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	18	PRO
2	B	181	PRO
1	A	158	HIS
2	B	41	PHE
3	C	59	PRO
3	C	226	PRO

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Mol	Chain	Res	Type
1	A	255	GLY
1	A	205	GLU
3	C	62	PRO
1	A	213	LEU
3	C	135	PRO
2	B	52	GLY
2	B	37	VAL
3	C	18	PRO
1	A	267	ASN

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	186/320 (58%)	126 (68%)	60 (32%)	0	2
2	B	54/381 (14%)	36 (67%)	18 (33%)	0	2
3	C	58/380 (15%)	38 (66%)	20 (34%)	0	2
All	All	298/1081 (28%)	200 (67%)	98 (33%)	0	2

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	28	HIS
1	A	34	LYS
1	A	39	THR
1	A	48	LEU
1	A	56	SER
1	A	61	ASP
1	A	62	LEU
1	A	85	THR
1	A	86	VAL
1	A	87	GLU
1	A	98	THR
1	A	119	ILE

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Mol	Chain	Res	Type
1	A	122	ILE
1	A	127	GLU
1	A	134	SER
1	A	146	VAL
1	A	148	CYS
1	A	149	CYS
1	A	151	TYR
1	A	153	ILE
1	A	154	SER
1	A	158	HIS
1	A	160	LEU
1	A	163	LEU
1	A	164	ASP
1	A	165	VAL
1	A	167	PHE
1	A	176	ASN
1	A	183	LYS
1	A	187	LEU
1	A	188	THR
1	A	189	LEU
1	A	195	LEU
1	A	197	LYS
1	A	200	LEU
1	A	201	ASP
1	A	206	HIS
1	A	208	ILE
1	A	211	TYR
1	A	224	PHE
1	A	229	ARG
1	A	231	LEU
1	A	235	ILE
1	A	237	PHE
1	A	239	VAL
1	A	245	LEU
1	A	246	ILE
1	A	254	ARG
1	A	257	LEU
1	A	262	VAL
1	A	266	GLU
1	A	270	HIS
1	A	272	ASP
1	A	274	LEU

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Mol	Chain	Res	Type
1	A	277	ARG
1	A	279	MET
1	A	283	HIS
1	A	286	ASP
1	A	293	ASP
2	B	57	THR
2	B	58	LEU
2	B	60	ASP
2	B	61	THR
2	B	67	PHE
2	B	151	CYS
2	B	152	LEU
2	B	155	ILE
2	B	164	SER
2	B	166	ASP
2	B	168	VAL
2	B	169	THR
2	B	174	ASP
2	B	192	SER
2	B	210	VAL
2	B	251	MET
2	B	283	MET
2	B	306	MET
3	C	34	LEU
3	C	37	VAL
3	C	40	SER
3	C	44	LYS
3	C	46	THR
3	C	50	SER
3	C	51	LEU
3	C	52	PHE
3	C	53	LEU
3	C	54	THR
3	C	55	ASP
3	C	56	LEU
3	C	57	TYR
3	C	61	TYR
3	C	134	MET
3	C	141	CYS
3	C	174	ILE
3	C	178	ASP
3	C	181	THR

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Mol	Chain	Res	Type
3	C	255	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	131	HIS
1	A	172	HIS
1	A	173	ASN
1	A	206	HIS
1	A	212	HIS
1	A	270	HIS
1	A	283	HIS
1	A	285	GLN
1	A	295	HIS
1	A	298	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GDP	A	362	-	25,30,30	1.24	2 (8%)	27,47,47	2.08	7 (25%)
5	GTP	B	428	-	27,34,34	0.91	1 (3%)	29,54,54	1.91	7 (24%)
4	GDP	C	419	-	25,30,30	1.23	2 (8%)	27,47,47	2.08	7 (25%)

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	GDP	A	362	-	-	0/12/32/32	0/3/3/3
5	GTP	B	428	-	-	0/18/38/38	0/3/3/3
4	GDP	C	419	-	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	428	GTP	C6-N1	2.98	1.38	1.33
4	C	419	GDP	C5-C4	3.10	1.47	1.40
4	A	362	GDP	C5-C4	3.14	1.47	1.40
4	C	419	GDP	C6-C5	4.06	1.48	1.41
4	A	362	GDP	C6-C5	4.09	1.48	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	428	GTP	N3-C2-N1	-4.91	120.22	127.41
4	C	419	GDP	C5-C6-N1	-3.83	118.03	123.47
4	A	362	GDP	C5-C6-N1	-3.81	118.05	123.47
4	A	362	GDP	C6-C5-C4	-3.70	117.21	120.85
4	C	419	GDP	C6-C5-C4	-3.67	117.25	120.85
5	B	428	GTP	PB-O3B-PG	-3.61	120.48	132.63
4	C	419	GDP	PA-O3A-PB	-3.61	120.50	132.63
4	A	362	GDP	PA-O3A-PB	-3.61	120.50	132.63
5	B	428	GTP	PA-O3A-PB	-3.61	120.50	132.63
4	A	362	GDP	N3-C2-N1	-3.09	122.87	127.41
4	C	419	GDP	N3-C2-N1	-3.08	122.89	127.41
4	C	419	GDP	C4-C5-N7	-2.94	106.57	109.41
4	A	362	GDP	C4-C5-N7	-2.92	106.59	109.41
5	B	428	GTP	C5-C6-N1	-2.73	119.59	123.47
5	B	428	GTP	C4'-O4'-C1'	2.33	112.26	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	428	GTP	C6-N1-C2	2.64	119.86	116.06
4	C	419	GDP	C6-N1-C2	4.32	122.27	116.06
4	A	362	GDP	C6-N1-C2	4.33	122.28	116.06
5	B	428	GTP	C2-N3-C4	4.38	120.27	115.16
4	C	419	GDP	C2-N3-C4	4.99	120.98	115.16
4	A	362	GDP	C2-N3-C4	4.99	120.98	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	362	GDP	14	0
5	B	428	GTP	18	0
4	C	419	GDP	15	0

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	232/361 (64%)	-0.36	0 100 100	2, 81, 122, 148	0
2	B	246/427 (57%)	-0.59	0 100 100	3, 60, 134, 139	0
3	C	224/418 (53%)	-0.56	1 (0%) 92 87	26, 80, 134, 156	0
All	All	702/1206 (58%)	-0.51	1 (0%) 95 94	2, 73, 130, 156	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	134	MET	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 carbohydrates 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
4	GDP	C	419	28/28	0.84	0.19	83,89,97,100	0
4	GDP	A	362	28/28	0.88	0.21	53,75,81,81	0
5	GTP	B	428	32/32	0.89	0.18	35,56,65,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.