



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:43 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

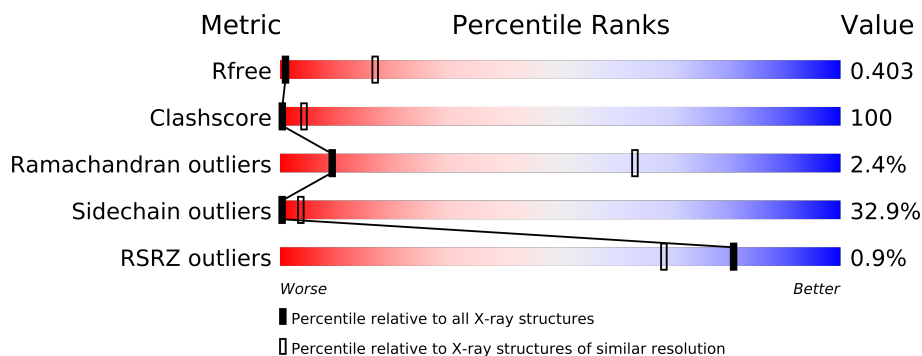
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance




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}	66092	1035 (4.52-3.46)
Clashscore	79885	1235 (4.50-3.50)
Ramachandran outliers	78287	1170 (4.50-3.50)
Sidechain outliers	78261	1156 (4.50-3.50)
RSRZ outliers	66119	1035 (4.52-3.46)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	361	
2	B	427	
3	C	418	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 4495 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

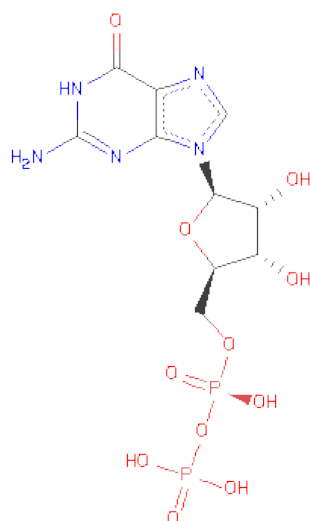
- Molecule 2 is a protein called Septin-6.

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.

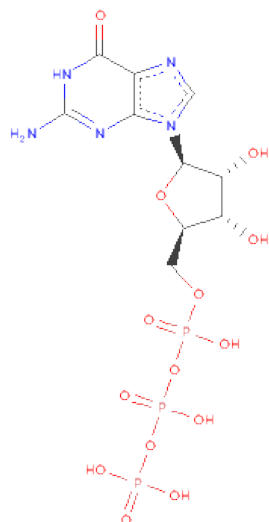
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	224	Total	C	N	O	S	0	0	0
			1273	788	230	247	8			

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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: $C_{10}H_{16}N_5O_{14}P_3$).



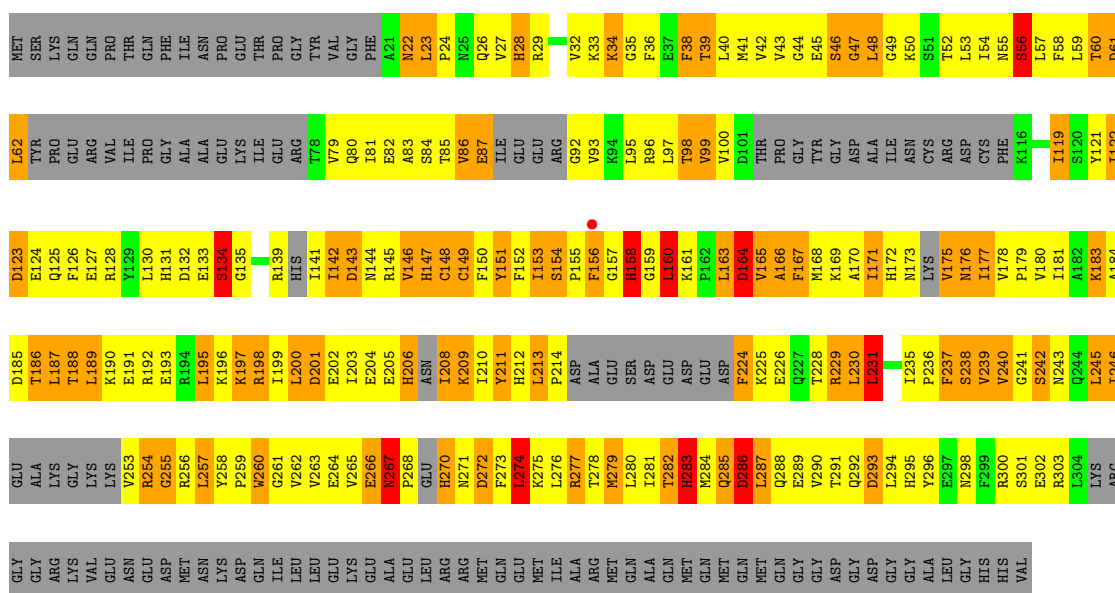
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

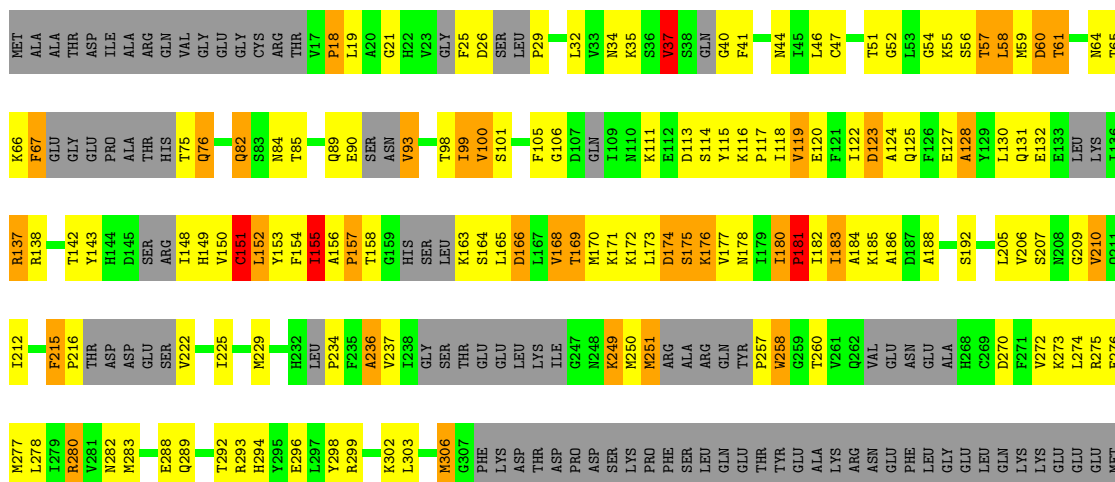
• Molecule 1: Septin-2

Chain A:



• Molecule 2: Septin-6

Chain B:



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

- Molecule 3: Septin-7

Chain C: 

[illegible]

P62		S65	HIS	ARG	ILE	LYS	LYS	T71	V72	G73	V74	E76	Q76	S77	K78	V79	L80	ILE	LYS	GLU	GLY	GLY	VAL	Q87	L88	T91	I92	I93	D94	T95	P96	GLY	PHI	GLY	GLY	ASP	ALA	VAL	VAL	ASP	ASN	SER	CYS	T108	Q109	P110	Y114	I115	D116	S117	K118	F119	E120	D121	Y122	A125
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R128	R129	R130	R131	R132	R133	R134	R135	R136	R137	ARG	R139	Q140	C141	C142	C143	V144	F145	I146	A147	P148	SER	G150	K154	D157	I158	M161	K162	R163	L164	H165	E166	K167	V168	M169	L173	I174	A175	K176	A177	D178	T179	L180	T181	P182	E183	F184	C185	F188	I192	M193	K194	E195	I196
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I203	Y204	P207	GLJ	THR	ASP	ASP	GLJ	GLJ	GLJ	ASN	LVS	LEU	VAL	LVS	LVS	ASP	ASP	ARG	ARG	L225	P226	L227	A228	V229	V230	G231	SER	ASN	THR	ILE	ILE	ILE	GLJ	VAL	ASN	GLY	LVS	ARG	VAL	ARG	ARG	G245	E246	Q247	Y248	P249	P250	G251	V252	V253	A254	E254	V255	GLJ	ASN	G258	H259	E260	H261	L266
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[illegible]

GLU GLN VAL VAL PHE GLU MET LYS VAL VAL LYS LYS LYS VAL VAL GLN LYS LYS LEU LEU LYS ASP SER GLU GLU ALA ALA GLU LEU LEU GLN ARG ARG HIS HIS LYS LYS LYS LYS LYS ASN ASN LEU LEU GLU GLU ALA ALA GLN LYS HIS HIS LYS LYS GLU GLU LEU LEU GLU GLU LYS LYS ASP ASP ARG ARG LYS LYS ALA ALA TRP TRP GLU GLU ALA ALA GLN GLN LYS LYS ARG ARG 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	2122 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	96.4	Xtriage
Anisotropy	1.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 131.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 42484 reflections	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.

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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 100.

All (791) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:185:LYS:HE3	5:B:428:GTP:C4	1.85	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
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:239:VAL:HG12	1:A:273:PHE:HA	1.24	1.07
1:A:130:LEU:HB2	1:A:295:HIS:HE1	1.19	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
1:A:143:ASP:OD2	1:A:145:ARG:HD3	1.53	1.05

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:155:ILE:N	2:B:155:ILE:HD13	1.75	1.00
2:B:113:ASP:O	2:B:117:PRO:HG3	1.62	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:42:LEU:CA	4:C:419:GDP:H5'	1.93	0.98
3:C:179:THR:HG23	3:C:180:LEU:CD2	1.93	0.98
1:A:175:VAL:CG1	1:A:176:ASN:HB2	1.92	0.98
1:A:284:MET:O	1:A:287:LEU:HG	1.63	0.98
1:A:258:TYR:HB2	1:A:261:GLY:O	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
1:A:282:THR:HG23	1:A:283:HIS:N	1.80	0.96
3:C:42:LEU:HA	4:C:419:GDP:C5'	1.93	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:249:LYS:CB	2:B:250:MET:SD	2.54	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
2:B:58:LEU:O	2:B:61:THR:HG22	1.67	0.94
1:A:271:ASN:ND2	1:A:273:PHE:HB2	1.82	0.94
3:C:43:GLY:CA	3:C:46:THR:HG22	1.95	0.94
1:A:177:ILE:HB	1:A:210:ILE:HG22	1.48	0.94
1:A:39:THR:O	1:A:147:HIS:HB2	1.66	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
2:B:54:GLY:HA3	2:B:57:THR:HG23	1.50	0.93
1:A:29:ARG:O	1:A:32:VAL:HB	1.65	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:H	1:A:237:PHE:HD2	0.99	0.92
1:A:265:VAL:HG12	1:A:266:GLU:HG2	0.92	0.92
1:A:237:PHE:N	1:A:237:PHE:CD2	2.36	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:H	1:A:283:HIS:HD2	1.26	0.82
1:A:211:TYR:CZ	1:A:214:PRO:HD2	2.15	0.82
3:C:41:GLY:O	4:C:419:GDP:H5"	1.80	0.81
2:B:294:HIS:O	2:B:298:TYR:CB	2.27	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:CD2	1:A:211:TYR:O	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
3:C:40:SER:HA	3:C:44:LYS:HZ3	1.45	0.80
1:A:55:ASN:CA	1:A:60:THR:O	2.29	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:C:173:LEU:CB	3:C:227:LEU:O	2.31	0.79
2:B:44:ASN:O	2:B:149:HIS:HB2	1.83	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
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:250:MET:O	2:B:251:MET:HG3	1.84	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
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:43:GLY:C	3:C:46:THR:CG2	2.54	0.75
3:C:34:LEU:C	3:C:34:LEU:HD22	2.06	0.75
1:A:211:TYR:HD2	1:A:211:TYR:O	1.70	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:36:PHE:O	1:A:93:VAL:CG2	2.34	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
1:A:181:ILE:HD11	1:A:236:PRO:HG2	1.69	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:N	1:A:153:ILE:HD13	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
2:B:257:PRO:HB2	2:B:258:TRP:HD1	1.47	0.73
1:A:47:GLY:HA2	2:B:158:THR:HG21	1.70	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:49:GLY:CA	1:A:52:THR:HG22	2.19	0.72
1:A:271:ASN:HD21	1:A:273:PHE:HB2	1.52	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: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:132:ASP:O	1:A:135:GLY:N	2.24	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:44:LYS:O	3:C:48:ILE:HG13	1.92	0.70
3:C:181:THR:O	3:C:185:CYS:N	2.23	0.70
3:C:174:ILE:N	3:C:174:ILE:HD12	2.05	0.70
1:A:172:HIS:CD2	1:A:209:LYS:HB2	2.26	0.70
1:A:288:GLN:O	1:A:291:THR:HG22	1.92	0.70
1:A:257:LEU:CD2	1:A:257:LEU:C	2.59	0.70
1:A:139:ARG:H	1:A:141:ILE:CG2	1.90	0.70
2:B:153:TYR:CE1	2:B:169:THR:HG21	2.27	0.70
1:A:279:MET:O	1:A:282:THR:CG2	2.27	0.70
1:A:57:LEU:HD11	1:A:277:ARG:HA	1.74	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:N	2:B:155:ILE:CD1	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:149:CYS:N	1:A:176:ASN:O	2.20	0.69
1:A:237:PHE:HB2	1:A:272:ASP:HB3	1.74	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:57:THR:CG2	5:B:428:GTP:O1A	2.37	0.68
2:B:251:MET:SD	2:B:251:MET:N	2.65	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:274:LEU:HD23	1:A:277:ARG:HG2	1.74	0.68
1:A:257:LEU:HD23	1:A:258:TYR:N	2.08	0.68
1:A:211:TYR:C	1:A:211:TYR:CD2	2.67	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:258:TYR:HD2	1:A:260:TRP:CE3	2.12	0.67
1:A:139:ARG:CB	1:A:141:ILE:N	2.58	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:149:CYS:SG	1:A:150:PHE:O	2.53	0.66
1:A:42:VAL:O	1:A:100:VAL:HG23	1.96	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
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
2:B:60:ASP:O	2:B:64:ASN:N	2.30	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
1:A:147:HIS:O	1:A:286:ASP:HB2	1.98	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:179:PRO:CD	1:A:210:ILE:CD1	2.76	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:79:VAL:HA	3:C:87:GLN:HA	1.80	0.63
3:C:141:CYS:HB2	3:C:169:ASN:O	1.99	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
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
1:A:54:ILE:CG2	1:A:55:ASN:N	2.63	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:211:TYR:CZ	1:A:214:PRO:CD	2.82	0.62
1:A:119:ILE:HD11	1:A:170:ALA:O	1.98	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:C:148:PRO:CG	3:C:150:GLY:CA	2.65	0.61
2:B:19:LEU:CB	3:C:77:SER:O	2.48	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:196:LYS:O	1:A:200:LEU:CD1	2.47	0.60
1:A:180:VAL:HG22	1:A:181:ILE:N	2.15	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:279:MET:SD	1:A:279:MET:C	2.79	0.60
1:A:213:LEU:O	1:A:213:LEU:CD2	2.44	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:265:VAL:HG12	1:A:266:GLU:N	2.15	0.60
1:A:173:ASN:HA	1:A:294:LEU:HD21	1.79	0.60
3:C:43:GLY:O	3:C:46:THR:CG2	2.39	0.60
2:B:185:LYS:HG3	5:B:428:GTP:C5	2.37	0.60
1:A:268:PRO:CG	1:A:271:ASN:O	2.50	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:240:VAL:CG1	4:A:362:GDP:O6	2.50	0.59
1:A:279:MET:SD	1:A:280:LEU:HA	2.42	0.59
2:B:153:TYR:HB3	2:B:170:MET:HE3	1.84	0.59
2:B:206:VAL:HA	2:B:209:GLY:CA	2.27	0.59
2:B:19:LEU:CB	3:C:77:SER:N	2.65	0.59
3:C:259:GLU:N	3:C:260:HIS:CB	2.66	0.59
3:C:140:GLN:O	3:C:168:VAL:CB	2.51	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:47:LEU:O	3:C:51:LEU:HB2	2.02	0.58
1:A:49:GLY:HA2	4:A:362:GDP:O1A	2.04	0.58
3:C:42:LEU:CA	4:C:419:GDP:C5'	2.69	0.58
1:A:45:GLU:O	1:A:47:GLY:HA3	2.03	0.58
2:B:85:THR:CB	2:B:98:THR:HA	2.34	0.58
1:A:38:PHE:CE1	1:A:147:HIS:HB3	2.38	0.58
1:A:263:VAL:HG13	2:B:257:PRO:CG	2.33	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:277:MET:HG3	2:B:278:LEU:N	2.18	0.57
2:B:225:ILE:O	2:B:229:MET:HG2	2.04	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
2:B:171:LYS:O	2:B:174:ASP:CB	2.52	0.57
1:A:229:ARG:NH2	1:A:230:LEU:CD1	2.67	0.57
3:C:34:LEU:O	3:C:34:LEU:CD1	2.42	0.57
3:C:174:ILE:N	3:C:174:ILE:CD1	2.67	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
3:C:43:GLY:HA2	4:C:419:GDP:O1A	2.04	0.56
1:A:47:GLY:HA2	2:B:158:THR:CG2	2.35	0.56
2:B:257:PRO:C	2:B:258:TRP:CD1	2.79	0.56
3:C:157:ASP:O	3:C:161:MET:HG3	2.05	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
3:C:51:LEU:HD12	3:C:51:LEU:O	2.06	0.56
2:B:120:GLU:O	2:B:124:ALA:CB	2.54	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:34:LEU:O	3:C:92:ILE:HA	2.07	0.55
3:C:141:CYS:HA	3:C:168:VAL:CB	2.37	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
3:C:41:GLY:C	4:C:419:GDP:H5''	2.28	0.53
1:A:87:GLU:C	1:A:92:GLY:HA2	2.28	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:29:ARG:O	1:A:32:VAL:HG23	2.08	0.53
1:A:298:ASN:O	1:A:302:GLU:CB	2.56	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:210:VAL:HG23	2.09	0.53
2:B:205:LEU:O	2:B:209:GLY:HA2	2.09	0.53
3:C:176:LYS:O	3:C:179:THR:N	2.38	0.53
2:B:166:ASP:HA	2:B:169:THR:HG21	1.88	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:212:HIS:O	1:A:214:PRO:CD	2.54	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:242:SER:HB3	1:A:255:GLY:O	2.09	0.52
1:A:242:SER:CB	1:A:255:GLY:O	2.56	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
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
3:C:60:GLU:HG2	4:C:419:GDP:O3B	2.10	0.52
1:A:245:LEU:CA	1:A:246:ILE:HD13	2.39	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:265:VAL:C	1:A:266:GLU:HG3	2.29	0.52
1:A:175:VAL:CG1	1:A:176:ASN:N	2.56	0.52
1:A:125:GLN:CB	1:A:144:ASN:O	2.58	0.52
1:A:285:GLN:HB3	1:A:288:GLN:NE2	2.25	0.51
1:A:131:HIS:HD2	1:A:132:ASP:OD1	1.93	0.51
3:C:42:LEU:N	4:C:419:GDP:H5"	2.25	0.51
3:C:34:LEU:HD22	3:C:35:MET:N	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:B:153:TYR:HE2	2:B:155:ILE:CG2	2.25	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
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: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:181:ILE:HB	1:A:238:SER:OG	2.13	0.49
1:A:206:HIS:CD2	1:A:208:ILE:CG1	2.95	0.49
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:156:PHE:CE2	2:B:185:LYS:CB	2.96	0.49
2:B:114:SER:C	2:B:117:PRO:HG2	2.33	0.49
1:A:54:ILE:HG13	1:A:58:PHE:CD2	2.45	0.49
1:A:148:CYS:SG	1:A:149:CYS:C	2.91	0.49
1:A:57:LEU:HD22	1:A:276:LEU:HD21	1.88	0.49
1:A:258:TYR:CE2	1:A:260:TRP:CZ3	3.00	0.49
2:B:116:LYS:H	2:B:117:PRO:CD	2.04	0.49
1:A:139:ARG:CA	1:A:141:ILE:N	2.76	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:CD1	1:A:153:ILE:H	2.05	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:197:LYS:O	1:A:200:LEU:HB2	2.13	0.48
1:A:183:LYS:HG3	4:A:362:GDP:C6	2.47	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:49:GLY:HA2	1:A:52:THR:HG22	1.95	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
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:195:LEU:O	1:A:199:ILE:HG13	2.13	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: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:257:PRO:C	2:B:258:TRP:CG	2.88	0.47
2:B:153:TYR:HB3	2:B:170:MET:HE2	1.97	0.47
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: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
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
1:A:121:TYR:HA	1:A:124:GLU:HB3	1.97	0.47
3:C:26:VAL:O	3:C:27:LYS:O	2.31	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:163:LEU:C	1:A:163:LEU:HD13	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
3:C:23:ARG:C	3:C:25:SER:N	2.68	0.45
2:B:84:ASN:O	2:B:99:ILE:O	2.34	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:HA	1:A:231:LEU:HD12	1.67	0.45
1:A:164:ASP:O	1:A:168:MET:HG3	2.16	0.45
2:B:169:THR:CG2	2:B:170:MET:N	2.79	0.45
1:A:82:GLU:O	1:A:97:LEU:N	2.49	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:160:LEU:CD1	1:A:199:ILE:HG12	2.35	0.45
3:C:46:THR:O	3:C:50:SER:N	2.44	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:60:ASP:HA	2:B:65:THR: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
2:B:25:PHE:O	2:B:26:ASP:O	2.35	0.45
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
2:B:180:ILE:HA	2:B:181:PRO:HD3	1.37	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:231:GLY:HA3	4:C:419:GDP:N7	2.32	0.44
3:C:192:ILE:O	3:C:195:GLU:N	2.50	0.44
1:A:150:PHE:CD1	1:A:150:PHE:N	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
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
2:B:64:ASN:C	2:B:65:THR:HG23	2.35	0.43
1:A:54:ILE:HG22	1:A:55:ASN:N	2.34	0.43
1:A:163:LEU:HA	1:A:163:LEU:HD22	1.64	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:150:PHE:CB	1:A:152:PHE:CE1	3.02	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
3:C:179:THR:HG23	3:C:180:LEU:N	2.34	0.42
2:B:149:HIS:O	2:B:178:ASN:CB	2.67	0.42
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.75	0.42
1:A:119:ILE:O	1:A:119:ILE:CG2	2.64	0.42
1:A:204:GLU:C	1:A:206:HIS:N	2.73	0.42
2:B:57:THR:HG21	5:B:428:GTP:H5'	2.01	0.42
2:B:182:ILE:HD12	2:B:183:ILE:N	2.24	0.42
1:A:29:ARG:HA	1:A:32:VAL:CG2	2.49	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:185:LYS:CG	5:B:428:GTP:C5	3.01	0.42
2:B:289:GLN:O	2:B:293:ARG:N	2.52	0.42
2:B:55:LYS:O	2:B:59:MET:HG2	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
1:A:226:GLU:O	1:A:230:LEU:HB2	2.19	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
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:56:SER:OG	1:A:254:ARG:NH2	2.41	0.41
1:A:193:GLU:HA	1:A:196:LYS:HE3	2.02	0.41
1:A:134:SER:HA	1:A:135:GLY:HA3	1.79	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
2:B:182:ILE:HD11	2:B:237:VAL:CB	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:237:PHE:CB	1:A:272:ASP:HB3	2.47	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:HB3	1:A:197:LYS:HE2	1.80	0.41
1:A:197:LYS:HA	1:A:200:LEU:HD13	2.03	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: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
2:B:206:VAL:CA	2:B:209:GLY:HA2	2.33	0.41
1:A:81:ILE:CD1	1:A:81:ILE:C	2.88	0.41
1:A:181:ILE:HD13	1:A:238:SER:OG	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:119:ILE:O	1:A:119:ILE:HG23	2.21	0.41
1:A:254:ARG:O	1:A:265:VAL:HG23	2.21	0.41
2:B:170:MET:O	2:B:173:LEU:C	2.59	0.41
1:A:36:PHE:H	1:A:93:VAL:HG23	1.86	0.41
1:A:26:GLN:HA	1:A:26:GLN:NE2	2.35	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
1:A:126:PHE:CZ	1:A:175:VAL:HG22	2.56	0.40
2:B:54:GLY:CA	2:B:57:THR:HG21	2.39	0.40
1:A:271:ASN:C	1:A:273:PHE:H	2.24	0.40
1:A:165:VAL:O	1:A:169:LYS:N	2.53	0.40
1:A:156:PHE:CZ	2:B:185:LYS:HG2	2.56	0.40
1:A:258:TYR:O	1:A:261:GLY:O	2.40	0.40
1:A:224:PHE:O	1:A:224:PHE:CD2	2.42	0.40
1:A:150:PHE:HD1	1:A:150:PHE:N	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

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/361 (59%)	189 (89%)	18 (8%)	5 (2%)	9	63
2	B	216/427 (51%)	190 (88%)	21 (10%)	5 (2%)	10	64
3	C	202/418 (48%)	172 (85%)	25 (12%)	5 (2%)	9	62
All	All	630/1206 (52%)	551 (88%)	64 (10%)	15 (2%)	9	63

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
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	4
2	B	54/381 (14%)	36 (67%)	18 (33%)	0	3
3	C	58/380 (15%)	38 (66%)	20 (34%)	0	3
All	All	298/1081 (28%)	200 (67%)	98 (33%)	0	4

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	30,30,30	1.44	5 (16%)	44,47,47	2.93	8 (18%)
5	GTP	B	428	-	34,34,34	0.98	1 (2%)	51,54,54	2.47	9 (17%)
4	GDP	C	419	-	30,30,30	1.43	5 (16%)	44,47,47	2.92	8 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GDP	A	362	-	-	0/16/32/32	0/1/3/3
5	GTP	B	428	-	-	0/22/38/38	0/1/3/3
4	GDP	C	419	-	-	0/16/32/32	0/1/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	362	GDP	C6-C5	4.53	1.48	1.41
4	C	419	GDP	C6-C5	4.50	1.48	1.41
5	B	428	GTP	C2-N3	4.01	1.38	1.33
4	A	362	GDP	C5-C4	3.14	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	419	GDP	C5-C4	3.10	1.47	1.40
4	C	419	GDP	C4-N9	-2.55	1.34	1.37
4	A	362	GDP	C4-N9	-2.54	1.34	1.37
4	C	419	GDP	C2-N2	2.30	1.36	1.32
4	A	362	GDP	C2-N2	2.28	1.36	1.32
4	A	362	GDP	C2-N3	2.20	1.36	1.33
4	C	419	GDP	C2-N3	2.19	1.36	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	362	GDP	C6-C5-N7	15.27	136.20	134.14
4	C	419	GDP	C6-C5-N7	15.19	136.19	134.14
5	B	428	GTP	C6-C5-N7	-13.58	132.31	134.14
4	A	362	GDP	N3-C4-N9	5.59	135.10	126.91
4	C	419	GDP	N3-C4-N9	5.56	135.07	126.91
4	C	419	GDP	C5-C4-N3	-5.08	118.58	125.94
4	A	362	GDP	C5-C4-N3	-5.07	118.60	125.94
4	A	362	GDP	C2-N3-C4	4.20	120.98	115.09
4	C	419	GDP	C2-N3-C4	4.19	120.98	115.09
5	B	428	GTP	C5-C4-N3	-3.89	120.30	125.94
5	B	428	GTP	PB-O3B-PG	-3.82	120.48	131.68
4	C	419	GDP	PA-O3A-PB	-3.81	120.50	131.68
4	A	362	GDP	PA-O3A-PB	-3.81	120.50	131.68
5	B	428	GTP	PA-O3A-PB	-3.81	120.50	131.68
5	B	428	GTP	N3-C4-N9	3.81	132.50	126.91
5	B	428	GTP	C2-N3-C4	3.69	120.27	115.09
4	C	419	GDP	C4-C5-N7	-3.45	106.57	109.52
4	C	419	GDP	C3'-C2'-C1'	3.42	106.27	100.91
4	A	362	GDP	C4-C5-N7	-3.42	106.59	109.52
4	A	362	GDP	C3'-C2'-C1'	3.41	106.24	100.91
5	B	428	GTP	C3'-C2'-C1'	3.16	105.86	100.91
5	B	428	GTP	C4'-O4'-C1'	2.31	112.26	109.75
4	A	362	GDP	C8-N9-C4	2.10	108.50	106.90
5	B	428	GTP	N7-C8-N9	-2.04	108.58	114.36
4	C	419	GDP	C8-N9-C4	2.02	108.44	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.12	1 (0%) 90 82	2, 81, 122, 148	0
2	B	246/427 (57%)	-0.07	0 100 100	3, 60, 134, 139	0
3	C	224/418 (53%)	-0.02	5 (2%) 59 46	26, 80, 134, 156	0
All	All	702/1206 (58%)	0.01	6 (0%) 81 68	2, 73, 130, 156	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	134	MET	3.4
3	C	175	ALA	3.0
1	A	156	PHE	2.5
3	C	176	LYS	2.3
3	C	179	THR	2.3
3	C	41	GLY	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GTP	B	428	32/32	0.19	-0.99	35,56,65,67	0
4	GDP	A	362	28/28	0.20	-1.26	53,75,81,81	0
4	GDP	C	419	28/28	0.24	-1.35	83,89,97,100	0

6.5 Other polymers ⓘ

There are no such residues in this entry.