Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 10:28 PM EDT

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

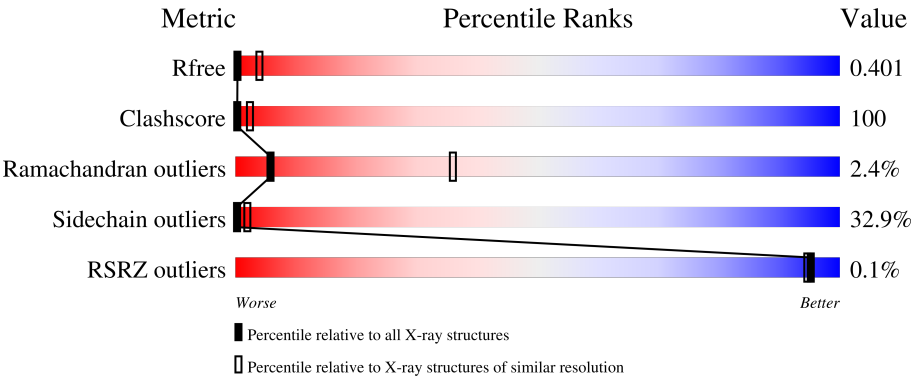
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	361	8% 33% 21% • 36%
2	B	427	24% 25% 8% • 42%
3	C	418	21% 24% 8% • 46%

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
			Total	C	N	O	S			
1	A	232	1765	1129	302	328	6	0	0	0

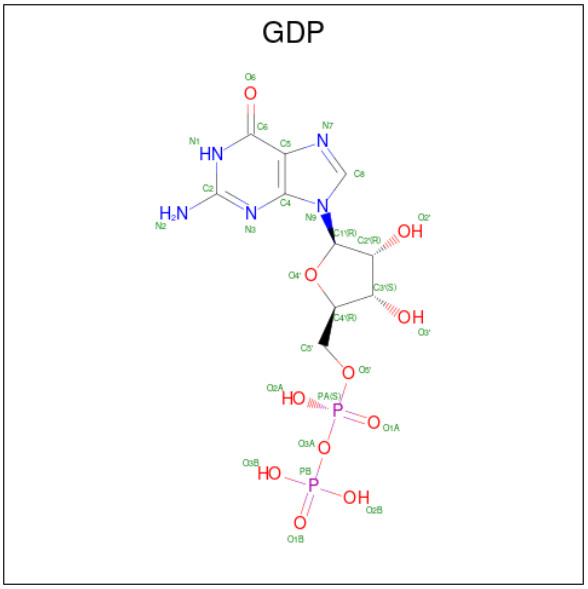
- Molecule 2 is a protein called Septin-6.

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

- Molecule 3 is a protein called Septin-7.

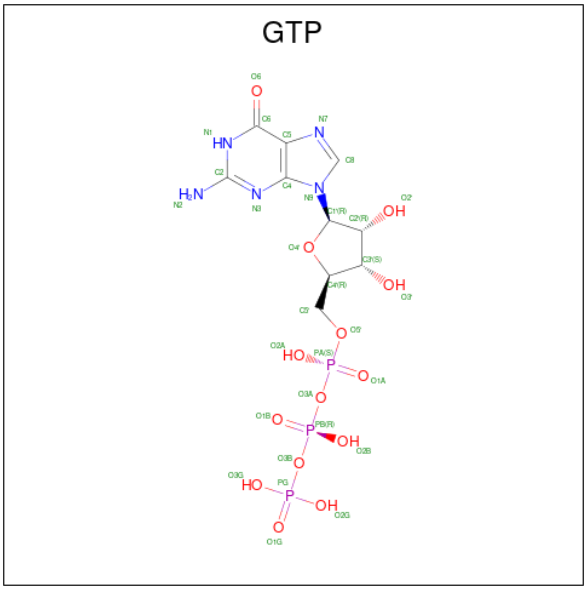
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	224	1273	788	230	247	8	0	0	0

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



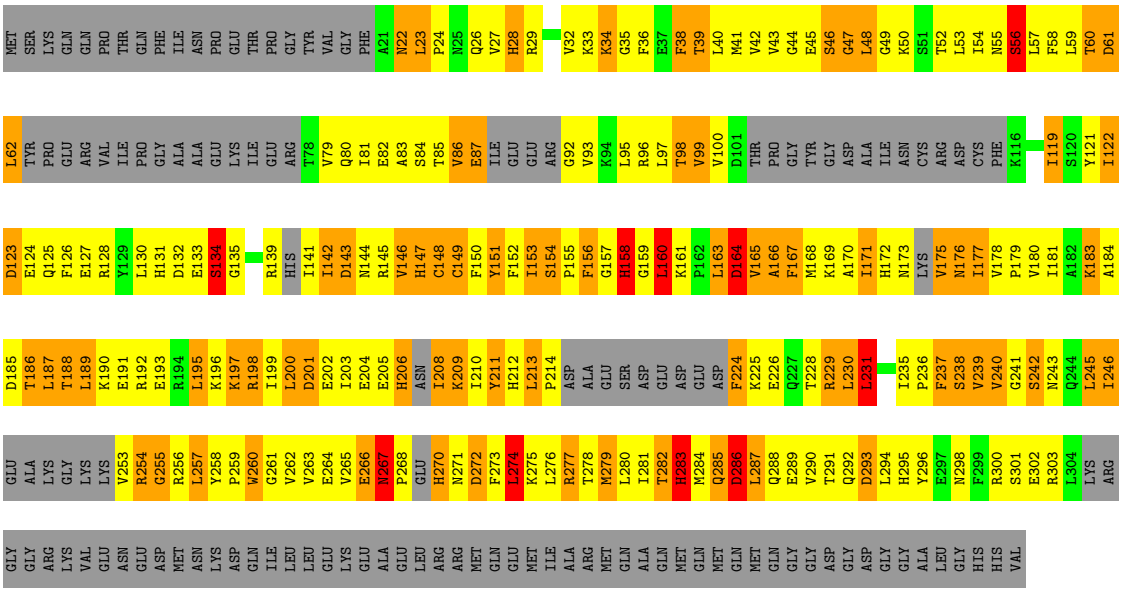
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

3 Residue-property plots (i)

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

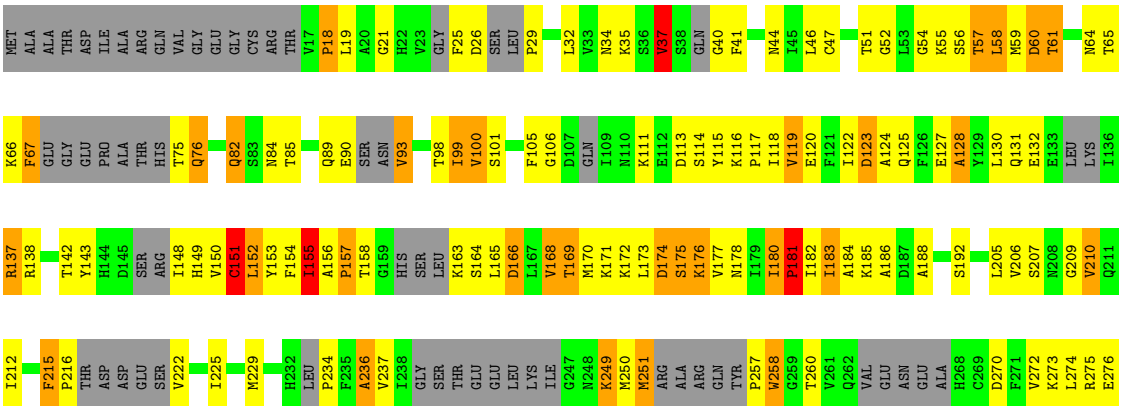
- Molecule 1: Septin-2

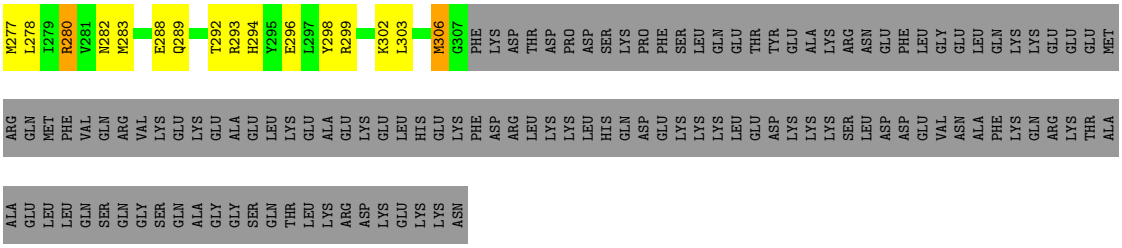
Chain A:



- Molecule 2: Septin-6

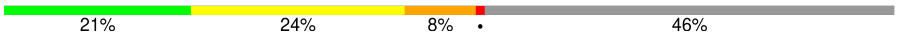
Chain B:

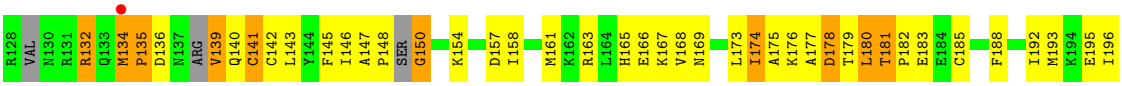


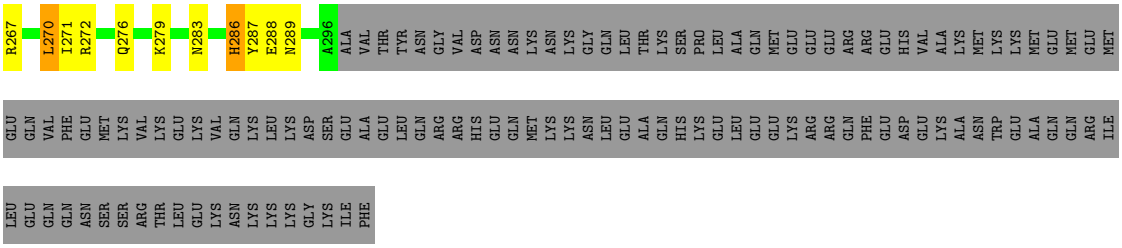


• Molecule 3: Septin-7

Chain C:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	252.51Å 252.51Å 156.49Å 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
$< I/\sigma(I) >$ [1]	3.89 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.376 , 0.392 0.399 , 0.401	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 , 213.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.54	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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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
1:A:139:ARG:H	1:A:141:ILE:HG23	0.96	1.11
2:B:116:LYS:N	2:B:117:PRO:HD2	1.57	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:C	1:A:224:PHE:CD2	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:HD13	3:C:34:LEU:O	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:HD23	1:A:213:LEU:O	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:55:ASN:HA	1:A:60:THR:O	1.61	1.01
1:A:201:ASP:O	1:A:204:GLU:HB2	1.59	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:HD13	2:B:155:ILE:N	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: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: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:H	1:A:237:PHE:HD2	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:C	1:A:224:PHE:HD2	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:39:THR:HA	1:A:96:ARG:O	1.72	0.90
1:A:240:VAL:HG22	4:A:362:GDP:O6	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:PHE:HD2	1:A:224:PHE:O	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:HD13	1:A:153:ILE:H	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:60:ASP:HB3	2:B:65:THR:O	1.75	0.84
2:B:116:LYS:N	2:B:117:PRO:CD	2.39	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
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: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

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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:36:PHE:O	1:A:93:VAL:CG2	2.34	0.74
1:A:211:TYR:O	1:A:211:TYR:HD2	1.70	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:79:VAL:CG2	1:A:99:VAL:O	2.34	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: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:47:GLY:HA2	2:B:158:THR:HG21	1.70	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: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:55:ASN:CG	1:A:61:ASP:HA	2.11	0.71
1:A:173:ASN:CA	1:A:294:LEU:CD2	2.50	0.71
1:A:34:LYS:HD2	1:A:34:LYS:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASP:O	1:A:135:GLY:N	2.24	0.71
1:A:208:ILE:CD1	1:A:209:LYS:N	2.44	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:C	1:A:257:LEU:CD2	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: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:57:THR:CG2	5:B:428:GTP:O1A	2.37	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
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:CD2	1:A:211:TYR:C	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:156:PHE:CE1	2:B:185:LYS:HG2	2.30	0.67
1:A:198:ARG:O	1:A:202:GLU:CG	2.43	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:O	1:A:59:LEU:HG	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:55:ASN:O	1:A:59:LEU:N	2.30	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
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
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:29:ARG:O	1:A:32:VAL:CG2	2.46	0.63
1:A:175:VAL:HG12	1:A:176:ASN:CA	2.28	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:81:ILE:HD12	1:A:81:ILE:C	2.19	0.63
1:A:285:GLN:CA	1:A:288:GLN:HG3	2.28	0.63
1:A:122:ILE:HD12	1:A:175:VAL:HG23	1.81	0.62
1:A:54:ILE:CG2	1:A:55:ASN:N	2.63	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
2:B:236:ALA:O	2:B:270:ASP:CB	2.48	0.62
1:A:55:ASN:CB	1:A:60:THR:O	2.47	0.62
1:A:265:VAL:CG1	1:A:266:GLU:HG3	2.11	0.62
1:A:119:ILE:HD11	1:A:170:ALA:O	1.98	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: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:61:ASP:O	1:A:62:LEU:HD23	2.01	0.61
1:A:177:ILE:HG22	1:A:179:PRO:CD	2.31	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:O	1:A:213:LEU:CD2	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: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

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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: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: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: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:41:MET:HA	1:A:98:THR:O	2.05	0.57
1:A:80:GLN:HA	1:A:80:GLN:OE1	2.04	0.57
1:A:265:VAL:CB	1:A:266:GLU:HG3	2.34	0.57
1:A:47:GLY:HA2	2:B:158:THR:CG2	2.35	0.56
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
2:B:257:PRO:C	2:B:258:TRP:CD1	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N	2:B:67:PHE:CD1	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: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:38:PHE:CE2	1:A:40:LEU:HB3	2.41	0.55
1:A:206:HIS:CD2	1:A:208:ILE:HG13	2.42	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:HD12	1:A:203:ILE:H	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:87:GLU:C	1:A:92:GLY:HA2	2.28	0.53
1:A:274:LEU:CD2	1:A:277:ARG:HG2	2.37	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: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
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:45:GLU:O	1:A:48:LEU:HG	2.09	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: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:C	1:A:28:HIS:CD2	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:61:ASP:OD2	1:A:62:LEU:N	2.44	0.51
1:A:189:LEU:HD12	1:A:190:LYS:H	1.75	0.51
1:A:151:TYR:HD2	1:A:151:TYR:C	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:54:ILE:HG13	1:A:58:PHE:CZ	2.45	0.50
1:A:186:THR:O	5:B:428:GTP:N2	2.44	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:82:GLU:CB	1:A:97:LEU:O	2.59	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
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:57:LEU:CD2	1:A:276:LEU:CD2	2.83	0.50
1:A:122:ILE:HG13	1:A:126:PHE:HD1	1.76	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:181:ILE:HB	1:A:238:SER:OG	2.13	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
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:57:LEU:HD22	1:A:276:LEU:HD21	1.88	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
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:49:GLY:HA2	1:A:52:THR:HG22	1.95	0.48
1:A:130:LEU:CD1	1:A:295:HIS:CE1	2.96	0.48
1:A:141:ILE:HD12	1:A:142:ILE:H	1.74	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:C	1:A:97:LEU:HD23	2.34	0.48
1:A:130:LEU:HD12	1:A:295:HIS:CE1	2.49	0.47
1:A:179:PRO:HD2	1:A:210:ILE:HD12	1.95	0.47
3:C:154:LYS:O	3:C:158:ILE:N	2.45	0.47
1:A:163:LEU:HD13	1:A:163:LEU:O	2.13	0.47
1:A:195:LEU:O	1:A:199:ILE:HG13	2.13	0.47
1:A:23:LEU:O	1:A:27:VAL:N	2.29	0.47
1:A:195:LEU:O	1:A:199:ILE:CG1	2.62	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:49:GLY:O	1:A:53:LEU:HB3	2.15	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
2:B:75:THR:O	2:B:76:GLN:CB	2.61	0.47
2:B:153:TYR:OH	2:B:166:ASP:CB	2.59	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
1:A:121:TYR:HA	1:A:124:GLU:HB3	1.97	0.47
2:B:35:LYS:C	2:B:37:VAL:H	2.17	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
3:C:26:VAL:O	3:C:27:LYS:O	2.31	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:52:THR:HG23	1:A:53:LEU:N	2.31	0.46
1:A:240:VAL:CG1	4:A:362:GDP:C6	2.93	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:29:ARG:C	1:A:32:VAL:HG23	2.36	0.45
1:A:163:LEU:HD13	1:A:163:LEU:C	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:46:SER:HB3	1:A:50:LYS:NZ	2.31	0.45
1:A:286:ASP:OD1	1:A:286:ASP:N	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:34:LYS:HD2	1:A:34:LYS:C	2.35	0.45
1:A:172:HIS:CD2	1:A:209:LYS:HG3	2.50	0.45
1:A:231:LEU:HD12	1:A:231:LEU:HA	1.67	0.45
1:A:82:GLU:O	1:A:97:LEU:N	2.49	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:143:ASP:HB2	1:A:145:ARG:HD3	1.97	0.45
3:C:79:VAL:CB	3:C:87:GLN:CB	2.95	0.45
3:C:148:PRO:CB	3:C:150:GLY:HA3	2.47	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:57:LEU:HD21	1:A:276:LEU:CD2	2.33	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
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:247:GLN:CB	3:C:252:VAL:CB	2.97	0.43
3:C:249:PRO:HB2	3:C:250:TRP:CE3	2.53	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
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:39:GLU:O	3:C:44:LYS:CE	2.67	0.43
3:C:43:GLY:H	4:C:419:GDP:PA	2.41	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:82:GLN:O	2:B:101:SER:O	2.37	0.43
2:B:186:ALA:CB	2:B:237:VAL:O	2.65	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:HD12	1:A:187:LEU:HA	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:29:ARG:HA	1:A:32:VAL:CG2	2.49	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:156:PHE:CD1	2:B:185:LYS:HE2	2.55	0.42
1:A:164:ASP:O	1:A:168:MET:N	2.46	0.42
2:B:55:LYS:O	2:B:59:MET:HG2	2.19	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
1:A:226:GLU:O	1:A:230:LEU:HB2	2.19	0.42
1:A:284:MET:HE3	1:A:284:MET:HB3	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:38:PHE:O	1:A:95:LEU:HD23	2.20	0.42
1:A:149:CYS:O	1:A:177:ILE:HA	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: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: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:36:PHE:O	1:A:93:VAL:HG23	2.17	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:81:ILE:C	1:A:81:ILE:CD1	2.88	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
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: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
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:43:VAL:HG21	1:A:167:PHE:CE2	2.57	0.40
1:A:173:ASN:HD22	1:A:294:LEU:CD2	2.34	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:156:PHE:CZ	2:B:185:LYS:HG2	2.56	0.40
1:A:165:VAL:O	1:A:169:LYS:N	2.53	0.40
1:A:224:PHE:CD2	1:A:224:PHE:O	2.42	0.40
1:A:258:TYR:O	1:A:261:GLY:O	2.40	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	36
2	B	216/427 (51%)	190 (88%)	21 (10%)	5 (2%)	6	37
3	C	202/418 (48%)	172 (85%)	25 (12%)	5 (2%)	5	35
All	All	630/1206 (52%)	551 (88%)	64 (10%)	15 (2%)	6	36

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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	1
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

Sometimes 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 molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides 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	$\#\|Z\|>2$
5	GTP	B	428	-	29,34,34	1.23	2 (6%)	35,54,54	1.37	5 (14%)
4	GDP	A	362	-	25,30,30	1.00	1 (4%)	30,47,47	1.15	3 (10%)
4	GDP	C	419	-	25,30,30	0.99	1 (4%)	30,47,47	1.14	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	B	428	-	-	4/18/38/38	0/3/3/3
4	GDP	A	362	-	-	2/12/32/32	0/3/3/3
4	GDP	C	419	-	-	5/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	428	GTP	C5-C6	-4.12	1.39	1.47
4	A	362	GDP	C6-N1	-2.29	1.34	1.37
4	C	419	GDP	C6-N1	-2.23	1.34	1.37
5	B	428	GTP	C2-N3	2.20	1.38	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	428	GTP	C8-N7-C5	3.60	108.68	102.55
4	C	419	GDP	C8-N7-C5	2.91	107.50	102.55
4	A	362	GDP	C8-N7-C5	2.90	107.49	102.55
5	B	428	GTP	C5-C6-N1	2.89	119.59	114.07
5	B	428	GTP	C2-N1-C6	-2.87	119.86	125.11
5	B	428	GTP	C4'-O4'-C1'	2.55	112.26	109.92
4	A	362	GDP	C4'-O4'-C1'	2.16	111.90	109.92
4	C	419	GDP	C4'-O4'-C1'	2.15	111.89	109.92
4	A	362	GDP	C5-C6-N1	2.09	118.05	114.07
5	B	428	GTP	O6-C6-C5	-2.08	120.20	124.32
4	C	419	GDP	C5-C6-N1	2.07	118.03	114.07

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	419	GDP	C5'-O5'-PA-O3A
4	C	419	GDP	C5'-O5'-PA-O1A
4	A	362	GDP	O4'-C4'-C5'-O5'
4	A	362	GDP	C3'-C4'-C5'-O5'
5	B	428	GTP	O4'-C4'-C5'-O5'
5	B	428	GTP	PA-O3A-PB-O1B
4	C	419	GDP	C5'-O5'-PA-O2A
4	C	419	GDP	PB-O3A-PA-O1A
4	C	419	GDP	C4'-C5'-O5'-PA
5	B	428	GTP	C3'-C4'-C5'-O5'
5	B	428	GTP	PB-O3A-PA-O2A

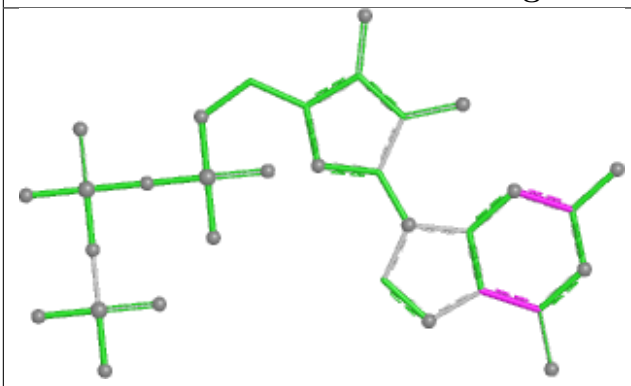
There are no ring outliers.

3 monomers are involved in 47 short contacts:

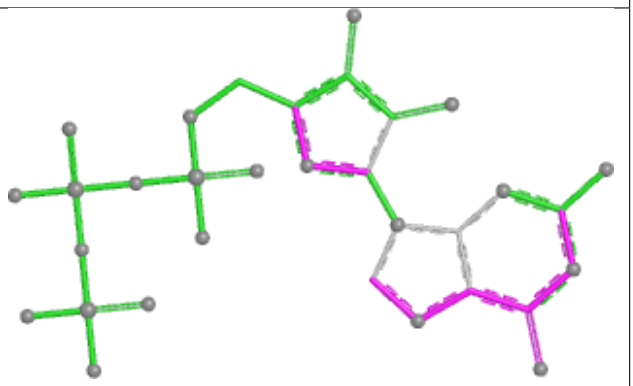
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	428	GTP	18	0
4	A	362	GDP	14	0
4	C	419	GDP	15	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

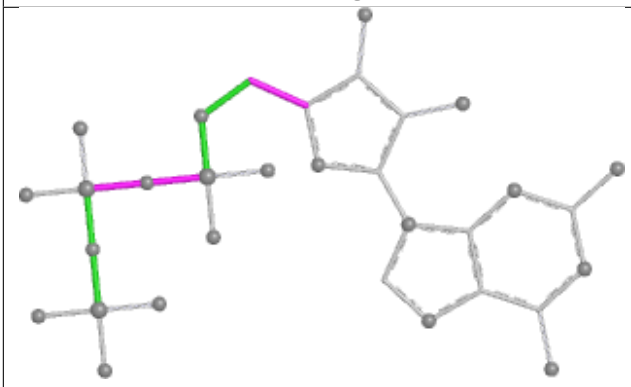
Ligand GTP B 428



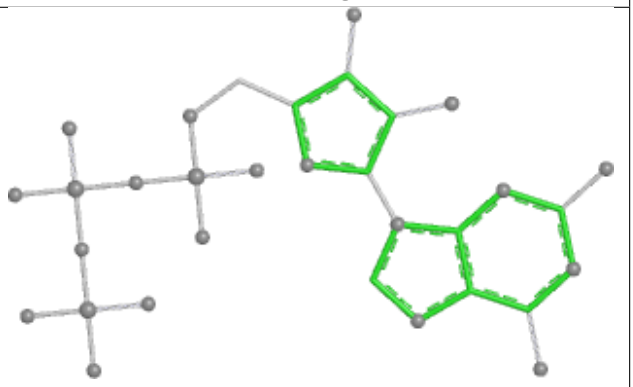
Bond lengths



Bond angles

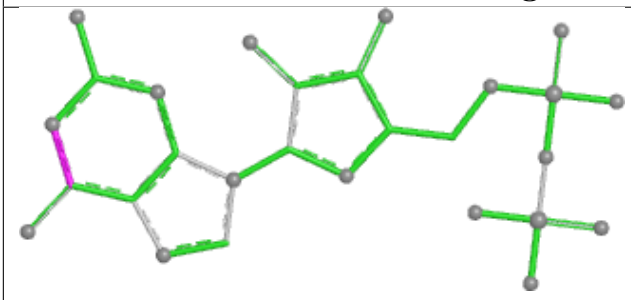


Torsions

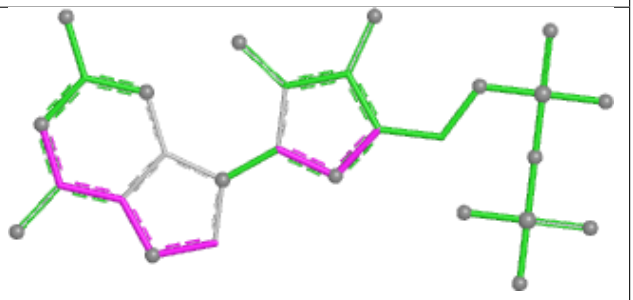


Rings

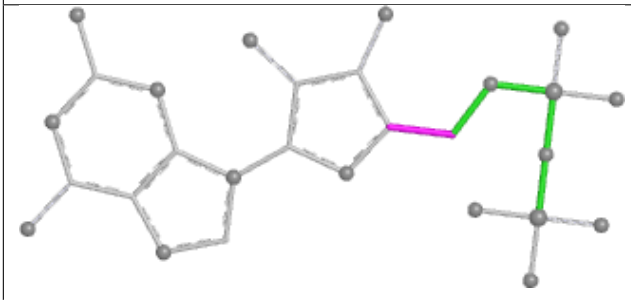
Ligand GDP A 362



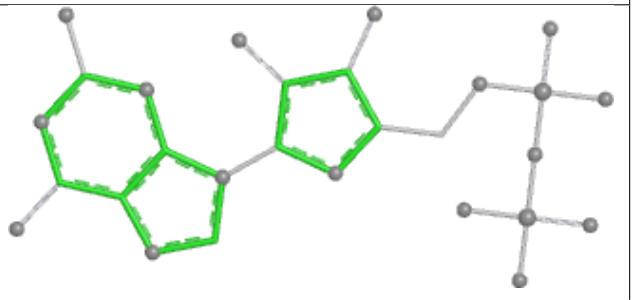
Bond lengths



Bond angles

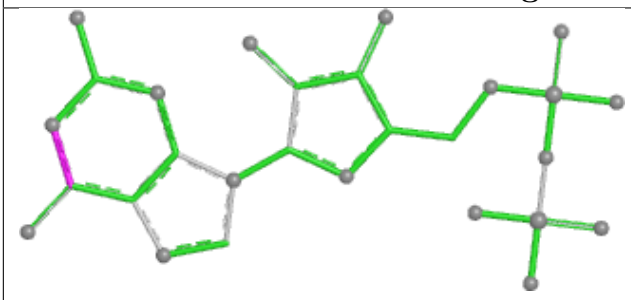


Torsions

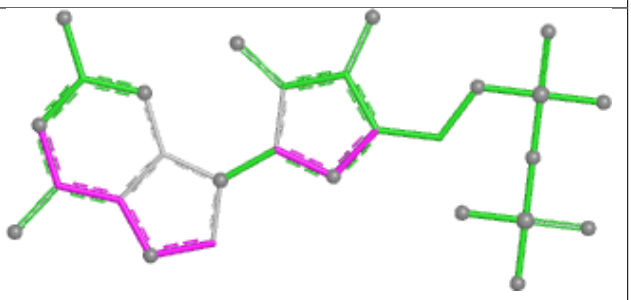


Rings

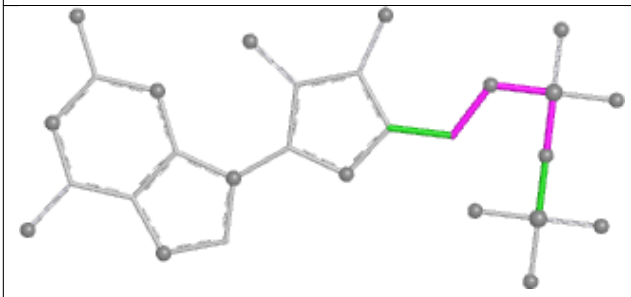
Ligand GDP C 419



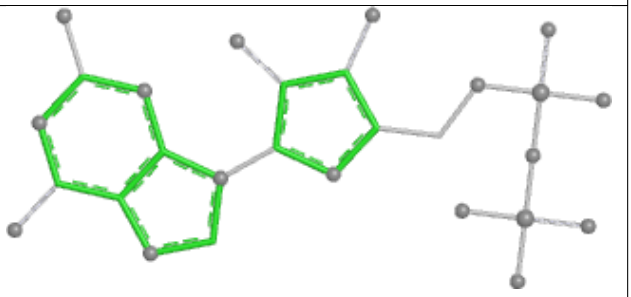
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.50	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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

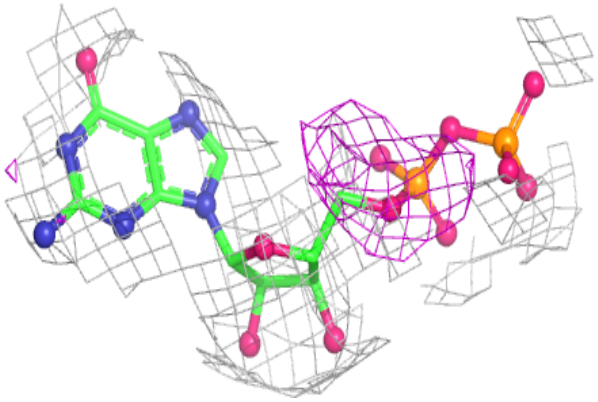
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

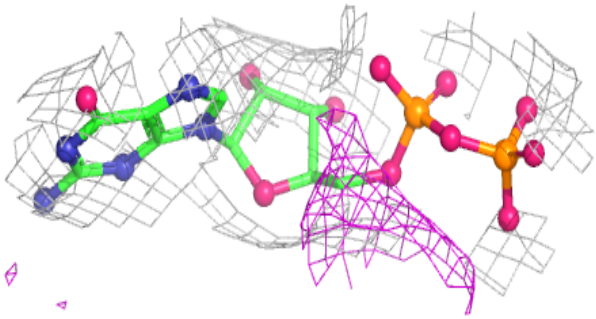
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GDP	C	419	28/28	0.84	0.19	83,89,97,100	0
4	GDP	A	362	28/28	0.88	0.21	53,75,81,81	0
5	GTP	B	428	32/32	0.89	0.19	35,56,65,67	0

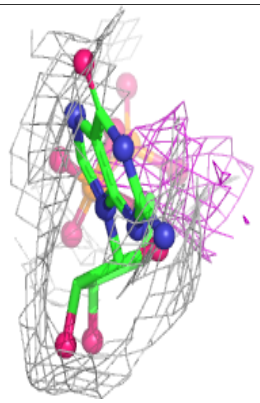
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP C 419:

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

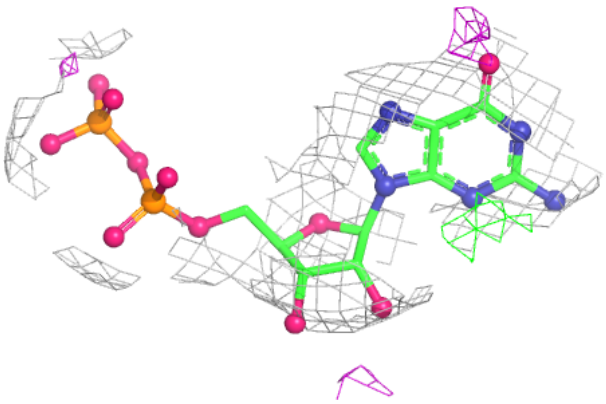


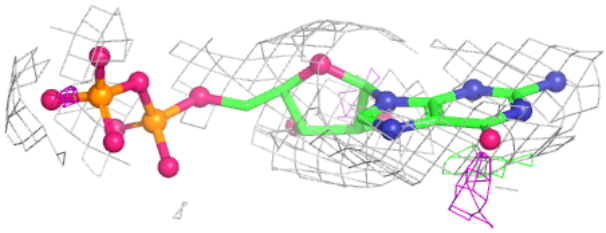


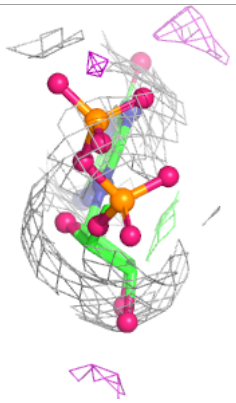


Electron density around GDP A 362:

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

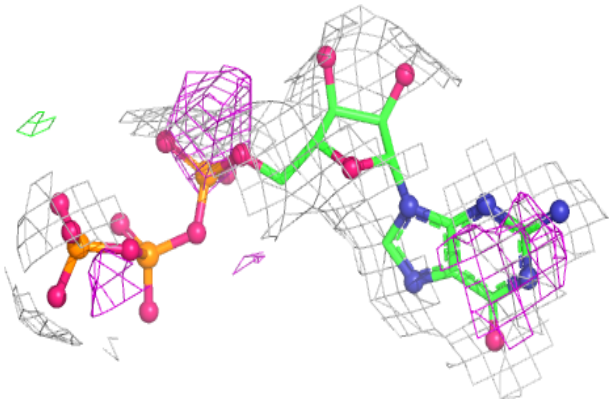


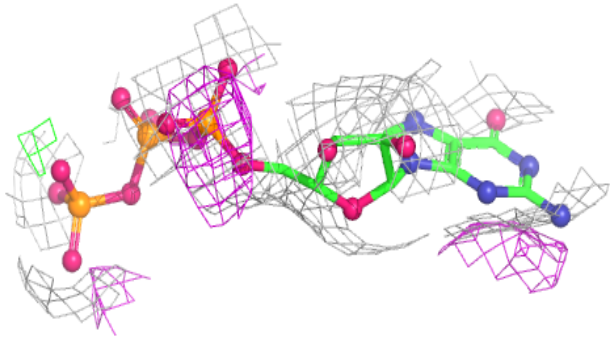


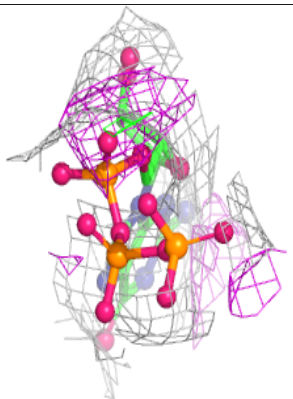


Electron density around GTP B 428:

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







6.5 Other polymers (i)

There are no such residues in this entry.