



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:54 PM UTC

PDB ID : 1HI0 / pdb_00001hi0
Title : RNA dependent RNA polymerase from dsRNA bacteriophage phi6 plus initiation complex
Authors : Grimes, J.M.; Butcher, S.J.; Makeyev, E.V.; Bamford, D.H.; Stuart, D.I.
Deposited on : 2000-12-31
Resolution : 3.00 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

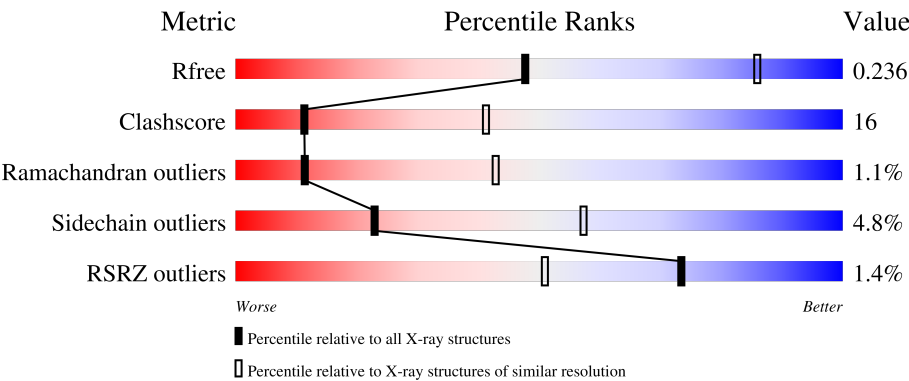
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	5	40% 40% 20% 20% 20%
1	E	5	40% 40% 20% 20% 20%
1	F	5	20% 40% 20% 20% 20%
2	P	664	% 63% 33% .
2	Q	664	% 63% 33% .

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Mol	Chain	Length	Quality of chain
2	R	664	% 64% 33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16221 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 DNA chain called DNA (5'-(**TP*TP*TP*CP*C*)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	4	Total	C	N	O	P	0	0	0
			75	38	10	24	3			
1	E	4	Total	C	N	O	P	0	0	0
			75	38	10	24	3			
1	F	4	Total	C	N	O	P	0	0	0
			75	38	10	24	3			

- Molecule 2 is a protein called P2 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
2	Q	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
2	R	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	456	MET	ILE	conflict	UNP P11124
Q	456	MET	ILE	conflict	UNP P11124
R	456	MET	ILE	conflict	UNP P11124

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

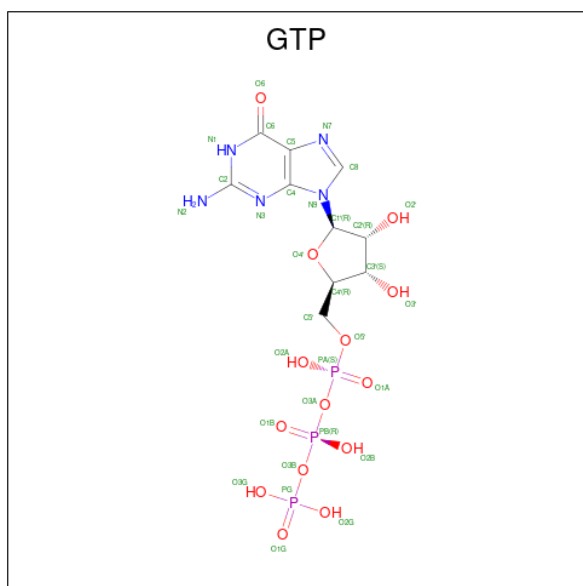
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Mn	0	0
			1	1		
3	Q	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	R	1	Total	Mn	0	0
			1	1		

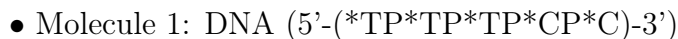
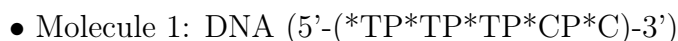
- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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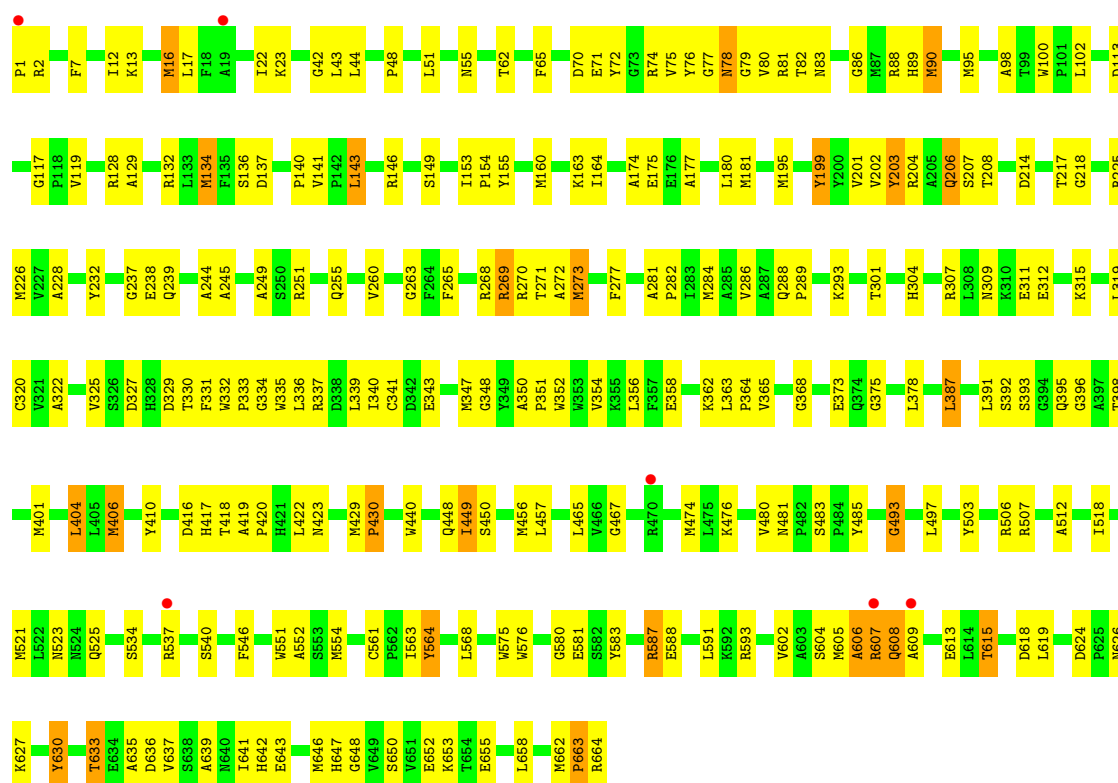
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	R	2	Total	Mg	0	0
			2	2		

- Molecule 1: DNA (5'-(*TP*TP*TP*CP*C)-3')

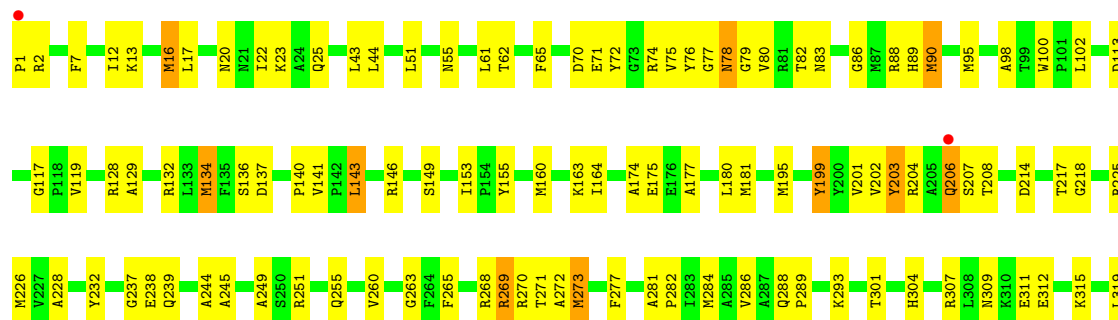


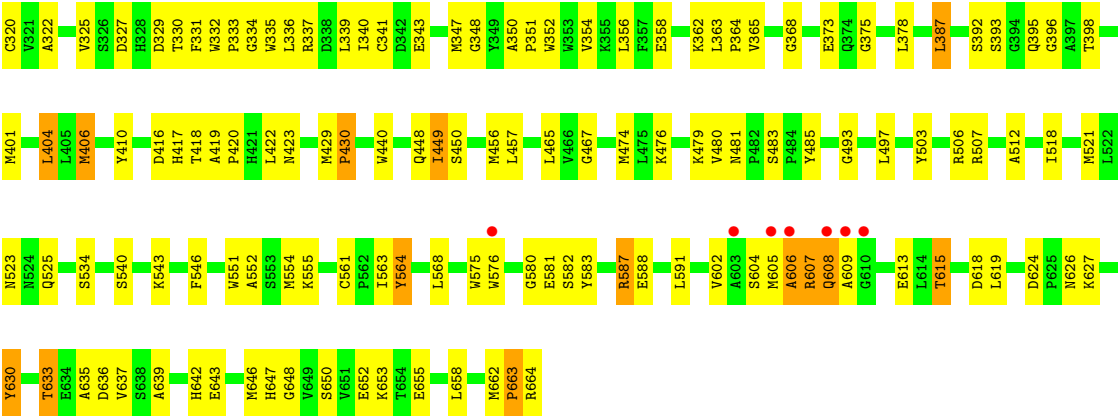


• Molecule 2: P2 PROTEIN



• Molecule 2: P2 PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.65Å 92.70Å 140.79Å 90.00° 101.09° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.00) 99.6 (20.00-3.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.19 (at 2.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.214 , 0.239 0.211 , 0.236	Depositor DCC
R_{free} test set	2711 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.716	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16221	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, MG, 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	D	0.38	0/82	1.19	1/124 (0.8%)
1	E	0.38	0/82	1.19	1/124 (0.8%)
1	F	0.39	0/82	1.19	1/124 (0.8%)
2	P	0.60	2/5396 (0.0%)	1.06	34/7297 (0.5%)
2	Q	0.60	2/5396 (0.0%)	1.06	34/7297 (0.5%)
2	R	0.60	2/5396 (0.0%)	1.06	34/7297 (0.5%)
All	All	0.60	6/16434 (0.0%)	1.06	105/22263 (0.5%)

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	D	0	1
1	E	0	1
1	F	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	90	MET	SD-CE	-5.72	1.65	1.79
2	Q	90	MET	SD-CE	-5.71	1.65	1.79
2	R	90	MET	SD-CE	-5.70	1.65	1.79
2	P	406	MET	SD-CE	-5.43	1.66	1.79
2	Q	406	MET	SD-CE	-5.43	1.66	1.79
2	R	406	MET	SD-CE	-5.41	1.66	1.79

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	100	TRP	N-CA-C	-7.66	100.15	109.72
2	P	100	TRP	N-CA-C	-7.65	100.16	109.72
2	Q	100	TRP	N-CA-C	-7.65	100.16	109.72
2	P	450	SER	N-CA-C	7.41	119.99	108.96
2	R	450	SER	N-CA-C	7.39	119.97	108.96
2	Q	450	SER	N-CA-C	7.39	119.97	108.96
2	Q	155	TYR	N-CA-C	7.29	120.66	111.69
2	P	155	TYR	N-CA-C	7.28	120.65	111.69
2	R	155	TYR	N-CA-C	7.25	120.61	111.69
2	P	95	MET	N-CA-C	-7.17	101.06	110.53
2	Q	95	MET	N-CA-C	-7.16	101.08	110.53
2	R	95	MET	N-CA-C	-7.15	101.10	110.53
2	P	329	ASP	N-CA-C	6.61	118.49	111.28
2	Q	329	ASP	N-CA-C	6.61	118.48	111.28
2	P	493	GLY	N-CA-C	-6.59	97.55	113.18
2	Q	493	GLY	N-CA-C	-6.59	97.55	113.18
2	R	493	GLY	N-CA-C	-6.58	97.58	113.18
2	R	329	ASP	N-CA-C	6.58	118.45	111.28
2	R	406	MET	N-CA-C	6.54	118.41	111.28
2	P	406	MET	N-CA-C	6.51	118.38	111.28
2	Q	406	MET	N-CA-C	6.49	118.35	111.28
2	P	206	GLN	N-CA-C	-6.40	99.51	108.54
2	R	206	GLN	N-CA-C	-6.40	99.52	108.54
2	Q	206	GLN	N-CA-C	-6.39	99.53	108.54
2	R	606	ALA	N-CA-C	-6.32	101.06	110.23
2	P	606	ALA	N-CA-C	-6.29	101.11	110.23
2	Q	606	ALA	N-CA-C	-6.28	101.13	110.23
2	R	129	ALA	N-CA-C	-6.19	104.61	111.36
2	Q	129	ALA	N-CA-C	-6.19	104.61	111.36
2	P	129	ALA	N-CA-C	-6.18	104.62	111.36
2	P	648	GLY	N-CA-C	6.18	121.34	112.81
2	R	648	GLY	N-CA-C	6.18	121.33	112.81
2	Q	648	GLY	N-CA-C	6.17	121.32	112.81
2	P	22	ILE	N-CA-C	6.05	116.52	110.23
2	R	22	ILE	N-CA-C	6.05	116.52	110.23
2	Q	22	ILE	N-CA-C	6.03	116.50	110.23
2	Q	98	ALA	N-CA-C	-6.02	101.86	110.59
2	P	98	ALA	N-CA-C	-6.01	101.88	110.59
2	R	485	TYR	N-CA-C	6.01	120.69	112.04
2	R	98	ALA	N-CA-C	-6.00	101.89	110.59
2	P	485	TYR	N-CA-C	5.97	120.64	112.04
2	R	245	ALA	N-CA-C	-5.96	102.67	110.53
2	Q	485	TYR	N-CA-C	5.95	120.60	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	245	ALA	N-CA-C	-5.94	102.69	110.53
2	R	203	TYR	N-CA-C	5.93	119.40	107.41
2	P	203	TYR	N-CA-C	5.93	119.39	107.41
2	Q	203	TYR	N-CA-C	5.93	119.39	107.41
2	Q	245	ALA	N-CA-C	-5.93	102.71	110.53
2	Q	521	MET	N-CA-C	-5.91	104.75	111.07
2	R	521	MET	N-CA-C	-5.90	104.76	111.07
2	P	521	MET	N-CA-C	-5.90	104.76	111.07
2	Q	393	SER	N-CA-C	5.85	121.02	111.37
2	R	393	SER	N-CA-C	5.84	121.00	111.37
2	R	218	GLY	N-CA-C	-5.84	106.90	115.30
2	P	393	SER	N-CA-C	5.83	120.98	111.37
2	P	218	GLY	N-CA-C	-5.81	106.93	115.30
2	Q	218	GLY	N-CA-C	-5.81	106.93	115.30
2	Q	449	ILE	N-CA-C	-5.77	99.81	108.12
2	R	449	ILE	N-CA-C	-5.77	99.81	108.12
2	P	449	ILE	N-CA-C	-5.75	99.84	108.12
2	P	277	PHE	N-CA-C	5.72	117.52	111.28
2	Q	277	PHE	N-CA-C	5.71	117.50	111.28
2	R	277	PHE	N-CA-C	5.71	117.50	111.28
2	R	201	VAL	N-CA-C	5.64	116.28	108.84
2	Q	201	VAL	N-CA-C	5.63	116.28	108.84
2	P	201	VAL	N-CA-C	5.63	116.28	108.84
2	P	333	PRO	N-CA-C	5.54	119.20	110.50
2	Q	333	PRO	N-CA-C	5.54	119.20	110.50
2	R	333	PRO	N-CA-C	5.53	119.19	110.50
2	R	525	GLN	N-CA-C	5.46	118.15	111.82
2	Q	525	GLN	N-CA-C	5.45	118.14	111.82
2	P	525	GLN	N-CA-C	5.44	118.13	111.82
2	Q	416	ASP	N-CA-C	5.31	117.76	111.33
2	P	416	ASP	N-CA-C	5.28	117.72	111.33
2	R	416	ASP	N-CA-C	5.27	117.71	111.33
2	R	199	TYR	N-CA-C	-5.22	102.03	110.32
2	Q	199	TYR	N-CA-C	-5.21	102.03	110.32
2	P	199	TYR	N-CA-C	-5.20	102.05	110.32
2	Q	134	MET	N-CA-C	5.17	117.00	111.36
2	R	546	PHE	CA-C-N	5.17	125.21	119.32
2	R	546	PHE	C-N-CA	5.17	125.21	119.32
2	P	546	PHE	CA-C-N	5.16	125.21	119.32
2	P	546	PHE	C-N-CA	5.16	125.21	119.32
2	Q	546	PHE	CA-C-N	5.16	125.20	119.32
2	Q	546	PHE	C-N-CA	5.16	125.20	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	134	MET	N-CA-C	5.15	116.98	111.36
2	R	134	MET	N-CA-C	5.13	116.96	111.36
2	P	141	VAL	CA-C-N	-5.11	114.52	119.78
2	P	141	VAL	C-N-CA	-5.11	114.52	119.78
2	Q	637	VAL	N-CA-C	5.10	115.25	108.11
2	Q	141	VAL	CA-C-N	-5.09	114.53	119.78
2	Q	141	VAL	C-N-CA	-5.09	114.53	119.78
2	P	637	VAL	N-CA-C	5.09	115.24	108.11
2	R	637	VAL	N-CA-C	5.09	115.23	108.11
2	R	141	VAL	CA-C-N	-5.08	114.55	119.78
2	R	141	VAL	C-N-CA	-5.08	114.55	119.78
2	Q	575	TRP	N-CA-C	-5.08	105.93	111.82
2	P	575	TRP	N-CA-C	-5.05	105.96	111.82
2	R	575	TRP	N-CA-C	-5.05	105.96	111.82
1	E	5	DC	N1-C1'-C2'	-5.05	105.93	113.50
1	F	5	DC	N1-C1'-C2'	-5.04	105.93	113.50
1	D	5	DC	N1-C1'-C2'	-5.04	105.94	113.50
2	P	396	GLY	N-CA-C	5.04	120.43	113.99
2	R	396	GLY	N-CA-C	5.03	120.43	113.99
2	Q	396	GLY	N-CA-C	5.00	120.39	113.99

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	5	DC	Sidechain
1	E	5	DC	Sidechain
1	F	5	DC	Sidechain

5.2 Too-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 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	D	75	0	48	2	0
1	E	75	0	48	1	0
1	F	75	0	48	2	0
2	P	5265	0	5165	181	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	5265	0	5165	177	1
2	R	5265	0	5165	173	15
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
4	P	64	0	22	2	0
4	Q	64	0	22	3	0
4	R	64	0	22	3	0
5	P	2	0	0	0	0
5	Q	2	0	0	0	0
5	R	2	0	0	0	0
All	All	16221	0	15705	517	15

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 16.

All (517) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:608:GLN:HE22	2:Q:593:ARG:CZ	1.51	1.22
2:P:608:GLN:HE22	2:Q:593:ARG:NH1	1.50	1.08
2:R:325:VAL:HG21	2:R:406:MET:HE2	1.43	0.99
2:Q:203:TYR:HE1	2:Q:271:THR:HG22	1.27	0.99
2:Q:325:VAL:HG21	2:Q:406:MET:HE2	1.44	0.99
2:P:608:GLN:NE2	2:Q:593:ARG:NH1	2.10	0.99
2:P:325:VAL:HG21	2:P:406:MET:HE2	1.44	0.98
2:R:203:TYR:HE1	2:R:271:THR:HG22	1.27	0.97
2:P:203:TYR:HE1	2:P:271:THR:HG22	1.28	0.96
2:R:251:ARG:HH11	2:R:255:GLN:HE22	1.14	0.95
2:P:608:GLN:NE2	2:Q:593:ARG:CZ	2.30	0.94
2:Q:251:ARG:HH11	2:Q:255:GLN:HE22	1.14	0.91
2:R:364:PRO:HA	2:R:387:LEU:HD22	1.51	0.90
2:P:364:PRO:HA	2:P:387:LEU:HD22	1.51	0.90
2:Q:364:PRO:HA	2:Q:387:LEU:HD22	1.51	0.88
2:P:251:ARG:HH11	2:P:255:GLN:HE22	1.14	0.88
2:R:615:THR:HG23	2:R:618:ASP:OD2	1.75	0.87
2:P:615:THR:HG23	2:P:618:ASP:OD2	1.75	0.87
2:Q:615:THR:HG23	2:Q:618:ASP:OD2	1.75	0.87
2:P:606:ALA:HB3	2:P:609:ALA:HB2	1.56	0.87
2:Q:606:ALA:HB3	2:Q:609:ALA:HB2	1.56	0.87
2:R:606:ALA:HB3	2:R:609:ALA:HB2	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:203:TYR:CE1	2:R:271:THR:HG22	2.13	0.84
2:P:203:TYR:CE1	2:P:271:THR:HG22	2.13	0.84
2:Q:203:TYR:CE1	2:Q:271:THR:HG22	2.13	0.81
2:R:419:ALA:HB1	2:R:422:LEU:HD12	1.64	0.80
2:Q:419:ALA:HB1	2:Q:422:LEU:HD12	1.64	0.79
2:P:419:ALA:HB1	2:P:422:LEU:HD12	1.64	0.78
2:R:181:MET:CE	2:R:356:LEU:HD23	2.14	0.78
2:Q:181:MET:CE	2:Q:356:LEU:HD23	2.14	0.77
2:P:181:MET:CE	2:P:356:LEU:HD23	2.14	0.77
2:P:427:LYS:HE3	2:R:12:ILE:HG21	1.67	0.76
2:R:226:MET:HE1	2:R:244:ALA:HB2	1.67	0.75
2:P:226:MET:HE1	2:P:244:ALA:HB2	1.67	0.74
2:P:608:GLN:HE22	2:Q:593:ARG:NE	1.82	0.74
2:Q:226:MET:HE1	2:Q:244:ALA:HB2	1.67	0.74
2:R:132:ARG:NH1	2:R:343:GLU:OE2	2.21	0.73
2:Q:132:ARG:NH1	2:Q:343:GLU:OE2	2.21	0.73
2:P:132:ARG:NH1	2:P:343:GLU:OE2	2.21	0.73
2:P:518:ILE:HB	2:P:561:CYS:SG	2.29	0.73
2:R:518:ILE:HB	2:R:561:CYS:SG	2.29	0.72
2:Q:288:GLN:HB3	2:Q:289:PRO:HD3	1.72	0.72
2:Q:518:ILE:HB	2:Q:561:CYS:SG	2.29	0.72
2:Q:181:MET:HE3	2:Q:356:LEU:HD23	1.72	0.71
2:R:181:MET:HE3	2:R:356:LEU:HD23	1.72	0.71
2:P:288:GLN:HB3	2:P:289:PRO:HD3	1.72	0.71
2:Q:652:GLU:CD	2:Q:652:GLU:H	1.99	0.71
2:P:652:GLU:CD	2:P:652:GLU:H	1.99	0.70
2:P:627:LYS:HA	2:P:630:TYR:CE2	2.26	0.70
2:Q:627:LYS:HA	2:Q:630:TYR:CE2	2.27	0.70
2:R:658:LEU:HG	2:R:662:MET:HE2	1.74	0.70
2:R:652:GLU:CD	2:R:652:GLU:H	1.99	0.70
2:R:288:GLN:HB3	2:R:289:PRO:HD3	1.72	0.70
2:P:181:MET:HE3	2:P:356:LEU:HD23	1.72	0.69
2:R:137:ASP:H	2:R:293:LYS:NZ	1.90	0.69
2:R:627:LYS:HA	2:R:630:TYR:CE2	2.26	0.69
2:P:137:ASP:H	2:P:293:LYS:NZ	1.90	0.69
2:Q:273:MET:HE3	2:Q:392:SER:OG	1.93	0.69
2:P:225:ARG:NH1	2:P:268:ARG:NH1	2.40	0.69
2:P:273:MET:HE3	2:P:392:SER:OG	1.93	0.69
2:P:658:LEU:HG	2:P:662:MET:HE2	1.74	0.69
2:Q:225:ARG:NH1	2:Q:268:ARG:NH1	2.40	0.69
2:Q:137:ASP:H	2:Q:293:LYS:NZ	1.90	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:658:LEU:HG	2:Q:662:MET:HE2	1.74	0.68
2:R:273:MET:HE3	2:R:392:SER:OG	1.93	0.68
2:R:225:ARG:NH1	2:R:268:ARG:NH1	2.40	0.68
2:P:364:PRO:HA	2:P:387:LEU:CD2	2.25	0.67
2:Q:137:ASP:H	2:Q:293:LYS:HZ2	1.42	0.67
2:P:225:ARG:HD2	2:P:268:ARG:HD2	1.77	0.67
2:Q:90:MET:HE2	2:Q:90:MET:HA	1.77	0.67
2:R:225:ARG:HD2	2:R:268:ARG:HD2	1.77	0.66
2:P:90:MET:HA	2:P:90:MET:HE2	1.77	0.66
2:R:90:MET:HA	2:R:90:MET:HE2	1.77	0.66
2:Q:552:ALA:HB3	2:Q:619:LEU:HD13	1.78	0.66
2:Q:364:PRO:HA	2:Q:387:LEU:CD2	2.25	0.66
2:Q:225:ARG:HD2	2:Q:268:ARG:HD2	1.77	0.66
2:R:552:ALA:HB3	2:R:619:LEU:HD13	1.78	0.66
2:P:465:LEU:HD12	2:P:465:LEU:O	1.97	0.65
2:R:78:ASN:ND2	2:R:80:VAL:H	1.94	0.65
2:P:78:ASN:ND2	2:P:80:VAL:H	1.94	0.65
2:Q:78:ASN:ND2	2:Q:80:VAL:H	1.93	0.65
2:R:465:LEU:HD12	2:R:465:LEU:O	1.97	0.65
2:P:552:ALA:HB3	2:P:619:LEU:HD13	1.78	0.64
2:Q:465:LEU:HD12	2:Q:465:LEU:O	1.97	0.64
2:P:417:HIS:ND1	2:P:474:MET:HE1	2.13	0.64
2:Q:417:HIS:ND1	2:Q:474:MET:HE1	2.13	0.64
2:R:175:GLU:HA	2:R:352:TRP:CE3	2.33	0.64
2:R:160:MET:O	2:R:164:ILE:HG12	1.98	0.64
2:P:251:ARG:HB2	2:P:255:GLN:HE21	1.64	0.63
2:R:364:PRO:HA	2:R:387:LEU:CD2	2.25	0.63
2:R:251:ARG:HB2	2:R:255:GLN:HE21	1.64	0.63
2:Q:175:GLU:HA	2:Q:352:TRP:CE3	2.33	0.63
2:R:74:ARG:HB3	2:R:503:TYR:CD2	2.34	0.63
1:D:3:DT:H5"	2:P:23:LYS:HE3	1.80	0.63
1:F:3:DT:H5"	2:R:23:LYS:HE3	1.80	0.63
2:R:417:HIS:ND1	2:R:474:MET:HE1	2.13	0.63
2:P:55:ASN:OD1	2:P:88:ARG:NH2	2.31	0.63
2:P:74:ARG:HB3	2:P:503:TYR:CD2	2.34	0.63
2:R:606:ALA:C	2:R:608:GLN:H	2.07	0.62
2:Q:429:MET:HB2	2:Q:430:PRO:HD3	1.82	0.62
2:R:137:ASP:H	2:R:293:LYS:HZ2	1.46	0.62
2:Q:606:ALA:C	2:Q:608:GLN:H	2.07	0.62
2:P:175:GLU:HA	2:P:352:TRP:CE3	2.33	0.62
2:P:429:MET:HB2	2:P:430:PRO:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:181:MET:HE1	2:P:356:LEU:HD23	1.82	0.62
1:E:3:DT:H5"	2:Q:23:LYS:HE3	1.81	0.62
2:P:160:MET:O	2:P:164:ILE:HG12	1.98	0.62
2:P:633:THR:HG23	2:P:635:ALA:H	1.65	0.62
2:Q:606:ALA:CB	2:Q:609:ALA:HB2	2.29	0.62
2:Q:160:MET:O	2:Q:164:ILE:HG12	1.98	0.62
2:Q:251:ARG:HB2	2:Q:255:GLN:HE21	1.64	0.61
2:P:606:ALA:C	2:P:608:GLN:H	2.07	0.61
2:P:251:ARG:HH11	2:P:255:GLN:NE2	1.93	0.61
2:Q:74:ARG:HB3	2:Q:503:TYR:CD2	2.34	0.61
2:Q:55:ASN:OD1	2:Q:88:ARG:NH2	2.31	0.61
2:Q:663:PRO:HG2	2:Q:664:ARG:H	1.65	0.61
2:Q:251:ARG:HH11	2:Q:255:GLN:NE2	1.93	0.61
2:R:633:THR:HG23	2:R:635:ALA:H	1.65	0.61
2:Q:633:THR:HG23	2:Q:635:ALA:H	1.65	0.61
2:R:181:MET:HE1	2:R:356:LEU:HD23	1.82	0.61
2:P:663:PRO:HG2	2:P:664:ARG:H	1.65	0.61
2:R:606:ALA:O	2:R:608:GLN:N	2.31	0.60
2:P:72:TYR:CE1	2:P:476:LYS:HD3	2.36	0.60
2:Q:181:MET:HE1	2:Q:356:LEU:HD23	1.82	0.60
2:R:72:TYR:CE1	2:R:476:LYS:HD3	2.36	0.60
2:R:251:ARG:HH11	2:R:255:GLN:NE2	1.93	0.60
2:R:663:PRO:HG2	2:R:664:ARG:H	1.65	0.60
2:R:606:ALA:CB	2:R:609:ALA:HB2	2.29	0.60
2:Q:72:TYR:CE1	2:Q:476:LYS:HD3	2.36	0.59
2:P:71:GLU:H	2:P:71:GLU:CD	2.10	0.59
2:R:429:MET:HB2	2:R:430:PRO:HD3	1.82	0.59
2:P:417:HIS:CE1	2:P:474:MET:HE1	2.38	0.59
2:Q:401:MET:HA	2:Q:401:MET:HE2	1.85	0.59
2:Q:417:HIS:CE1	2:Q:474:MET:HE1	2.37	0.59
2:P:122:ARG:NH2	2:R:20:ASN:ND2	2.51	0.59
2:Q:71:GLU:CD	2:Q:71:GLU:H	2.10	0.59
2:R:417:HIS:CE1	2:R:474:MET:HE1	2.38	0.59
2:P:401:MET:HE2	2:P:401:MET:HA	1.85	0.59
2:R:72:TYR:CZ	2:R:476:LYS:HD3	2.38	0.59
2:P:72:TYR:CZ	2:P:476:LYS:HD3	2.38	0.59
2:Q:72:TYR:CZ	2:Q:476:LYS:HD3	2.38	0.59
2:Q:132:ARG:HD2	2:Q:429:MET:HE2	1.85	0.58
2:P:132:ARG:HD2	2:P:429:MET:HE2	1.85	0.58
2:R:55:ASN:OD1	2:R:88:ARG:NH2	2.31	0.58
2:R:650:SER:HB2	2:R:652:GLU:OE1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:606:ALA:CB	2:P:609:ALA:HB2	2.29	0.58
2:R:132:ARG:HD2	2:R:429:MET:HE2	1.86	0.58
2:R:71:GLU:CD	2:R:71:GLU:H	2.10	0.58
2:Q:650:SER:HB2	2:Q:652:GLU:OE1	2.03	0.58
2:R:128:ARG:HG3	2:R:339:LEU:HD21	1.86	0.58
2:R:420:PRO:HA	2:R:423:ASN:ND2	2.19	0.57
2:P:70:ASP:OD1	2:P:74:ARG:NH1	2.37	0.57
2:P:143:LEU:HD21	2:P:284:MET:HE2	1.86	0.57
2:P:420:PRO:HA	2:P:423:ASN:ND2	2.19	0.57
2:Q:70:ASP:OD1	2:Q:74:ARG:NH1	2.37	0.57
2:Q:420:PRO:HA	2:Q:423:ASN:ND2	2.19	0.57
2:Q:606:ALA:O	2:Q:608:GLN:N	2.31	0.57
2:P:650:SER:HB2	2:P:652:GLU:OE1	2.03	0.57
2:P:606:ALA:O	2:P:608:GLN:N	2.31	0.57
2:Q:78:ASN:HD22	2:Q:79:GLY:N	2.03	0.57
2:P:128:ARG:HG3	2:P:339:LEU:HD21	1.86	0.57
2:R:363:LEU:HG	2:R:364:PRO:HD2	1.87	0.57
2:R:401:MET:HE2	2:R:401:MET:HA	1.84	0.57
2:R:78:ASN:HD22	2:R:79:GLY:N	2.03	0.57
2:Q:128:ARG:HG3	2:Q:339:LEU:HD21	1.86	0.57
2:Q:143:LEU:HD21	2:Q:284:MET:HE2	1.86	0.56
2:R:143:LEU:HD21	2:R:284:MET:HE2	1.86	0.56
2:P:363:LEU:HG	2:P:364:PRO:HD2	1.87	0.56
2:R:70:ASP:OD1	2:R:74:ARG:NH1	2.37	0.56
2:R:203:TYR:HB3	2:R:269:ARG:HD2	1.88	0.56
2:P:137:ASP:H	2:P:293:LYS:HZ2	1.52	0.56
2:P:134:MET:SD	2:P:404:LEU:HD23	2.46	0.56
2:Q:86:GLY:O	2:Q:89:HIS:HD2	1.89	0.56
2:P:78:ASN:HD22	2:P:79:GLY:N	2.03	0.56
2:P:301:THR:HG22	2:P:448:GLN:O	2.06	0.56
2:P:327:ASP:OD1	2:P:330:THR:HG23	2.06	0.56
2:R:86:GLY:O	2:R:89:HIS:HD2	1.89	0.56
2:P:203:TYR:HB3	2:P:269:ARG:HD2	1.88	0.56
2:P:427:LYS:HE3	2:R:12:ILE:CG2	2.35	0.56
2:R:327:ASP:OD1	2:R:330:THR:HG23	2.06	0.56
2:Q:363:LEU:HG	2:Q:364:PRO:HD2	1.87	0.56
2:Q:607:ARG:O	2:Q:608:GLN:HG3	2.06	0.56
2:Q:203:TYR:HB3	2:Q:269:ARG:HD2	1.88	0.56
2:Q:301:THR:HG22	2:Q:448:GLN:O	2.06	0.56
2:P:607:ARG:O	2:P:608:GLN:HG3	2.06	0.55
2:Q:419:ALA:CB	2:Q:422:LEU:HD12	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:134:MET:SD	2:Q:404:LEU:HD23	2.46	0.55
2:R:134:MET:SD	2:R:404:LEU:HD23	2.46	0.55
2:P:1:PRO:HG2	2:P:238:GLU:OE1	2.07	0.55
2:P:78:ASN:HD22	2:P:78:ASN:C	2.15	0.55
2:R:1:PRO:HG2	2:R:238:GLU:OE1	2.07	0.55
2:P:86:GLY:O	2:P:89:HIS:HD2	1.89	0.55
2:Q:327:ASP:OD1	2:Q:330:THR:HG23	2.06	0.55
2:R:339:LEU:C	2:R:339:LEU:HD23	2.32	0.55
2:R:607:ARG:O	2:R:608:GLN:HG3	2.06	0.55
2:P:174:ALA:HA	2:P:195:MET:HE1	1.89	0.55
2:R:301:THR:HG22	2:R:448:GLN:O	2.06	0.55
2:Q:174:ALA:HA	2:Q:195:MET:HE1	1.89	0.54
2:R:78:ASN:HD22	2:R:78:ASN:C	2.15	0.54
2:P:652:GLU:CD	2:P:652:GLU:N	2.64	0.54
2:P:149:SER:OG	2:P:163:LYS:HE3	2.08	0.54
2:Q:1:PRO:HG2	2:Q:238:GLU:OE1	2.07	0.54
2:R:174:ALA:HA	2:R:195:MET:HE1	1.89	0.54
2:Q:339:LEU:C	2:Q:339:LEU:HD23	2.32	0.54
2:R:149:SER:OG	2:R:163:LYS:HE3	2.08	0.54
2:R:419:ALA:CB	2:R:422:LEU:HD12	2.36	0.54
2:P:419:ALA:CB	2:P:422:LEU:HD12	2.36	0.54
2:Q:149:SER:OG	2:Q:163:LYS:HE3	2.08	0.54
2:Q:652:GLU:CD	2:Q:652:GLU:N	2.64	0.54
2:P:596:LEU:HD12	2:Q:42:GLY:HA3	1.90	0.54
2:P:339:LEU:HD23	2:P:339:LEU:C	2.32	0.54
2:R:652:GLU:CD	2:R:652:GLU:N	2.64	0.54
2:P:17:LEU:HB3	2:P:153:ILE:HD13	1.90	0.53
2:R:177:ALA:O	2:R:180:LEU:HB2	2.08	0.53
2:R:663:PRO:O	2:R:664:ARG:CZ	2.56	0.53
2:P:608:GLN:HE22	2:Q:593:ARG:CD	2.21	0.53
2:R:17:LEU:HB3	2:R:153:ILE:HD13	1.90	0.53
2:R:88:ARG:HD3	2:R:263:GLY:O	2.09	0.53
2:Q:177:ALA:O	2:Q:180:LEU:HB2	2.08	0.53
2:Q:203:TYR:HE1	2:Q:271:THR:CG2	2.13	0.53
2:P:51:LEU:CD2	2:P:90:MET:HE1	2.39	0.53
2:P:663:PRO:O	2:P:664:ARG:CZ	2.56	0.53
2:Q:51:LEU:CD2	2:Q:90:MET:HE1	2.39	0.53
2:Q:62:THR:HG23	2:Q:83:ASN:HB2	1.91	0.53
2:P:88:ARG:HD3	2:P:263:GLY:O	2.09	0.53
2:R:225:ARG:NH1	2:R:268:ARG:CZ	2.72	0.53
2:P:177:ALA:O	2:P:180:LEU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:663:PRO:O	2:Q:664:ARG:CZ	2.56	0.53
2:P:225:ARG:NH1	2:P:268:ARG:CZ	2.72	0.52
2:Q:88:ARG:HD3	2:Q:263:GLY:O	2.09	0.52
2:R:7:PHE:CE2	2:R:13:LYS:HD2	2.44	0.52
2:P:7:PHE:CE2	2:P:13:LYS:HD2	2.45	0.52
2:Q:7:PHE:CE2	2:Q:13:LYS:HD2	2.45	0.52
2:Q:17:LEU:HB3	2:Q:153:ILE:HD13	1.91	0.52
2:Q:78:ASN:HD22	2:Q:78:ASN:C	2.15	0.52
2:Q:286:VAL:C	2:Q:289:PRO:HD2	2.35	0.52
2:P:650:SER:OG	2:P:653:LYS:HG3	2.09	0.52
2:R:51:LEU:HD22	2:R:90:MET:HE1	1.91	0.52
2:R:286:VAL:C	2:R:289:PRO:HD2	2.34	0.52
2:R:51:LEU:CD2	2:R:90:MET:HE1	2.39	0.52
2:R:650:SER:OG	2:R:653:LYS:HG3	2.09	0.52
2:Q:51:LEU:HD22	2:Q:90:MET:HE1	1.91	0.52
2:Q:225:ARG:NH1	2:Q:268:ARG:CZ	2.73	0.52
2:R:62:THR:HG23	2:R:83:ASN:HB2	1.91	0.52
2:Q:650:SER:OG	2:Q:653:LYS:HG3	2.09	0.52
2:Q:65:PHE:CD1	2:Q:563:ILE:HG21	2.45	0.52
2:Q:481:ASN:ND2	2:Q:483:SER:O	2.43	0.52
2:R:304:HIS:HA	2:R:309:ASN:ND2	2.25	0.52
2:Q:304:HIS:HA	2:Q:309:ASN:ND2	2.25	0.52
2:P:51:LEU:HD22	2:P:90:MET:HE1	1.91	0.51
2:P:62:THR:HG23	2:P:83:ASN:HB2	1.91	0.51
2:P:304:HIS:HA	2:P:309:ASN:ND2	2.25	0.51
2:P:481:ASN:ND2	2:P:483:SER:O	2.43	0.51
2:R:65:PHE:CD1	2:R:563:ILE:HG21	2.45	0.51
2:P:286:VAL:C	2:P:289:PRO:HD2	2.35	0.51
2:Q:225:ARG:HH12	2:Q:268:ARG:NH1	2.09	0.51
2:R:481:ASN:ND2	2:R:483:SER:O	2.43	0.51
2:P:65:PHE:CD1	2:P:563:ILE:HG21	2.45	0.51
2:Q:307:ARG:HB2	2:Q:307:ARG:CZ	2.41	0.51
2:R:203:TYR:HE1	2:R:271:THR:CG2	2.13	0.51
2:R:232:TYR:CE2	2:R:237:GLY:HA2	2.46	0.51
2:R:251:ARG:NH1	2:R:255:GLN:HE22	1.96	0.51
2:P:232:TYR:CE2	2:P:237:GLY:HA2	2.46	0.51
2:R:307:ARG:HB2	2:R:307:ARG:CZ	2.41	0.51
2:P:225:ARG:HH12	2:P:268:ARG:NH1	2.09	0.50
2:Q:642:HIS:CE1	2:Q:646:MET:HG3	2.46	0.50
2:P:203:TYR:HE1	2:P:271:THR:CG2	2.13	0.50
2:P:642:HIS:CE1	2:P:646:MET:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:307:ARG:HB2	2:P:307:ARG:CZ	2.41	0.50
2:R:315:LYS:HE2	2:R:512:ALA:O	2.12	0.50
2:P:315:LYS:HE2	2:P:512:ALA:O	2.12	0.49
2:Q:232:TYR:CE2	2:Q:237:GLY:HA2	2.46	0.49
2:R:642:HIS:CE1	2:R:646:MET:HG3	2.46	0.49
2:R:225:ARG:HH12	2:R:268:ARG:NH1	2.09	0.49
2:R:202:VAL:CG2	2:R:272:ALA:HB3	2.43	0.49
2:P:613:GLU:HA	2:P:613:GLU:OE1	2.13	0.49
2:P:664:ARG:HH11	2:P:664:ARG:HG2	1.78	0.49
2:P:119:VAL:O	2:R:25:GLN:HG3	2.12	0.49
2:P:416:ASP:CG	2:R:20:ASN:HD22	2.21	0.49
2:Q:613:GLU:OE1	2:Q:613:GLU:HA	2.13	0.49
2:Q:315:LYS:HE2	2:Q:512:ALA:O	2.12	0.48
2:P:202:VAL:CG2	2:P:272:ALA:HB3	2.43	0.48
2:P:214:ASP:HB3	2:P:217:THR:OG1	2.13	0.48
2:P:322:ALA:HB2	2:P:456:MET:HE2	1.95	0.48
2:Q:214:ASP:HB3	2:Q:217:THR:OG1	2.13	0.48
2:R:214:ASP:HB3	2:R:217:THR:OG1	2.13	0.48
2:P:1:PRO:O	2:P:2:ARG:HB3	2.13	0.48
2:R:1:PRO:O	2:R:2:ARG:HB3	2.13	0.48
2:R:251:ARG:HB2	2:R:255:GLN:NE2	2.29	0.48
2:R:664:ARG:HG2	2:R:664:ARG:HH11	1.78	0.48
2:Q:251:ARG:HB2	2:Q:255:GLN:NE2	2.29	0.48
2:Q:664:ARG:HG2	2:Q:664:ARG:HH11	1.78	0.48
2:Q:202:VAL:CG2	2:Q:272:ALA:HB3	2.43	0.48
2:R:613:GLU:OE1	2:R:613:GLU:HA	2.13	0.48
2:R:322:ALA:HB2	2:R:456:MET:HE2	1.95	0.48
2:P:350:ALA:HB1	2:P:352:TRP:NE1	2.29	0.47
2:P:336:LEU:O	2:P:340:ILE:HG13	2.14	0.47
2:Q:350:ALA:HB1	2:Q:352:TRP:NE1	2.29	0.47
2:P:181:MET:HE3	2:P:356:LEU:CD2	2.42	0.47
2:Q:322:ALA:HB2	2:Q:456:MET:HE2	1.95	0.47
2:Q:1:PRO:O	2:Q:2:ARG:HB3	2.13	0.47
2:R:281:ALA:HB3	2:R:282:PRO:CD	2.45	0.47
2:P:132:ARG:HA	2:P:347:MET:SD	2.55	0.47
2:Q:181:MET:HE3	2:Q:356:LEU:CD2	2.42	0.47
2:R:350:ALA:HB1	2:R:352:TRP:NE1	2.29	0.47
2:P:251:ARG:HB2	2:P:255:GLN:NE2	2.29	0.47
2:Q:368:GLY:O	2:Q:375:GLY:HA3	2.15	0.47
2:P:136:SER:OG	2:P:293:LYS:NZ	2.41	0.46
2:R:132:ARG:HA	2:R:347:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:336:LEU:O	2:R:340:ILE:HG13	2.14	0.46
2:P:368:GLY:O	2:P:375:GLY:HA3	2.15	0.46
2:P:153:ILE:HA	2:P:154:PRO:HA	1.75	0.46
2:Q:336:LEU:O	2:Q:340:ILE:HG13	2.14	0.46
2:P:606:ALA:C	2:P:608:GLN:N	2.74	0.46
2:P:664:ARG:HG2	2:P:664:ARG:NH1	2.31	0.46
2:Q:281:ALA:HB3	2:Q:282:PRO:CD	2.45	0.46
2:Q:606:ALA:C	2:Q:608:GLN:N	2.74	0.46
2:R:664:ARG:HG2	2:R:664:ARG:NH1	2.31	0.46
2:P:286:VAL:O	2:P:289:PRO:HD2	2.16	0.46
2:Q:136:SER:OG	2:Q:293:LYS:NZ	2.41	0.46
2:R:181:MET:HE3	2:R:356:LEU:CD2	2.42	0.46
2:R:199:TYR:HB3	2:R:273:MET:HB3	1.97	0.46
2:Q:251:ARG:CB	2:Q:255:GLN:HE21	2.29	0.46
2:Q:664:ARG:HG2	2:Q:664:ARG:NH1	2.31	0.46
2:P:281:ALA:HB3	2:P:282:PRO:CD	2.45	0.46
2:Q:117:GLY:HA2	2:Q:335:TRP:CD2	2.51	0.46
2:R:368:GLY:O	2:R:375:GLY:HA3	2.15	0.46
2:P:580:GLY:C	2:P:581:GLU:HG2	2.41	0.45
2:Q:551:TRP:CH2	2:Q:554:MET:HE1	2.51	0.45
2:R:117:GLY:HA2	2:R:335:TRP:CD2	2.51	0.45
2:Q:132:ARG:HA	2:Q:347:MET:SD	2.55	0.45
2:Q:251:ARG:NH1	2:Q:255:GLN:HE22	1.97	0.45
2:R:551:TRP:CH2	2:R:554:MET:HE1	2.51	0.45
2:Q:160:MET:HE3	2:Q:647:HIS:HB3	1.99	0.45
2:Q:395:GLN:HB3	2:Q:398:THR:HG23	1.99	0.45
2:Q:449:ILE:HG13	2:Q:449:ILE:O	2.16	0.45
2:P:160:MET:HE3	2:P:647:HIS:HB3	1.99	0.45
2:P:449:ILE:HG13	2:P:449:ILE:O	2.16	0.45
2:Q:286:VAL:O	2:Q:289:PRO:HD2	2.16	0.45
2:Q:332:TRP:CZ2	2:Q:401:MET:HB3	2.51	0.45
2:R:136:SER:OG	2:R:293:LYS:NZ	2.41	0.45
2:P:117:GLY:HA2	2:P:335:TRP:CD2	2.51	0.45
2:P:551:TRP:CH2	2:P:554:MET:HE1	2.51	0.45
2:Q:204:ARG:NH1	2:Q:270:ARG:CD	2.80	0.45
2:R:332:TRP:CZ2	2:R:401:MET:HB3	2.51	0.45
2:P:199:TYR:HB3	2:P:273:MET:HB3	1.97	0.45
2:Q:146:ARG:NH2	2:Q:540:SER:O	2.50	0.45
2:Q:199:TYR:HB3	2:Q:273:MET:HB3	1.97	0.45
2:R:140:PRO:HB3	2:R:655:GLU:HA	1.99	0.45
2:R:564:TYR:CZ	2:R:568:LEU:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:DC:OP2	2:R:543:LYS:NZ	2.48	0.45
2:P:564:TYR:CZ	2:P:568:LEU:HD11	2.52	0.45
2:Q:580:GLY:C	2:Q:581:GLU:HG2	2.42	0.45
2:R:449:ILE:HG13	2:R:449:ILE:O	2.16	0.45
2:P:332:TRP:CZ2	2:P:401:MET:HB3	2.51	0.45
2:P:391:LEU:HD23	2:P:391:LEU:HA	1.69	0.45
2:R:146:ARG:NH2	2:R:540:SER:O	2.50	0.45
2:R:160:MET:HE3	2:R:647:HIS:HB3	1.99	0.45
2:P:146:ARG:NH2	2:P:540:SER:O	2.50	0.45
2:Q:662:MET:HB3	2:Q:663:PRO:HD2	1.99	0.45
2:R:286:VAL:O	2:R:289:PRO:HD2	2.16	0.45
2:P:204:ARG:NH1	2:P:270:ARG:CD	2.80	0.45
2:R:204:ARG:NH1	2:R:270:ARG:CD	2.80	0.45
2:R:639:ALA:O	2:R:643:GLU:HG3	2.17	0.45
2:P:251:ARG:NH1	2:P:255:GLN:HE22	1.96	0.44
2:R:580:GLY:C	2:R:581:GLU:HG2	2.41	0.44
2:R:662:MET:HB3	2:R:663:PRO:HD2	1.99	0.44
2:P:301:THR:HG23	2:P:440:TRP:O	2.18	0.44
2:P:639:ALA:O	2:P:643:GLU:HG3	2.17	0.44
2:Q:564:TYR:CZ	2:Q:568:LEU:HD11	2.52	0.44
2:R:249:ALA:O	2:R:260:VAL:HG21	2.17	0.44
2:R:395:GLN:HB3	2:R:398:THR:HG23	1.99	0.44
2:P:62:THR:CG2	2:P:83:ASN:HB2	2.48	0.44
2:Q:62:THR:CG2	2:Q:83:ASN:HB2	2.48	0.44
2:Q:249:ALA:O	2:Q:260:VAL:HG21	2.18	0.44
2:Q:630:TYR:CE1	4:Q:666:GTP:H1'	2.53	0.44
2:R:401:MET:HE2	2:R:401:MET:CA	2.47	0.44
2:P:251:ARG:CB	2:P:255:GLN:HE21	2.29	0.44
2:P:395:GLN:HB3	2:P:398:THR:HG23	1.99	0.44
2:P:630:TYR:CE1	4:P:666:GTP:H1'	2.53	0.44
2:R:301:THR:HG23	2:R:440:TRP:O	2.18	0.44
2:P:81:ARG:NH1	2:P:493:GLY:O	2.51	0.44
2:P:242:LEU:HD12	2:P:242:LEU:HA	1.75	0.44
2:P:401:MET:HE2	2:P:401:MET:CA	2.47	0.44
2:P:427:LYS:CE	2:R:12:ILE:HG21	2.42	0.44
2:P:662:MET:HB3	2:P:663:PRO:HD2	1.99	0.44
2:R:62:THR:CG2	2:R:83:ASN:HB2	2.48	0.44
2:P:630:TYR:HB3	4:P:666:GTP:N2	2.33	0.44
2:Q:153:ILE:HA	2:Q:154:PRO:HA	1.75	0.44
2:Q:319:LEU:HD12	2:Q:320:CYS:H	1.83	0.44
2:Q:325:VAL:CG2	2:Q:406:MET:HE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:61:LEU:HA	2:R:61:LEU:HD23	1.78	0.43
2:R:606:ALA:C	2:R:608:GLN:N	2.74	0.43
2:P:122:ARG:HH21	2:R:20:ASN:ND2	2.14	0.43
2:Q:301:THR:HG23	2:Q:440:TRP:O	2.18	0.43
2:Q:639:ALA:O	2:Q:643:GLU:HG3	2.17	0.43
2:R:331:PHE:O	2:R:332:TRP:C	2.62	0.43
2:R:418:THR:HG22	2:R:467:GLY:C	2.44	0.43
2:R:602:VAL:HB	2:R:605:MET:HB2	2.00	0.43
2:P:7:PHE:CD1	2:P:7:PHE:N	2.87	0.43
2:P:12:ILE:O	2:P:16:MET:HG3	2.19	0.43
2:P:249:ALA:O	2:P:260:VAL:HG21	2.17	0.43
2:Q:602:VAL:HB	2:Q:605:MET:HB2	2.00	0.43
2:P:140:PRO:HB3	2:P:655:GLU:HA	1.99	0.43
2:P:341:CYS:SG	2:P:358:GLU:HB2	2.58	0.43
2:P:418:THR:HG22	2:P:467:GLY:C	2.44	0.43
2:P:602:VAL:HB	2:P:605:MET:HB2	2.00	0.43
2:P:633:THR:HG23	2:P:635:ALA:N	2.32	0.43
2:R:348:GLY:O	2:R:663:PRO:HB3	2.18	0.43
2:P:348:GLY:O	2:P:663:PRO:HB3	2.18	0.43
2:R:7:PHE:CD1	2:R:7:PHE:N	2.87	0.43
2:R:12:ILE:O	2:R:16:MET:HG3	2.19	0.43
2:R:341:CYS:SG	2:R:358:GLU:HB2	2.58	0.43
2:R:630:TYR:CE1	4:R:666:GTP:H1'	2.53	0.43
2:P:506:ARG:O	2:P:507:ARG:HB2	2.19	0.43
2:Q:132:ARG:HD2	2:Q:429:MET:CE	2.47	0.43
2:Q:140:PRO:HB3	2:Q:655:GLU:HA	1.99	0.43
2:R:78:ASN:ND2	2:R:78:ASN:C	2.77	0.43
2:R:208:THR:HG21	2:R:523:ASN:OD1	2.19	0.43
2:P:608:GLN:NE2	2:Q:593:ARG:CD	2.82	0.43
2:R:630:TYR:HB3	4:R:666:GTP:N2	2.33	0.43
2:P:331:PHE:O	2:P:332:TRP:C	2.61	0.43
2:Q:265:PHE:CD1	2:Q:265:PHE:N	2.87	0.43
2:Q:341:CYS:SG	2:Q:358:GLU:HB2	2.58	0.43
2:P:208:THR:HG21	2:P:523:ASN:OD1	2.19	0.43
2:Q:7:PHE:N	2:Q:7:PHE:CD1	2.87	0.43
2:Q:208:THR:HG21	2:Q:523:ASN:OD1	2.19	0.43
2:Q:401:MET:HE2	2:Q:401:MET:CA	2.47	0.43
2:Q:630:TYR:HB3	4:Q:666:GTP:N2	2.33	0.43
2:R:319:LEU:HD12	2:R:320:CYS:H	1.83	0.43
2:P:663:PRO:CG	2:P:664:ARG:H	2.32	0.43
2:Q:76:TYR:CD1	2:Q:77:GLY:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:265:PHE:CD1	2:R:265:PHE:N	2.87	0.43
2:R:132:ARG:HD2	2:R:429:MET:CE	2.47	0.42
2:P:265:PHE:CD1	2:P:265:PHE:N	2.87	0.42
2:P:633:THR:HG22	2:P:636:ASP:OD2	2.19	0.42
2:Q:81:ARG:NH1	2:Q:493:GLY:O	2.51	0.42
2:Q:82:THR:OG1	2:Q:83:ASN:N	2.52	0.42
2:Q:348:GLY:O	2:Q:663:PRO:HB3	2.18	0.42
2:R:76:TYR:CD1	2:R:77:GLY:N	2.87	0.42
2:R:350:ALA:O	2:R:354:VAL:HG23	2.19	0.42
2:R:633:THR:HG22	2:R:636:ASP:OD2	2.19	0.42
2:P:534:SER:O	2:Q:48:PRO:HG2	2.19	0.42
2:Q:331:PHE:O	2:Q:332:TRP:C	2.61	0.42
2:R:82:THR:OG1	2:R:83:ASN:N	2.52	0.42
2:R:506:ARG:O	2:R:507:ARG:HB2	2.19	0.42
2:P:132:ARG:HD2	2:P:429:MET:CE	2.47	0.42
2:P:334:GLY:O	2:P:337:ARG:HB3	2.19	0.42
2:P:350:ALA:O	2:P:354:VAL:HG23	2.19	0.42
2:Q:350:ALA:O	2:Q:354:VAL:HG23	2.19	0.42
2:Q:418:THR:HG22	2:Q:467:GLY:C	2.44	0.42
2:R:273:MET:HE1	2:R:365:VAL:HG11	2.02	0.42
2:R:663:PRO:CG	2:R:664:ARG:H	2.32	0.42
2:Q:410:TYR:HB3	2:Q:457:LEU:HD21	2.02	0.42
2:P:82:THR:OG1	2:P:83:ASN:N	2.52	0.42
2:P:319:LEU:HD12	2:P:320:CYS:H	1.83	0.42
2:Q:334:GLY:O	2:Q:337:ARG:HB3	2.19	0.42
2:R:251:ARG:CB	2:R:255:GLN:HE21	2.29	0.42
2:P:76:TYR:CD1	2:P:77:GLY:N	2.87	0.42
2:Q:78:ASN:ND2	2:Q:78:ASN:C	2.77	0.42
2:Q:633:THR:HG23	2:Q:635:ALA:N	2.32	0.42
2:R:17:LEU:HD11	2:R:378:LEU:HD22	2.02	0.42
2:Q:137:ASP:N	2:Q:293:LYS:HZ2	2.13	0.42
2:Q:273:MET:HE1	2:Q:365:VAL:HG11	2.02	0.42
2:P:392:SER:O	2:P:398:THR:HG21	2.20	0.42
2:Q:12:ILE:O	2:Q:16:MET:HG3	2.19	0.42
2:Q:429:MET:CB	2:Q:430:PRO:HD3	2.49	0.42
2:R:658:LEU:CG	2:R:662:MET:HE2	2.48	0.42
2:P:17:LEU:HD11	2:P:378:LEU:HD22	2.02	0.41
2:P:348:GLY:C	2:P:663:PRO:HB3	2.45	0.41
2:Q:506:ARG:O	2:Q:507:ARG:HB2	2.19	0.41
4:R:666:GTP:H2'	4:R:666:GTP:N3	2.36	0.41
2:P:358:GLU:HG2	2:P:362:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:17:LEU:O	2:Q:153:ILE:HG23	2.20	0.41
2:Q:348:GLY:C	2:Q:663:PRO:HB3	2.45	0.41
2:Q:633:THR:HG22	2:Q:636:ASP:OD2	2.19	0.41
2:Q:663:PRO:HG2	2:Q:664:ARG:N	2.34	0.41
2:P:17:LEU:O	2:P:153:ILE:HG23	2.20	0.41
2:P:410:TYR:HB3	2:P:457:LEU:HD21	2.02	0.41
2:Q:358:GLU:HG2	2:Q:362:LYS:HD3	2.02	0.41
2:Q:392:SER:O	2:Q:398:THR:HG21	2.20	0.41
2:R:17:LEU:O	2:R:153:ILE:HG23	2.20	0.41
2:P:181:MET:CE	2:P:356:LEU:CD2	2.94	0.41
2:Q:17:LEU:HD11	2:Q:378:LEU:HD22	2.02	0.41
2:Q:583:TYR:CE2	2:Q:587:ARG:HD3	2.56	0.41
2:R:334:GLY:O	2:R:337:ARG:HB3	2.19	0.41
2:R:624:ASP:OD1	2:R:626:ASN:HB2	2.21	0.41
2:R:137:ASP:N	2:R:293:LYS:HZ2	2.15	0.41
2:P:624:ASP:OD1	2:P:626:ASN:HB2	2.21	0.41
2:P:641:ILE:HD13	2:P:641:ILE:HA	1.84	0.41
2:R:392:SER:O	2:R:398:THR:HG21	2.20	0.41
2:Q:391:LEU:HD23	2:Q:391:LEU:HA	1.69	0.41
2:R:140:PRO:HG3	2:R:658:LEU:HD23	2.03	0.41
2:Q:140:PRO:HG3	2:Q:658:LEU:HD23	2.03	0.41
2:Q:228:ALA:HB1	2:Q:232:TYR:HB3	2.03	0.41
2:R:348:GLY:C	2:R:663:PRO:HB3	2.45	0.41
2:R:358:GLU:HG2	2:R:362:LYS:HD3	2.02	0.41
2:R:583:TYR:CE2	2:R:587:ARG:HD3	2.56	0.41
2:R:633:THR:HG23	2:R:635:ALA:N	2.32	0.41
1:D:5:DC:OP2	2:P:543:LYS:NZ	2.48	0.41
2:P:140:PRO:HG3	2:P:658:LEU:HD23	2.03	0.41
2:Q:624:ASP:OD1	2:Q:626:ASN:HB2	2.21	0.41
4:Q:666:GTP:N3	4:Q:666:GTP:H2'	2.35	0.41
2:P:583:TYR:CE2	2:P:587:ARG:HD3	2.56	0.40
2:Q:663:PRO:CG	2:Q:664:ARG:H	2.32	0.40
2:R:175:GLU:HA	2:R:352:TRP:CD2	2.56	0.40
2:P:273:MET:HE1	2:P:365:VAL:HG11	2.02	0.40
2:Q:311:GLU:O	2:Q:312:GLU:C	2.65	0.40
2:R:410:TYR:HB3	2:R:457:LEU:HD21	2.02	0.40
2:P:555:LYS:HA	2:P:564:TYR:OH	2.22	0.40
2:Q:641:ILE:HD13	2:Q:641:ILE:HA	1.84	0.40
2:R:555:LYS:HA	2:R:564:TYR:OH	2.22	0.40
2:P:50:PHE:O	2:P:53:PHE:HB3	2.22	0.40
2:Q:175:GLU:HA	2:Q:352:TRP:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:228:ALA:HB1	2:R:232:TYR:HB3	2.03	0.40
2:R:311:GLU:O	2:R:312:GLU:C	2.64	0.40
2:R:429:MET:CB	2:R:430:PRO:HD3	2.49	0.40

All (15) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:479:LYS:NZ	2:R:608:GLN:N[2_445]	0.78	1.42
2:R:479:LYS:NZ	2:R:607:ARG:C[2_445]	1.27	0.93
2:R:479:LYS:NZ	2:R:608:GLN:CA[2_445]	1.50	0.70
2:R:479:LYS:CE	2:R:608:GLN:CA[2_445]	1.55	0.65
2:R:479:LYS:CD	2:R:608:GLN:CB[2_445]	1.58	0.62
2:R:479:LYS:CE	2:R:608:GLN:N[2_445]	1.70	0.50
2:R:479:LYS:CE	2:R:608:GLN:C[2_445]	1.71	0.49
2:R:479:LYS:NZ	2:R:607:ARG:O[2_445]	1.91	0.29
2:R:479:LYS:NZ	2:R:608:GLN:CB[2_445]	1.99	0.21
2:R:479:LYS:CE	2:R:608:GLN:CB[2_445]	2.02	0.18
2:Q:537:ARG:NH2	2:R:582:SER:N[1_655]	2.03	0.17
2:R:479:LYS:CE	2:R:609:ALA:N[2_445]	2.10	0.10
2:P:569:GLU:OE2	2:R:1:PRO:CB[2_555]	2.16	0.04
2:R:479:LYS:CD	2:R:608:GLN:CA[2_445]	2.19	0.01
2:R:479:LYS:CD	2:R:608:GLN:C[2_445]	2.19	0.01

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	
2	P	662/664 (100%)	612 (92%)	43 (6%)	7 (1%)	11	43
2	Q	662/664 (100%)	612 (92%)	43 (6%)	7 (1%)	11	43
2	R	662/664 (100%)	612 (92%)	43 (6%)	7 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1986/1992 (100%)	1836 (92%)	129 (6%)	21 (1%)	11	43

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	608	GLN
2	Q	608	GLN
2	R	608	GLN
2	P	207	SER
2	P	607	ARG
2	P	630	TYR
2	Q	207	SER
2	Q	607	ARG
2	Q	630	TYR
2	R	207	SER
2	R	607	ARG
2	R	630	TYR
2	P	604	SER
2	Q	604	SER
2	R	604	SER
2	P	564	TYR
2	Q	564	TYR
2	R	564	TYR
2	P	663	PRO
2	Q	663	PRO
2	R	663	PRO

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	
2	P	557/557 (100%)	530 (95%)	27 (5%)	23	57
2	Q	557/557 (100%)	530 (95%)	27 (5%)	23	57
2	R	557/557 (100%)	530 (95%)	27 (5%)	23	57
All	All	1671/1671 (100%)	1590 (95%)	81 (5%)	23	57

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	16	MET
2	P	43	LEU
2	P	44	LEU
2	P	75	VAL
2	P	78	ASN
2	P	102	LEU
2	P	113	ASP
2	P	119	VAL
2	P	143	LEU
2	P	206	GLN
2	P	239	GLN
2	P	269	ARG
2	P	273	MET
2	P	351	PRO
2	P	373	GLU
2	P	387	LEU
2	P	404	LEU
2	P	430	PRO
2	P	480	VAL
2	P	497	LEU
2	P	534	SER
2	P	576	TRP
2	P	587	ARG
2	P	588	GLU
2	P	591	LEU
2	P	615	THR
2	P	633	THR
2	Q	16	MET
2	Q	43	LEU
2	Q	44	LEU
2	Q	75	VAL
2	Q	78	ASN
2	Q	102	LEU
2	Q	113	ASP
2	Q	119	VAL
2	Q	143	LEU
2	Q	206	GLN
2	Q	239	GLN
2	Q	269	ARG
2	Q	273	MET
2	Q	351	PRO
2	Q	373	GLU

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Mol	Chain	Res	Type
2	Q	387	LEU
2	Q	404	LEU
2	Q	430	PRO
2	Q	480	VAL
2	Q	497	LEU
2	Q	534	SER
2	Q	576	TRP
2	Q	587	ARG
2	Q	588	GLU
2	Q	591	LEU
2	Q	615	THR
2	Q	633	THR
2	R	16	MET
2	R	43	LEU
2	R	44	LEU
2	R	75	VAL
2	R	78	ASN
2	R	102	LEU
2	R	113	ASP
2	R	119	VAL
2	R	143	LEU
2	R	206	GLN
2	R	239	GLN
2	R	269	ARG
2	R	273	MET
2	R	351	PRO
2	R	373	GLU
2	R	387	LEU
2	R	404	LEU
2	R	430	PRO
2	R	480	VAL
2	R	497	LEU
2	R	534	SER
2	R	576	TRP
2	R	587	ARG
2	R	588	GLU
2	R	591	LEU
2	R	615	THR
2	R	633	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
2	P	26	GLN
2	P	78	ASN
2	P	89	HIS
2	P	91	ASN
2	P	158	ASN
2	P	191	GLN
2	P	193	HIS
2	P	255	GLN
2	P	309	ASN
2	P	328	HIS
2	P	448	GLN
2	P	519	ASN
2	P	524	ASN
2	P	525	GLN
2	P	608	GLN
2	P	642	HIS
2	Q	15	GLN
2	Q	26	GLN
2	Q	78	ASN
2	Q	89	HIS
2	Q	91	ASN
2	Q	158	ASN
2	Q	191	GLN
2	Q	193	HIS
2	Q	255	GLN
2	Q	309	ASN
2	Q	328	HIS
2	Q	448	GLN
2	Q	519	ASN
2	Q	524	ASN
2	Q	525	GLN
2	Q	642	HIS
2	R	26	GLN
2	R	78	ASN
2	R	89	HIS
2	R	91	ASN
2	R	158	ASN
2	R	191	GLN
2	R	193	HIS
2	R	255	GLN
2	R	309	ASN
2	R	328	HIS
2	R	448	GLN

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Mol	Chain	Res	Type
2	R	519	ASN
2	R	524	ASN
2	R	525	GLN
2	R	642	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GTP	R	667	5	33,34,34	3.53	12 (36%)	50,54,54	2.69	14 (28%)
4	GTP	R	666	-	33,34,34	3.57	15 (45%)	50,54,54	2.75	15 (30%)
4	GTP	Q	666	-	33,34,34	3.57	14 (42%)	50,54,54	2.76	15 (30%)
4	GTP	Q	667	5	33,34,34	3.53	13 (39%)	50,54,54	2.70	14 (28%)
4	GTP	P	667	5	33,34,34	3.53	12 (36%)	50,54,54	2.69	14 (28%)
4	GTP	P	666	-	33,34,34	3.57	15 (45%)	50,54,54	2.76	15 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	R	667	5	-	6/22/38/38	0/3/3/3
4	GTP	R	666	-	-	6/22/38/38	0/3/3/3
4	GTP	Q	666	-	-	6/22/38/38	0/3/3/3
4	GTP	Q	667	5	-	6/22/38/38	0/3/3/3
4	GTP	P	667	5	-	6/22/38/38	0/3/3/3
4	GTP	P	666	-	-	6/22/38/38	0/3/3/3

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	667	GTP	PB-O3B	11.50	1.71	1.59
4	P	667	GTP	PB-O3B	11.49	1.71	1.59
4	Q	667	GTP	PB-O3B	11.44	1.71	1.59
4	R	666	GTP	PB-O3B	11.01	1.71	1.59
4	P	666	GTP	PB-O3B	11.01	1.71	1.59
4	Q	666	GTP	PB-O3B	10.96	1.71	1.59
4	P	666	GTP	C6-N1	8.76	1.55	1.38
4	Q	666	GTP	C6-N1	8.76	1.55	1.38
4	R	666	GTP	C6-N1	8.74	1.55	1.38
4	Q	667	GTP	C6-N1	8.49	1.54	1.38
4	P	667	GTP	C6-N1	8.45	1.54	1.38
4	R	667	GTP	C6-N1	8.42	1.54	1.38
4	Q	666	GTP	C2-N2	7.26	1.51	1.34
4	P	666	GTP	C2-N2	7.24	1.51	1.34
4	R	666	GTP	C2-N2	7.22	1.51	1.34
4	Q	667	GTP	C2-N2	6.89	1.50	1.34
4	P	667	GTP	C2-N2	6.87	1.50	1.34
4	R	667	GTP	C2-N2	6.84	1.50	1.34
4	Q	666	GTP	PA-O3A	5.84	1.65	1.59
4	P	666	GTP	PA-O3A	5.84	1.65	1.59
4	R	666	GTP	PA-O3A	5.84	1.65	1.59
4	Q	667	GTP	C2'-C1'	5.54	1.70	1.53
4	P	667	GTP	C2'-C1'	5.53	1.70	1.53
4	R	667	GTP	C2'-C1'	5.52	1.70	1.53
4	Q	666	GTP	C2'-C1'	4.95	1.69	1.53
4	P	666	GTP	C2'-C1'	4.94	1.69	1.53
4	R	666	GTP	C2'-C1'	4.93	1.69	1.53
4	R	667	GTP	C5'-C4'	4.28	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	667	GTP	C5'-C4'	4.26	1.64	1.51
4	Q	667	GTP	C5'-C4'	4.24	1.64	1.51
4	Q	666	GTP	O2'-C2'	-4.18	1.32	1.43
4	P	666	GTP	O2'-C2'	-4.15	1.32	1.43
4	R	666	GTP	O2'-C2'	-4.13	1.32	1.43
4	Q	667	GTP	C5-C6	-4.09	1.29	1.44
4	P	667	GTP	C5-C6	-4.08	1.29	1.44
4	R	667	GTP	C5-C6	-4.06	1.29	1.44
4	P	666	GTP	C5-C6	-3.96	1.30	1.44
4	Q	666	GTP	C5-C6	-3.94	1.30	1.44
4	R	666	GTP	C5-C6	-3.94	1.30	1.44
4	R	666	GTP	C5'-C4'	3.82	1.63	1.51
4	P	666	GTP	C5'-C4'	3.78	1.62	1.51
4	Q	666	GTP	C5'-C4'	3.77	1.62	1.51
4	R	667	GTP	O2'-C2'	-3.54	1.34	1.43
4	R	667	GTP	C1'-N9	3.53	1.57	1.47
4	P	667	GTP	C1'-N9	3.52	1.57	1.47
4	P	667	GTP	O2'-C2'	-3.52	1.34	1.43
4	Q	667	GTP	O2'-C2'	-3.51	1.34	1.43
4	Q	667	GTP	C1'-N9	3.50	1.57	1.47
4	Q	667	GTP	PA-O3A	3.30	1.63	1.59
4	R	667	GTP	PA-O5'	3.27	1.72	1.59
4	Q	667	GTP	PA-O5'	3.27	1.72	1.59
4	P	667	GTP	PA-O5'	3.26	1.72	1.59
4	P	667	GTP	PA-O3A	3.25	1.63	1.59
4	R	667	GTP	PA-O3A	3.25	1.63	1.59
4	P	666	GTP	C2-N1	-2.85	1.30	1.37
4	R	666	GTP	C2-N1	-2.84	1.30	1.37
4	Q	666	GTP	C2-N1	-2.83	1.30	1.37
4	P	666	GTP	C1'-N9	2.71	1.55	1.47
4	R	666	GTP	C1'-N9	2.71	1.55	1.47
4	Q	666	GTP	C1'-N9	2.69	1.55	1.47
4	P	667	GTP	C2-N1	-2.67	1.31	1.37
4	R	666	GTP	C3'-C4'	-2.67	1.46	1.53
4	Q	667	GTP	C2-N1	-2.67	1.31	1.37
4	R	667	GTP	C2-N1	-2.65	1.31	1.37
4	P	666	GTP	C3'-C4'	-2.65	1.46	1.53
4	Q	666	GTP	C3'-C4'	-2.65	1.46	1.53
4	P	667	GTP	O6-C6	2.46	1.28	1.23
4	R	667	GTP	O6-C6	2.46	1.28	1.23
4	Q	667	GTP	O6-C6	2.44	1.28	1.23
4	P	666	GTP	PA-O5'	2.23	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	666	GTP	PA-O5'	2.22	1.68	1.59
4	Q	666	GTP	PA-O5'	2.21	1.68	1.59
4	Q	666	GTP	PG-O3G	-2.16	1.46	1.54
4	P	666	GTP	PG-O3G	-2.15	1.46	1.54
4	R	666	GTP	PG-O3G	-2.14	1.46	1.54
4	P	666	GTP	C4-N3	2.10	1.39	1.34
4	R	666	GTP	C4-N3	2.10	1.39	1.34
4	Q	666	GTP	C4-N3	2.09	1.39	1.34
4	P	666	GTP	O6-C6	2.02	1.27	1.23
4	R	666	GTP	O6-C6	2.01	1.27	1.23
4	Q	667	GTP	PG-O3G	-2.01	1.47	1.54

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	666	GTP	N9-C8-N7	-7.87	98.81	113.40
4	P	666	GTP	N9-C8-N7	-7.86	98.83	113.40
4	R	666	GTP	N9-C8-N7	-7.85	98.85	113.40
4	R	667	GTP	N9-C8-N7	-7.38	99.71	113.40
4	P	667	GTP	N9-C8-N7	-7.37	99.73	113.40
4	Q	667	GTP	N9-C8-N7	-7.36	99.74	113.40
4	R	667	GTP	C8-N7-C5	6.72	116.22	104.26
4	Q	667	GTP	C8-N7-C5	6.71	116.22	104.26
4	P	667	GTP	C8-N7-C5	6.71	116.21	104.26
4	P	666	GTP	C8-N7-C5	6.61	116.04	104.26
4	Q	666	GTP	C8-N7-C5	6.61	116.03	104.26
4	R	666	GTP	C8-N7-C5	6.60	116.01	104.26
4	P	666	GTP	O6-C6-N1	-6.11	108.63	120.11
4	Q	666	GTP	O6-C6-N1	-6.11	108.63	120.11
4	R	666	GTP	O6-C6-N1	-6.08	108.68	120.11
4	Q	667	GTP	O6-C6-N1	-5.76	109.28	120.11
4	P	667	GTP	O6-C6-N1	-5.73	109.34	120.11
4	R	667	GTP	O6-C6-N1	-5.72	109.36	120.11
4	Q	667	GTP	N1-C2-N3	5.41	133.23	123.32
4	P	667	GTP	N1-C2-N3	5.40	133.20	123.32
4	R	667	GTP	N1-C2-N3	5.39	133.18	123.32
4	Q	667	GTP	C6-C5-C4	5.32	126.83	118.83
4	P	666	GTP	C2-N1-C6	-5.32	115.46	125.11
4	Q	666	GTP	C2-N1-C6	-5.31	115.49	125.11
4	R	666	GTP	C2-N1-C6	-5.30	115.50	125.11
4	P	667	GTP	C6-C5-C4	5.29	126.79	118.83
4	R	667	GTP	C2'-C3'-C4'	5.28	112.82	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	667	GTP	C2'-C3'-C4'	5.27	112.78	102.61
4	P	667	GTP	C2'-C3'-C4'	5.26	112.78	102.61
4	R	667	GTP	C6-C5-C4	5.25	126.73	118.83
4	P	666	GTP	N1-C2-N3	5.24	132.91	123.32
4	Q	666	GTP	N1-C2-N3	5.24	132.91	123.32
4	R	666	GTP	N1-C2-N3	5.21	132.86	123.32
4	Q	666	GTP	C6-C5-C4	5.21	126.66	118.83
4	P	666	GTP	C6-C5-C4	5.21	126.66	118.83
4	R	666	GTP	C6-C5-C4	5.19	126.64	118.83
4	Q	667	GTP	C2-N1-C6	-5.18	115.71	125.11
4	P	667	GTP	C2-N1-C6	-5.16	115.75	125.11
4	R	667	GTP	C2-N1-C6	-5.16	115.75	125.11
4	Q	666	GTP	O6-C6-C5	5.05	139.87	126.53
4	P	666	GTP	O6-C6-C5	5.03	139.82	126.53
4	R	666	GTP	O6-C6-C5	5.01	139.76	126.53
4	Q	667	GTP	O6-C6-C5	4.89	139.46	126.53
4	P	667	GTP	O6-C6-C5	4.86	139.38	126.53
4	R	667	GTP	O6-C6-C5	4.84	139.32	126.53
4	Q	666	GTP	C2'-C3'-C4'	4.78	111.85	102.61
4	P	666	GTP	C2'-C3'-C4'	4.77	111.83	102.61
4	R	666	GTP	C2'-C3'-C4'	4.76	111.81	102.61
4	P	666	GTP	C4-C5-N7	-4.06	104.24	110.67
4	R	666	GTP	C4-C5-N7	-4.05	104.25	110.67
4	Q	666	GTP	C4-C5-N7	-4.02	104.30	110.67
4	Q	667	GTP	C4-C5-N7	-3.89	104.51	110.67
4	P	667	GTP	C4-C5-N7	-3.87	104.53	110.67
4	R	667	GTP	C4-C5-N7	-3.85	104.58	110.67
4	P	666	GTP	N2-C2-N3	-3.78	112.28	119.67
4	Q	666	GTP	N2-C2-N3	-3.78	112.29	119.67
4	R	666	GTP	N2-C2-N3	-3.76	112.33	119.67
4	R	666	GTP	C8-N9-C4	3.76	113.08	106.03
4	Q	666	GTP	C8-N9-C4	3.76	113.07	106.03
4	P	666	GTP	C8-N9-C4	3.75	113.06	106.03
4	P	667	GTP	N2-C2-N3	-3.75	112.36	119.67
4	Q	667	GTP	N2-C2-N3	-3.74	112.37	119.67
4	R	667	GTP	N2-C2-N3	-3.73	112.40	119.67
4	R	667	GTP	C8-N9-C4	3.33	112.27	106.03
4	P	667	GTP	C8-N9-C4	3.33	112.27	106.03
4	Q	667	GTP	C8-N9-C4	3.32	112.25	106.03
4	Q	667	GTP	C4'-O4'-C1'	3.18	116.49	109.47
4	P	667	GTP	C4'-O4'-C1'	3.17	116.45	109.47
4	R	667	GTP	C4'-O4'-C1'	3.16	116.45	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	667	GTP	C2-N3-C4	-3.02	107.09	112.30
4	R	667	GTP	C2-N3-C4	-3.02	107.10	112.30
4	Q	667	GTP	C2-N3-C4	-3.02	107.10	112.30
4	Q	666	GTP	C2-N3-C4	-2.84	107.40	112.30
4	P	666	GTP	C2-N3-C4	-2.82	107.43	112.30
4	R	666	GTP	C2-N3-C4	-2.78	107.50	112.30
4	P	666	GTP	O4'-C4'-C5'	2.77	118.21	109.33
4	R	666	GTP	O4'-C4'-C5'	2.77	118.19	109.33
4	Q	666	GTP	O4'-C4'-C5'	2.76	118.17	109.33
4	R	666	GTP	O5'-C5'-C4'	-2.70	99.79	108.99
4	P	666	GTP	O5'-C5'-C4'	-2.69	99.83	108.99
4	Q	666	GTP	O5'-C5'-C4'	-2.68	99.86	108.99
4	P	666	GTP	C4'-O4'-C1'	2.55	115.10	109.47
4	R	666	GTP	C4'-O4'-C1'	2.54	115.08	109.47
4	Q	666	GTP	C4'-O4'-C1'	2.54	115.08	109.47
4	R	667	GTP	O5'-C5'-C4'	-2.54	100.34	108.99
4	Q	667	GTP	O5'-C5'-C4'	-2.54	100.35	108.99
4	P	667	GTP	O5'-C5'-C4'	-2.53	100.38	108.99

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	666	GTP	O4'-C4'-C5'-O5'
4	Q	666	GTP	O4'-C4'-C5'-O5'
4	R	666	GTP	O4'-C4'-C5'-O5'
4	R	666	GTP	C3'-C4'-C5'-O5'
4	P	666	GTP	C3'-C4'-C5'-O5'
4	Q	666	GTP	C3'-C4'-C5'-O5'
4	P	667	GTP	PB-O3A-PA-O5'
4	Q	667	GTP	PB-O3A-PA-O5'
4	R	667	GTP	PB-O3A-PA-O5'
4	P	666	GTP	PA-O3A-PB-O2B
4	P	667	GTP	PA-O3A-PB-O2B
4	Q	666	GTP	PA-O3A-PB-O2B
4	Q	667	GTP	PA-O3A-PB-O2B
4	R	666	GTP	PA-O3A-PB-O2B
4	R	667	GTP	PA-O3A-PB-O2B
4	P	667	GTP	PG-O3B-PB-O3A
4	Q	667	GTP	PG-O3B-PB-O3A
4	R	667	GTP	PG-O3B-PB-O3A
4	P	666	GTP	PG-O3B-PB-O3A

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Mol	Chain	Res	Type	Atoms
4	Q	666	GTP	PG-O3B-PB-O3A
4	R	666	GTP	PG-O3B-PB-O3A
4	P	666	GTP	PG-O3B-PB-O2B
4	P	666	GTP	PA-O3A-PB-O1B
4	P	667	GTP	PG-O3B-PB-O1B
4	P	667	GTP	PA-O3A-PB-O1B
4	Q	666	GTP	PG-O3B-PB-O2B
4	Q	666	GTP	PA-O3A-PB-O1B
4	Q	667	GTP	PG-O3B-PB-O1B
4	Q	667	GTP	PA-O3A-PB-O1B
4	R	666	GTP	PG-O3B-PB-O2B
4	R	666	GTP	PA-O3A-PB-O1B
4	R	667	GTP	PG-O3B-PB-O1B
4	R	667	GTP	PA-O3A-PB-O1B
4	P	667	GTP	PG-O3B-PB-O2B
4	Q	667	GTP	PG-O3B-PB-O2B
4	R	667	GTP	PG-O3B-PB-O2B

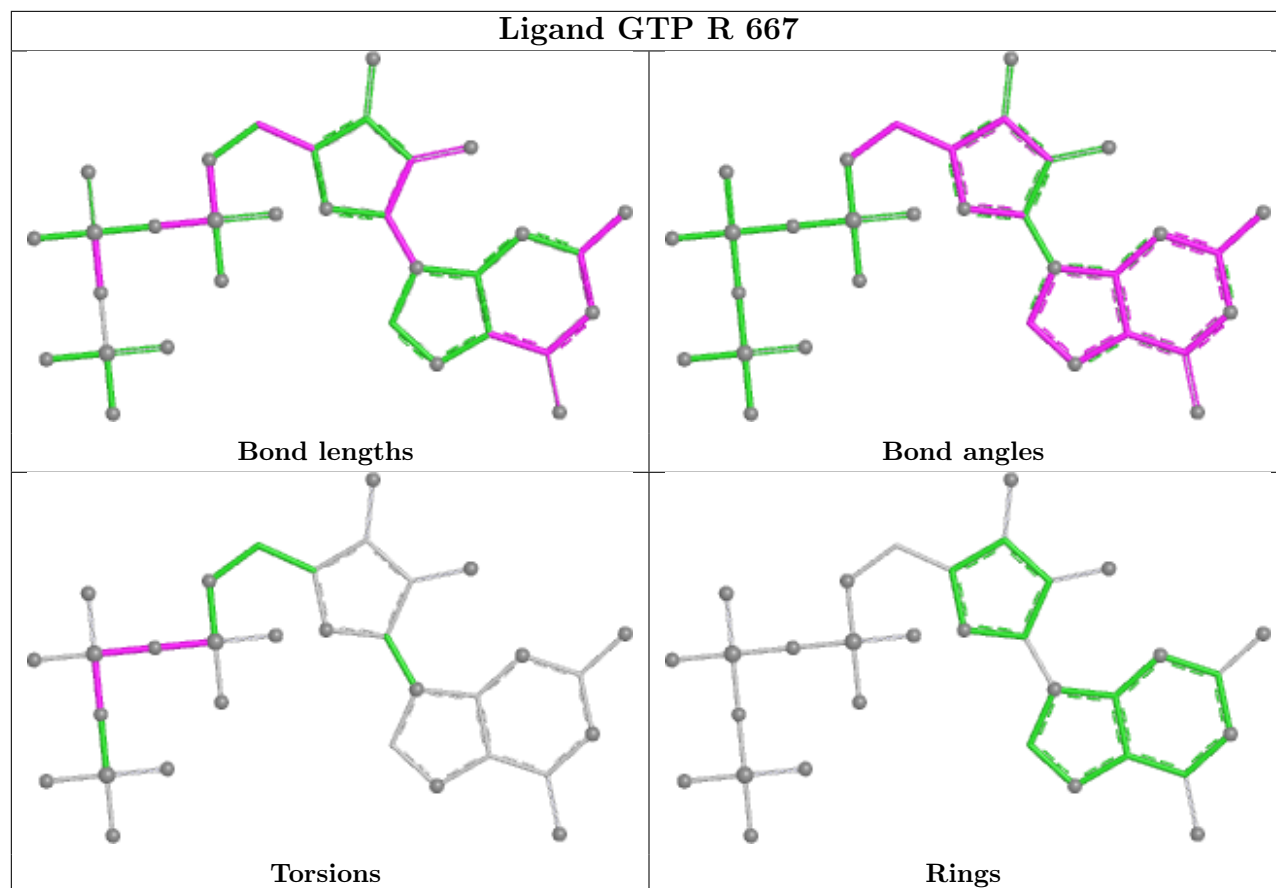
There are no ring outliers.

3 monomers are involved in 8 short contacts:

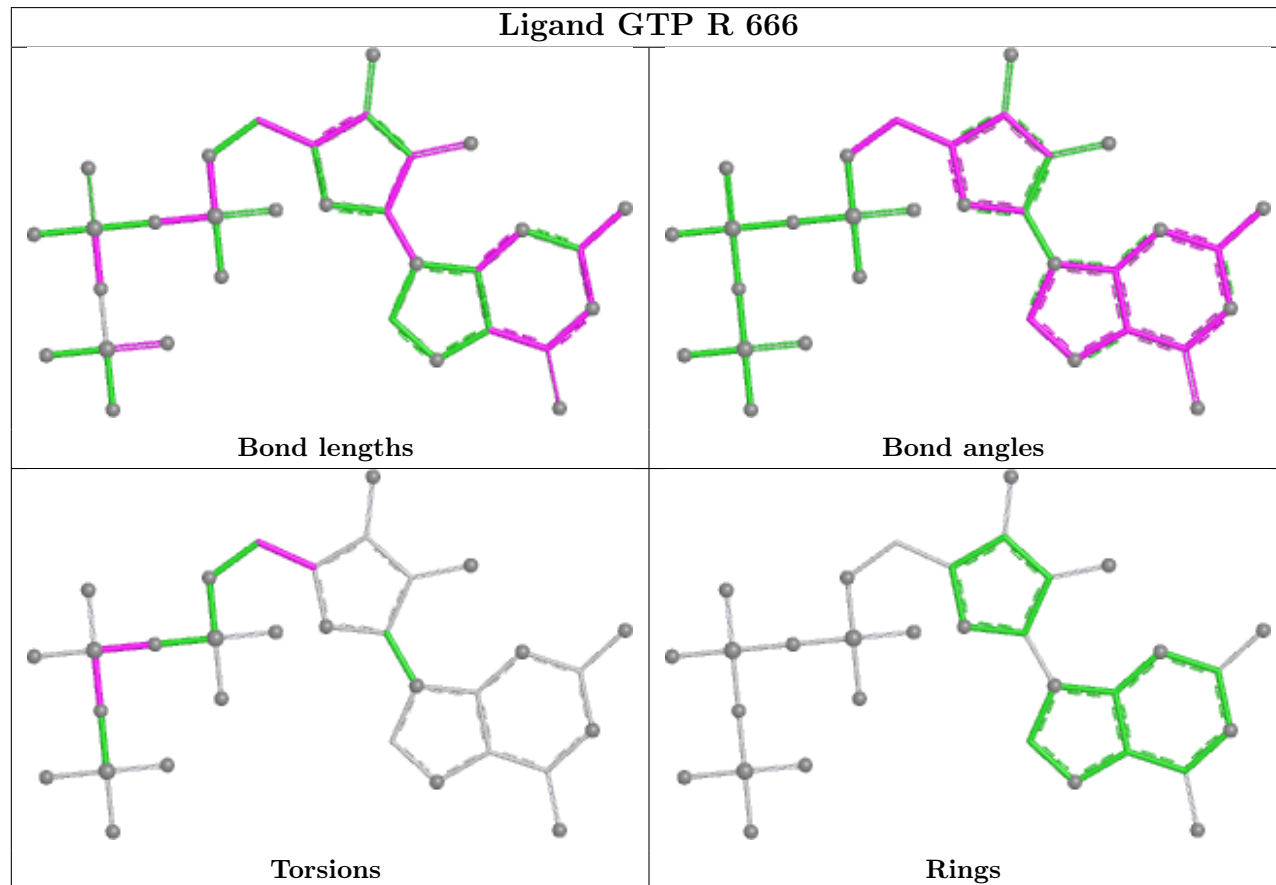
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	666	GTP	3	0
4	Q	666	GTP	3	0
4	P	666	GTP	2	0

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

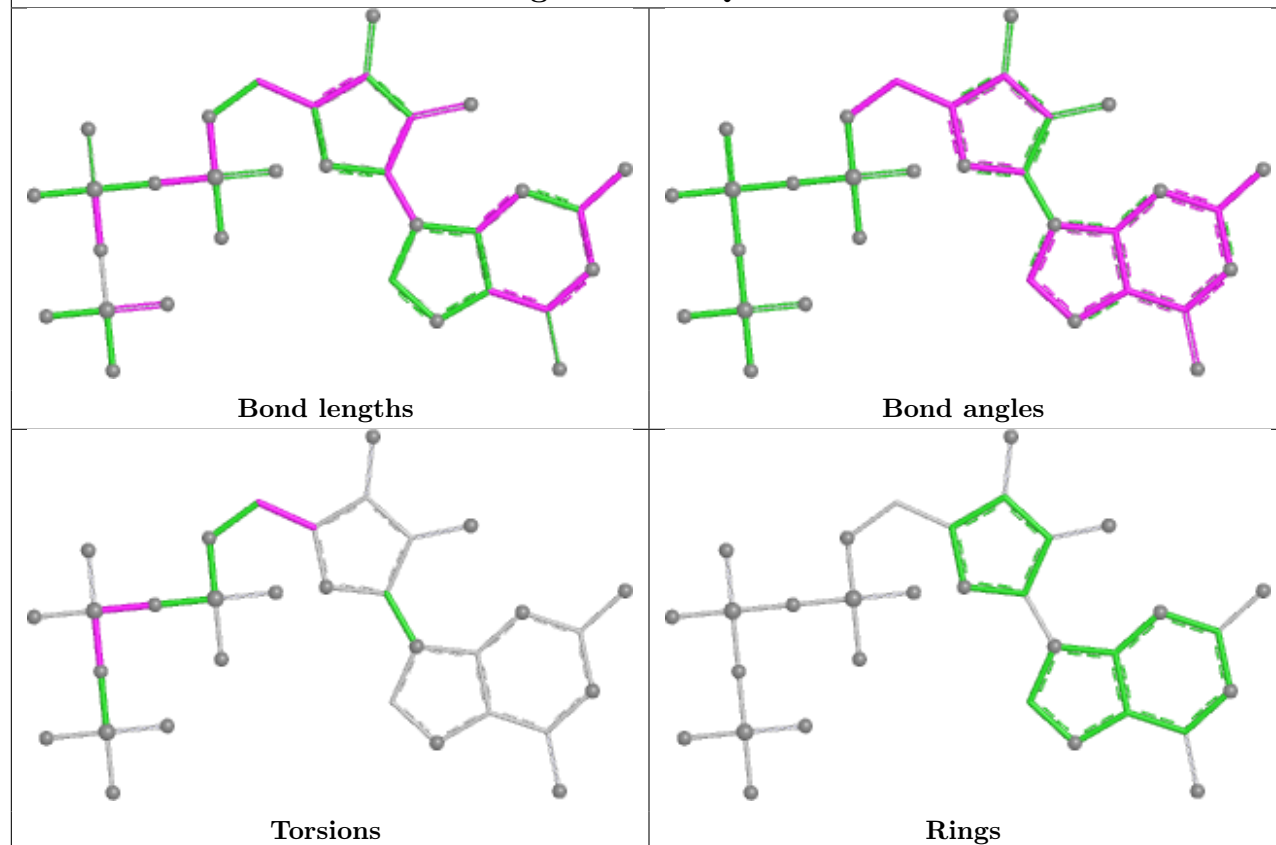
Ligand GTP R 667



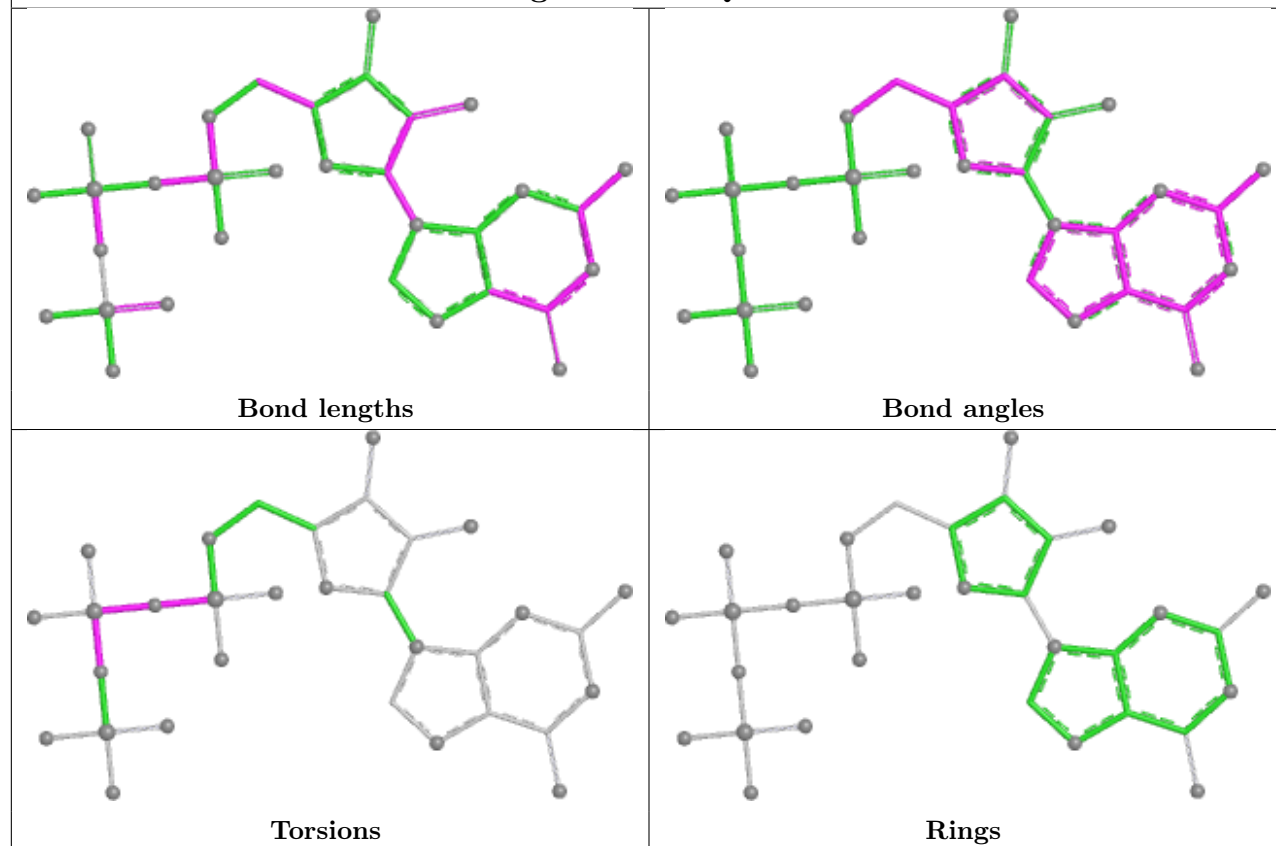
Ligand GTP R 666



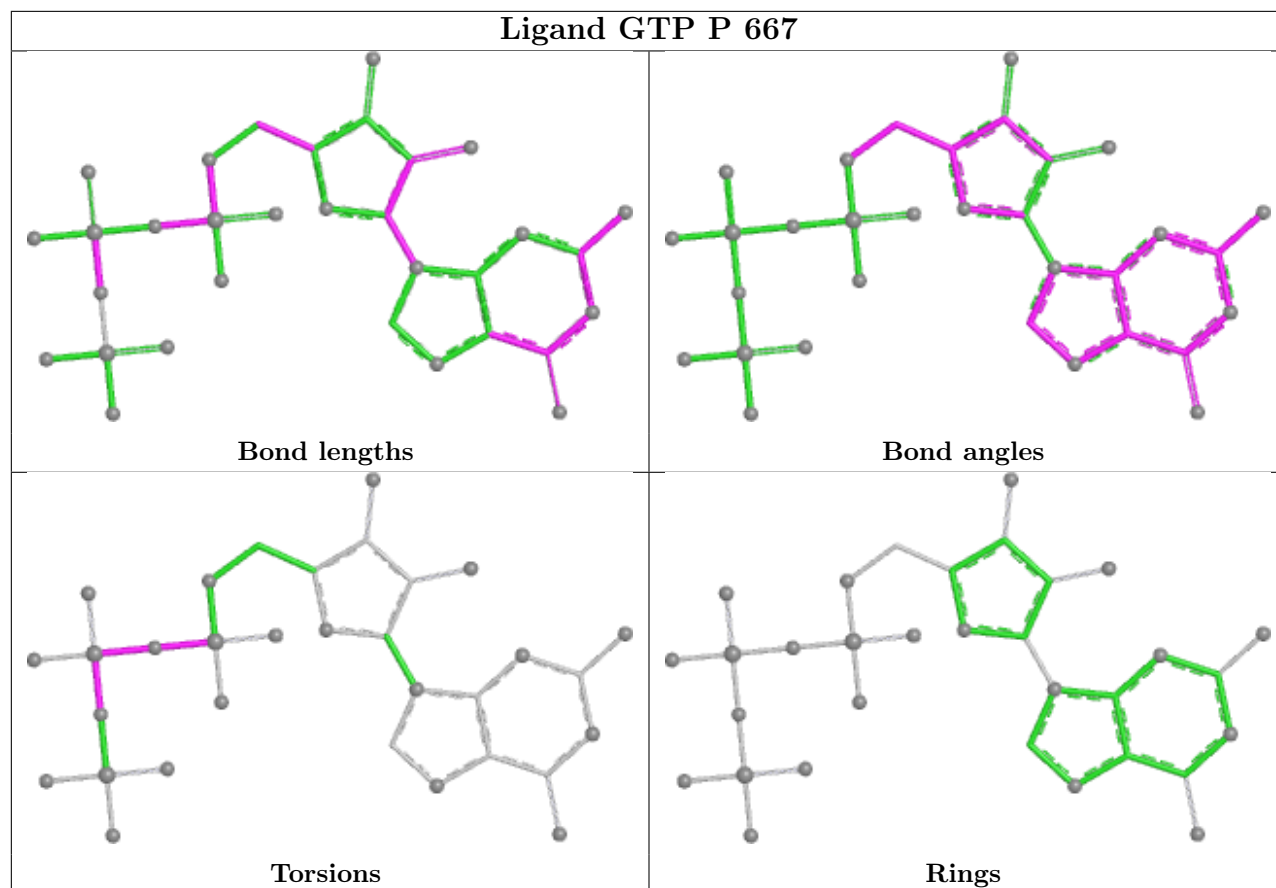
Ligand GTP Q 666



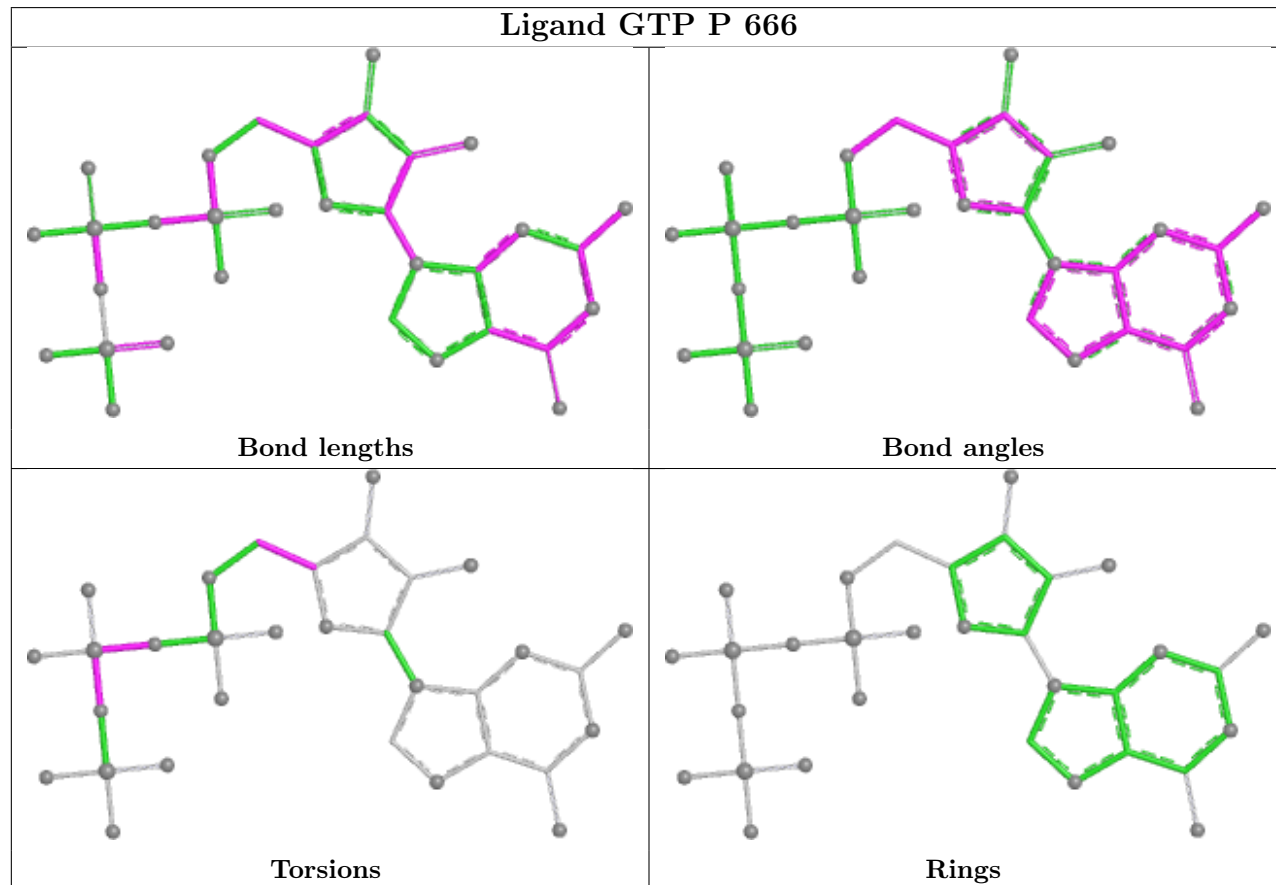
Ligand GTP Q 667



Ligand GTP P 667



Ligand GTP P 666



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	D	4/5 (80%)	1.60	2 (50%) 0 0	74, 83, 104, 154	0
1	E	4/5 (80%)	1.95	2 (50%) 0 0	74, 83, 104, 154	0
1	F	4/5 (80%)	1.30	1 (25%) 2 1	74, 83, 104, 154	0
2	P	664/664 (100%)	-0.32	9 (1%) 73 51	28, 48, 78, 140	0
2	Q	664/664 (100%)	-0.18	6 (0%) 81 61	28, 48, 78, 140	0
2	R	664/664 (100%)	-0.33	9 (1%) 73 51	28, 48, 78, 140	0
All	All	2004/2007 (99%)	-0.27	29 (1%) 73 51	28, 48, 79, 154	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	609	ALA	4.6
2	R	606	ALA	4.0
1	E	3	DT	3.8
2	Q	607	ARG	3.6
1	F	3	DT	3.3
2	P	606	ALA	3.2
2	Q	1	PRO	3.1
2	P	1	PRO	3.0
2	R	608	GLN	2.9
1	D	3	DT	2.9
2	P	610	GLY	2.8
2	R	576	TRP	2.5
2	R	610	GLY	2.5
2	R	1	PRO	2.5
2	Q	609	ALA	2.5
2	R	605	MET	2.4
2	P	609	ALA	2.4
2	Q	537	ARG	2.4
2	R	206	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	P	664	ARG	2.3
2	P	604	SER	2.2
2	P	608	GLN	2.2
2	P	605	MET	2.1
1	E	4	DT	2.1
2	Q	19	ALA	2.1
2	P	207	SER	2.1
2	R	603	ALA	2.1
2	Q	470	ARG	2.1
1	D	4	DT	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

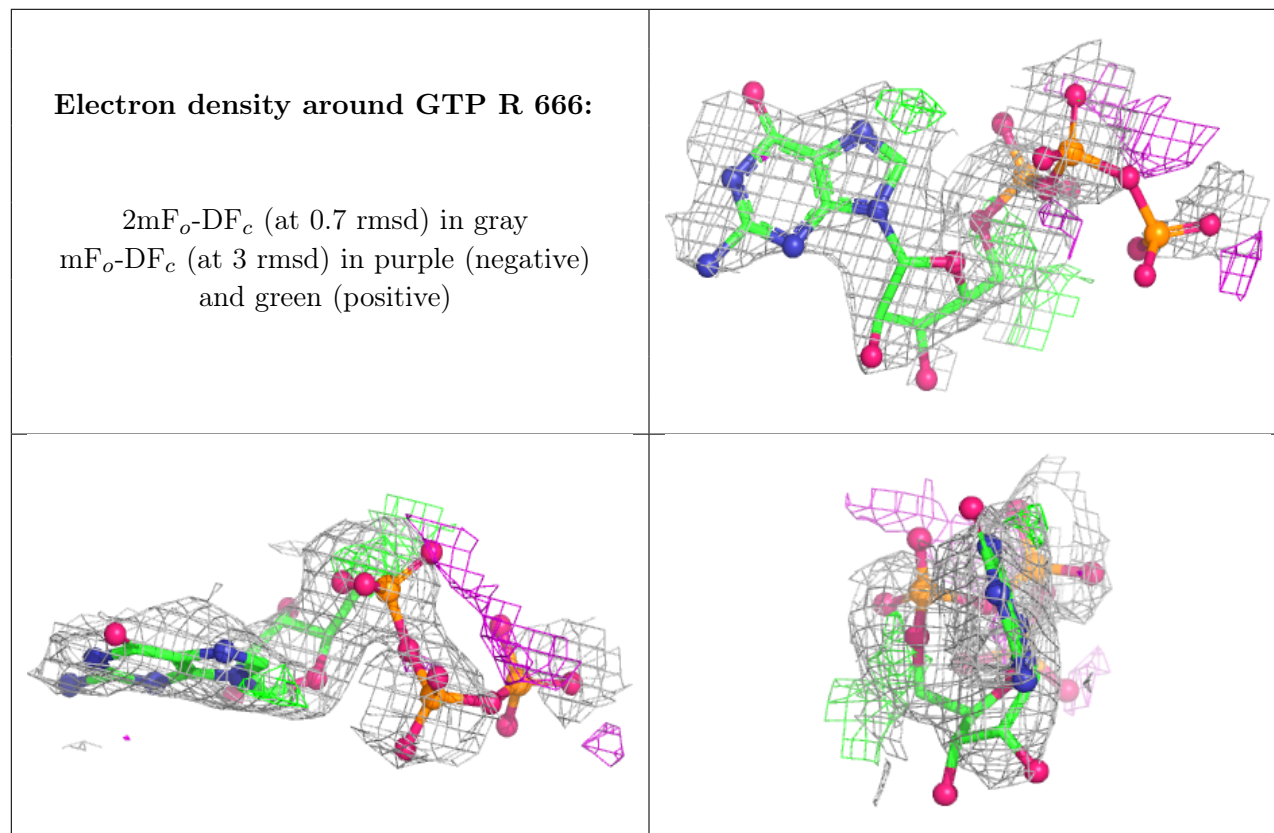
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GTP	R	666	32/32	0.58	0.19	99,125,165,170	0
4	GTP	Q	666	32/32	0.59	0.19	99,125,165,170	0
4	GTP	P	666	32/32	0.64	0.17	99,125,165,170	0
5	MG	P	669	1/1	0.66	0.31	83,83,83,83	0
5	MG	Q	669	1/1	0.68	0.13	83,83,83,83	0
4	GTP	Q	667	32/32	0.69	0.18	84,109,140,144	0
4	GTP	R	667	32/32	0.72	0.17	84,109,140,144	0
5	MG	R	669	1/1	0.76	0.36	83,83,83,83	0
5	MG	P	668	1/1	0.80	0.09	73,73,73,73	0
4	GTP	P	667	32/32	0.80	0.18	84,109,140,144	0
5	MG	R	668	1/1	0.85	0.11	73,73,73,73	0
5	MG	Q	668	1/1	0.90	0.08	73,73,73,73	0
3	MN	R	665	1/1	0.93	0.06	67,67,67,67	0

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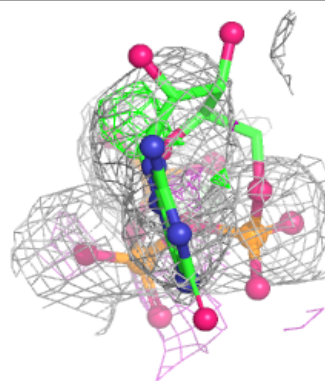
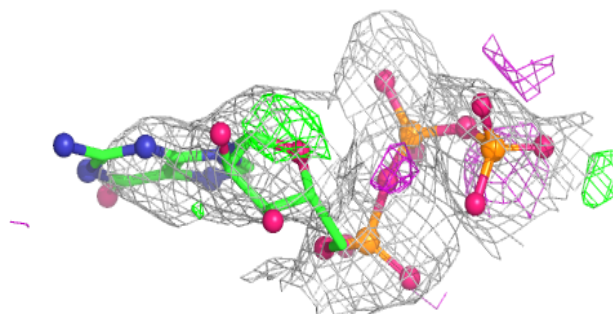
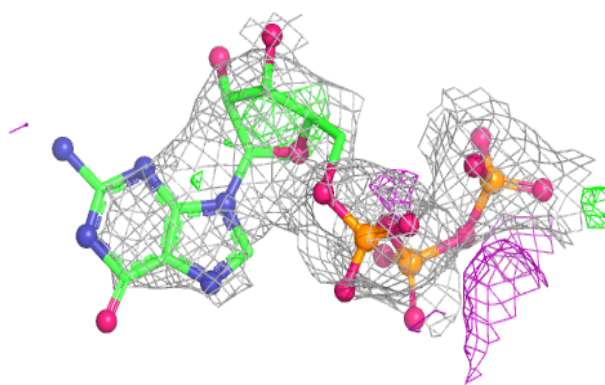
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MN	Q	665	1/1	0.96	0.05	67,67,67,67	0
3	MN	P	665	1/1	0.97	0.04	67,67,67,67	0

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.

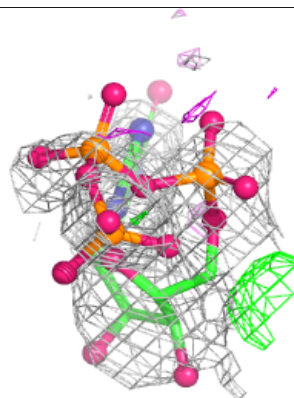
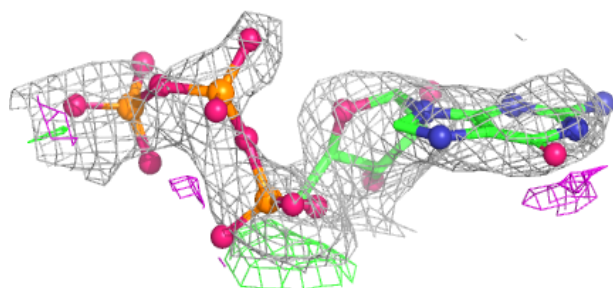
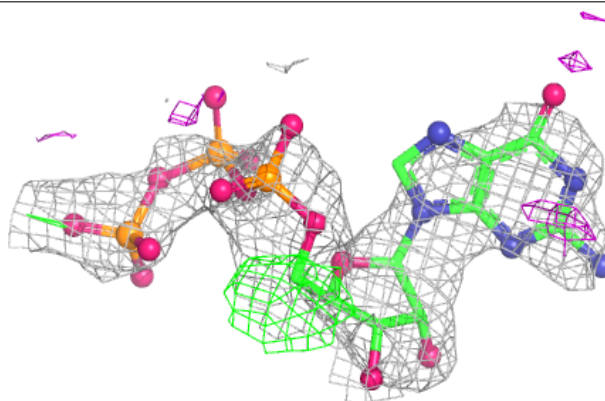


Electron density around GTP Q 666:

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

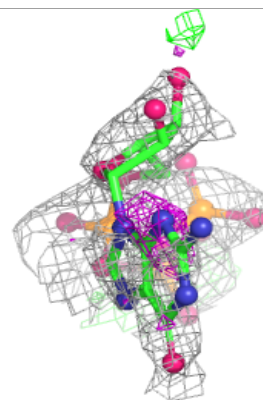
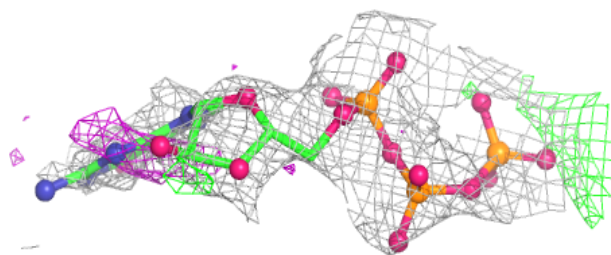
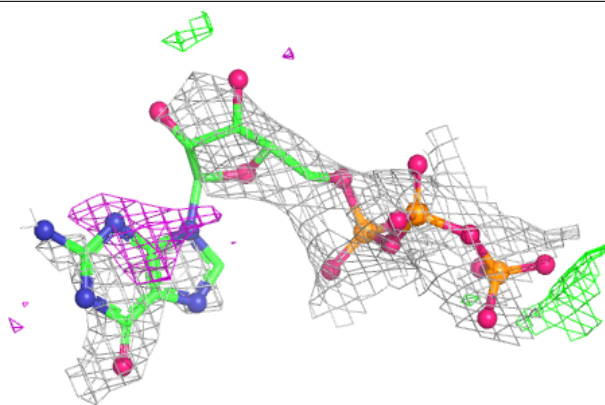
**Electron density around GTP P 666:**

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

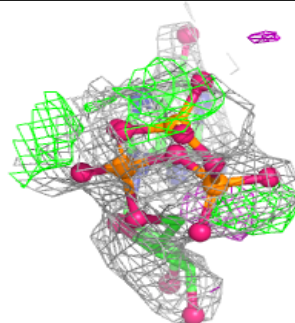
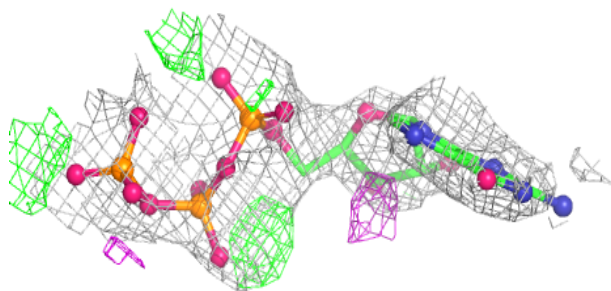
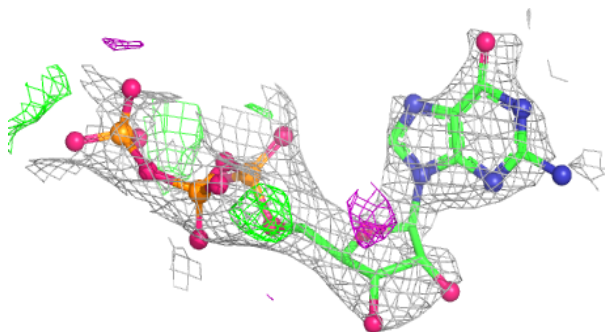


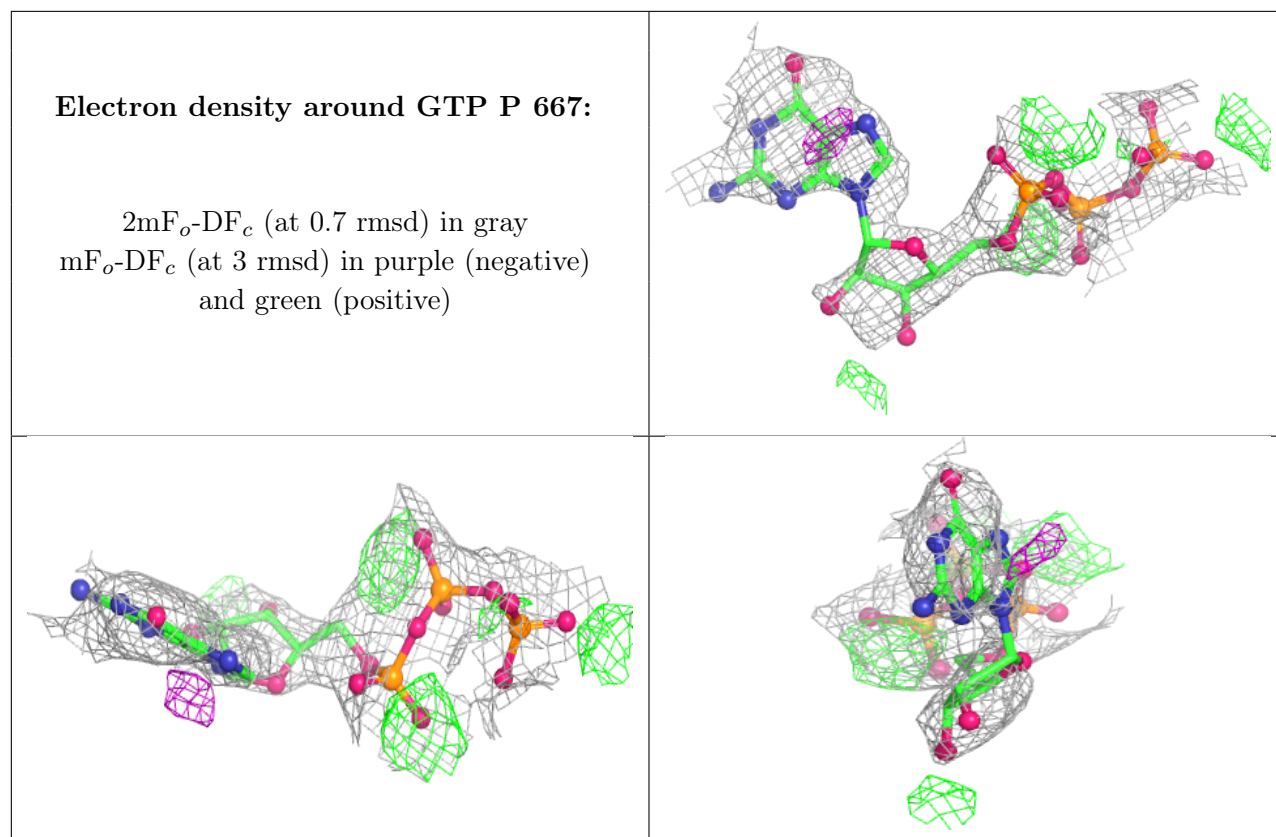
Electron density around GTP Q 667:

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

**Electron density around GTP R 667:**

$2mF_o-DF_c$ (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.