



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:51 PM UTC

PDB ID : 4HDG / pdb_00004hdg
Title : Crystal Structure of viral RdRp in complex with GTP
Authors : Surana, P.; Nair, D.T.
Deposited on : 2012-10-02
Resolution : 2.38 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

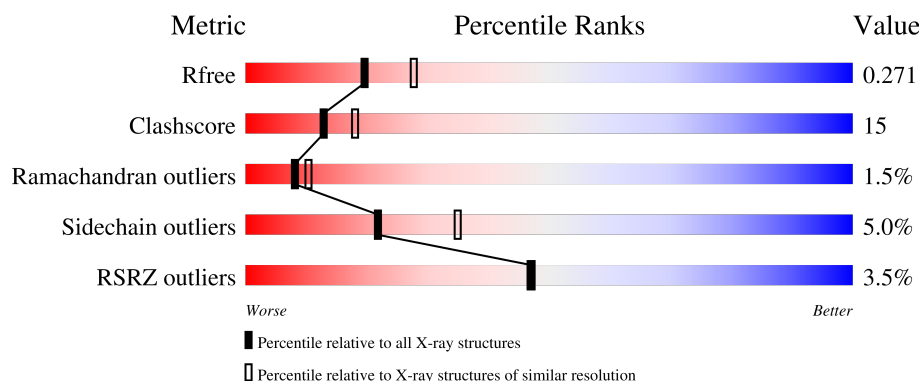
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

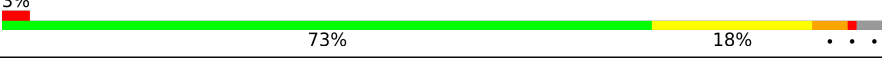
The reported resolution of this entry is 2.38 Å.

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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	A	639	
1	B	639	

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
2	GTP	A	1001	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10361 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 Polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	0	0	0
			4924	3105	889	900	30			
1	B	612	Total	C	N	O	S	0	0	0
			4914	3100	884	899	31			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	267	GLY	-	expression tag	UNP G3LHD9
A	268	PRO	-	expression tag	UNP G3LHD9
A	269	LEU	-	expression tag	UNP G3LHD9
A	270	GLY	-	expression tag	UNP G3LHD9
A	271	SER	-	expression tag	UNP G3LHD9
A	373	ARG	LYS	conflict	UNP G3LHD9
A	429	ASN	ASP	conflict	UNP G3LHD9
A	836	ALA	THR	conflict	UNP G3LHD9
B	267	GLY	-	expression tag	UNP G3LHD9
B	268	PRO	-	expression tag	UNP G3LHD9
B	269	LEU	-	expression tag	UNP G3LHD9
B	270	GLY	-	expression tag	UNP G3LHD9
B	271	SER	-	expression tag	UNP G3LHD9
B	373	ARG	LYS	conflict	UNP G3LHD9
B	429	ASN	ASP	conflict	UNP G3LHD9
B	836	ALA	THR	conflict	UNP G3LHD9

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0

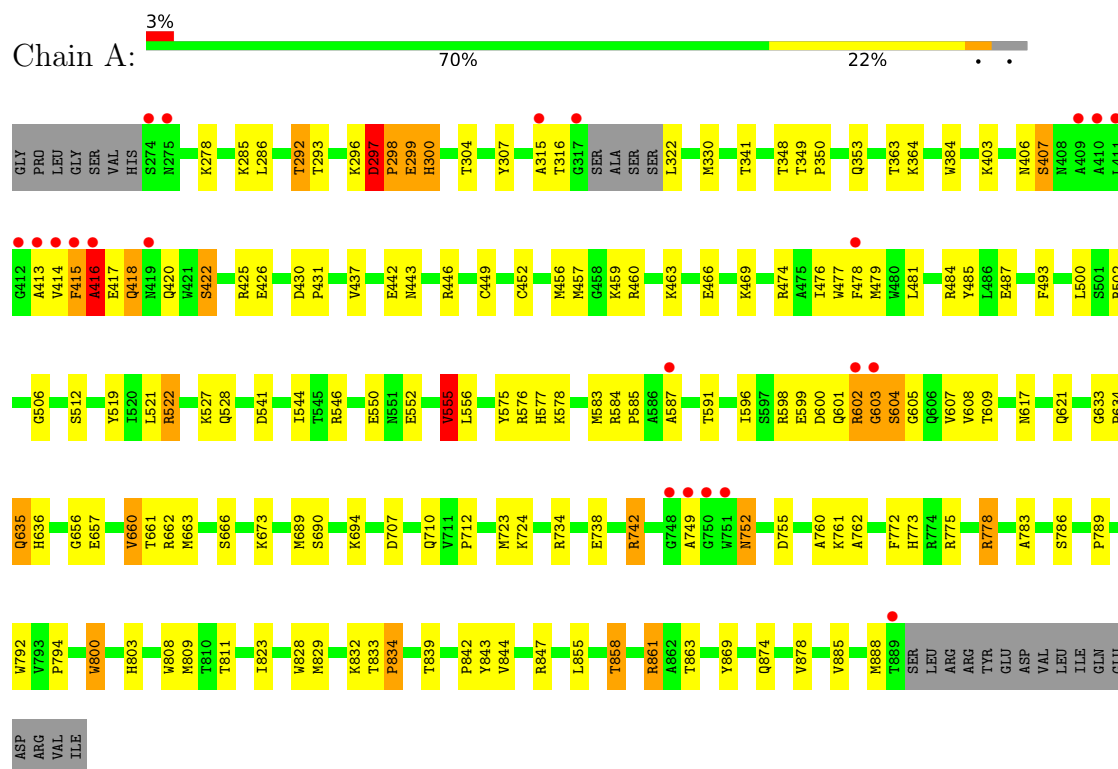
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	211	Total O 211 211	0	0
4	B	244	Total O 244 244	0	0

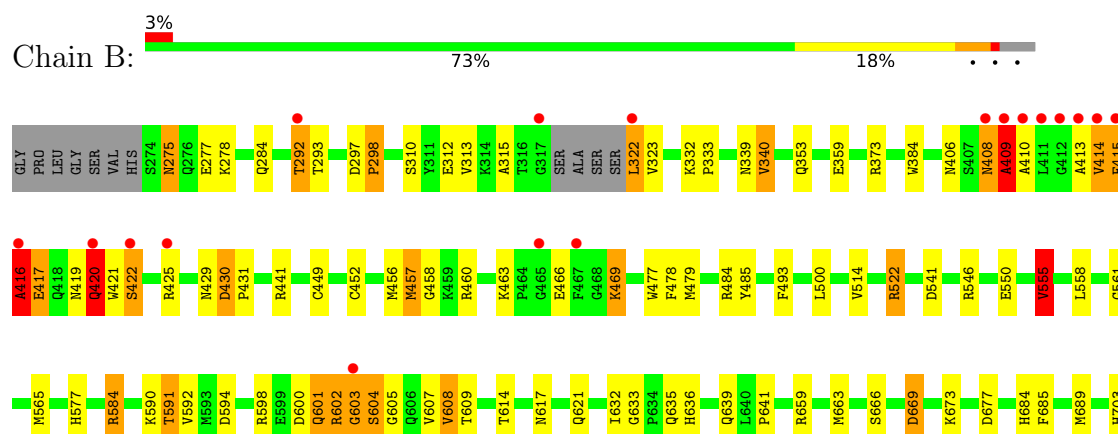
3 Residue-property plots

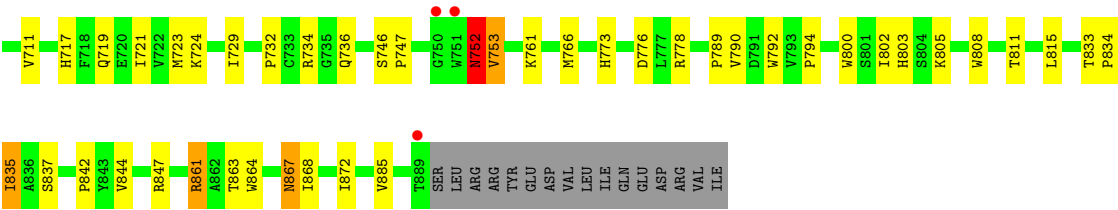
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Polyprotein



• Molecule 1: Polyprotein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	144.57Å 86.55Å 112.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.38 50.00 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.38) 99.7 (50.00-2.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.276 0.216 , 0.271	Depositor DCC
R_{free} test set	4034 reflections (7.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.780	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.3	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	0.95	EDS
Total number of atoms	10361	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4982e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	4/5041 (0.1%)	1.09	16/6823 (0.2%)
1	B	0.98	3/5031 (0.1%)	1.05	16/6811 (0.2%)
All	All	0.99	7/10072 (0.1%)	1.07	32/13634 (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	2
1	B	0	2
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	416	ALA	CA-CB	8.29	1.67	1.53
1	B	298	PRO	N-CD	7.51	1.58	1.47
1	A	834	PRO	N-CD	7.20	1.57	1.47
1	A	422	SER	CB-OG	6.72	1.55	1.42
1	B	340	VAL	CA-CB	5.85	1.61	1.54
1	A	760	ALA	CA-CB	-5.45	1.44	1.53
1	B	673	LYS	C-O	-5.29	1.19	1.24

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ASP	CA-C-N	-13.35	106.27	119.89
1	A	297	ASP	C-N-CA	-13.35	106.27	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	555	VAL	CB-CA-C	-8.08	101.46	112.04
1	B	409	ALA	N-CA-C	8.01	127.86	110.80
1	A	555	VAL	CB-CA-C	-7.99	101.58	112.04
1	B	430	ASP	CA-C-N	6.79	128.33	119.84
1	B	430	ASP	C-N-CA	6.79	128.33	119.84
1	A	420	GLN	N-CA-C	-6.65	103.39	113.89
1	A	298	PRO	N-CA-C	-6.46	100.83	111.11
1	A	833	THR	CA-C-N	6.19	126.21	119.90
1	A	833	THR	C-N-CA	6.19	126.21	119.90
1	A	603	GLY	N-CA-C	-6.16	106.58	115.27
1	B	323	VAL	N-CA-C	5.89	116.79	108.36
1	B	458	GLY	N-CA-C	5.89	118.11	110.45
1	B	608	VAL	N-CA-C	5.89	117.15	111.91
1	A	673	LYS	CA-C-N	5.74	126.20	120.52
1	A	673	LYS	C-N-CA	5.74	126.20	120.52
1	A	416	ALA	CA-C-N	-5.69	114.76	122.95
1	A	416	ALA	C-N-CA	-5.69	114.76	122.95
1	B	275	ASN	N-CA-C	-5.62	106.34	113.43
1	B	417	GLU	CB-CA-C	5.41	119.99	111.77
1	A	749	ALA	N-CA-C	-5.31	99.49	110.80
1	B	584	ARG	CA-C-N	5.30	125.55	119.83
1	B	584	ARG	C-N-CA	5.30	125.55	119.83
1	B	677	ASP	N-CA-C	5.23	119.53	113.20
1	B	753	VAL	N-CA-C	-5.18	98.58	109.34
1	B	663	MET	N-CA-C	5.13	117.47	109.52
1	B	711	VAL	CA-C-N	5.12	125.52	119.99
1	B	711	VAL	C-N-CA	5.12	125.52	119.99
1	A	800	TRP	N-CA-C	-5.10	107.11	113.38
1	A	297	ASP	N-CA-C	5.09	121.06	109.81
1	A	500	LEU	CA-CB-CG	-5.04	98.65	116.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300	HIS	Mainchain
1	A	416	ALA	Peptide
1	B	408	ASN	Peptide
1	B	416	ALA	Peptide

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	A	4924	0	4826	157	0
1	B	4914	0	4808	136	0
2	A	32	0	12	9	0
2	B	32	0	12	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	211	0	0	8	0
4	B	244	0	0	15	0
All	All	10361	0	9658	295	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 15.

All (295) 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:487:GLU:CD	1:A:607:VAL:HG12	1.70	1.15
1:A:527:LYS:NZ	1:A:661:THR:OG1	1.79	1.13
1:A:742:ARG:HH11	1:A:742:ARG:HG2	0.96	1.12
1:A:416:ALA:HB3	1:A:478:PHE:CE2	1.86	1.10
1:A:414:VAL:HG11	1:A:478:PHE:CE1	1.86	1.09
1:B:284:GLN:HG3	4:B:1297:HOH:O	1.51	1.07
1:A:298:PRO:HB2	1:A:584:ARG:HH12	1.20	1.07
1:A:457:MET:HG3	1:A:478:PHE:CD1	1.89	1.06
1:A:602:ARG:HG2	1:A:603:GLY:H	1.21	1.04
1:A:416:ALA:HB3	1:A:478:PHE:HE2	1.19	0.98
1:A:808:TRP:CD1	1:A:809:MET:HE3	1.99	0.97
1:B:602:ARG:HG3	1:B:604:SER:H	1.27	0.97
1:A:742:ARG:HG2	1:A:742:ARG:NH1	1.74	0.97
1:A:633:GLY:H	1:A:636:HIS:HD2	1.13	0.94
1:A:603:GLY:HA3	4:A:1280:HOH:O	1.68	0.93
1:A:330:MET:HE2	1:A:783:ALA:HB1	1.48	0.91
1:B:292:THR:HG22	1:B:293:THR:HG23	1.50	0.91
1:B:633:GLY:H	1:B:636:HIS:CD2	1.90	0.89
1:A:633:GLY:H	1:A:636:HIS:CD2	1.92	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:GLY:H	1:B:636:HIS:HD2	1.18	0.88
1:A:600:ASP:CG	1:A:601:GLN:H	1.81	0.88
1:B:600:ASP:CG	1:B:601:GLN:H	1.79	0.86
1:A:808:TRP:HD1	1:A:809:MET:HE3	1.38	0.86
1:A:634:PRO:HD2	1:A:635:GLN:HE21	1.41	0.85
1:A:416:ALA:HA	1:A:418:GLN:HE21	1.41	0.84
1:A:414:VAL:HG11	1:A:478:PHE:CZ	2.12	0.83
1:B:766:MET:HG3	1:B:808:TRP:CE2	2.13	0.83
1:A:809:MET:HA	1:A:809:MET:HE2	1.62	0.82
1:B:406:ASN:OD1	1:B:425:ARG:NH1	2.12	0.82
1:A:330:MET:HE2	1:A:783:ALA:CB	2.10	0.81
1:B:359:GLU:OE1	4:B:1217:HOH:O	1.98	0.81
1:B:790:VAL:HG21	1:B:885:VAL:HG23	1.64	0.80
1:B:602:ARG:HG3	1:B:604:SER:N	1.96	0.80
1:B:414:VAL:HG11	1:B:478:PHE:CE2	2.15	0.80
1:B:373:ARG:CD	4:B:1273:HOH:O	2.29	0.80
1:A:762:ALA:CB	1:A:809:MET:HE1	2.11	0.80
1:A:602:ARG:HG2	1:A:603:GLY:N	1.97	0.79
1:B:310:SER:HB3	1:B:592:VAL:CG1	2.13	0.79
1:B:466:GLU:HB2	1:B:469:LYS:HE3	1.64	0.79
1:A:449:CYS:SG	1:A:452:CYS:HB2	2.23	0.79
1:A:330:MET:CE	1:A:783:ALA:HB1	2.12	0.79
1:A:487:GLU:OE2	1:A:607:VAL:HG12	1.83	0.78
1:A:855:LEU:O	1:A:858:THR:HB	1.84	0.78
1:B:546:ARG:NH2	4:B:1259:HOH:O	2.17	0.78
1:B:598:ARG:HE	1:B:600:ASP:HB3	1.48	0.77
1:A:602:ARG:HG3	1:A:604:SER:H	1.48	0.77
1:B:414:VAL:CG1	1:B:478:PHE:CZ	2.68	0.77
1:A:742:ARG:HH11	1:A:742:ARG:CG	1.88	0.76
1:A:600:ASP:CG	1:A:601:GLN:N	2.44	0.74
1:A:723:MET:HG2	1:A:842:PRO:HG3	1.70	0.74
1:B:449:CYS:SG	1:B:452:CYS:HB2	2.29	0.73
1:B:721:ILE:HD12	1:B:721:ILE:O	1.88	0.73
1:A:762:ALA:HB1	1:A:809:MET:HE1	1.69	0.73
1:B:297:ASP:OD2	1:B:584:ARG:NH2	2.20	0.72
1:A:602:ARG:CG	1:A:603:GLY:H	1.94	0.72
1:B:457:MET:SD	1:B:478:PHE:CE2	2.82	0.72
1:B:666:SER:OG	1:B:803:HIS:HE1	1.72	0.72
1:A:487:GLU:CG	1:A:607:VAL:HG12	2.19	0.72
1:B:373:ARG:HD2	4:B:1273:HOH:O	1.87	0.72
1:B:600:ASP:CG	1:B:601:GLN:N	2.48	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:VAL:CG1	1:B:478:PHE:CE2	2.74	0.71
1:B:607:VAL:HG13	1:B:608:VAL:HG13	1.72	0.71
1:A:414:VAL:CG1	1:A:478:PHE:CE1	2.71	0.70
1:A:487:GLU:OE2	1:A:575:TYR:OH	2.08	0.70
1:A:633:GLY:N	1:A:636:HIS:HD2	1.87	0.70
1:B:584:ARG:HD3	1:B:594:ASP:OD2	1.92	0.70
1:B:604:SER:OG	1:B:605:GLY:N	2.24	0.69
1:A:775:ARG:NH2	1:A:844:VAL:O	2.24	0.69
1:B:373:ARG:HD3	4:B:1273:HOH:O	1.92	0.69
1:A:298:PRO:CB	1:A:584:ARG:HH12	2.04	0.68
1:A:602:ARG:CG	1:A:603:GLY:N	2.53	0.68
1:A:607:VAL:HG13	1:A:608:VAL:HG13	1.76	0.67
1:B:721:ILE:HD11	1:B:729:ILE:CG1	2.25	0.67
1:A:292:THR:HG22	1:A:293:THR:HG23	1.75	0.67
1:B:310:SER:HB3	1:B:592:VAL:HG11	1.77	0.66
1:A:298:PRO:HB2	1:A:584:ARG:NH1	2.02	0.66
1:A:416:ALA:HA	1:A:418:GLN:NE2	2.09	0.66
1:B:313:VAL:HG23	1:B:591:THR:HG22	1.78	0.66
1:B:717:HIS:CD2	1:B:719:GLN:HE21	2.14	0.65
1:A:457:MET:HG3	1:A:478:PHE:CG	2.31	0.65
1:A:457:MET:CG	1:A:478:PHE:CD1	2.74	0.65
1:B:633:GLY:N	1:B:636:HIS:HD2	1.92	0.65
1:A:384:TRP:CH2	1:A:555:VAL:HG13	2.32	0.65
1:B:598:ARG:HG2	1:B:600:ASP:HB3	1.78	0.65
1:B:815:LEU:HD21	1:B:837:SER:HA	1.77	0.65
1:B:790:VAL:HG21	1:B:885:VAL:CG2	2.27	0.64
1:A:315:ALA:HB2	1:A:591:THR:HG21	1.80	0.63
1:A:522:ARG:HD2	4:A:1108:HOH:O	1.97	0.63
1:A:406:ASN:ND2	1:A:425:ARG:HG2	2.14	0.63
1:B:603:GLY:O	1:B:604:SER:HB3	1.99	0.63
1:B:456:MET:HB2	1:B:477:TRP:CZ3	2.33	0.63
1:A:457:MET:HG3	1:A:478:PHE:CE1	2.33	0.63
1:A:858:THR:HG22	1:A:861:ARG:H	1.62	0.63
1:B:734:ARG:NH1	2:B:1001:GTP:O2G	2.29	0.62
1:A:414:VAL:CG1	1:A:478:PHE:CZ	2.82	0.62
2:A:1001:GTP:C5'	2:A:1001:GTP:O2B	2.47	0.62
1:B:863:THR:O	1:B:867:ASN:ND2	2.31	0.61
1:A:666:SER:OG	1:A:803:HIS:HE1	1.83	0.61
1:A:474:ARG:NH1	2:A:1001:GTP:H2'	2.16	0.61
2:A:1001:GTP:O2B	2:A:1001:GTP:O1G	2.18	0.61
1:B:752:ASN:ND2	4:B:1330:HOH:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ILE:HG21	1:A:601:GLN:CG	2.31	0.61
1:A:541:ASP:HB3	1:A:603:GLY:HA2	1.83	0.61
1:A:602:ARG:CG	1:A:604:SER:H	2.13	0.61
1:A:416:ALA:HB3	1:A:478:PHE:CD2	2.35	0.60
1:B:766:MET:HG3	1:B:808:TRP:CZ2	2.36	0.60
1:B:406:ASN:CG	1:B:425:ARG:HH11	2.08	0.60
1:B:800:TRP:HB2	2:B:1001:GTP:O2B	2.02	0.59
1:B:684:HIS:HD2	4:B:1286:HOH:O	1.85	0.59
1:A:297:ASP:OD1	1:A:298:PRO:O	2.20	0.59
1:B:761:LYS:HG2	1:B:794:PRO:HG3	1.84	0.59
1:A:502:ARG:NH2	1:A:663:MET:O	2.30	0.59
1:B:414:VAL:HG11	1:B:478:PHE:CZ	2.35	0.59
1:B:666:SER:OG	1:B:803:HIS:CE1	2.55	0.59
1:A:457:MET:HE2	1:A:478:PHE:CE2	2.38	0.58
1:A:460:ARG:HB2	1:A:476:ILE:HD11	1.86	0.58
1:A:578:LYS:HZ1	1:A:602:ARG:H	1.49	0.58
1:B:466:GLU:HB2	1:B:469:LYS:CE	2.34	0.57
1:A:506:GLY:HA3	1:A:660:VAL:CG1	2.34	0.57
1:A:576:ARG:O	1:A:599:GLU:HA	2.02	0.57
1:B:717:HIS:HD2	1:B:719:GLN:HE21	1.50	0.57
1:A:297:ASP:C	1:A:298:PRO:O	2.43	0.57
1:B:522:ARG:HD2	4:B:1113:HOH:O	2.04	0.57
1:A:487:GLU:HG2	1:A:607:VAL:CG1	2.35	0.57
1:A:446:ARG:O	1:A:446:ARG:HG2	2.04	0.56
1:B:416:ALA:HB3	1:B:478:PHE:HE1	1.69	0.56
1:B:598:ARG:HE	1:B:600:ASP:CB	2.16	0.56
1:A:598:ARG:HG2	1:A:600:ASP:HB2	1.86	0.56
1:A:633:GLY:N	1:A:636:HIS:CD2	2.69	0.56
1:B:425:ARG:HH21	1:B:429:ASN:CG	2.14	0.55
1:B:384:TRP:CH2	1:B:555:VAL:HG13	2.41	0.55
1:B:312:GLU:OE2	1:B:590:LYS:HE3	2.07	0.55
1:B:602:ARG:C	1:B:604:SER:H	2.13	0.55
2:A:1001:GTP:O2B	2:A:1001:GTP:H5'	2.07	0.54
1:A:297:ASP:CG	1:A:298:PRO:O	2.51	0.54
1:B:721:ILE:HD11	1:B:729:ILE:HD11	1.89	0.54
1:A:710:GLN:NE2	4:A:1120:HOH:O	2.39	0.54
1:B:802:ILE:C	1:B:802:ILE:HD12	2.32	0.54
1:A:544:ILE:HG21	1:A:601:GLN:HG3	1.88	0.54
1:B:632:ILE:HD12	1:B:685:PHE:CZ	2.43	0.54
1:A:422:SER:OG	1:A:426:GLU:OE2	2.25	0.54
1:A:752:ASN:HB2	1:A:755:ASP:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:GLU:CG	1:A:607:VAL:CG1	2.87	0.53
1:A:617:ASN:O	1:A:621:GLN:HG2	2.09	0.53
1:A:809:MET:HE2	1:A:809:MET:CA	2.38	0.53
1:B:600:ASP:C	1:B:601:GLN:OE1	2.52	0.53
1:B:284:GLN:CG	4:B:1297:HOH:O	2.30	0.52
1:B:723:MET:HG2	1:B:842:PRO:HG3	1.91	0.52
1:A:544:ILE:HG21	1:A:601:GLN:HG2	1.92	0.51
1:B:546:ARG:NH1	1:B:550:GLU:OE2	2.44	0.51
1:A:707:ASP:HB3	1:A:710:GLN:HE21	1.74	0.51
1:B:773:HIS:H	1:B:773:HIS:CD2	2.28	0.51
1:A:578:LYS:HZ1	1:A:602:ARG:N	2.09	0.51
1:A:296:LYS:O	1:A:297:ASP:HB3	2.11	0.51
1:B:406:ASN:ND2	1:B:425:ARG:HH11	2.09	0.51
1:A:493:PHE:HD2	4:A:1270:HOH:O	1.92	0.51
1:B:315:ALA:HB2	1:B:591:THR:OG1	2.10	0.51
1:A:474:ARG:HH12	2:A:1001:GTP:H2'	1.74	0.51
1:B:602:ARG:HD2	1:B:609:THR:HG23	1.93	0.50
1:B:421:TRP:O	1:B:422:SER:CB	2.59	0.50
1:B:721:ILE:HD11	1:B:729:ILE:HG13	1.93	0.50
1:B:736:GLN:OE1	1:B:776:ASP:HB2	2.12	0.50
1:B:441:ARG:HD3	4:B:1302:HOH:O	2.12	0.50
1:B:721:ILE:HD12	1:B:721:ILE:C	2.36	0.50
1:B:868:ILE:O	1:B:872:ILE:HG13	2.12	0.49
1:A:761:LYS:HG2	1:A:794:PRO:HG3	1.93	0.49
1:B:732:PRO:O	1:B:773:HIS:CE1	2.65	0.49
1:A:414:VAL:CG1	1:A:478:PHE:CD1	2.95	0.49
1:A:633:GLY:HA3	1:A:635:GLN:NE2	2.27	0.49
1:B:633:GLY:N	1:B:636:HIS:CD2	2.69	0.49
1:A:415:PHE:O	1:A:417:GLU:N	2.44	0.49
1:A:414:VAL:HG11	1:A:478:PHE:CD1	2.46	0.49
1:B:602:ARG:C	1:B:604:SER:N	2.71	0.48
1:B:602:ARG:HH11	1:B:602:ARG:HB2	1.77	0.48
1:A:457:MET:HE2	1:A:478:PHE:CD2	2.49	0.48
1:A:603:GLY:CA	4:A:1280:HOH:O	2.42	0.48
1:B:561:GLY:O	1:B:565:MET:HG3	2.13	0.48
1:B:632:ILE:HD12	1:B:685:PHE:CE1	2.48	0.48
1:B:861:ARG:HD2	1:B:864:TRP:CZ3	2.48	0.48
1:A:634:PRO:HD2	1:A:635:GLN:NE2	2.20	0.48
1:B:721:ILE:HD13	1:B:842:PRO:CG	2.43	0.47
1:A:415:PHE:CD2	1:A:415:PHE:N	2.70	0.47
1:A:578:LYS:NZ	1:A:602:ARG:H	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:721:ILE:HD11	1:B:729:ILE:CD1	2.44	0.47
1:A:552:GLU:O	1:A:555:VAL:HG22	2.15	0.47
1:B:721:ILE:HG21	1:B:844:VAL:HG12	1.95	0.47
1:A:657:GLU:HG3	4:A:1182:HOH:O	2.14	0.47
1:A:734:ARG:NH1	2:A:1001:GTP:O3G	2.43	0.47
1:B:373:ARG:HH11	1:B:373:ARG:HB3	1.79	0.47
1:A:443:ASN:OD1	1:A:446:ARG:NH1	2.47	0.47
1:B:278:LYS:HD2	1:B:577:HIS:CD2	2.50	0.47
1:A:742:ARG:NH1	1:A:742:ARG:CG	2.57	0.47
1:B:332:LYS:HB3	1:B:333:PRO:HD3	1.97	0.47
1:B:414:VAL:CG1	1:B:478:PHE:CE1	2.98	0.47
1:B:500:LEU:HD22	1:B:614:THR:CG2	2.44	0.47
1:A:341:THR:OG1	1:B:703:HIS:CD2	2.68	0.47
1:A:487:GLU:HG2	1:A:607:VAL:HG12	1.92	0.47
1:A:789:PRO:HG2	1:A:792:TRP:CE2	2.50	0.47
1:A:832:LYS:O	1:A:834:PRO:HD3	2.15	0.47
1:B:617:ASN:O	1:B:621:GLN:HG2	2.14	0.46
1:A:666:SER:OG	1:A:803:HIS:CE1	2.68	0.46
1:B:322:LEU:HD13	1:B:322:LEU:N	2.31	0.46
1:B:604:SER:HA	1:B:609:THR:OG1	2.16	0.46
1:B:479:MET:HB2	1:B:484:ARG:CD	2.46	0.46
1:B:603:GLY:O	1:B:604:SER:CB	2.63	0.46
1:B:685:PHE:O	1:B:689:MET:HG3	2.15	0.46
1:B:425:ARG:HH21	1:B:429:ASN:CB	2.28	0.46
1:A:742:ARG:NH2	2:A:1001:GTP:O1B	2.48	0.46
1:B:598:ARG:NE	1:B:600:ASP:HB3	2.25	0.46
1:A:519:TYR:HB3	1:A:828:TRP:CE2	2.51	0.46
1:B:416:ALA:HB3	1:B:478:PHE:CE1	2.50	0.46
1:B:456:MET:HE3	1:B:456:MET:O	2.15	0.46
1:A:874:GLN:O	1:A:878:VAL:HG23	2.16	0.46
1:B:789:PRO:HG2	1:B:792:TRP:CE2	2.50	0.46
1:A:307:TYR:HA	1:A:596:ILE:HG22	1.98	0.45
1:A:506:GLY:HA3	1:A:660:VAL:HG13	1.99	0.45
1:B:456:MET:CB	1:B:477:TRP:CZ3	2.99	0.45
1:B:460:ARG:NH2	1:B:463:LYS:HD2	2.31	0.45
1:B:752:ASN:OD1	1:B:752:ASN:N	2.49	0.45
1:A:316:THR:HG23	1:A:583:MET:HE1	1.98	0.45
1:A:601:GLN:HE21	1:A:602:ARG:CZ	2.30	0.45
1:B:721:ILE:CD1	1:B:729:ILE:CG1	2.92	0.45
1:B:353:GLN:HA	1:B:456:MET:HE1	1.99	0.45
1:A:446:ARG:O	1:A:446:ARG:CG	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:LYS:NZ	2:A:1001:GTP:O3B	2.50	0.45
1:A:601:GLN:HE21	1:A:602:ARG:NH2	2.15	0.45
1:A:406:ASN:HD22	1:A:425:ARG:HG2	1.79	0.45
1:A:694:LYS:HB2	1:A:694:LYS:HE3	1.78	0.45
1:B:639:GLN:O	1:B:641:PRO:HD3	2.17	0.45
1:A:349:THR:O	1:A:353:GLN:HG3	2.17	0.45
1:A:689:MET:O	1:A:690:SER:HB2	2.16	0.45
1:B:419:ASN:O	1:B:420:GLN:HB3	2.17	0.45
1:A:602:ARG:HD3	1:A:609:THR:HG23	1.99	0.44
1:B:430:ASP:HA	1:B:431:PRO:HD2	1.80	0.44
1:A:773:HIS:CD2	1:A:773:HIS:H	2.36	0.44
1:A:304:THR:O	1:A:598:ARG:HD2	2.16	0.44
1:A:430:ASP:HA	1:A:431:PRO:HD2	1.92	0.44
1:A:578:LYS:NZ	1:A:602:ARG:N	2.66	0.44
1:B:441:ARG:NE	4:B:1302:HOH:O	2.51	0.44
1:A:479:MET:HB2	1:A:484:ARG:CD	2.48	0.44
1:A:546:ARG:O	1:A:550:GLU:HG3	2.18	0.44
1:A:512:SER:O	1:A:803:HIS:HD2	2.00	0.44
1:B:297:ASP:OD1	1:B:298:PRO:HD2	2.17	0.44
1:B:636:HIS:HE1	4:B:1307:HOH:O	2.00	0.44
1:A:556:LEU:HD23	1:A:556:LEU:HA	1.88	0.44
1:B:635:GLN:HG2	1:B:636:HIS:CE1	2.52	0.44
1:B:805:LYS:HB2	4:B:1265:HOH:O	2.17	0.44
1:A:322:LEU:HD12	1:A:322:LEU:O	2.17	0.44
1:A:823:ILE:HA	1:A:829:MET:HG2	2.00	0.43
1:A:528:GLN:O	1:A:662:ARG:NH2	2.35	0.43
1:A:298:PRO:O	1:A:300:HIS:N	2.51	0.43
1:A:418:GLN:HG2	1:A:481:LEU:HD22	2.00	0.43
1:A:734:ARG:HH21	1:A:738:GLU:CD	2.25	0.43
1:A:278:LYS:HD2	1:A:577:HIS:CD2	2.53	0.43
1:B:493:PHE:HD2	4:B:1127:HOH:O	2.02	0.43
1:A:403:LYS:O	1:A:407:SER:OG	2.37	0.43
1:A:584:ARG:HA	1:A:585:PRO:HD3	1.91	0.43
1:A:469:LYS:HE2	1:A:712:PRO:HB2	2.01	0.43
1:B:275:ASN:C	1:B:277:GLU:N	2.76	0.42
1:B:789:PRO:HD2	1:B:792:TRP:CE3	2.54	0.42
1:A:292:THR:HG22	1:A:293:THR:N	2.34	0.42
1:B:313:VAL:CG2	1:B:591:THR:HG22	2.47	0.42
1:A:773:HIS:HA	1:A:843:TYR:HA	2.01	0.42
1:A:869:TYR:OH	1:A:888:MET:HB2	2.19	0.42
1:A:353:GLN:HA	1:A:456:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:TRP:N	2:A:1001:GTP:O1B	2.38	0.42
1:B:746:SER:HA	1:B:747:PRO:HD3	1.91	0.42
1:A:656:GLY:O	1:A:660:VAL:HB	2.20	0.42
1:B:339:ASN:HD22	1:B:339:ASN:HA	1.67	0.42
1:B:541:ASP:HB3	1:B:603:GLY:HA2	2.02	0.42
1:A:479:MET:HB2	1:A:484:ARG:NE	2.35	0.42
1:A:832:LYS:NZ	4:A:1142:HOH:O	2.53	0.42
1:A:437:VAL:HG11	1:A:485:TYR:CD2	2.54	0.42
1:A:772:PHE:O	1:A:778:ARG:HD3	2.20	0.42
1:B:721:ILE:CD1	1:B:729:ILE:HG13	2.50	0.42
1:B:414:VAL:HG13	1:B:478:PHE:CZ	2.52	0.41
1:A:786:SER:HA	1:A:885:VAL:O	2.20	0.41
1:A:789:PRO:HG2	1:A:792:TRP:CZ2	2.55	0.41
1:A:442:GLU:HG3	4:A:1248:HOH:O	2.20	0.41
1:A:601:GLN:NE2	1:A:602:ARG:CZ	2.84	0.41
1:B:297:ASP:OD1	1:B:297:ASP:C	2.62	0.41
1:B:415:PHE:O	1:B:417:GLU:N	2.52	0.41
1:A:297:ASP:O	1:A:298:PRO:C	2.53	0.41
1:B:322:LEU:HB2	1:B:746:SER:O	2.20	0.41
1:B:485:TYR:CD2	1:B:485:TYR:C	2.98	0.41
1:B:601:GLN:HG2	1:B:601:GLN:O	2.21	0.41
1:B:723:MET:SD	1:B:835:ILE:HD11	2.60	0.41
1:B:766:MET:HG3	1:B:808:TRP:CD2	2.55	0.41
1:A:477:TRP:HB2	1:A:605:GLY:HA3	2.03	0.41
1:A:457:MET:CG	1:A:478:PHE:CG	3.02	0.40
1:A:350:PRO:HG2	1:A:591:THR:HG21	2.04	0.40
1:B:666:SER:O	1:B:669:ASP:HB2	2.21	0.40
1:B:833:THR:HA	1:B:834:PRO:HD3	1.93	0.40
1:B:409:ALA:HB1	1:B:410:ALA:H	1.51	0.40
1:B:602:ARG:HB2	1:B:602:ARG:NH1	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	608/639 (95%)	572 (94%)	28 (5%)	8 (1%)	9	12
1	B	608/639 (95%)	570 (94%)	28 (5%)	10 (2%)	7	9
All	All	1216/1278 (95%)	1142 (94%)	56 (5%)	18 (2%)	8	10

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	ASP
1	A	416	ALA
1	B	409	ALA
1	B	416	ALA
1	B	420	GLN
1	B	752	ASN
1	A	299	GLU
1	A	587	ALA
1	A	604	SER
1	A	752	ASN
1	B	422	SER
1	B	604	SER
1	B	408	ASN
1	A	602	ARG
1	A	413	ALA
1	B	601	GLN
1	B	413	ALA
1	B	603	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	516/544 (95%)	490 (95%)	26 (5%)	22	35
1	B	514/544 (94%)	489 (95%)	25 (5%)	22	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1030/1088 (95%)	979 (95%)	51 (5%)	22	35

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	LYS
1	A	286	LEU
1	A	292	THR
1	A	299	GLU
1	A	348	THR
1	A	363	THR
1	A	364	LYS
1	A	407	SER
1	A	415	PHE
1	A	418	GLN
1	A	459	LYS
1	A	466	GLU
1	A	521	LEU
1	A	522	ARG
1	A	555	VAL
1	A	635	GLN
1	A	660	VAL
1	A	724	LYS
1	A	742	ARG
1	A	778	ARG
1	A	811	THR
1	A	839	THR
1	A	847	ARG
1	A	858	THR
1	A	861	ARG
1	A	863	THR
1	B	292	THR
1	B	322	LEU
1	B	340	VAL
1	B	414	VAL
1	B	415	PHE
1	B	420	GLN
1	B	457	MET
1	B	469	LYS
1	B	514	VAL
1	B	522	ARG
1	B	555	VAL

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Mol	Chain	Res	Type
1	B	558	LEU
1	B	591	THR
1	B	602	ARG
1	B	659	ARG
1	B	669	ASP
1	B	724	LYS
1	B	752	ASN
1	B	753	VAL
1	B	778	ARG
1	B	811	THR
1	B	835	ILE
1	B	847	ARG
1	B	861	ARG
1	B	867	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	406	ASN
1	A	408	ASN
1	A	419	ASN
1	A	450	HIS
1	A	528	GLN
1	A	551	ASN
1	A	621	GLN
1	A	635	GLN
1	A	636	HIS
1	A	687	ASN
1	A	703	HIS
1	A	706	HIS
1	A	710	GLN
1	A	717	HIS
1	A	803	HIS
1	B	339	ASN
1	B	354	GLN
1	B	495	ASN
1	B	528	GLN
1	B	551	ASN
1	B	563	HIS
1	B	621	GLN
1	B	636	HIS
1	B	684	HIS

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Mol	Chain	Res	Type
1	B	687	ASN
1	B	703	HIS
1	B	717	HIS
1	B	719	GLN
1	B	773	HIS
1	B	803	HIS
1	B	867	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
2	GTP	B	1001	-	33,34,34	1.71	7 (21%)	50,54,54	1.80	10 (20%)
2	GTP	A	1001	-	33,34,34	2.02	9 (27%)	50,54,54	1.62	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GTP	B	1001	-	-	6/22/38/38	0/3/3/3
2	GTP	A	1001	-	-	9/22/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	GTP	PB-O3B	-7.28	1.51	1.59
2	B	1001	GTP	PB-O3A	5.14	1.65	1.59
2	A	1001	GTP	O4'-C1'	3.81	1.50	1.42
2	A	1001	GTP	PB-O3A	3.53	1.63	1.59
2	B	1001	GTP	PG-O3G	2.87	1.65	1.54
2	A	1001	GTP	PG-O3G	2.72	1.64	1.54
2	B	1001	GTP	O4'-C1'	2.71	1.48	1.42
2	B	1001	GTP	C1'-N9	2.66	1.55	1.47
2	A	1001	GTP	C5-N7	-2.41	1.34	1.39
2	B	1001	GTP	C5-N7	-2.35	1.34	1.39
2	B	1001	GTP	PA-O5'	2.26	1.68	1.59
2	B	1001	GTP	C5'-C4'	2.26	1.58	1.51
2	A	1001	GTP	PA-O3A	2.19	1.61	1.59
2	A	1001	GTP	PG-O2G	2.18	1.62	1.54
2	A	1001	GTP	C1'-N9	2.07	1.53	1.47
2	A	1001	GTP	O2'-C2'	2.01	1.47	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	GTP	C2-N3-C4	5.48	121.73	112.30
2	B	1001	GTP	C2-N3-C4	5.38	121.57	112.30
2	B	1001	GTP	C5-C4-N3	-4.77	120.80	128.39
2	A	1001	GTP	C5-C4-N3	-4.30	121.54	128.39
2	B	1001	GTP	N9-C4-N3	3.54	133.04	125.95
2	A	1001	GTP	N9-C4-N3	3.38	132.72	125.95
2	B	1001	GTP	C2-N1-C6	-3.21	119.28	125.11
2	B	1001	GTP	O3A-PA-O1A	-3.20	101.07	110.70
2	B	1001	GTP	O3A-PB-O1B	-2.90	101.97	110.70
2	B	1001	GTP	C5-C6-N1	2.85	120.51	113.25
2	A	1001	GTP	N1-C2-N3	-2.78	118.24	123.32
2	B	1001	GTP	O6-C6-C5	-2.68	119.47	126.53
2	A	1001	GTP	O6-C6-C5	-2.64	119.55	126.53
2	B	1001	GTP	O2A-PA-O3A	2.37	113.69	107.27
2	A	1001	GTP	C5-C6-N1	2.32	119.16	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	GTP	O3A-PA-O1A	-2.26	103.89	110.70
2	A	1001	GTP	C2-N1-C6	-2.23	121.07	125.11
2	B	1001	GTP	N1-C2-N3	-2.12	119.44	123.32
2	A	1001	GTP	O4'-C1'-N9	2.01	112.91	108.36

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	GTP	C5'-O5'-PA-O3A
2	A	1001	GTP	C5'-O5'-PA-O1A
2	A	1001	GTP	C5'-O5'-PA-O2A
2	B	1001	GTP	C5'-O5'-PA-O3A
2	B	1001	GTP	C4'-C5'-O5'-PA
2	A	1001	GTP	C4'-C5'-O5'-PA
2	B	1001	GTP	PB-O3A-PA-O1A
2	A	1001	GTP	PB-O3A-PA-O5'
2	B	1001	GTP	PB-O3A-PA-O5'
2	A	1001	GTP	C3'-C4'-C5'-O5'
2	A	1001	GTP	PA-O3A-PB-O2B
2	B	1001	GTP	C5'-O5'-PA-O1A
2	B	1001	GTP	PG-O3B-PB-O2B
2	A	1001	GTP	O4'-C4'-C5'-O5'
2	A	1001	GTP	PA-O3A-PB-O1B

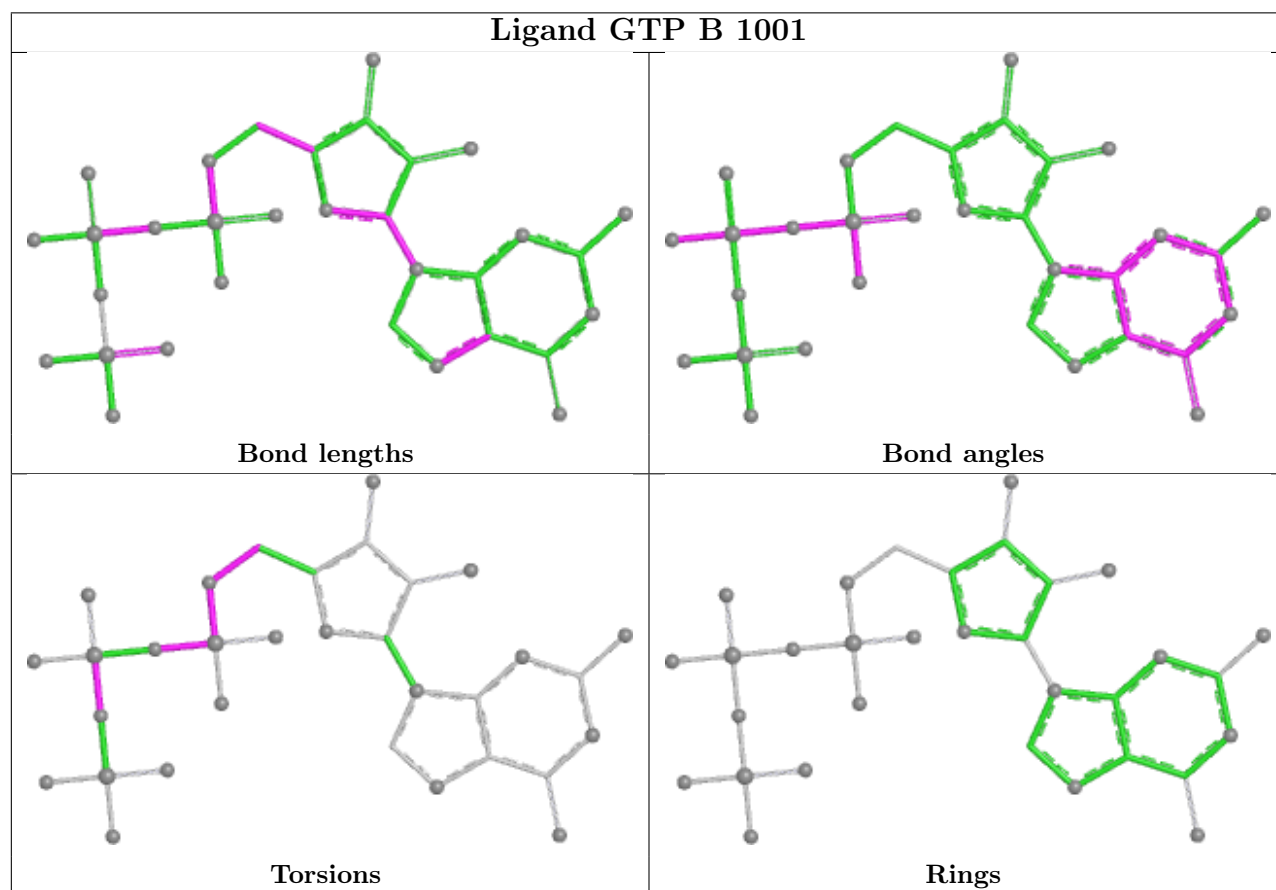
There are no ring outliers.

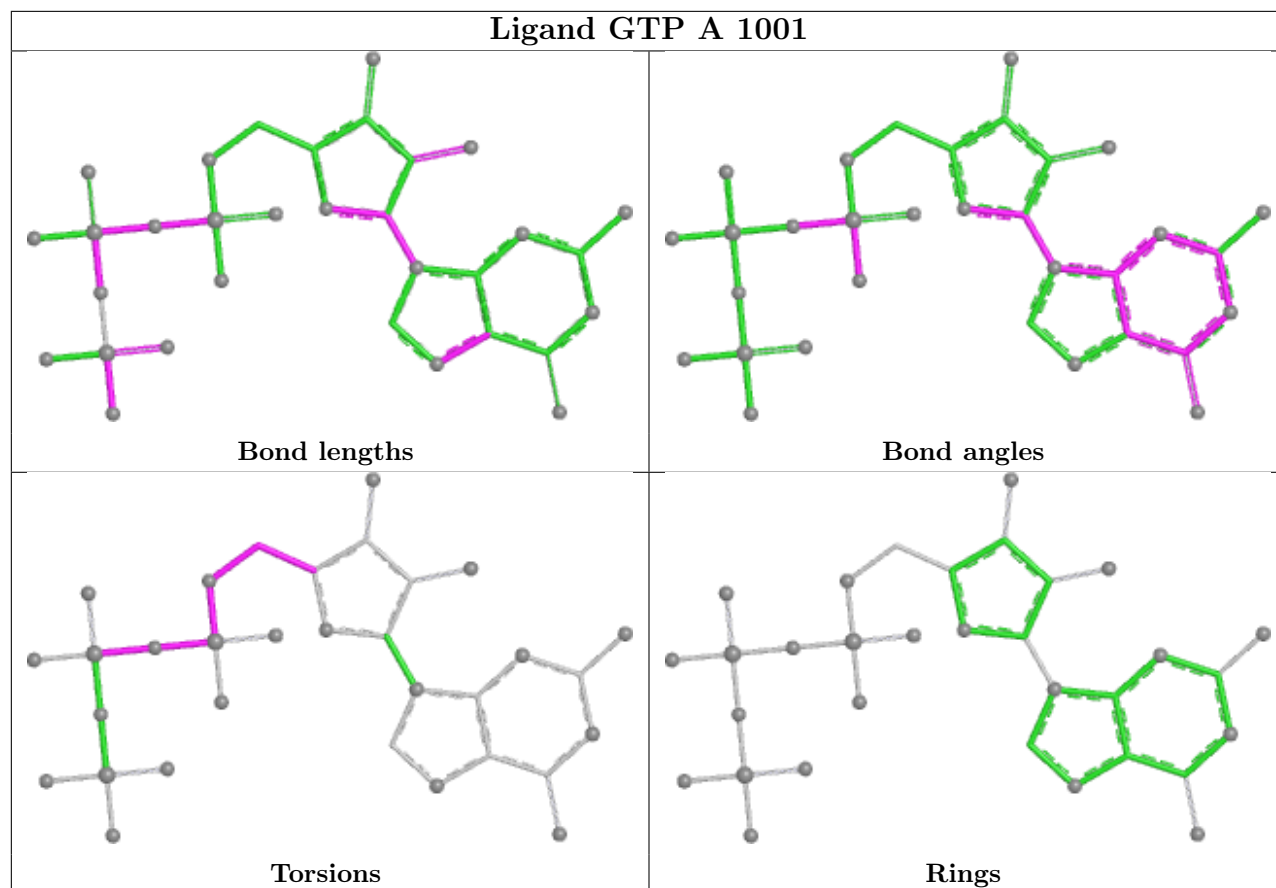
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	GTP	2	0
2	A	1001	GTP	9	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.





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	A	612/639 (95%)	-0.03	22 (3%) 46 46	15, 33, 60, 81	0
1	B	612/639 (95%)	-0.06	21 (3%) 48 48	16, 33, 57, 76	0
All	All	1224/1278 (95%)	-0.04	43 (3%) 47 47	15, 33, 58, 81	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	415	PHE	5.9
1	A	412	GLY	5.8
1	B	411	LEU	5.4
1	A	416	ALA	5.1
1	B	410	ALA	5.0
1	B	416	ALA	4.7
1	B	414	VAL	4.5
1	A	411	LEU	4.4
1	A	889	THR	4.4
1	B	413	ALA	4.4
1	A	413	ALA	4.3
1	B	751	TRP	4.3
1	A	410	ALA	4.2
1	B	415	PHE	4.2
1	A	414	VAL	3.7
1	A	751	TRP	3.3
1	A	275	ASN	3.0
1	B	408	ASN	3.0
1	B	603	GLY	3.0
1	B	412	GLY	3.0
1	A	317	GLY	2.6
1	A	603	GLY	2.6
1	B	750	GLY	2.6
1	A	478	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	889	THR	2.6
1	B	409	ALA	2.6
1	A	750	GLY	2.6
1	A	602	ARG	2.5
1	A	749	ALA	2.5
1	A	409	ALA	2.4
1	B	322	LEU	2.4
1	A	274	SER	2.3
1	B	422	SER	2.3
1	B	420	GLN	2.2
1	A	748	GLY	2.2
1	A	587	ALA	2.2
1	B	425	ARG	2.1
1	B	465	GLY	2.1
1	B	292	THR	2.1
1	B	467	PHE	2.1
1	A	419	ASN	2.1
1	B	317	GLY	2.0
1	A	315	ALA	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.

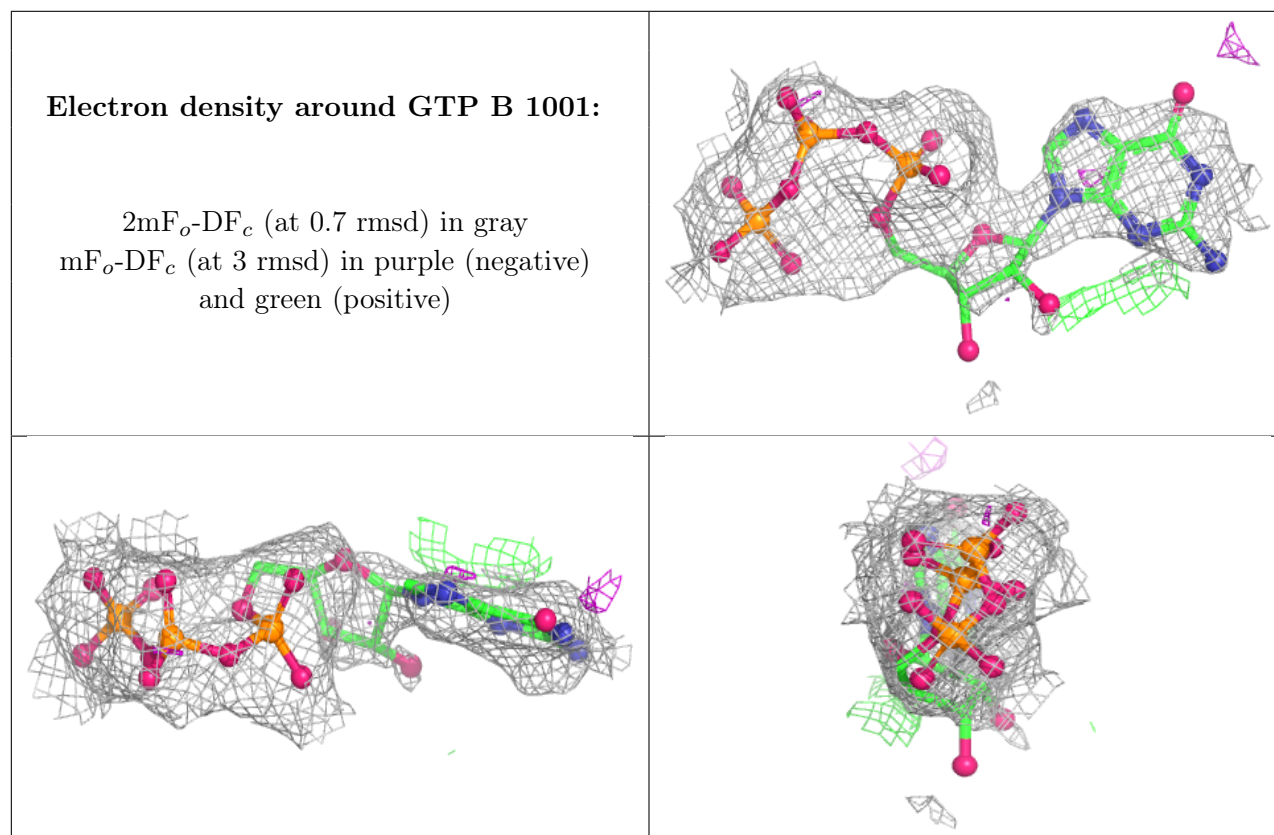
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GTP	B	1001	32/32	0.84	0.14	52,71,78,78	0
2	GTP	A	1001	32/32	0.86	0.14	44,72,78,80	0
3	ZN	A	1003	1/1	0.99	0.03	36,36,36,36	1
3	ZN	B	1002	1/1	0.99	0.02	31,31,31,31	0

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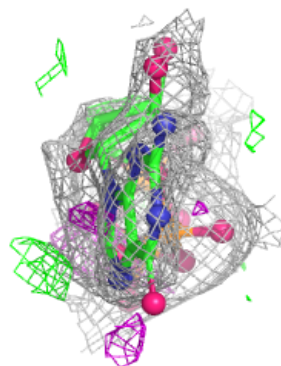
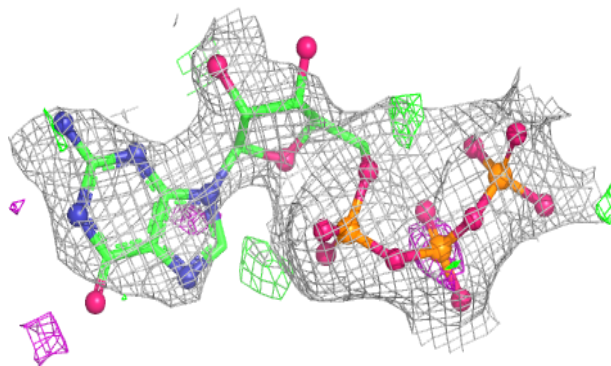
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	B	1003	1/1	0.99	0.03	37,37,37,37	1
3	ZN	A	1002	1/1	1.00	0.02	33,33,33,33	0

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 A 1001:

$2mF_o-DF_c$ (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.