WORLDWIDE
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:32 pm GMT

PDB ID	:	2JH9
Title	:	The structure of bluetongue virus VP4 reveals a multifunctional RNA- capping production-line
Authors	:	Sutton, G.; Grimes, J.M.; Stuart, D.I.; Roy, P.
Deposited on	:	2007-02-21
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949
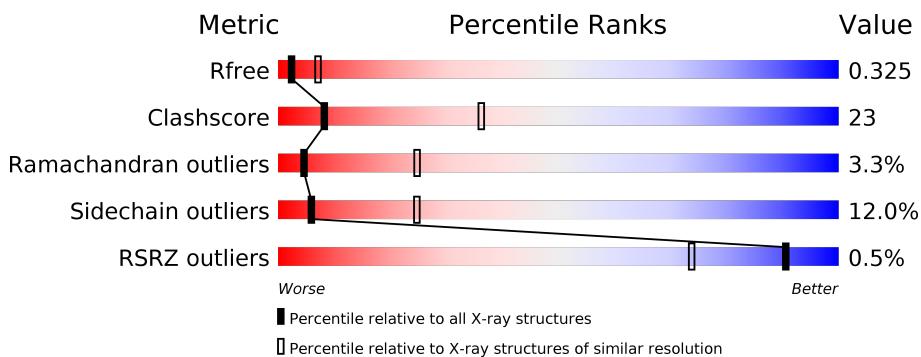
1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
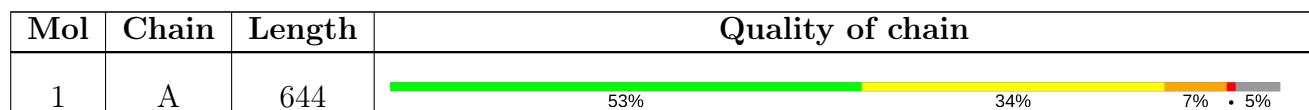
The reported resolution of this entry is 3.00 Å.

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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	644	53% 34% 7% · 5%

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
3	GUN	A	1646	-	-	-	X
3	GUN	A	1647	-	-	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 5094 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.
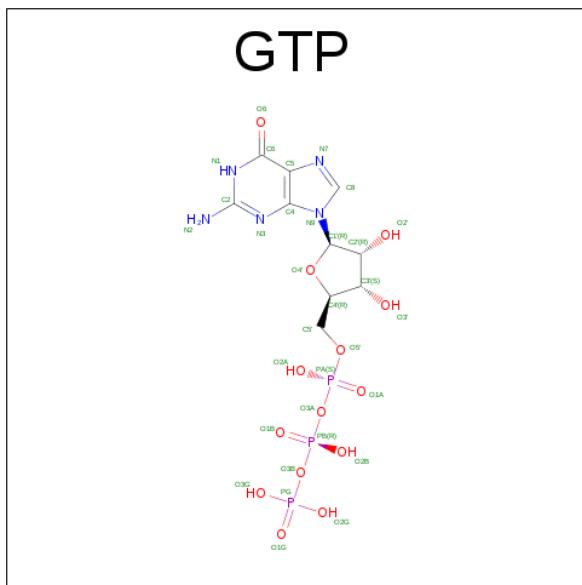
- Molecule 1 is a protein called VP4 CORE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total 5040	C 3219	N 892	O 901	S 28	0	0	0

There is a discrepancy between the modelled and reference sequences:
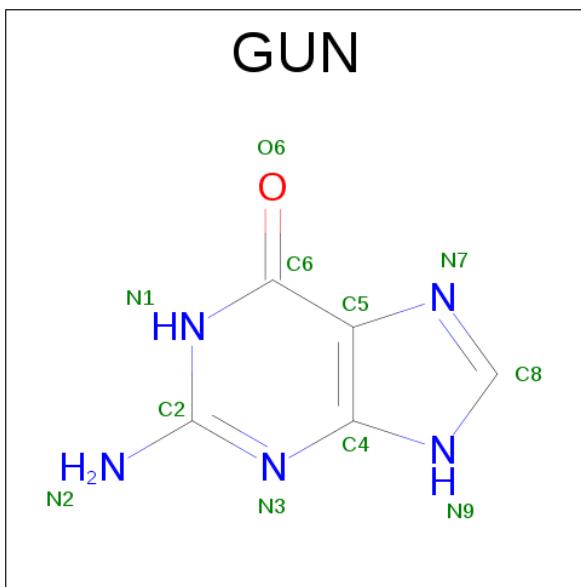
Chain	Residue	Modelled	Actual	Comment	Reference
A	261	LEU	PRO	CONFLICT	UNP P07132

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: 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

- Molecule 3 is GUANINE (three-letter code: GUN) (formula: $C_5H_5N_5O$).

GUN

O6
O

C6   N7
N1   C5   N
HN   C8

C2   C4
H₂N   N   N
N2   N3   N9
                                H
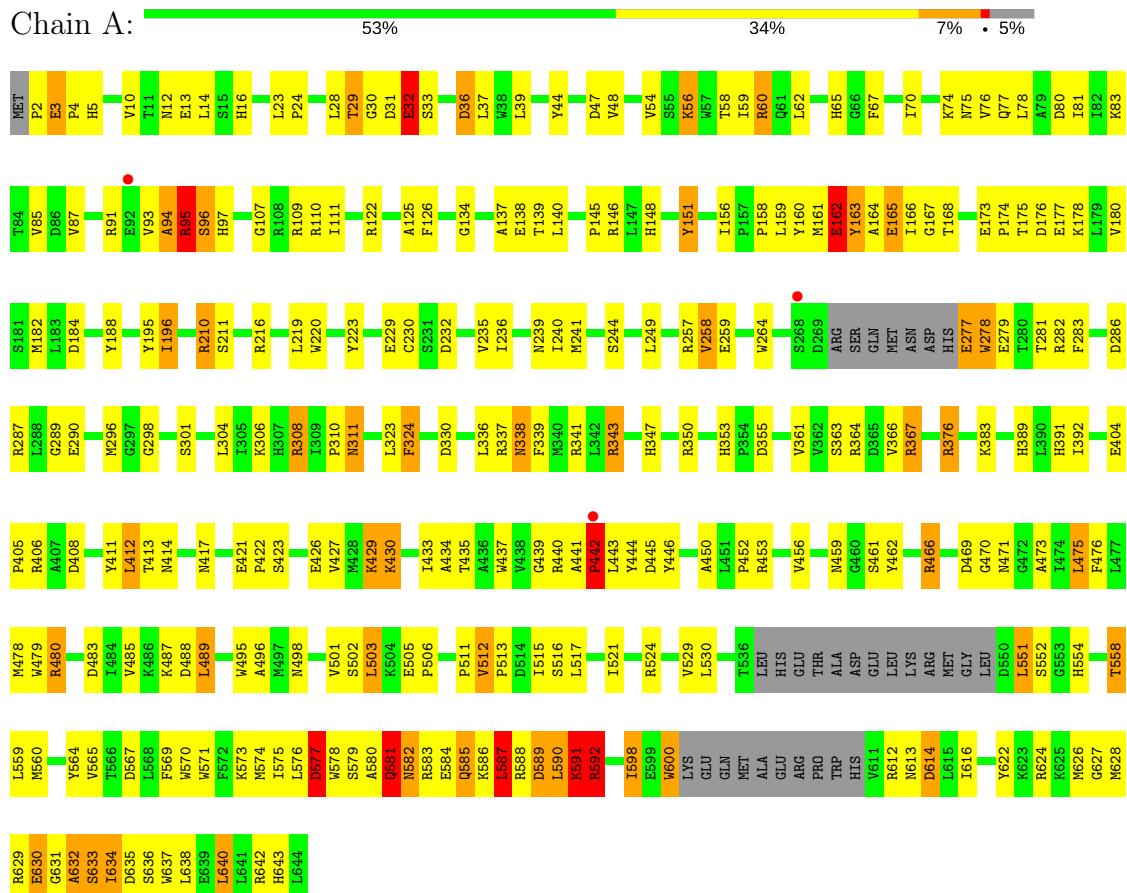
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 11	C 5	N 5	O 1	0	0
3	A	1	Total 11	C 5	N 5	O 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: VP4 CORE PROTEIN

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	75.54Å　75.54Å　423.42Å 90.00°　90.00°　120.00°	Depositor
Resolution (Å)	25.00　–　3.00 24.93　–　3.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (25.00-3.00) 96.8 (24.93-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.99Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.248　,　0.330 0.239　,　0.325	Depositor DCC
R_{free} test set	716 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	74.6	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 46.2	EDS
L-test for twinning[2]	$< |L| > = 0.41, < L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5094	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.96	24/5167 (0.5%)	0.86	12/6981 (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	4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	GLU	CD-OE2	20.32	1.48	1.25
1	A	592	ARG	NE-CZ	17.37	1.55	1.33
1	A	279	GLU	CD-OE2	16.74	1.44	1.25
1	A	584	GLU	CD-OE2	14.61	1.41	1.25
1	A	229	GLU	CD-OE2	14.23	1.41	1.25
1	A	56	LYS	CE-NZ	11.49	1.77	1.49
1	A	581	GLN	CD-OE1	10.23	1.46	1.24
1	A	162	GLU	CD-OE1	9.97	1.36	1.25
1	A	584	GLU	CD-OE1	8.31	1.34	1.25
1	A	429	LYS	CD-CE	7.68	1.70	1.51
1	A	229	GLU	CD-OE1	7.48	1.33	1.25
1	A	429	LYS	CE-NZ	7.38	1.67	1.49
1	A	277	GLU	C-O	7.25	1.37	1.23
1	A	480	ARG	CZ-NH1	7.14	1.42	1.33
1	A	279	GLU	CD-OE1	6.86	1.33	1.25
1	A	60	ARG	CZ-NH1	6.79	1.41	1.33
1	A	277	GLU	CD-OE2	6.33	1.32	1.25
1	A	592	ARG	CZ-NH1	-6.10	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	GLU	CB-CG	6.04	1.63	1.52
1	A	577	ASP	CG-OD1	5.90	1.39	1.25
1	A	279	GLU	CG-CD	5.70	1.60	1.51
1	A	239	ASN	CG-ND2	5.59	1.46	1.32
1	A	589	ASP	CG-OD2	5.56	1.38	1.25
1	A	589	ASP	CG-OD1	5.21	1.37	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	592	ARG	NE-CZ-NH1	-17.39	111.61	120.30
1	A	592	ARG	NH1-CZ-NH2	10.14	130.56	119.40
1	A	480	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	A	60	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	577	ASP	CB-CG-OD1	-6.75	112.22	118.30
1	A	589	ASP	CB-CG-OD1	-6.51	112.44	118.30
1	A	592	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	429	LYS	CD-CE-NZ	-5.68	98.63	111.70
1	A	442	PRO	N-CA-C	5.48	126.36	112.10
1	A	591	LYS	N-CA-C	5.22	125.11	111.00
1	A	32	GLU	N-CA-C	5.12	124.81	111.00
1	A	39	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	442	PRO	Peptide
1	A	483	ASP	Peptide
1	A	587	LEU	Peptide
1	A	591	LYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5040	0	4985	235	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	32	0	12	1	0
3	A	22	0	10	5	0
All	All	5094	0	5007	236	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 23.

All (236) 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:429:LYS:CE	1:A:429:LYS:NZ	1.67	1.52
1:A:56:LYS:NZ	1:A:56:LYS:CE	1.77	1.47
1:A:632:ALA:CB	1:A:633:SER:HB2	1.49	1.39
1:A:580:ALA:HB1	1:A:581:GLN:O	1.27	1.32
1:A:632:ALA:HB3	1:A:633:SER:CB	1.61	1.29
1:A:630:GLU:HB3	1:A:631:GLY:CA	1.74	1.17
1:A:630:GLU:CB	1:A:631:GLY:HA2	1.72	1.16
1:A:2:PRO:HG3	1:A:453:ARG:NH1	1.68	1.09
1:A:441:ALA:HB1	1:A:442:PRO:HD3	1.20	1.08
1:A:631:GLY:O	1:A:633:SER:HB3	1.54	1.08
1:A:2:PRO:HG3	1:A:453:ARG:HH12	0.88	1.03
1:A:94:ALA:HB3	1:A:95:ARG:CB	1.93	0.99
1:A:2:PRO:CG	1:A:453:ARG:HH12	1.76	0.97
1:A:28:LEU:HA	1:A:29:THR:HG22	1.48	0.94
1:A:552:SER:HB3	1:A:614:ASP:HB3	1.49	0.93
1:A:495:TRP:HE1	3:A:1647:GUN:HN21	0.94	0.93
1:A:3:GLU:H	1:A:4:PRO:CD	1.83	0.92
1:A:94:ALA:HB3	1:A:95:ARG:HG3	1.52	0.91
1:A:95:ARG:N	1:A:96:SER:HB2	1.85	0.90
1:A:634:ILE:HG22	1:A:635:ASP:H	1.35	0.90
1:A:582:ASN:O	1:A:586:LYS:HG2	1.73	0.89
1:A:94:ALA:HB3	1:A:95:ARG:CG	2.03	0.88
1:A:587:LEU:H	1:A:588:ARG:HB2	1.41	0.86
1:A:282:ARG:HD2	1:A:308:ARG:HG3	1.58	0.84
1:A:3:GLU:H	1:A:4:PRO:HD2	1.42	0.84
1:A:95:ARG:H	1:A:96:SER:CB	1.90	0.84
1:A:441:ALA:CB	1:A:442:PRO:HD3	2.06	0.83
1:A:437:TRP:HZ2	1:A:443:LEU:HD13	1.43	0.83
1:A:633:SER:H	1:A:635:ASP:N	1.76	0.82
1:A:122:ARG:HG2	1:A:126:PHE:CE1	2.14	0.81
1:A:95:ARG:H	1:A:96:SER:HB2	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ALA:HB1	1:A:442:PRO:CD	2.07	0.79
1:A:122:ARG:HG2	1:A:126:PHE:HE1	1.47	0.78
1:A:631:GLY:O	1:A:633:SER:CB	2.32	0.76
1:A:210:ARG:HG3	1:A:210:ARG:HH11	1.50	0.76
1:A:94:ALA:HB3	1:A:95:ARG:HB2	1.66	0.76
1:A:2:PRO:HD3	1:A:439:GLY:HA2	1.67	0.76
1:A:176:ASP:HB3	1:A:180:VAL:CG2	2.15	0.76
1:A:600:TRP:CE3	1:A:600:TRP:HA	2.21	0.75
1:A:634:ILE:HG22	1:A:635:ASP:N	1.99	0.75
1:A:28:LEU:HA	1:A:29:THR:CG2	2.17	0.74
1:A:323:LEU:HD23	1:A:338:ASN:HA	1.71	0.73
1:A:600:TRP:HE3	1:A:600:TRP:HA	1.53	0.73
1:A:630:GLU:HB3	1:A:631:GLY:HA2	0.82	0.72
1:A:95:ARG:H	1:A:96:SER:CA	2.03	0.72
1:A:338:ASN:HD22	1:A:339:PHE:N	1.88	0.71
1:A:5:HIS:CE1	1:A:44:TYR:O	2.44	0.71
1:A:95:ARG:N	1:A:97:HIS:H	1.89	0.70
1:A:429:LYS:CD	1:A:429:LYS:NZ	2.56	0.69
1:A:632:ALA:CA	1:A:633:SER:HB2	2.21	0.69
1:A:44:TYR:CG	1:A:48:VAL:HG11	2.28	0.69
1:A:587:LEU:N	1:A:588:ARG:HB2	2.08	0.68
1:A:210:ARG:CG	1:A:210:ARG:HH11	2.06	0.67
1:A:210:ARG:HG3	1:A:210:ARG:NH1	2.06	0.67
1:A:580:ALA:CB	1:A:581:GLN:O	2.24	0.66
1:A:140:LEU:HD21	1:A:392:ILE:HG12	1.78	0.65
1:A:589:ASP:HB3	1:A:592:ARG:NH1	2.12	0.65
1:A:517:LEU:HD13	1:A:570:TRP:CE3	2.31	0.65
1:A:95:ARG:H	1:A:97:HIS:H	1.45	0.65
1:A:75:ASN:HA	1:A:85:VAL:HG23	1.79	0.64
1:A:629:ARG:O	1:A:630:GLU:HB2	1.98	0.64
1:A:633:SER:H	1:A:635:ASP:H	1.42	0.63
1:A:286:ASP:O	1:A:290:GLU:HG3	1.99	0.63
1:A:554:HIS:O	1:A:558:THR:HG23	1.98	0.63
1:A:28:LEU:CA	1:A:29:THR:HG22	2.26	0.62
1:A:580:ALA:HB1	1:A:581:GLN:C	2.18	0.62
1:A:156:ILE:HG12	1:A:389:HIS:CD2	2.35	0.62
1:A:634:ILE:CG2	1:A:635:ASP:N	2.62	0.61
1:A:75:ASN:HB2	1:A:83:LYS:O	2.00	0.61
1:A:257:ARG:O	1:A:258:VAL:HG13	2.01	0.61
1:A:16:HIS:HE2	1:A:97:HIS:CD2	2.18	0.60
1:A:574:MET:O	1:A:578:TRP:HB3	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:TRP:CZ2	1:A:443:LEU:HD13	2.32	0.60
1:A:441:ALA:O	1:A:443:LEU:HB2	2.02	0.60
1:A:470:GLY:HA3	1:A:496:ALA:O	2.02	0.60
1:A:578:TRP:O	1:A:581:GLN:HB2	2.02	0.60
1:A:311:ASN:ND2	1:A:311:ASN:H	2.01	0.59
1:A:632:ALA:CB	1:A:633:SER:CB	2.46	0.58
1:A:95:ARG:H	1:A:97:HIS:N	2.01	0.58
1:A:426:GLU:O	1:A:430:LYS:HE3	2.05	0.57
1:A:184:ASP:C	3:A:1646:GUN:HN21	2.08	0.57
1:A:364:ARG:HB3	1:A:364:ARG:NH1	2.19	0.57
1:A:173:GLU:HB3	1:A:174:PRO:HD2	1.84	0.57
1:A:632:ALA:HB3	1:A:633:SER:HB2	0.67	0.56
1:A:94:ALA:HB3	1:A:95:ARG:CA	2.35	0.56
1:A:24:PRO:HB2	1:A:48:VAL:HG12	1.87	0.56
1:A:435:THR:HG22	1:A:501:VAL:HG22	1.87	0.56
1:A:591:LYS:N	1:A:592:ARG:HB3	2.20	0.55
1:A:441:ALA:CB	1:A:442:PRO:CD	2.78	0.55
1:A:591:LYS:H	1:A:592:ARG:HB3	1.72	0.55
1:A:94:ALA:CB	1:A:95:ARG:HG3	2.32	0.54
1:A:512:VAL:HG23	1:A:513:PRO:HD2	1.90	0.54
1:A:452:PRO:O	1:A:456:VAL:HG23	2.07	0.54
1:A:3:GLU:N	1:A:4:PRO:CD	2.58	0.54
1:A:433:ILE:HA	1:A:502:SER:O	2.07	0.54
1:A:530:LEU:HD21	1:A:560:MET:HB3	1.90	0.54
1:A:62:LEU:O	1:A:67:PHE:HB2	2.07	0.54
1:A:587:LEU:HD23	1:A:600:TRP:HZ2	1.72	0.53
1:A:176:ASP:HB3	1:A:180:VAL:HG23	1.90	0.53
1:A:230:CYS:SG	1:A:232:ASP:HB2	2.48	0.53
1:A:408:ASP:HB2	1:A:434:ALA:HB2	1.90	0.53
1:A:158:PRO:O	1:A:159:LEU:HD23	2.09	0.53
1:A:515:ILE:HD11	1:A:598:ILE:HG12	1.91	0.52
1:A:2:PRO:CG	1:A:453:ARG:NH1	2.52	0.52
1:A:470:GLY:O	1:A:473:ALA:HB3	2.09	0.52
1:A:58:THR:HB	1:A:80:ASP:OD2	2.09	0.52
1:A:259:GLU:HG3	1:A:301:SER:HB3	1.92	0.51
1:A:5:HIS:HB2	1:A:47:ASP:HA	1.92	0.51
1:A:423:SER:O	1:A:427:VAL:HG23	2.11	0.51
1:A:56:LYS:CD	1:A:56:LYS:NZ	2.69	0.50
1:A:138:GLU:HG2	1:A:139:THR:N	2.26	0.50
1:A:629:ARG:O	1:A:630:GLU:CB	2.59	0.50
1:A:87:VAL:HG22	1:A:109:ARG:CG	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:HD12	1:A:338:ASN:O	2.12	0.50
1:A:406:ARG:NH2	1:A:408:ASP:OD1	2.44	0.49
1:A:249:LEU:HD22	1:A:296:MET:CE	2.42	0.49
1:A:2:PRO:HD3	1:A:440:ARG:H	1.77	0.49
1:A:632:ALA:O	1:A:635:ASP:HB2	2.11	0.49
1:A:126:PHE:HD2	1:A:148:HIS:CE1	2.31	0.49
1:A:32:GLU:HG2	1:A:37:LEU:HD23	1.95	0.49
1:A:10:VAL:HA	1:A:70:ILE:O	2.12	0.49
1:A:94:ALA:CB	1:A:95:ARG:HB2	2.39	0.49
1:A:383:LYS:HG2	3:A:1646:GUN:HN22	1.77	0.49
1:A:350:ARG:NH2	1:A:391:HIS:ND1	2.61	0.49
1:A:91:ARG:O	1:A:95:ARG:HB2	2.13	0.49
1:A:249:LEU:HD22	1:A:296:MET:HE3	1.95	0.48
1:A:589:ASP:HA	1:A:592:ARG:HG2	1.96	0.48
1:A:219:LEU:HD11	1:A:236:ILE:HD12	1.95	0.48
1:A:306:LYS:HD3	1:A:308:ARG:HD2	1.96	0.48
1:A:521:ILE:O	1:A:564:TYR:OH	2.30	0.48
1:A:159:LEU:CD2	1:A:324:PHE:HD2	2.26	0.47
1:A:613:ASN:O	1:A:616:ILE:HG13	2.15	0.47
1:A:278:TRP:O	1:A:278:TRP:HE3	1.97	0.47
1:A:298:GLY:N	1:A:343:ARG:O	2.45	0.47
1:A:122:ARG:HH22	3:A:1647:GUN:HN9	1.63	0.47
1:A:33:SER:O	1:A:36:ASP:HB2	2.14	0.47
1:A:122:ARG:NH2	3:A:1647:GUN:C8	2.77	0.47
1:A:282:ARG:HG2	1:A:308:ARG:NH2	2.30	0.47
1:A:125:ALA:HB2	1:A:433:ILE:HG21	1.97	0.47
1:A:162:GLU:HB3	1:A:163:TYR:CB	2.45	0.47
1:A:421:GLU:O	1:A:422:PRO:C	2.52	0.47
1:A:512:VAL:HG23	1:A:590:LEU:HD12	1.95	0.47
1:A:87:VAL:HG22	1:A:109:ARG:HG3	1.97	0.46
1:A:74:LYS:HE3	1:A:75:ASN:HD22	1.79	0.46
1:A:511:PRO:O	1:A:574:MET:HB3	2.16	0.46
1:A:56:LYS:HA	1:A:56:LYS:HE2	1.97	0.46
1:A:282:ARG:HD2	1:A:308:ARG:CG	2.39	0.46
1:A:31:ASP:O	1:A:31:ASP:OD1	2.34	0.46
1:A:2:PRO:HG2	1:A:4:PRO:HD2	1.96	0.46
1:A:633:SER:H	1:A:634:ILE:C	2.18	0.46
1:A:459:ASN:O	1:A:462:TYR:CE1	2.68	0.46
1:A:13:GLU:OE1	1:A:13:GLU:N	2.50	0.45
1:A:633:SER:HA	1:A:636:SER:HB2	1.98	0.45
1:A:341:ARG:HD3	1:A:353:HIS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ALA:CB	1:A:95:ARG:CB	2.82	0.45
1:A:137:ALA:HA	1:A:140:LEU:HD12	1.99	0.45
1:A:574:MET:SD	1:A:575:ILE:N	2.90	0.45
1:A:466:ARG:NE	1:A:567:ASP:OD2	2.49	0.45
1:A:75:ASN:CB	1:A:83:LYS:O	2.65	0.45
1:A:412:LEU:O	1:A:417:ASN:ND2	2.47	0.44
1:A:151:TYR:N	1:A:151:TYR:CD1	2.84	0.44
1:A:282:ARG:HG2	1:A:308:ARG:CZ	2.47	0.44
1:A:529:VAL:O	1:A:530:LEU:C	2.56	0.44
1:A:638:LEU:C	1:A:640:LEU:H	2.19	0.44
1:A:598:ILE:O	1:A:598:ILE:HG22	2.18	0.44
1:A:94:ALA:CB	1:A:95:ARG:CA	2.96	0.44
1:A:77:GLN:HE21	1:A:78:LEU:N	2.14	0.44
1:A:196:ILE:HD13	1:A:223:TYR:CD1	2.53	0.44
1:A:338:ASN:ND2	1:A:339:PHE:N	2.63	0.43
1:A:581:GLN:HB3	1:A:582:ASN:H	1.58	0.43
1:A:632:ALA:CA	1:A:633:SER:CB	2.92	0.43
1:A:182:MET:HE3	1:A:337:ARG:HD2	2.00	0.43
1:A:505:GLU:OE1	1:A:506:PRO:HD2	2.17	0.43
1:A:579:SER:HA	1:A:580:ALA:HA	1.91	0.43
1:A:495:TRP:HA	1:A:498:ASN:HD22	1.83	0.43
1:A:573:LYS:O	1:A:577:ASP:HB2	2.18	0.43
1:A:627:GLY:O	1:A:628:MET:HB2	2.18	0.43
1:A:324:PHE:CZ	1:A:339:PHE:HB2	2.54	0.43
1:A:93:VAL:CG1	1:A:93:VAL:O	2.65	0.43
1:A:437:TRP:O	1:A:450:ALA:HA	2.18	0.43
1:A:65:HIS:HE2	1:A:598:ILE:HG21	1.82	0.43
1:A:574:MET:C	1:A:574:MET:SD	2.97	0.43
1:A:95:ARG:N	1:A:96:SER:CB	2.56	0.43
1:A:167:GLY:HA3	1:A:168:THR:HA	1.80	0.43
1:A:2:PRO:HG2	1:A:4:PRO:CD	2.49	0.42
1:A:107:GLY:O	1:A:111:ILE:HG13	2.20	0.42
1:A:146:ARG:HG2	1:A:347:HIS:CE1	2.55	0.42
1:A:165:GLU:O	1:A:165:GLU:HG2	2.20	0.42
1:A:145:PRO:HB3	1:A:188:TYR:CZ	2.55	0.42
1:A:495:TRP:HA	1:A:498:ASN:ND2	2.34	0.42
1:A:29:THR:O	1:A:32:GLU:OE1	2.38	0.42
1:A:559:LEU:HB3	1:A:622:TYR:CE1	2.54	0.42
1:A:160:TYR:HB3	1:A:323:LEU:HB2	2.02	0.42
1:A:95:ARG:N	1:A:97:HIS:N	2.60	0.42
1:A:478:MET:HG2	1:A:485:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ASN:HA	1:A:12:ASN:HD22	1.74	0.42
1:A:588:ARG:O	1:A:590:LEU:N	2.53	0.42
1:A:10:VAL:HG12	1:A:70:ILE:HB	2.02	0.42
1:A:281:THR:O	1:A:282:ARG:C	2.59	0.42
1:A:471:ASN:O	1:A:475:LEU:HD22	2.20	0.42
1:A:469:ASP:HB3	1:A:565:VAL:HB	2.02	0.42
1:A:630:GLU:CB	1:A:631:GLY:CA	2.56	0.42
1:A:278:TRP:CE3	1:A:278:TRP:O	2.73	0.41
1:A:633:SER:H	1:A:634:ILE:CA	2.33	0.41
1:A:177:GLU:O	1:A:178:LYS:C	2.58	0.41
1:A:220:TRP:HB2	1:A:235:VAL:HG22	2.01	0.41
1:A:283:PHE:CE1	1:A:310:PRO:HG3	2.55	0.41
1:A:578:TRP:CE3	1:A:579:SER:HB3	2.55	0.41
1:A:404:GLU:HB3	1:A:405:PRO:HD2	2.01	0.41
1:A:433:ILE:HG13	1:A:503:LEU:HD23	2.02	0.41
1:A:461:SER:HB3	1:A:637:TRP:CZ2	2.56	0.41
1:A:488:ASP:O	1:A:489:LEU:C	2.59	0.41
1:A:571:TRP:O	1:A:574:MET:HG3	2.19	0.41
1:A:330:ASP:OD1	1:A:376:ARG:HG3	2.21	0.41
1:A:633:SER:N	1:A:635:ASP:N	2.55	0.41
1:A:281:THR:C	1:A:283:PHE:N	2.71	0.41
1:A:264:TRP:CD2	1:A:289:GLY:HA3	2.55	0.41
1:A:134:GLY:HA3	1:A:411:TYR:CG	2.56	0.41
1:A:554:HIS:C	1:A:554:HIS:ND1	2.73	0.41
1:A:59:ILE:HG22	1:A:80:ASP:OD2	2.21	0.41
1:A:16:HIS:NE2	1:A:97:HIS:CD2	2.88	0.41
1:A:29:THR:O	1:A:31:ASP:N	2.53	0.41
1:A:433:ILE:HG23	1:A:433:ILE:O	2.20	0.41
1:A:60:ARG:CZ	1:A:479:TRP:HB2	2.51	0.41
2:A:1645:GTP:N3	2:A:1645:GTP:H5"	2.36	0.41
1:A:23:LEU:HD22	1:A:47:ASP:O	2.21	0.41
1:A:578:TRP:CD1	1:A:581:GLN:OE1	2.74	0.41
1:A:412:LEU:HA	1:A:412:LEU:HD12	1.92	0.40
1:A:414:ASN:HD22	1:A:414:ASN:N	2.18	0.40
1:A:585:GLN:HA	1:A:588:ARG:HD2	2.03	0.40
1:A:336:LEU:CD1	1:A:366:VAL:HG22	2.52	0.40
1:A:94:ALA:C	1:A:97:HIS:H	2.24	0.40
1:A:363:SER:O	1:A:367:ARG:HB2	2.22	0.40
1:A:551:LEU:HD11	1:A:575:ILE:HD12	2.03	0.40
1:A:364:ARG:HH11	1:A:364:ARG:HB3	1.83	0.40
1:A:476:PHE:HB2	1:A:516:SER:HB2	2.03	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	605/644 (94%)	499 (82%)	86 (14%)	20 (3%)	4	25

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	32	GLU
1	A	162	GLU
1	A	163	TYR
1	A	581	GLN
1	A	630	GLU
1	A	632	ALA
1	A	633	SER
1	A	3	GLU
1	A	95	ARG
1	A	643	HIS
1	A	94	ALA
1	A	96	SER
1	A	164	ALA
1	A	577	ASP
1	A	592	ARG
1	A	634	ILE
1	A	30	GLY
1	A	489	LEU
1	A	81	ILE

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	542/571 (95%)	477 (88%)	65 (12%)	6 25

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	36	ASP
1	A	54	VAL
1	A	76	VAL
1	A	95	ARG
1	A	110	ARG
1	A	151	TYR
1	A	161	MET
1	A	165	GLU
1	A	166	ILE
1	A	175	THR
1	A	195	TYR
1	A	196	ILE
1	A	210	ARG
1	A	211	SER
1	A	216	ARG
1	A	240	ILE
1	A	241	MET
1	A	244	SER
1	A	258	VAL
1	A	277	GLU
1	A	278	TRP
1	A	287	ARG
1	A	308	ARG
1	A	311	ASN
1	A	324	PHE
1	A	338	ASN
1	A	343	ARG
1	A	355	ASP
1	A	361	VAL
1	A	367	ARG
1	A	376	ARG
1	A	412	LEU
1	A	413	THR

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Mol	Chain	Res	Type
1	A	430	LYS
1	A	444	TYR
1	A	445	ASP
1	A	446	TYR
1	A	466	ARG
1	A	475	LEU
1	A	480	ARG
1	A	487	LYS
1	A	503	LEU
1	A	512	VAL
1	A	524	ARG
1	A	551	LEU
1	A	558	THR
1	A	569	PHE
1	A	576	LEU
1	A	581	GLN
1	A	582	ASN
1	A	583	ARG
1	A	585	GLN
1	A	587	LEU
1	A	590	LEU
1	A	591	LYS
1	A	592	ARG
1	A	598	ILE
1	A	600	TRP
1	A	612	ARG
1	A	614	ASP
1	A	624	ARG
1	A	626	MET
1	A	640	LEU
1	A	642	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	12	ASN
1	A	75	ASN
1	A	77	GLN
1	A	148	HIS
1	A	307	HIS
1	A	311	ASN

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Mol	Chain	Res	Type
1	A	338	ASN
1	A	389	HIS
1	A	414	ASN
1	A	471	ASN
1	A	498	ASN
1	A	582	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6   Ligand geometry ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	GTP	A	1645	-	27,34,34	2.04	8 (29%)	27,54,54	1.87	5 (18%)
3	GUN	A	1646	-	9,12,12	1.97	2 (22%)	8,17,17	3.48	5 (62%)
3	GUN	A	1647	-	9,12,12	1.65	2 (22%)	8,17,17	3.50	6 (75%)

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	A	1645	-	-	0/18/38/38	0/3/3/3
3	GUN	A	1646	-	-	0/0/0/0	0/2/2/2
3	GUN	A	1647	-	-	0/0/0/0	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1645	GTP	PG-O2G	2.19	1.63	1.54
3	A	1647	GUN	C5-C4	2.60	1.46	1.40
2	A	1645	GTP	C2-N1	2.87	1.40	1.35
2	A	1645	GTP	PA-O1A	3.03	1.62	1.50
2	A	1645	GTP	PB-O1B	3.30	1.63	1.50
3	A	1646	GUN	C5-C4	3.46	1.48	1.40
2	A	1645	GTP	PG-O1G	3.51	1.62	1.50
2	A	1645	GTP	O4'-C1'	3.56	1.46	1.41
3	A	1647	GUN	C6-C5	3.93	1.48	1.41
2	A	1645	GTP	C6-N1	4.40	1.41	1.33
3	A	1646	GUN	C6-C5	4.51	1.49	1.41
2	A	1645	GTP	PG-O3B	5.23	1.68	1.60

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1646	GUN	C5-C6-N1	-5.25	116.01	123.48
3	A	1647	GUN	C6-C5-C4	-5.15	115.72	120.84
2	A	1645	GTP	N3-C2-N1	-5.10	120.00	127.46
3	A	1646	GUN	C6-C5-C4	-4.28	116.59	120.84
3	A	1646	GUN	C4-C5-N7	-4.04	105.51	109.41
3	A	1647	GUN	C5-C6-N1	-3.78	118.10	123.48
3	A	1647	GUN	C4-C5-N7	-3.28	106.24	109.41
3	A	1647	GUN	N3-C2-N1	-3.15	122.86	127.46
2	A	1645	GTP	C5-C6-N1	-2.68	119.67	123.48
2	A	1645	GTP	C4-C5-N7	-2.20	107.29	109.41
3	A	1646	GUN	N3-C2-N1	-2.08	124.42	127.46
2	A	1645	GTP	N2-C2-N1	2.03	120.49	117.24
3	A	1647	GUN	C2-N3-C4	3.80	119.60	115.16
3	A	1647	GUN	C6-N1-C2	4.51	122.55	116.06
3	A	1646	GUN	C6-N1-C2	5.27	123.64	116.06
2	A	1645	GTP	C2-N3-C4	6.04	122.22	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1645	GTP	1	0
3	A	1646	GUN	2	0
3	A	1647	GUN	3	0

5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	613/644 (95%)	-0.36	3 (0%)	90	74	34, 51, 62, 69	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	442	PRO	2.2
1	A	268	SER	2.1
1	A	92	GLU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GUN	A	1646	11/11	0.79	0.43	7.93	97,98,98,98	0
3	GUN	A	1647	11/11	0.93	0.27	2.38	99,99,99,99	0
2	GTP	A	1645	32/32	0.78	0.26	0.43	146,147,155,156	0

6.5   Other polymers ⓘ

There are no such residues in this entry.