Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2024 – 06:16 pm GMT

PDB ID	:	2JH8
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	:	3.22 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

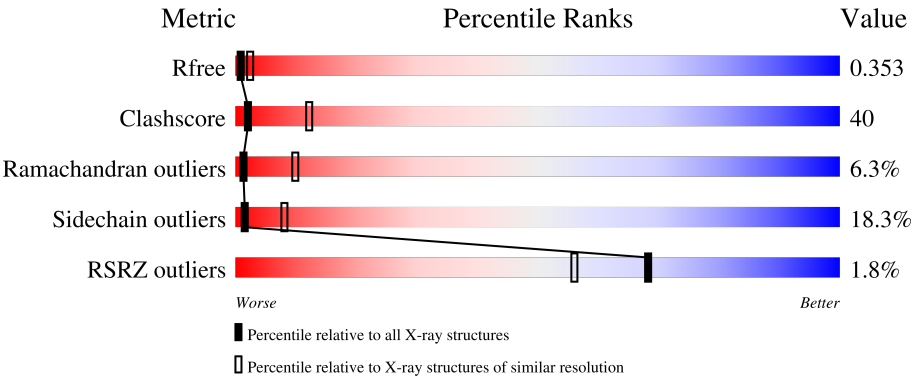
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.22 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	644	2% 36% 44% 14% • 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
2	M7G	A	1645	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5091 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.

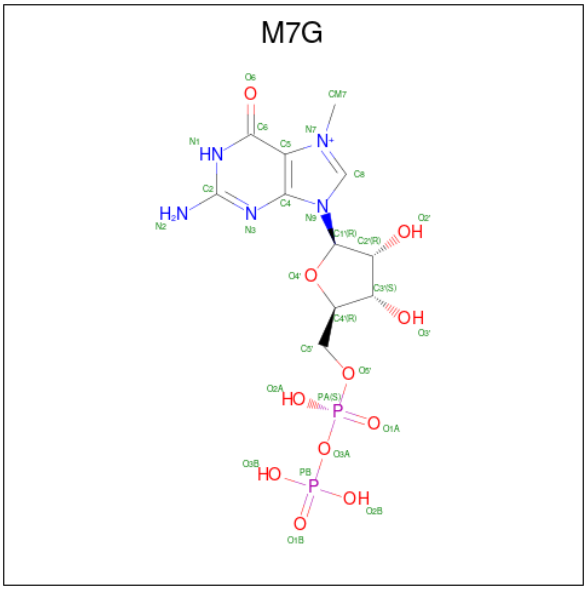
- Molecule 1 is a protein called VP4 CORE PROTEIN.

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

There is a discrepancy between the modelled and reference sequences:

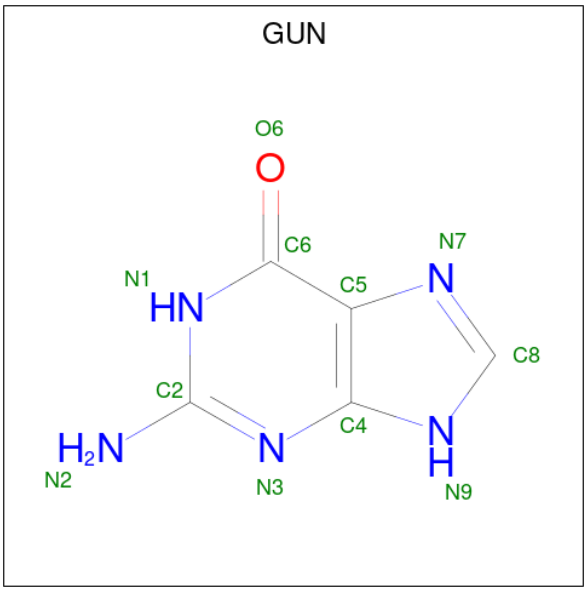
Chain	Residue	Modelled	Actual	Comment	Reference
A	261	LEU	PRO	conflict	UNP P07132

- Molecule 2 is 7N-METHYL-8-HYDROGUANOSINE-5'-DIPHOSPHATE (three-letter code: M7G) (formula: $C_{11}H_{18}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	11	5	11	2		

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



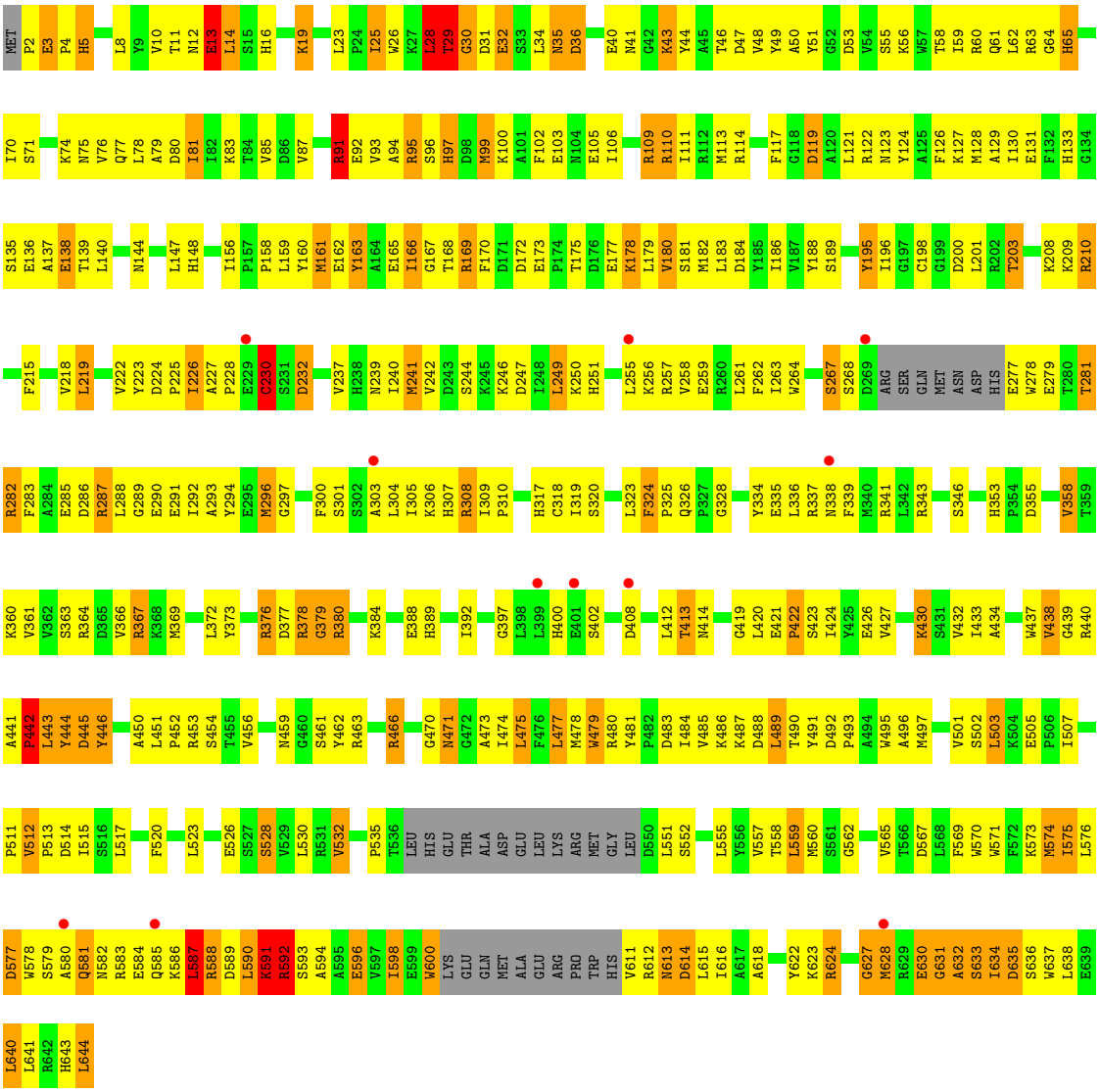
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 11 5 5 1	0	0
3	A	1	Total C N O 11 5 5 1	0	0

3 Residue-property plots (i)

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

- Molecule 1: VP4 CORE PROTEIN

Chain A: 2% 36% 44% 14% • 5%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	75.06Å 75.06Å 419.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 3.22 24.74 – 3.22	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-3.22) 99.8 (24.74-3.22)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 3.23Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.341 0.277 , 0.353	Depositor DCC
R_{free} test set	590 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	95.5	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 6.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5091	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M7G, 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	0.86	8/5167 (0.2%)	0.93	7/6981 (0.1%)

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	6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	GLU	CD-OE1	15.71	1.43	1.25
1	A	592	ARG	CZ-NH1	11.35	1.47	1.33
1	A	244	SER	CB-OG	10.52	1.55	1.42
1	A	92	GLU	CD-OE2	9.13	1.35	1.25
1	A	230	CYS	CB-SG	6.84	1.93	1.82
1	A	91	ARG	CZ-NH1	5.64	1.40	1.33
1	A	35	ASN	CG-ND2	5.39	1.46	1.32
1	A	239	ASN	CG-OD1	5.04	1.35	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	559	LEU	CB-CG-CD1	-7.44	98.36	111.00
1	A	32	GLU	N-CA-C	5.58	126.06	111.00
1	A	442	PRO	N-CA-C	5.20	125.63	112.10
1	A	627	GLY	N-CA-C	-5.15	100.22	113.10
1	A	30	GLY	N-CA-C	5.10	125.85	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	591	LYS	N-CA-C	5.07	124.70	111.00
1	A	587	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	LEU	Peptide
1	A	31	ASP	Peptide
1	A	442	PRO	Peptide
1	A	483	ASP	Peptide
1	A	587	LEU	Peptide
1	A	631	GLY	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	408	0
2	A	29	0	16	1	0
3	A	22	0	10	4	0
All	All	5091	0	5011	408	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 40.

All (408) 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:632:ALA:HB3	1:A:633:SER:CB	1.62	1.27
1:A:632:ALA:CB	1:A:633:SER:HB2	1.69	1.20
1:A:94:ALA:HB3	1:A:95:ARG:HB2	1.27	1.08
1:A:623:LYS:HD3	1:A:634:ILE:HG21	1.29	1.06
1:A:3:GLU:H	1:A:4:PRO:CD	1.69	1.05
1:A:94:ALA:HB3	1:A:95:ARG:CB	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:TRP:HA	1:A:600:TRP:CE3	1.98	0.98
1:A:122:ARG:HG2	1:A:126:PHE:HE1	1.33	0.94
1:A:600:TRP:HA	1:A:600:TRP:HE3	1.36	0.91
1:A:288:LEU:O	1:A:292:ILE:HG13	1.71	0.91
1:A:589:ASP:HA	1:A:592:ARG:HG2	1.54	0.89
1:A:23:LEU:HD12	1:A:49:TYR:CE2	2.07	0.89
1:A:2:PRO:HG3	1:A:453:ARG:HH22	1.37	0.87
1:A:495:TRP:HE1	3:A:1647:GUN:HN21	1.22	0.87
1:A:282:ARG:HG2	1:A:308:ARG:NH2	1.91	0.86
1:A:96:SER:O	1:A:97:HIS:HB2	1.74	0.85
1:A:2:PRO:CG	1:A:453:ARG:HH12	1.90	0.85
1:A:261:LEU:HD12	1:A:262:PHE:H	1.42	0.84
1:A:632:ALA:HB3	1:A:633:SER:HB2	0.88	0.84
1:A:94:ALA:CB	1:A:95:ARG:HB2	2.06	0.84
1:A:160:TYR:HB3	1:A:323:LEU:HB2	1.58	0.83
1:A:28:LEU:HA	1:A:29:THR:HG23	1.60	0.83
1:A:127:LYS:HE2	1:A:127:LYS:HA	1.59	0.83
1:A:2:PRO:CG	1:A:453:ARG:HH22	1.91	0.83
1:A:309:ILE:HD13	1:A:366:VAL:HG12	1.61	0.83
1:A:95:ARG:H	1:A:96:SER:CB	1.92	0.82
1:A:489:LEU:HG	1:A:490:THR:N	1.92	0.82
1:A:630:GLU:HB3	1:A:631:GLY:CA	2.11	0.81
1:A:634:ILE:HG22	1:A:635:ASP:N	1.94	0.81
1:A:459:ASN:O	1:A:462:TYR:HE1	1.64	0.81
1:A:634:ILE:HG22	1:A:635:ASP:H	1.44	0.81
1:A:632:ALA:CB	1:A:633:SER:CB	2.43	0.80
1:A:2:PRO:HB3	1:A:440:ARG:HB2	1.64	0.80
1:A:574:MET:O	1:A:578:TRP:HB3	1.82	0.80
1:A:95:ARG:H	1:A:96:SER:CA	1.95	0.79
1:A:437:TRP:HZ2	1:A:443:LEU:HD13	1.47	0.79
1:A:282:ARG:HD2	1:A:308:ARG:HG3	1.63	0.79
1:A:309:ILE:HD13	1:A:366:VAL:CG1	2.14	0.78
1:A:408:ASP:HB2	1:A:434:ALA:HB2	1.65	0.78
1:A:65:HIS:HE2	1:A:598:ILE:HG21	1.48	0.78
1:A:640:LEU:HG	1:A:640:LEU:O	1.83	0.78
1:A:3:GLU:H	1:A:4:PRO:HD2	1.48	0.77
1:A:633:SER:H	1:A:635:ASP:N	1.82	0.77
1:A:630:GLU:HB3	1:A:631:GLY:HA3	1.68	0.76
1:A:282:ARG:HG2	1:A:308:ARG:HH21	1.47	0.76
1:A:2:PRO:HG3	1:A:453:ARG:NH2	2.01	0.76
1:A:336:LEU:HD11	1:A:366:VAL:HG13	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:H	1:A:4:PRO:HD3	1.50	0.75
1:A:582:ASN:O	1:A:586:LYS:HG2	1.85	0.75
1:A:91:ARG:O	1:A:95:ARG:HB2	1.85	0.75
1:A:99:MET:O	1:A:103:GLU:HG3	1.87	0.75
1:A:16:HIS:NE2	1:A:97:HIS:NE2	2.35	0.74
1:A:478:MET:HG2	1:A:485:VAL:HG12	1.70	0.74
1:A:2:PRO:HG3	1:A:453:ARG:HH12	1.53	0.74
1:A:578:TRP:CE3	1:A:579:SER:HB3	2.23	0.74
1:A:631:GLY:O	1:A:633:SER:HB3	1.88	0.74
1:A:5:HIS:CE1	1:A:44:TYR:O	2.41	0.73
1:A:528:SER:O	1:A:532:VAL:HG13	1.88	0.73
1:A:3:GLU:N	1:A:4:PRO:CD	2.45	0.72
1:A:136:GLU:HB2	1:A:138:GLU:OE1	1.90	0.72
1:A:2:PRO:HD3	1:A:439:GLY:HA2	1.71	0.72
1:A:591:LYS:N	1:A:592:ARG:HB3	2.06	0.71
1:A:633:SER:H	1:A:635:ASP:H	1.38	0.71
1:A:5:HIS:HE1	1:A:44:TYR:O	1.72	0.71
1:A:517:LEU:HD22	1:A:570:TRP:CE2	2.25	0.71
1:A:623:LYS:HD3	1:A:634:ILE:CG2	2.14	0.71
1:A:210:ARG:HH11	1:A:210:ARG:CG	2.04	0.70
1:A:571:TRP:O	1:A:574:MET:HG3	1.92	0.69
1:A:478:MET:HG2	1:A:485:VAL:CG1	2.23	0.69
1:A:40:GLU:O	1:A:43:LYS:HB2	1.93	0.69
1:A:177:GLU:HG2	1:A:180:VAL:HG12	1.76	0.68
1:A:282:ARG:HH21	1:A:308:ARG:HB2	1.58	0.68
1:A:441:ALA:HB1	1:A:442:PRO:HD3	1.75	0.68
1:A:466:ARG:HA	1:A:567:ASP:OD1	1.94	0.68
1:A:580:ALA:HB1	1:A:581:GLN:O	1.93	0.68
1:A:630:GLU:CB	1:A:631:GLY:CA	2.70	0.68
1:A:470:GLY:HA3	1:A:496:ALA:O	1.94	0.68
1:A:210:ARG:HH11	1:A:210:ARG:HB2	1.59	0.67
1:A:25:ILE:HD12	1:A:25:ILE:H	1.59	0.67
1:A:160:TYR:HB2	1:A:369:MET:HE3	1.75	0.67
1:A:159:LEU:CD2	1:A:324:PHE:HD2	2.07	0.66
1:A:413:THR:HG21	1:A:437:TRP:H	1.59	0.66
1:A:25:ILE:HD12	1:A:25:ILE:N	2.10	0.66
1:A:28:LEU:HA	1:A:29:THR:CG2	2.24	0.66
1:A:279:GLU:C	1:A:281:THR:H	1.99	0.66
1:A:615:LEU:O	1:A:618:ALA:HB3	1.95	0.66
1:A:2:PRO:CD	1:A:453:ARG:HH12	2.09	0.66
1:A:138:GLU:OE2	1:A:139:THR:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TYR:HB2	1:A:369:MET:CE	2.25	0.66
1:A:75:ASN:HB2	1:A:83:LYS:O	1.95	0.65
1:A:210:ARG:HH11	1:A:210:ARG:HG3	1.61	0.65
1:A:408:ASP:HB2	1:A:434:ALA:CB	2.26	0.65
1:A:632:ALA:HB3	1:A:633:SER:HB3	1.73	0.65
1:A:261:LEU:HD12	1:A:262:PHE:N	2.11	0.65
1:A:517:LEU:HD13	1:A:570:TRP:CE3	2.32	0.65
1:A:441:ALA:O	1:A:443:LEU:HB2	1.96	0.65
1:A:170:PHE:O	1:A:378:ARG:NH1	2.26	0.64
1:A:507:ILE:HD11	1:A:569:PHE:HD2	1.63	0.64
1:A:507:ILE:HD13	1:A:570:TRP:HA	1.80	0.64
1:A:77:GLN:O	1:A:78:LEU:HD12	1.98	0.64
1:A:188:TYR:CD2	1:A:189:SER:HB3	2.33	0.64
1:A:2:PRO:HG3	1:A:453:ARG:NH1	2.12	0.64
1:A:3:GLU:N	1:A:4:PRO:HD3	2.13	0.64
1:A:95:ARG:N	1:A:96:SER:HB2	2.13	0.63
1:A:103:GLU:HA	1:A:106:ILE:HD12	1.81	0.63
1:A:341:ARG:HD3	1:A:353:HIS:O	1.99	0.63
1:A:627:GLY:O	1:A:628:MET:HB2	1.99	0.63
1:A:32:GLU:H	1:A:32:GLU:CD	2.02	0.63
1:A:2:PRO:CG	1:A:453:ARG:NH1	2.62	0.62
1:A:210:ARG:HH11	1:A:210:ARG:CB	2.12	0.62
1:A:552:SER:HB3	1:A:614:ASP:CB	2.30	0.62
1:A:5:HIS:HB2	1:A:47:ASP:HA	1.80	0.61
1:A:32:GLU:HB3	1:A:36:ASP:HB3	1.81	0.61
1:A:281:THR:O	1:A:282:ARG:C	2.38	0.61
1:A:633:SER:N	1:A:635:ASP:N	2.49	0.61
1:A:95:ARG:N	1:A:96:SER:CB	2.64	0.61
1:A:122:ARG:HG2	1:A:126:PHE:CE1	2.25	0.61
1:A:466:ARG:NE	1:A:567:ASP:OD1	2.33	0.60
1:A:44:TYR:CG	1:A:48:VAL:HG11	2.35	0.60
1:A:65:HIS:HE2	1:A:598:ILE:CG2	2.13	0.60
1:A:208:LYS:HG3	1:A:215:PHE:CD2	2.37	0.60
1:A:441:ALA:HB3	1:A:443:LEU:CD1	2.32	0.60
1:A:586:LYS:O	1:A:587:LEU:HB3	2.01	0.60
1:A:12:ASN:C	1:A:14:LEU:H	2.05	0.60
1:A:91:ARG:O	1:A:95:ARG:CB	2.51	0.59
1:A:58:THR:OG1	1:A:61:GLN:HG3	2.02	0.59
1:A:517:LEU:HB2	1:A:570:TRP:CH2	2.37	0.59
1:A:2:PRO:HD3	1:A:440:ARG:H	1.67	0.59
1:A:585:GLN:HA	1:A:588:ARG:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ALA:HB3	1:A:95:ARG:CA	2.33	0.59
1:A:591:LYS:CA	1:A:592:ARG:HB3	2.33	0.59
1:A:8:LEU:N	1:A:48:VAL:O	2.31	0.59
1:A:109:ARG:O	1:A:113:MET:HG3	2.03	0.59
1:A:420:LEU:O	1:A:423:SER:OG	2.20	0.59
1:A:326:GLN:NE2	1:A:335:GLU:O	2.28	0.58
1:A:93:VAL:HG12	1:A:93:VAL:O	2.04	0.58
1:A:282:ARG:HG2	1:A:308:ARG:CZ	2.33	0.58
1:A:474:ILE:HG21	1:A:491:TYR:CZ	2.38	0.58
1:A:640:LEU:O	1:A:644:LEU:HA	2.03	0.58
1:A:74:LYS:O	1:A:85:VAL:HB	2.03	0.58
1:A:413:THR:HG21	1:A:437:TRP:N	2.18	0.58
1:A:578:TRP:HE3	1:A:579:SER:HB3	1.66	0.58
1:A:224:ASP:OD1	1:A:226:ILE:HG12	2.04	0.57
1:A:437:TRP:O	1:A:450:ALA:HA	2.04	0.57
1:A:2:PRO:CG	1:A:453:ARG:NH2	2.63	0.57
1:A:286:ASP:HB3	1:A:287:ARG:NH2	2.18	0.57
1:A:432:VAL:O	1:A:503:LEU:HA	2.04	0.57
1:A:12:ASN:O	1:A:14:LEU:N	2.38	0.56
1:A:131:GLU:OE2	1:A:400:HIS:HE1	1.87	0.56
1:A:421:GLU:O	1:A:422:PRO:C	2.42	0.56
1:A:634:ILE:CG2	1:A:635:ASP:N	2.66	0.56
1:A:26:TRP:O	1:A:50:ALA:HA	2.05	0.56
1:A:281:THR:C	1:A:283:PHE:N	2.57	0.56
1:A:26:TRP:HB3	1:A:50:ALA:HB2	1.87	0.56
1:A:582:ASN:O	1:A:586:LYS:CG	2.51	0.56
1:A:633:SER:H	1:A:634:ILE:CB	2.18	0.56
1:A:633:SER:N	1:A:635:ASP:H	2.04	0.56
1:A:323:LEU:HD23	1:A:338:ASN:HA	1.87	0.56
1:A:560:MET:HE2	1:A:622:TYR:CD1	2.41	0.56
1:A:282:ARG:NH2	1:A:308:ARG:HB2	2.20	0.56
1:A:507:ILE:HD11	1:A:569:PHE:CD2	2.40	0.56
1:A:452:PRO:O	1:A:456:VAL:HG23	2.05	0.56
1:A:65:HIS:NE2	1:A:598:ILE:HG21	2.19	0.56
1:A:208:LYS:HG3	1:A:215:PHE:CG	2.41	0.56
1:A:379:GLY:O	1:A:380:ARG:C	2.44	0.56
1:A:100:LYS:O	1:A:103:GLU:N	2.39	0.55
1:A:83:LYS:NZ	1:A:488:ASP:O	2.39	0.55
1:A:555:LEU:HD13	1:A:571:TRP:CZ3	2.42	0.55
1:A:182:MET:HE3	1:A:337:ARG:HD2	1.89	0.55
1:A:433:ILE:HA	1:A:502:SER:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:SER:O	1:A:633:SER:OG	2.22	0.55
1:A:552:SER:HB3	1:A:614:ASP:HB2	1.88	0.55
1:A:286:ASP:CB	1:A:287:ARG:NH2	2.70	0.55
1:A:304:LEU:HD12	1:A:338:ASN:O	2.06	0.55
1:A:585:GLN:HA	1:A:588:ARG:CD	2.37	0.55
1:A:162:GLU:N	1:A:163:TYR:CB	2.69	0.55
1:A:560:MET:CE	1:A:622:TYR:CD1	2.91	0.54
1:A:426:GLU:O	1:A:430:LYS:HE3	2.07	0.54
1:A:511:PRO:O	1:A:574:MET:HB2	2.07	0.54
1:A:632:ALA:CA	1:A:633:SER:CB	2.85	0.54
1:A:2:PRO:HG3	1:A:453:ARG:CZ	2.38	0.54
1:A:633:SER:H	1:A:634:ILE:CA	2.20	0.54
1:A:324:PHE:HB2	1:A:325:PRO:HD2	1.90	0.54
1:A:119:ASP:O	1:A:123:ASN:HB2	2.07	0.54
1:A:156:ILE:HG12	1:A:389:HIS:CD2	2.43	0.54
1:A:264:TRP:CE3	1:A:289:GLY:HA2	2.43	0.54
1:A:471:ASN:HB2	1:A:497:MET:HG3	1.90	0.54
1:A:567:ASP:OD2	1:A:567:ASP:C	2.44	0.54
1:A:230:CYS:SG	1:A:232:ASP:HB2	2.47	0.54
1:A:177:GLU:O	1:A:178:LYS:C	2.46	0.54
1:A:633:SER:N	1:A:634:ILE:HB	2.23	0.54
1:A:459:ASN:O	1:A:462:TYR:CE1	2.53	0.53
1:A:589:ASP:CA	1:A:592:ARG:HG2	2.34	0.53
1:A:635:ASP:HA	1:A:638:LEU:HD12	1.91	0.53
1:A:169:ARG:NE	1:A:372:LEU:O	2.42	0.53
1:A:576:LEU:C	1:A:578:TRP:H	2.13	0.53
1:A:614:ASP:OD1	1:A:614:ASP:N	2.41	0.53
1:A:59:ILE:HG22	1:A:80:ASP:OD2	2.09	0.52
1:A:282:ARG:HA	1:A:308:ARG:CZ	2.39	0.52
1:A:63:ARG:C	1:A:65:HIS:N	2.61	0.52
1:A:102:PHE:O	1:A:105:GLU:HB3	2.10	0.52
1:A:119:ASP:HA	1:A:122:ARG:NH1	2.25	0.52
1:A:166:ILE:HG22	1:A:167:GLY:HA2	1.92	0.52
1:A:292:ILE:O	1:A:296:MET:HG3	2.09	0.52
1:A:515:ILE:HD11	1:A:598:ILE:HG12	1.92	0.52
1:A:598:ILE:HG22	1:A:598:ILE:O	2.10	0.52
1:A:201:LEU:HD12	1:A:228:PRO:HD2	1.92	0.52
1:A:317:HIS:CE1	1:A:360:LYS:HB2	2.44	0.52
1:A:210:ARG:HB2	1:A:210:ARG:NH1	2.25	0.52
1:A:110:ARG:NH1	1:A:492:ASP:OD2	2.43	0.52
1:A:454:SER:HB2	1:A:622:TYR:OH	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:HIS:CD2	1:A:97:HIS:CD2	2.98	0.52
1:A:293:ALA:O	1:A:294:TYR:C	2.48	0.51
1:A:317:HIS:HE1	1:A:360:LYS:HB2	1.73	0.51
1:A:218:VAL:CG1	1:A:219:LEU:N	2.71	0.51
1:A:384:LYS:O	1:A:388:GLU:HG3	2.10	0.51
1:A:600:TRP:CE3	1:A:600:TRP:CA	2.84	0.51
1:A:309:ILE:O	2:A:1645:M7G:N2	2.39	0.51
1:A:87:VAL:HG22	1:A:109:ARG:HG2	1.93	0.51
1:A:444:TYR:C	1:A:446:TYR:H	2.14	0.51
1:A:78:LEU:HB2	1:A:81:ILE:O	2.11	0.51
1:A:96:SER:O	1:A:97:HIS:CB	2.49	0.51
1:A:259:GLU:HG3	1:A:301:SER:HB3	1.91	0.51
1:A:290:GLU:HG3	1:A:305:ILE:HG21	1.92	0.51
1:A:58:THR:HG21	1:A:596:GLU:OE1	2.11	0.51
1:A:34:LEU:C	1:A:36:ASP:H	2.14	0.51
1:A:63:ARG:C	1:A:65:HIS:H	2.13	0.51
1:A:159:LEU:HD22	1:A:324:PHE:HD2	1.76	0.51
1:A:262:PHE:HB2	1:A:300:PHE:CE2	2.46	0.51
1:A:414:ASN:N	1:A:414:ASN:HD22	2.08	0.51
1:A:58:THR:HA	1:A:80:ASP:HB2	1.92	0.50
1:A:74:LYS:HE3	1:A:75:ASN:HD22	1.75	0.50
1:A:520:PHE:HB3	1:A:523:LEU:HD22	1.93	0.50
1:A:131:GLU:OE1	1:A:402:SER:HB3	2.11	0.50
1:A:178:LYS:HE2	1:A:179:LEU:HG	1.92	0.50
1:A:218:VAL:HG12	1:A:219:LEU:N	2.26	0.50
1:A:489:LEU:CG	1:A:490:THR:N	2.71	0.50
1:A:59:ILE:O	1:A:62:LEU:N	2.44	0.50
1:A:124:TYR:CD1	1:A:477:LEU:HD21	2.47	0.50
1:A:475:LEU:HD23	1:A:515:ILE:HG22	1.94	0.50
1:A:95:ARG:H	1:A:97:HIS:N	2.10	0.50
1:A:470:GLY:O	1:A:473:ALA:HB3	2.11	0.50
1:A:136:GLU:O	1:A:138:GLU:N	2.44	0.49
1:A:169:ARG:HB2	1:A:372:LEU:HD22	1.93	0.49
1:A:461:SER:HB3	1:A:637:TRP:CZ2	2.47	0.49
1:A:40:GLU:O	1:A:43:LYS:N	2.45	0.49
1:A:87:VAL:HG22	1:A:109:ARG:CG	2.42	0.49
1:A:246:LYS:HA	1:A:249:LEU:HD23	1.94	0.49
1:A:318:CYS:O	1:A:358:VAL:HA	2.12	0.49
1:A:306:LYS:HB2	1:A:337:ARG:NH1	2.28	0.49
1:A:124:TYR:O	1:A:127:LYS:HB2	2.11	0.49
1:A:144:ASN:H	1:A:148:HIS:HD2	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ARG:HH11	1:A:318:CYS:HB3	1.77	0.49
1:A:578:TRP:O	1:A:581:GLN:HB2	2.12	0.49
1:A:466:ARG:NH1	1:A:567:ASP:OD1	2.46	0.49
1:A:584:GLU:HB3	1:A:588:ARG:HH21	1.77	0.49
1:A:144:ASN:H	1:A:148:HIS:CD2	2.30	0.49
1:A:567:ASP:OD2	1:A:567:ASP:O	2.31	0.49
1:A:56:LYS:O	1:A:79:ALA:HB2	2.13	0.48
1:A:59:ILE:HG23	1:A:60:ARG:N	2.27	0.48
1:A:179:LEU:HB3	1:A:203:THR:HG21	1.94	0.48
1:A:282:ARG:HA	1:A:308:ARG:NH2	2.28	0.48
1:A:559:LEU:HB3	1:A:622:TYR:CE1	2.48	0.48
1:A:573:LYS:O	1:A:577:ASP:HB2	2.14	0.48
1:A:307:HIS:O	1:A:307:HIS:ND1	2.43	0.48
1:A:279:GLU:HB3	1:A:282:ARG:HB2	1.95	0.48
1:A:210:ARG:HG3	1:A:210:ARG:NH1	2.26	0.48
1:A:575:ILE:HG22	1:A:576:LEU:HG	1.95	0.48
1:A:635:ASP:O	1:A:636:SER:C	2.52	0.48
1:A:28:LEU:C	1:A:29:THR:HG22	2.34	0.48
1:A:184:ASP:C	3:A:1646:GUN:HN21	2.17	0.48
1:A:19:LYS:NZ	1:A:51:TYR:OH	2.43	0.48
1:A:28:LEU:CA	1:A:29:THR:CG2	2.91	0.48
1:A:58:THR:HB	1:A:80:ASP:OD2	2.14	0.48
1:A:172:ASP:O	1:A:173:GLU:HG3	2.14	0.48
1:A:294:TYR:CD1	1:A:319:ILE:HG21	2.49	0.48
1:A:364:ARG:HA	1:A:367:ARG:HD2	1.96	0.48
1:A:421:GLU:O	1:A:424:ILE:HB	2.14	0.47
1:A:574:MET:SD	1:A:575:ILE:N	2.87	0.47
1:A:588:ARG:O	1:A:590:LEU:N	2.47	0.47
1:A:75:ASN:CB	1:A:83:LYS:O	2.63	0.47
1:A:122:ARG:HH22	3:A:1647:GUN:HN9	1.61	0.47
1:A:198:CYS:SG	1:A:222:VAL:HB	2.54	0.47
1:A:13:GLU:N	1:A:13:GLU:OE1	2.48	0.47
1:A:224:ASP:HB3	1:A:227:ALA:HB2	1.97	0.47
1:A:309:ILE:HD12	1:A:334:TYR:HB3	1.96	0.47
1:A:264:TRP:CD2	1:A:289:GLY:CA	2.98	0.47
1:A:53:ASP:OD1	1:A:55:SER:OG	2.29	0.47
1:A:256:LYS:HG2	1:A:257:ARG:N	2.30	0.47
1:A:267:SER:HB3	1:A:308:ARG:NH2	2.30	0.47
1:A:466:ARG:CZ	1:A:567:ASP:OD1	2.62	0.47
1:A:474:ILE:HG21	1:A:491:TYR:CE2	2.50	0.47
1:A:613:ASN:O	1:A:614:ASP:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:C	1:A:36:ASP:N	2.68	0.47
1:A:41:ASN:C	1:A:43:LYS:H	2.18	0.47
1:A:366:VAL:O	1:A:369:MET:HB2	2.14	0.47
1:A:630:GLU:CB	1:A:631:GLY:HA2	2.45	0.47
1:A:613:ASN:O	1:A:616:ILE:HG13	2.14	0.46
1:A:44:TYR:CD2	1:A:48:VAL:HG11	2.49	0.46
1:A:177:GLU:HG2	1:A:180:VAL:CG1	2.43	0.46
1:A:641:LEU:C	1:A:643:HIS:H	2.19	0.46
1:A:453:ARG:HD2	1:A:562:GLY:O	2.15	0.46
1:A:223:TYR:O	1:A:224:ASP:HB2	2.15	0.46
1:A:63:ARG:O	1:A:65:HIS:N	2.49	0.46
1:A:75:ASN:HA	1:A:85:VAL:HG23	1.97	0.46
1:A:124:TYR:HA	1:A:484:ILE:HG21	1.98	0.46
1:A:222:VAL:HG23	1:A:222:VAL:O	2.16	0.46
1:A:215:PHE:CD2	1:A:215:PHE:C	2.88	0.46
1:A:633:SER:HA	1:A:636:SER:H	1.80	0.45
1:A:552:SER:HB3	1:A:614:ASP:HB3	1.97	0.45
1:A:95:ARG:H	1:A:96:SER:HB2	1.68	0.45
1:A:589:ASP:HB3	1:A:592:ARG:NH1	2.32	0.45
1:A:264:TRP:HB3	1:A:305:ILE:HD13	1.98	0.45
1:A:570:TRP:CD1	1:A:570:TRP:C	2.90	0.45
1:A:585:GLN:HA	1:A:588:ARG:HE	1.82	0.45
1:A:589:ASP:CB	1:A:592:ARG:NH1	2.79	0.45
1:A:324:PHE:CB	1:A:325:PRO:CD	2.93	0.45
1:A:438:VAL:HG12	1:A:451:LEU:O	2.17	0.45
1:A:10:VAL:HA	1:A:70:ILE:O	2.17	0.45
1:A:200:ASP:O	1:A:201:LEU:HB2	2.17	0.45
1:A:641:LEU:O	1:A:644:LEU:N	2.43	0.45
1:A:261:LEU:CD1	1:A:262:PHE:N	2.80	0.45
1:A:281:THR:O	1:A:283:PHE:N	2.50	0.45
1:A:470:GLY:HA2	1:A:501:VAL:HG21	1.98	0.45
1:A:462:TYR:O	1:A:463:ARG:C	2.54	0.44
1:A:584:GLU:O	1:A:587:LEU:HD12	2.18	0.44
1:A:12:ASN:C	1:A:14:LEU:N	2.70	0.44
1:A:633:SER:HA	1:A:636:SER:N	2.33	0.44
1:A:119:ASP:OD1	1:A:122:ARG:NH1	2.50	0.44
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.79	0.44
1:A:264:TRP:CD2	1:A:289:GLY:HA3	2.52	0.44
1:A:324:PHE:HB2	1:A:325:PRO:CD	2.46	0.44
1:A:26:TRP:HB2	1:A:44:TYR:CE1	2.53	0.44
1:A:426:GLU:O	1:A:426:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ARG:N	1:A:97:HIS:N	2.66	0.44
1:A:512:VAL:HG23	1:A:590:LEU:HD12	2.00	0.44
1:A:328:GLY:O	1:A:376:ARG:HG2	2.17	0.44
1:A:585:GLN:HA	1:A:588:ARG:NE	2.33	0.44
1:A:188:TYR:CE2	1:A:189:SER:HB3	2.53	0.44
1:A:93:VAL:O	1:A:93:VAL:CG1	2.65	0.43
1:A:166:ILE:H	1:A:166:ILE:HG13	1.49	0.43
1:A:388:GLU:O	1:A:389:HIS:C	2.56	0.43
1:A:515:ILE:HD11	1:A:598:ILE:CG1	2.48	0.43
1:A:557:VAL:O	1:A:558:THR:C	2.57	0.43
1:A:338:ASN:HD22	1:A:339:PHE:N	2.16	0.43
1:A:282:ARG:HD2	1:A:308:ARG:CG	2.41	0.43
1:A:195:TYR:HA	1:A:263:ILE:HB	2.01	0.43
1:A:186:ILE:HD12	1:A:186:ILE:HA	1.87	0.43
1:A:129:ALA:C	1:A:130:ILE:HD12	2.39	0.43
1:A:133:HIS:ND1	1:A:397:GLY:HA2	2.34	0.42
1:A:478:MET:O	1:A:479:TRP:C	2.57	0.42
1:A:489:LEU:HD23	1:A:491:TYR:CD2	2.54	0.42
1:A:363:SER:O	1:A:366:VAL:HB	2.19	0.42
1:A:576:LEU:C	1:A:578:TRP:N	2.72	0.42
1:A:60:ARG:NH2	1:A:479:TRP:HB2	2.34	0.42
1:A:268:SER:OG	1:A:285:GLU:OE2	2.31	0.42
1:A:304:LEU:HD12	1:A:304:LEU:HA	1.66	0.42
1:A:423:SER:O	1:A:427:VAL:HG23	2.19	0.42
1:A:11:THR:HG23	1:A:71:SER:HB2	2.01	0.42
1:A:131:GLU:OE1	1:A:402:SER:CB	2.67	0.42
1:A:74:LYS:HB3	1:A:75:ASN:HD22	1.83	0.42
1:A:441:ALA:HB1	1:A:442:PRO:CD	2.46	0.42
1:A:513:PRO:HD3	1:A:574:MET:HE3	2.01	0.42
1:A:514:ASP:OD2	1:A:515:ILE:N	2.52	0.42
1:A:32:GLU:HB3	1:A:36:ASP:CB	2.47	0.42
1:A:471:ASN:C	1:A:471:ASN:HD22	2.22	0.42
1:A:256:LYS:HG2	1:A:257:ARG:H	1.84	0.42
1:A:287:ARG:NH1	1:A:318:CYS:HB3	2.34	0.42
1:A:310:PRO:O	1:A:367:ARG:NH2	2.53	0.42
1:A:419:GLY:C	1:A:421:GLU:OE1	2.58	0.42
1:A:526:GLU:HA	1:A:526:GLU:OE1	2.19	0.42
1:A:160:TYR:HB2	1:A:369:MET:HE1	2.00	0.42
1:A:581:GLN:HB3	1:A:582:ASN:H	1.74	0.42
1:A:631:GLY:HA3	1:A:634:ILE:HD12	2.02	0.42
1:A:241:MET:HG3	1:A:242:VAL:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:SER:H	1:A:634:ILE:HB	1.79	0.41
1:A:121:LEU:O	1:A:122:ARG:C	2.59	0.41
1:A:453:ARG:HD3	1:A:565:VAL:HG23	2.01	0.41
1:A:461:SER:HB3	1:A:637:TRP:CH2	2.56	0.41
1:A:135:SER:O	1:A:136:GLU:HG3	2.21	0.41
1:A:637:TRP:O	1:A:638:LEU:C	2.58	0.41
1:A:113:MET:O	1:A:114:ARG:C	2.59	0.41
1:A:264:TRP:CD2	1:A:289:GLY:HA2	2.55	0.41
1:A:262:PHE:O	1:A:303:ALA:HA	2.20	0.41
1:A:63:ARG:O	1:A:64:GLY:C	2.58	0.41
1:A:110:ARG:O	1:A:113:MET:HB2	2.20	0.41
1:A:127:LYS:C	1:A:128:MET:HG2	2.40	0.41
1:A:147:LEU:HA	1:A:147:LEU:HD12	1.69	0.41
1:A:25:ILE:N	1:A:25:ILE:CD1	2.75	0.41
1:A:624:ARG:HE	1:A:624:ARG:C	2.24	0.41
1:A:611:VAL:O	1:A:614:ASP:OD1	2.38	0.41
1:A:471:ASN:ND2	1:A:491:TYR:OH	2.54	0.41
1:A:555:LEU:HA	1:A:558:THR:OG1	2.21	0.41
1:A:589:ASP:HB3	1:A:592:ARG:HH11	1.86	0.41
1:A:282:ARG:HG2	1:A:308:ARG:NE	2.36	0.40
1:A:287:ARG:HD3	1:A:290:GLU:OE1	2.21	0.40
1:A:451:LEU:HA	1:A:451:LEU:HD23	1.74	0.40
1:A:117:PHE:HD2	3:A:1647:GUN:N2	2.19	0.40
1:A:140:LEU:HD11	1:A:392:ILE:HG13	2.03	0.40
1:A:224:ASP:HA	1:A:225:PRO:HD3	2.00	0.40
1:A:338:ASN:ND2	1:A:339:PHE:N	2.68	0.40
1:A:511:PRO:O	1:A:574:MET:CB	2.69	0.40
1:A:158:PRO:HB3	1:A:373:TYR:CE2	2.56	0.40
1:A:466:ARG:HD2	1:A:505:GLU:O	2.21	0.40
1:A:574:MET:SD	1:A:574:MET:C	3.00	0.40
1:A:631:GLY:O	1:A:633:SER:CB	2.64	0.40
1:A:250:LYS:HG3	1:A:251:HIS:CE1	2.57	0.40
1:A:578:TRP:CZ2	1:A:586:LYS:HB2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	605/644 (94%)	451 (74%)	116 (19%)	38 (6%)	1 10

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	97	HIS
1	A	163	TYR
1	A	489	LEU
1	A	587	LEU
1	A	592	ARG
1	A	630	GLU
1	A	632	ALA
1	A	633	SER
1	A	19	LYS
1	A	30	GLY
1	A	81	ILE
1	A	95	ARG
1	A	137	ALA
1	A	282	ARG
1	A	380	ARG
1	A	442	PRO
1	A	535	PRO
1	A	612	ARG
1	A	634	ILE
1	A	3	GLU
1	A	13	GLU
1	A	161	MET
1	A	178	LYS
1	A	181	SER
1	A	588	ARG
1	A	183	LEU
1	A	232	ASP

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Mol	Chain	Res	Type
1	A	297	GLY
1	A	355	ASP
1	A	377	ASP
1	A	379	GLY
1	A	422	PRO
1	A	594	ALA
1	A	635	ASP
1	A	445	ASP
1	A	479	TRP
1	A	628	MET

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	542/571 (95%)	443 (82%)	99 (18%)	1 8

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	13	GLU
1	A	14	LEU
1	A	25	ILE
1	A	28	LEU
1	A	29	THR
1	A	35	ASN
1	A	36	ASP
1	A	43	LYS
1	A	46	THR
1	A	65	HIS
1	A	76	VAL
1	A	91	ARG
1	A	99	MET
1	A	109	ARG
1	A	110	ARG

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Mol	Chain	Res	Type
1	A	111	ILE
1	A	119	ASP
1	A	138	GLU
1	A	161	MET
1	A	165	GLU
1	A	166	ILE
1	A	168	THR
1	A	169	ARG
1	A	175	THR
1	A	180	VAL
1	A	195	TYR
1	A	196	ILE
1	A	203	THR
1	A	209	LYS
1	A	210	ARG
1	A	219	LEU
1	A	226	ILE
1	A	230	CYS
1	A	237	VAL
1	A	240	ILE
1	A	241	MET
1	A	247	ASP
1	A	249	LEU
1	A	255	LEU
1	A	258	VAL
1	A	267	SER
1	A	277	GLU
1	A	278	TRP
1	A	281	THR
1	A	287	ARG
1	A	291	GLU
1	A	296	MET
1	A	308	ARG
1	A	320	SER
1	A	324	PHE
1	A	343	ARG
1	A	346	SER
1	A	358	VAL
1	A	361	VAL
1	A	367	ARG
1	A	376	ARG
1	A	378	ARG

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Mol	Chain	Res	Type
1	A	412	LEU
1	A	413	THR
1	A	430	LYS
1	A	438	VAL
1	A	443	LEU
1	A	444	TYR
1	A	445	ASP
1	A	446	TYR
1	A	466	ARG
1	A	471	ASN
1	A	475	LEU
1	A	477	LEU
1	A	480	ARG
1	A	481	TYR
1	A	486	LYS
1	A	487	LYS
1	A	493	PRO
1	A	503	LEU
1	A	512	VAL
1	A	528	SER
1	A	530	LEU
1	A	532	VAL
1	A	551	LEU
1	A	574	MET
1	A	575	ILE
1	A	577	ASP
1	A	581	GLN
1	A	583	ARG
1	A	587	LEU
1	A	590	LEU
1	A	591	LYS
1	A	592	ARG
1	A	593	SER
1	A	596	GLU
1	A	598	ILE
1	A	600	TRP
1	A	613	ASN
1	A	614	ASP
1	A	624	ARG
1	A	640	LEU
1	A	644	LEU

Sometimes 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	133	HIS
1	A	141	ASN
1	A	148	HIS
1	A	317	HIS
1	A	338	ASN
1	A	389	HIS
1	A	400	HIS
1	A	414	ASN
1	A	471	ASN
1	A	581	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\|>2$
3	GUN	A	1646	-	7,12,12	1.39	1 (14%)	8,17,17	1.45	1 (12%)
2	M7G	A	1645	-	26,31,31	1.77	7 (26%)	28,49,49	1.50	7 (25%)
3	GUN	A	1647	-	7,12,12	1.16	1 (14%)	8,17,17	1.41	2 (25%)

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
3	GUN	A	1646	-	-	-	0/2/2/2
2	M7G	A	1645	-	2/2/6/6	3/12/32/32	0/3/3/3
3	GUN	A	1647	-	-	-	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1645	M7G	O4'-C1'	4.65	1.47	1.41
2	A	1645	M7G	PB-O1B	3.49	1.61	1.50
2	A	1645	M7G	PA-O1A	2.81	1.60	1.50
2	A	1645	M7G	C5'-C4'	2.62	1.59	1.51
2	A	1645	M7G	C5-C6	-2.53	1.39	1.45
3	A	1646	GUN	C6-N1	-2.47	1.34	1.37
2	A	1645	M7G	PB-O2B	2.42	1.64	1.54
2	A	1645	M7G	C6-N1	2.12	1.41	1.37
3	A	1647	GUN	C6-N1	-2.11	1.34	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1646	GUN	C8-N7-C5	3.07	108.84	102.99
2	A	1645	M7G	PA-O3A-PB	-2.87	122.99	132.83
2	A	1645	M7G	C2-N1-C6	-2.85	119.85	125.10
2	A	1645	M7G	N2-C2-N1	2.54	122.13	116.71
2	A	1645	M7G	O3B-PB-O3A	2.51	113.06	104.64
2	A	1645	M7G	O3B-PB-O2B	2.36	116.66	107.64
2	A	1645	M7G	C5'-C4'-C3'	2.35	123.98	115.18
2	A	1645	M7G	O2B-PB-O1B	-2.25	101.87	110.68
3	A	1647	GUN	C8-N7-C5	2.21	107.19	102.99
3	A	1647	GUN	C5-C6-N1	2.16	117.77	113.95

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1645	M7G	C1'
2	A	1645	M7G	C4'

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1645	M7G	C4'-C5'-O5'-PA
2	A	1645	M7G	C3'-C4'-C5'-O5'
2	A	1645	M7G	O4'-C4'-C5'-O5'

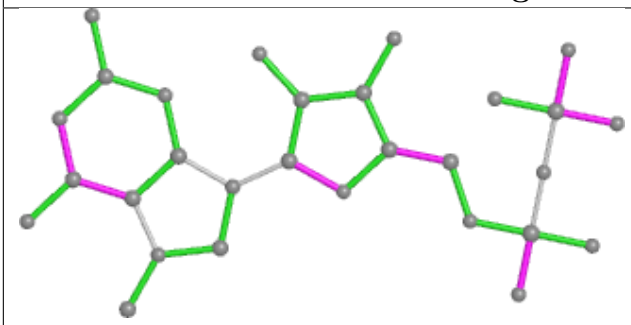
There are no ring outliers.

3 monomers are involved in 5 short contacts:

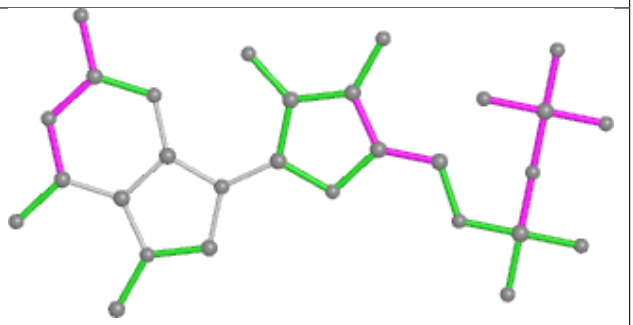
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1646	GUN	1	0
2	A	1645	M7G	1	0
3	A	1647	GUN	3	0

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

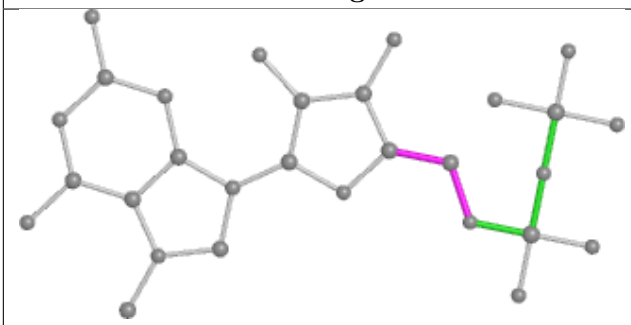
Ligand M7G A 1645



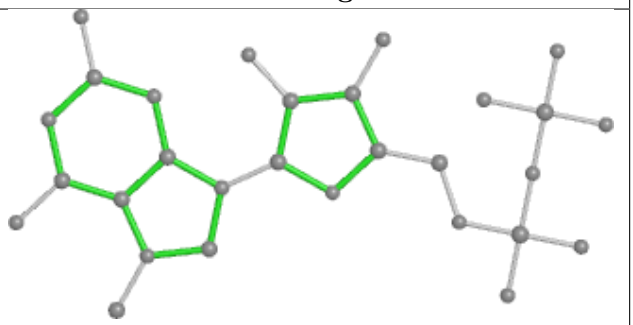
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	613/644 (95%)	-0.04	11 (1%) 68 56	53, 71, 87, 96	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	ASN	3.7
1	A	399	LEU	3.0
1	A	303	ALA	2.9
1	A	229	GLU	2.8
1	A	401	GLU	2.6
1	A	269	ASP	2.5
1	A	585	GLN	2.3
1	A	628	MET	2.2
1	A	255	LEU	2.1
1	A	408	ASP	2.0
1	A	580	ALA	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

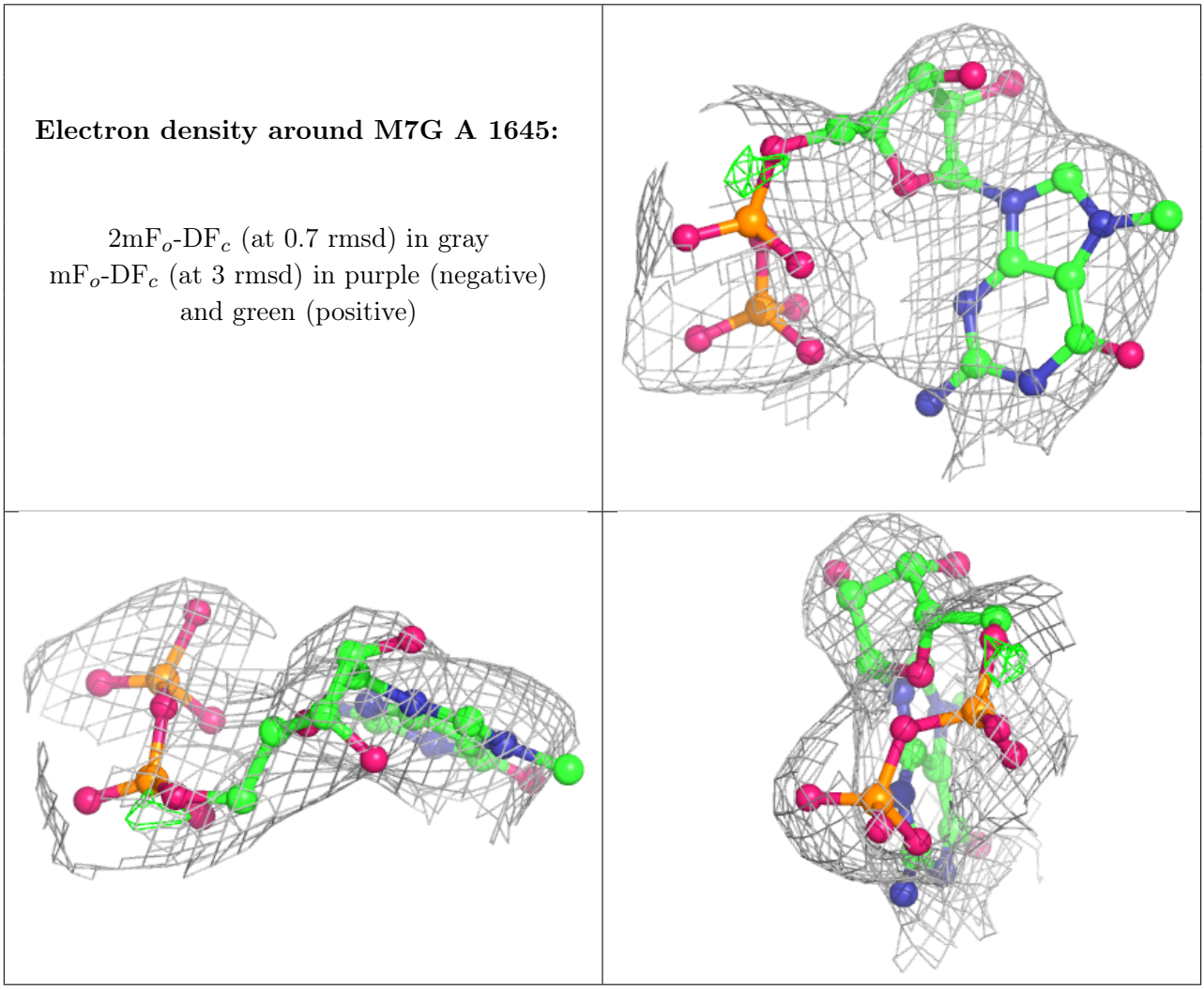
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	M7G	A	1645	29/29	0.83	0.22	120,123,125,125	0
3	GUN	A	1646	11/11	0.84	0.52	154,154,154,154	0
3	GUN	A	1647	11/11	0.89	0.38	128,128,129,129	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 M7G A 1645:

$2mF_o$-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.