Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:11 am BST

PDB ID	:	2JHA
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	:	3.40 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 following versions of software and data (see references ⓘ) were used in the production of this report:

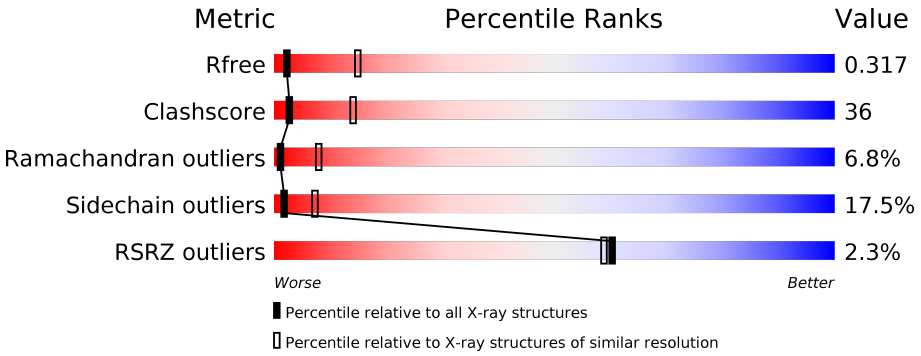
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 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% 39% 43% 11% • 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	GP3	A	1645	-	-	-	X
3	GUN	A	1646	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5113 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.

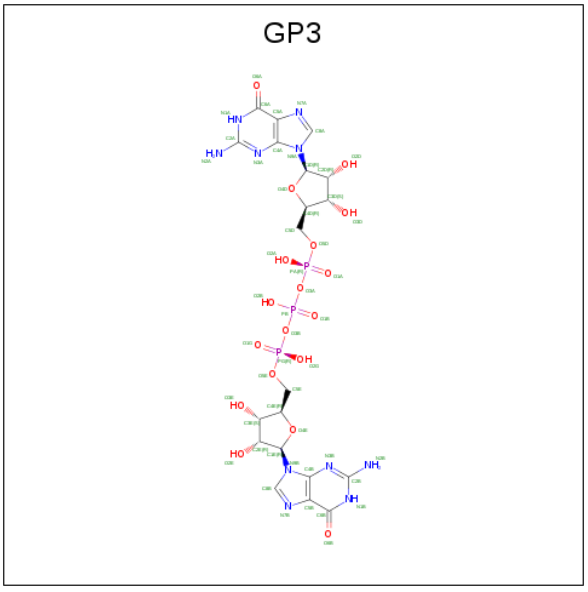
- Molecule 1 is a protein called VP4 CORE PROTEIN.

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:

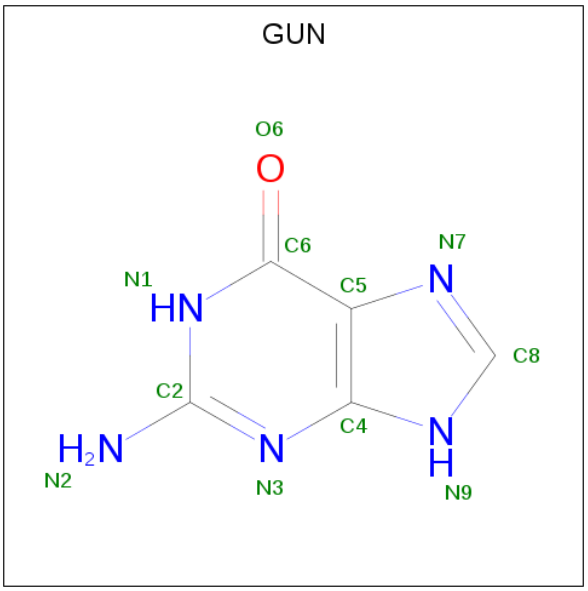
Chain	Residue	Modelled	Actual	Comment	Reference
A	261	LEU	PRO	conflict	UNP P07132

- Molecule 2 is DIGUANOSINE-5'-TRIPHOSPHATE (three-letter code: GP3) (formula: $C_{20}H_{27}N_{10}O_{18}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			51	20	10	18	3		

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



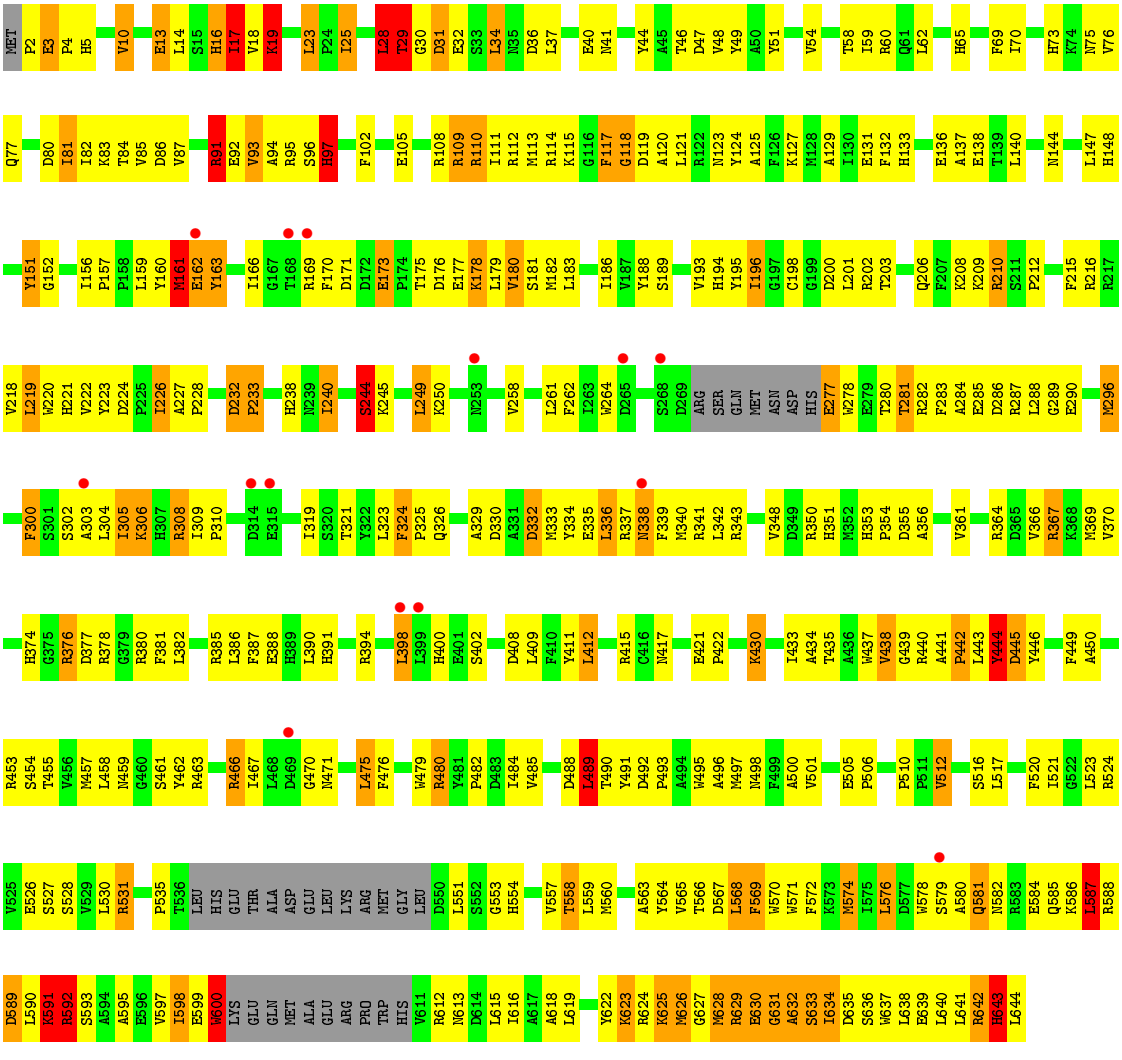
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 11 5 5 1	0	0
3	A	1	Total C N O 11 5 5 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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

Chain A: 2% 39% 43% 11% 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	75.40Å 75.40Å 422.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 3.40 24.88 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.00-3.40) 99.6 (24.88-3.40)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 3.38Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.331 0.232 , 0.317	Depositor DCC
R_{free} test set	516 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	105.8	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 79.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5113	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: GUN, GP3

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	1.03	20/5167 (0.4%)	0.97	8/6981 (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	5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	592	ARG	CZ-NH1	34.13	1.77	1.33
1	A	592	ARG	CZ-NH2	14.16	1.51	1.33
1	A	380	ARG	NE-CZ	12.34	1.49	1.33
1	A	92	GLU	CG-CD	9.97	1.67	1.51
1	A	589	ASP	CG-OD1	9.91	1.48	1.25
1	A	277	GLU	CG-CD	9.58	1.66	1.51
1	A	92	GLU	CD-OE2	9.44	1.36	1.25
1	A	592	ARG	CD-NE	8.99	1.61	1.46
1	A	584	GLU	CD-OE2	8.52	1.35	1.25
1	A	244	SER	CB-OG	8.27	1.53	1.42
1	A	589	ASP	CG-OD2	7.86	1.43	1.25
1	A	277	GLU	CD-OE2	7.85	1.34	1.25
1	A	162	GLU	CD-OE1	7.79	1.34	1.25
1	A	92	GLU	CD-OE1	7.63	1.34	1.25
1	A	162	GLU	CD-OE2	7.57	1.33	1.25
1	A	380	ARG	CZ-NH1	7.53	1.42	1.33
1	A	600	TRP	C-O	7.51	1.37	1.23
1	A	592	ARG	NE-CZ	6.75	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	GLU	CD-OE2	-5.90	1.19	1.25
1	A	430	LYS	CD-CE	5.89	1.66	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	592	ARG	NE-CZ-NH2	-18.61	110.99	120.30
1	A	592	ARG	NE-CZ-NH1	16.16	128.38	120.30
1	A	380	ARG	NE-CZ-NH2	-15.14	112.73	120.30
1	A	589	ASP	CB-CG-OD1	-9.55	109.70	118.30
1	A	173	GLU	OE1-CD-OE2	-8.95	112.56	123.30
1	A	380	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	17	ILE	CB-CA-C	-5.13	101.33	111.60
1	A	23	LEU	CA-CB-CG	5.05	126.93	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	GLU	Sidechain
1	A	28	LEU	Peptide
1	A	442	PRO	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	364	0
2	A	51	0	24	1	0
3	A	22	0	10	1	0
All	All	5113	0	5019	365	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 36.

All (365) 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:240:ILE:CD1	1:A:240:ILE:CG1	1.76	1.63
1:A:592:ARG:NH1	1:A:592:ARG:CZ	1.77	1.44
1:A:632:ALA:HB3	1:A:633:SER:CB	1.45	1.43
1:A:632:ALA:CB	1:A:633:SER:HB2	1.66	1.25
1:A:441:ALA:HB3	1:A:443:LEU:HD12	1.32	1.04
1:A:262:PHE:HB2	1:A:300:PHE:CD2	1.93	1.03
1:A:210:ARG:HG3	1:A:210:ARG:HH11	1.23	1.03
1:A:580:ALA:HB1	1:A:581:GLN:O	1.59	1.02
1:A:28:LEU:HA	1:A:29:THR:HG22	1.40	1.01
1:A:632:ALA:HB3	1:A:633:SER:HB3	1.43	1.00
1:A:201:LEU:HD12	1:A:228:PRO:HD2	1.42	1.00
1:A:632:ALA:CB	1:A:633:SER:CB	2.30	0.99
1:A:262:PHE:HB2	1:A:300:PHE:CE2	2.01	0.95
1:A:3:GLU:H	1:A:4:PRO:CD	1.78	0.95
1:A:94:ALA:HB3	1:A:95:ARG:HA	1.53	0.91
1:A:94:ALA:HB3	1:A:95:ARG:CA	2.01	0.91
1:A:632:ALA:HB3	1:A:633:SER:HB2	0.92	0.90
1:A:94:ALA:HB3	1:A:95:ARG:CB	2.03	0.88
1:A:94:ALA:CB	1:A:95:ARG:HA	2.03	0.88
1:A:633:SER:H	1:A:635:ASP:N	1.75	0.85
1:A:95:ARG:H	1:A:96:SER:CB	1.91	0.83
1:A:633:SER:H	1:A:635:ASP:H	1.27	0.82
1:A:2:PRO:HD3	1:A:439:GLY:HA2	1.62	0.82
1:A:2:PRO:HB3	1:A:440:ARG:HB2	1.61	0.81
1:A:591:LYS:HB3	1:A:592:ARG:CB	2.09	0.81
1:A:177:GLU:HG2	1:A:180:VAL:CG1	2.12	0.80
1:A:144:ASN:H	1:A:148:HIS:HD2	1.30	0.79
1:A:201:LEU:HD12	1:A:228:PRO:CD	2.13	0.78
1:A:2:PRO:HG3	1:A:453:ARG:HH22	1.48	0.78
1:A:95:ARG:N	1:A:96:SER:HB2	2.00	0.77
1:A:210:ARG:HG3	1:A:210:ARG:NH1	1.87	0.77
1:A:574:MET:O	1:A:578:TRP:HB3	1.85	0.76
1:A:264:TRP:CD2	1:A:289:GLY:HA2	2.21	0.76
1:A:2:PRO:CD	1:A:453:ARG:HH12	1.99	0.76
1:A:282:ARG:HG2	1:A:308:ARG:NH2	2.01	0.76
1:A:95:ARG:H	1:A:96:SER:CA	1.99	0.76
1:A:176:ASP:HB2	1:A:181:SER:OG	1.86	0.74
1:A:336:LEU:HD11	1:A:366:VAL:HG13	1.69	0.73
1:A:94:ALA:CB	1:A:95:ARG:CA	2.65	0.73
1:A:177:GLU:CG	1:A:180:VAL:HG12	2.20	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:LYS:HB3	1:A:592:ARG:HB3	1.72	0.71
1:A:633:SER:N	1:A:635:ASP:N	2.38	0.71
1:A:3:GLU:H	1:A:4:PRO:HD3	1.55	0.71
1:A:3:GLU:N	1:A:4:PRO:CD	2.51	0.71
1:A:589:ASP:HA	1:A:592:ARG:HG2	1.73	0.71
1:A:198:CYS:SG	1:A:222:VAL:HB	2.31	0.70
1:A:441:ALA:HB1	1:A:442:PRO:CD	2.21	0.70
1:A:201:LEU:CD1	1:A:228:PRO:HD2	2.18	0.70
1:A:94:ALA:HB3	1:A:95:ARG:HB2	1.74	0.70
1:A:249:LEU:HD22	1:A:296:MET:CE	2.22	0.70
1:A:87:VAL:HG13	1:A:109:ARG:HG2	1.74	0.69
1:A:2:PRO:CG	1:A:453:ARG:HH22	2.04	0.69
1:A:310:PRO:O	1:A:367:ARG:NH2	2.24	0.69
1:A:177:GLU:HG3	1:A:180:VAL:HG12	1.74	0.69
1:A:441:ALA:CB	1:A:443:LEU:HD12	2.18	0.69
1:A:495:TRP:HA	1:A:498:ASN:HD22	1.57	0.69
1:A:591:LYS:HB3	1:A:592:ARG:HB2	1.73	0.69
1:A:309:ILE:HD13	1:A:366:VAL:HG12	1.75	0.68
1:A:160:TYR:HB2	1:A:369:MET:HE1	1.75	0.68
1:A:249:LEU:HD22	1:A:296:MET:HE1	1.75	0.68
1:A:341:ARG:HD3	1:A:353:HIS:O	1.93	0.68
1:A:93:VAL:HG12	1:A:93:VAL:O	1.94	0.67
1:A:3:GLU:H	1:A:4:PRO:HD2	1.57	0.67
1:A:212:PRO:HB2	1:A:216:ARG:HH22	1.60	0.67
1:A:633:SER:N	1:A:635:ASP:H	1.93	0.67
1:A:208:LYS:HD3	1:A:215:PHE:CE2	2.30	0.67
1:A:471:ASN:ND2	1:A:491:TYR:OH	2.28	0.66
1:A:160:TYR:HB3	1:A:323:LEU:HB2	1.76	0.66
1:A:244:SER:OG	1:A:245:LYS:N	2.28	0.66
1:A:591:LYS:CA	1:A:592:ARG:HB3	2.25	0.66
1:A:210:ARG:CG	1:A:210:ARG:HH11	2.04	0.65
1:A:110:ARG:HG3	1:A:113:MET:HE3	1.78	0.65
1:A:587:LEU:H	1:A:588:ARG:HB3	1.59	0.65
1:A:338:ASN:HD22	1:A:339:PHE:N	1.95	0.65
1:A:510:PRO:O	1:A:512:VAL:HG12	1.97	0.65
1:A:182:MET:HE3	1:A:337:ARG:HD2	1.78	0.64
1:A:2:PRO:CG	1:A:453:ARG:HH12	2.09	0.64
1:A:321:THR:OG1	1:A:356:ALA:HB2	1.97	0.64
1:A:571:TRP:O	1:A:574:MET:HG3	1.96	0.64
1:A:264:TRP:CE3	1:A:289:GLY:HA2	2.33	0.64
1:A:495:TRP:HE1	3:A:1647:GUN:HN21	1.46	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ILE:HG23	1:A:60:ARG:H	1.63	0.64
1:A:160:TYR:HB2	1:A:369:MET:CE	2.27	0.64
1:A:505:GLU:HA	1:A:505:GLU:OE1	1.96	0.64
1:A:77:GLN:HA	1:A:77:GLN:OE1	1.99	0.63
1:A:531:ARG:NH2	1:A:531:ARG:HB2	2.14	0.63
1:A:326:GLN:HE22	1:A:335:GLU:HG2	1.63	0.63
1:A:5:HIS:HB2	1:A:47:ASP:HA	1.81	0.63
1:A:630:GLU:HB3	1:A:631:GLY:HA3	1.80	0.63
1:A:600:TRP:CE3	1:A:600:TRP:HA	2.33	0.62
1:A:628:MET:C	1:A:630:GLU:H	2.01	0.62
1:A:219:LEU:HD12	1:A:220:TRP:H	1.65	0.62
1:A:326:GLN:NE2	1:A:335:GLU:HG2	2.13	0.62
1:A:438:VAL:HA	1:A:450:ALA:HB1	1.81	0.62
1:A:453:ARG:HD3	1:A:565:VAL:HG23	1.80	0.62
1:A:162:GLU:N	1:A:163:TYR:CB	2.63	0.62
1:A:290:GLU:HG3	1:A:305:ILE:HG21	1.82	0.61
1:A:531:ARG:HB2	1:A:531:ARG:CZ	2.30	0.61
1:A:59:ILE:HG23	1:A:60:ARG:N	2.15	0.61
1:A:341:ARG:NH1	1:A:351:HIS:HA	2.15	0.61
1:A:186:ILE:HD13	1:A:304:LEU:HD22	1.83	0.61
1:A:29:THR:O	1:A:31:ASP:N	2.32	0.61
1:A:123:ASN:O	1:A:127:LYS:HG2	2.01	0.61
1:A:44:TYR:CG	1:A:48:VAL:HG11	2.35	0.60
1:A:177:GLU:CG	1:A:180:VAL:CG1	2.77	0.60
1:A:587:LEU:H	1:A:588:ARG:CB	2.14	0.60
1:A:264:TRP:CD2	1:A:289:GLY:CA	2.85	0.59
1:A:364:ARG:HA	1:A:367:ARG:HB2	1.83	0.59
1:A:623:LYS:HB3	1:A:634:ILE:HD13	1.84	0.59
1:A:109:ARG:HA	1:A:112:ARG:HB2	1.83	0.59
1:A:461:SER:OG	1:A:569:PHE:HB2	2.03	0.59
1:A:641:LEU:C	1:A:643:HIS:H	2.06	0.59
1:A:124:TYR:HA	1:A:484:ILE:HG21	1.84	0.58
1:A:93:VAL:CG1	1:A:93:VAL:O	2.50	0.58
1:A:188:TYR:CD2	1:A:189:SER:HB3	2.39	0.58
1:A:591:LYS:CB	1:A:592:ARG:HB3	2.32	0.58
1:A:102:PHE:O	1:A:105:GLU:HB3	2.03	0.58
1:A:114:ARG:HH12	1:A:445:ASP:HB3	1.68	0.58
1:A:330:ASP:O	1:A:333:MET:HB3	2.04	0.58
1:A:95:ARG:H	1:A:96:SER:HB2	1.56	0.58
1:A:2:PRO:HB3	1:A:440:ARG:CB	2.33	0.57
1:A:441:ALA:HB1	1:A:442:PRO:HD3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ALA:CA	1:A:633:SER:CB	2.81	0.57
1:A:282:ARG:HD2	1:A:308:ARG:HG3	1.85	0.57
1:A:586:LYS:O	1:A:586:LYS:HG3	2.04	0.57
1:A:200:ASP:O	1:A:201:LEU:HB2	2.03	0.57
1:A:324:PHE:HB2	1:A:325:PRO:CD	2.34	0.57
1:A:2:PRO:HG3	1:A:453:ARG:NH2	2.18	0.57
1:A:201:LEU:HD12	1:A:228:PRO:CG	2.35	0.57
1:A:437:TRP:HB3	1:A:449:PHE:O	2.05	0.57
1:A:563:ALA:HB3	1:A:564:TYR:CD1	2.39	0.57
1:A:58:THR:HA	1:A:80:ASP:HB2	1.86	0.57
1:A:633:SER:H	1:A:634:ILE:HB	1.70	0.56
1:A:86:ASP:OD2	1:A:490:THR:HG23	2.04	0.56
1:A:223:TYR:CE2	1:A:238:HIS:HD2	2.24	0.56
1:A:578:TRP:CE3	1:A:579:SER:HB3	2.40	0.56
1:A:627:GLY:O	1:A:629:ARG:N	2.37	0.56
1:A:136:GLU:HG2	1:A:388:GLU:OE2	2.05	0.56
1:A:480:ARG:C	1:A:482:PRO:HD3	2.26	0.56
1:A:634:ILE:O	1:A:637:TRP:N	2.39	0.56
1:A:578:TRP:O	1:A:581:GLN:HB2	2.05	0.56
1:A:628:MET:O	1:A:630:GLU:N	2.26	0.56
1:A:13:GLU:OE1	1:A:14:LEU:N	2.39	0.56
1:A:188:TYR:HB2	1:A:387:PHE:HE1	1.70	0.55
1:A:632:ALA:CB	1:A:633:SER:HB3	2.16	0.55
1:A:553:GLY:O	1:A:557:VAL:HG23	2.07	0.55
1:A:144:ASN:H	1:A:148:HIS:CD2	2.16	0.55
1:A:408:ASP:HB2	1:A:434:ALA:HB2	1.87	0.55
1:A:590:LEU:O	1:A:593:SER:N	2.38	0.55
1:A:59:ILE:O	1:A:62:LEU:N	2.39	0.55
1:A:324:PHE:CB	1:A:325:PRO:CD	2.84	0.54
1:A:563:ALA:HB3	1:A:564:TYR:CE1	2.42	0.54
1:A:91:ARG:HH11	1:A:95:ARG:HH22	1.56	0.54
1:A:382:LEU:HG	1:A:386:LEU:HD11	1.89	0.54
1:A:193:VAL:HG22	1:A:261:LEU:HB3	1.89	0.54
1:A:224:ASP:OD1	1:A:226:ILE:HG12	2.06	0.54
1:A:249:LEU:HD13	1:A:296:MET:HE3	1.89	0.54
1:A:17:ILE:HG23	1:A:97:HIS:HB3	1.90	0.54
1:A:262:PHE:O	1:A:303:ALA:HA	2.08	0.53
1:A:332:ASP:O	1:A:334:TYR:CD1	2.61	0.53
1:A:470:GLY:HA3	1:A:496:ALA:O	2.09	0.53
1:A:591:LYS:N	1:A:592:ARG:HB3	2.23	0.53
1:A:443:LEU:HD23	1:A:444:TYR:HD2	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ALA:CA	1:A:633:SER:HB3	2.39	0.53
1:A:179:LEU:O	1:A:182:MET:HB3	2.09	0.53
1:A:634:ILE:HG22	1:A:635:ASP:N	2.24	0.53
1:A:262:PHE:CB	1:A:300:PHE:CD2	2.82	0.52
1:A:512:VAL:HG21	1:A:595:ALA:CB	2.39	0.52
1:A:630:GLU:HB3	1:A:631:GLY:CA	2.39	0.52
1:A:554:HIS:C	1:A:554:HIS:ND1	2.62	0.52
1:A:569:PHE:O	1:A:572:PHE:HB2	2.10	0.52
1:A:177:GLU:HG2	1:A:180:VAL:HG11	1.91	0.51
1:A:488:ASP:O	1:A:489:LEU:C	2.48	0.51
1:A:458:LEU:HD23	1:A:568:LEU:HD11	1.92	0.51
1:A:16:HIS:CD2	1:A:97:HIS:CD2	2.98	0.51
1:A:466:ARG:HA	1:A:567:ASP:OD1	2.10	0.51
1:A:589:ASP:HB3	1:A:592:ARG:HH11	1.75	0.51
1:A:249:LEU:HD22	1:A:296:MET:HE3	1.93	0.51
1:A:589:ASP:CB	1:A:592:ARG:NH1	2.73	0.51
1:A:156:ILE:HG23	1:A:157:PRO:HD2	1.93	0.51
1:A:381:PHE:O	1:A:382:LEU:C	2.48	0.51
1:A:633:SER:N	1:A:634:ILE:HB	2.26	0.51
1:A:109:ARG:O	1:A:113:MET:N	2.41	0.50
1:A:3:GLU:OE1	1:A:3:GLU:HA	2.10	0.50
1:A:570:TRP:CD1	1:A:570:TRP:C	2.85	0.50
1:A:628:MET:C	1:A:630:GLU:N	2.64	0.50
1:A:65:HIS:NE2	1:A:598:ILE:HG21	2.26	0.50
1:A:2:PRO:HD2	1:A:453:ARG:HH12	1.72	0.50
1:A:136:GLU:HB3	1:A:138:GLU:OE1	2.12	0.50
1:A:111:ILE:HA	1:A:114:ARG:HG3	1.94	0.50
1:A:206:GLN:O	1:A:210:ARG:HB2	2.12	0.50
1:A:408:ASP:HB2	1:A:434:ALA:CB	2.42	0.49
1:A:615:LEU:O	1:A:618:ALA:HB3	2.12	0.49
1:A:224:ASP:HB3	1:A:227:ALA:HB2	1.94	0.49
1:A:110:ARG:HA	1:A:113:MET:HE2	1.94	0.49
1:A:282:ARG:HG2	1:A:308:ARG:CZ	2.42	0.49
1:A:96:SER:O	1:A:97:HIS:C	2.51	0.49
1:A:169:ARG:HD2	1:A:378:ARG:NH1	2.27	0.49
1:A:633:SER:H	1:A:634:ILE:CA	2.25	0.49
1:A:40:GLU:O	1:A:41:ASN:C	2.51	0.49
1:A:73:HIS:O	1:A:85:VAL:HG21	2.12	0.49
1:A:194:HIS:ND1	1:A:221:HIS:HB2	2.27	0.49
1:A:262:PHE:HB2	1:A:300:PHE:HD2	1.68	0.49
1:A:589:ASP:HB3	1:A:592:ARG:NH1	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:ASP:HA	1:A:638:LEU:HD12	1.94	0.49
1:A:625:LYS:C	1:A:626:MET:HG2	2.33	0.49
1:A:117:PHE:CE1	1:A:121:LEU:HD11	2.47	0.49
1:A:492:ASP:C	1:A:492:ASP:OD1	2.51	0.49
1:A:600:TRP:HE3	1:A:600:TRP:HA	1.78	0.49
1:A:559:LEU:HB3	1:A:622:TYR:CE1	2.48	0.48
1:A:300:PHE:CD1	1:A:300:PHE:N	2.82	0.48
1:A:329:ALA:HB1	1:A:333:MET:HG2	1.95	0.48
1:A:326:GLN:NE2	1:A:335:GLU:O	2.46	0.48
1:A:574:MET:HE1	1:A:578:TRP:HE3	1.79	0.48
1:A:264:TRP:CE2	1:A:289:GLY:CA	2.96	0.48
1:A:633:SER:H	1:A:634:ILE:CB	2.26	0.48
1:A:240:ILE:CD1	1:A:240:ILE:CB	2.84	0.48
1:A:591:LYS:CB	1:A:592:ARG:CB	2.86	0.48
1:A:382:LEU:HG	1:A:386:LEU:CD1	2.43	0.48
1:A:120:ALA:HB1	1:A:485:VAL:HG22	1.96	0.48
1:A:182:MET:HG2	1:A:183:LEU:N	2.28	0.48
1:A:25:ILE:HD12	1:A:25:ILE:H	1.78	0.48
1:A:162:GLU:CA	1:A:163:TYR:CB	2.92	0.47
1:A:201:LEU:HD12	1:A:228:PRO:HG2	1.94	0.47
1:A:437:TRP:CD1	1:A:450:ALA:HB2	2.49	0.47
1:A:117:PHE:CZ	1:A:121:LEU:HD11	2.49	0.47
1:A:219:LEU:HD12	1:A:220:TRP:N	2.29	0.47
1:A:589:ASP:CB	1:A:592:ARG:HH11	2.27	0.47
1:A:326:GLN:CD	1:A:337:ARG:HG2	2.34	0.47
1:A:443:LEU:HD23	1:A:444:TYR:CD2	2.48	0.47
1:A:23:LEU:HD12	1:A:49:TYR:CE2	2.49	0.47
1:A:495:TRP:HA	1:A:498:ASN:ND2	2.28	0.47
1:A:338:ASN:C	1:A:338:ASN:ND2	2.68	0.47
1:A:523:LEU:HA	1:A:526:GLU:HB2	1.96	0.47
1:A:140:LEU:HD13	1:A:387:PHE:CE2	2.50	0.47
1:A:188:TYR:CE2	1:A:189:SER:HB3	2.50	0.47
1:A:83:LYS:NZ	1:A:488:ASP:O	2.41	0.46
1:A:59:ILE:CG2	1:A:60:ARG:H	2.28	0.46
1:A:631:GLY:O	1:A:633:SER:C	2.53	0.46
1:A:125:ALA:O	1:A:129:ALA:N	2.43	0.46
1:A:94:ALA:HB1	1:A:95:ARG:HA	1.93	0.46
1:A:206:GLN:HB3	1:A:210:ARG:HH12	1.79	0.46
1:A:196:ILE:HD11	1:A:262:PHE:CE1	2.51	0.46
1:A:60:ARG:NH2	1:A:479:TRP:HB2	2.30	0.46
1:A:69:PHE:C	1:A:70:ILE:HG13	2.34	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:HIS:ND1	1:A:554:HIS:O	2.48	0.46
1:A:152:GLY:O	1:A:394:ARG:HA	2.16	0.46
1:A:517:LEU:HD12	1:A:566:THR:OG1	2.16	0.46
1:A:630:GLU:CB	1:A:631:GLY:CA	2.94	0.46
1:A:633:SER:H	1:A:634:ILE:C	2.19	0.46
1:A:520:PHE:HZ	1:A:566:THR:HG21	1.80	0.45
1:A:280:THR:O	1:A:283:PHE:HB3	2.16	0.45
1:A:364:ARG:CZ	1:A:364:ARG:HB3	2.45	0.45
1:A:376:ARG:NH1	1:A:376:ARG:O	2.50	0.45
1:A:557:VAL:O	1:A:559:LEU:N	2.50	0.45
1:A:531:ARG:CB	1:A:531:ARG:CZ	2.93	0.45
1:A:576:LEU:H	1:A:576:LEU:HG	1.57	0.45
1:A:300:PHE:HD1	1:A:300:PHE:N	2.14	0.45
1:A:309:ILE:HD13	1:A:366:VAL:CG1	2.46	0.45
1:A:421:GLU:HB2	1:A:422:PRO:HD3	1.97	0.45
1:A:444:TYR:CD2	1:A:444:TYR:N	2.82	0.45
1:A:633:SER:HA	1:A:636:SER:H	1.81	0.45
1:A:377:ASP:OD2	1:A:377:ASP:C	2.55	0.45
1:A:132:PHE:C	1:A:133:HIS:HD2	2.19	0.45
1:A:411:TYR:CZ	1:A:412:LEU:CD1	3.00	0.45
1:A:125:ALA:HB2	1:A:433:ILE:HG21	1.99	0.45
1:A:193:VAL:N	1:A:219:LEU:O	2.50	0.45
1:A:409:LEU:HD21	1:A:433:ILE:HG12	1.99	0.44
1:A:571:TRP:O	1:A:572:PHE:C	2.56	0.44
1:A:170:PHE:HD1	1:A:171:ASP:O	2.00	0.44
1:A:283:PHE:C	1:A:285:GLU:H	2.21	0.44
1:A:124:TYR:O	1:A:127:LYS:HB2	2.17	0.44
1:A:157:PRO:HG2	1:A:159:LEU:HD21	1.98	0.44
1:A:177:GLU:O	1:A:178:LYS:C	2.54	0.44
1:A:321:THR:HG23	1:A:354:PRO:O	2.17	0.44
1:A:13:GLU:O	1:A:16:HIS:CE1	2.71	0.44
1:A:641:LEU:O	1:A:643:HIS:N	2.42	0.44
1:A:232:ASP:HA	1:A:233:PRO:HD3	1.84	0.43
1:A:133:HIS:O	1:A:411:TYR:CE2	2.71	0.43
1:A:286:ASP:HB2	1:A:287:ARG:NH2	2.34	0.43
1:A:435:THR:HA	1:A:500:ALA:O	2.18	0.43
1:A:638:LEU:C	1:A:640:LEU:H	2.21	0.43
1:A:306:LYS:HD3	1:A:308:ARG:HD2	2.01	0.43
1:A:34:LEU:HD11	1:A:598:ILE:HG23	1.99	0.43
1:A:586:LYS:HA	1:A:589:ASP:OD2	2.18	0.43
1:A:592:ARG:HG3	1:A:593:SER:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:GLN:HB3	1:A:582:ASN:H	1.60	0.43
1:A:180:VAL:O	1:A:183:LEU:HB2	2.18	0.43
1:A:441:ALA:HB1	1:A:442:PRO:HD2	1.99	0.43
1:A:3:GLU:N	1:A:4:PRO:HD3	2.29	0.43
1:A:16:HIS:HA	1:A:19:LYS:HD3	2.01	0.43
1:A:25:ILE:HD12	1:A:25:ILE:N	2.32	0.43
1:A:324:PHE:HB2	1:A:325:PRO:HD2	2.00	0.43
1:A:455:THR:HG22	1:A:459:ASN:ND2	2.34	0.43
1:A:336:LEU:HD11	1:A:366:VAL:CG1	2.43	0.43
1:A:177:GLU:OE1	1:A:202:ARG:NH1	2.52	0.43
1:A:398:LEU:HD11	1:A:417:ASN:OD1	2.19	0.43
1:A:144:ASN:ND2	1:A:147:LEU:HB3	2.34	0.43
1:A:304:LEU:HA	1:A:304:LEU:HD12	1.88	0.43
1:A:480:ARG:O	1:A:482:PRO:HD3	2.19	0.43
1:A:631:GLY:O	1:A:633:SER:CA	2.67	0.43
1:A:75:ASN:N	1:A:75:ASN:OD1	2.52	0.43
1:A:162:GLU:HB3	1:A:163:TYR:CB	2.49	0.42
1:A:221:HIS:HD1	1:A:238:HIS:HE2	1.64	0.42
1:A:282:ARG:HG2	1:A:308:ARG:HH21	1.83	0.42
1:A:505:GLU:HA	1:A:506:PRO:HD2	1.69	0.42
1:A:381:PHE:O	1:A:385:ARG:HG3	2.19	0.42
2:A:1645:GP3:O3B	2:A:1645:GP3:H3E	2.19	0.42
1:A:218:VAL:HB	1:A:220:TRP:NE1	2.34	0.42
1:A:454:SER:O	1:A:458:LEU:HG	2.20	0.42
1:A:574:MET:SD	1:A:574:MET:C	2.98	0.42
1:A:437:TRP:HD1	1:A:450:ALA:HB2	1.85	0.42
1:A:579:SER:HA	1:A:580:ALA:HA	1.78	0.42
1:A:121:LEU:O	1:A:124:TYR:HB3	2.20	0.42
1:A:470:GLY:HA2	1:A:501:VAL:CG2	2.50	0.42
1:A:527:SER:O	1:A:530:LEU:HB3	2.19	0.42
1:A:629:ARG:O	1:A:630:GLU:HG3	2.19	0.42
1:A:161:MET:HE3	1:A:321:THR:O	2.19	0.42
1:A:338:ASN:ND2	1:A:339:PHE:N	2.64	0.42
1:A:133:HIS:HE1	1:A:400:HIS:ND1	2.17	0.42
1:A:631:GLY:O	1:A:633:SER:HB3	2.20	0.42
1:A:288:LEU:O	1:A:289:GLY:C	2.56	0.41
1:A:350:ARG:NH2	1:A:391:HIS:ND1	2.66	0.41
1:A:131:GLU:OE1	1:A:402:SER:HB3	2.20	0.41
1:A:151:TYR:N	1:A:151:TYR:CD1	2.88	0.41
1:A:348:VAL:HG12	1:A:350:ARG:HG2	2.01	0.41
1:A:117:PHE:O	1:A:118:GLY:C	2.58	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TYR:HB2	1:A:369:MET:HE3	2.03	0.41
1:A:580:ALA:HB1	1:A:581:GLN:C	2.34	0.41
1:A:281:THR:O	1:A:282:ARG:C	2.58	0.41
1:A:28:LEU:HA	1:A:29:THR:CG2	2.30	0.41
1:A:262:PHE:CE2	1:A:264:TRP:HB2	2.55	0.41
1:A:5:HIS:CE1	1:A:44:TYR:O	2.74	0.41
1:A:461:SER:HB2	1:A:467:ILE:CG2	2.51	0.41
1:A:521:ILE:HD13	1:A:521:ILE:HA	1.82	0.41
1:A:117:PHE:O	1:A:119:ASP:N	2.54	0.41
1:A:218:VAL:HG12	1:A:219:LEU:N	2.35	0.41
1:A:459:ASN:O	1:A:462:TYR:HE1	2.04	0.41
1:A:323:LEU:HD23	1:A:338:ASN:HA	2.03	0.41
1:A:10:VAL:HA	1:A:70:ILE:O	2.21	0.41
1:A:221:HIS:ND1	1:A:238:HIS:NE2	2.64	0.41
1:A:493:PRO:O	1:A:497:MET:HG3	2.21	0.41
1:A:586:LYS:CG	1:A:586:LYS:O	2.67	0.41
1:A:95:ARG:H	1:A:96:SER:C	2.25	0.41
1:A:133:HIS:O	1:A:411:TYR:CD2	2.74	0.41
1:A:475:LEU:HD12	1:A:475:LEU:HA	1.88	0.41
1:A:306:LYS:HD3	1:A:308:ARG:CD	2.51	0.40
1:A:415:ARG:HG3	1:A:415:ARG:HH11	1.86	0.40
1:A:2:PRO:HG2	1:A:453:ARG:HH22	1.84	0.40
1:A:62:LEU:HA	1:A:62:LEU:HD23	1.77	0.40
1:A:136:GLU:CB	1:A:138:GLU:OE1	2.69	0.40
1:A:390:LEU:HA	1:A:390:LEU:HD23	1.98	0.40
1:A:37:LEU:O	1:A:41:ASN:HB2	2.22	0.40
1:A:77:GLN:OE1	1:A:82:ILE:HG12	2.22	0.40
1:A:224:ASP:CG	1:A:226:ILE:HG12	2.42	0.40
1:A:370:VAL:O	1:A:374:HIS:HB2	2.20	0.40
1:A:476:PHE:N	1:A:516:SER:HB2	2.36	0.40
1:A:59:ILE:CG2	1:A:60:ARG:N	2.81	0.40
1:A:140:LEU:HD22	1:A:188:TYR:CE1	2.57	0.40
1:A:19:LYS:HE3	1:A:51:TYR:CE2	2.57	0.40
1:A:208:LYS:C	1:A:210:ARG:N	2.75	0.40
1:A:218:VAL:HB	1:A:220:TRP:HE1	1.86	0.40
1:A:303:ALA:HB3	1:A:340:MET:HB2	2.03	0.40
1:A:411:TYR:CZ	1:A:412:LEU:HD12	2.56	0.40
1:A:612:ARG:O	1:A:616:ILE:HG23	2.21	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%)	465 (77%)	99 (16%)	41 (7%)	1 8

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	29	THR
1	A	30	GLY
1	A	163	TYR
1	A	166	ILE
1	A	203	THR
1	A	444	TYR
1	A	558	THR
1	A	587	LEU
1	A	591	LYS
1	A	592	ARG
1	A	630	GLU
1	A	632	ALA
1	A	633	SER
1	A	19	LYS
1	A	31	ASP
1	A	93	VAL
1	A	97	HIS
1	A	161	MET
1	A	178	LYS
1	A	284	ALA
1	A	355	ASP
1	A	628	MET
1	A	629	ARG
1	A	634	ILE
1	A	642	ARG
1	A	32	GLU
1	A	81	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	91	ARG
1	A	117	PHE
1	A	118	GLY
1	A	250	LYS
1	A	489	LEU
1	A	643	HIS
1	A	3	GLU
1	A	639	GLU
1	A	108	ARG
1	A	137	ALA
1	A	535	PRO
1	A	568	LEU
1	A	18	VAL

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%)	447 (82%)	95 (18%)	2 7

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	13	GLU
1	A	17	ILE
1	A	19	LYS
1	A	25	ILE
1	A	28	LEU
1	A	29	THR
1	A	34	LEU
1	A	36	ASP
1	A	46	THR
1	A	54	VAL
1	A	76	VAL
1	A	81	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	84	THR
1	A	91	ARG
1	A	97	HIS
1	A	109	ARG
1	A	110	ARG
1	A	115	LYS
1	A	151	TYR
1	A	161	MET
1	A	175	THR
1	A	180	VAL
1	A	195	TYR
1	A	196	ILE
1	A	209	LYS
1	A	210	ARG
1	A	219	LEU
1	A	226	ILE
1	A	232	ASP
1	A	233	PRO
1	A	240	ILE
1	A	244	SER
1	A	249	LEU
1	A	258	VAL
1	A	277	GLU
1	A	278	TRP
1	A	281	THR
1	A	296	MET
1	A	300	PHE
1	A	302	SER
1	A	305	ILE
1	A	306	LYS
1	A	308	ARG
1	A	319	ILE
1	A	324	PHE
1	A	332	ASP
1	A	336	LEU
1	A	338	ASN
1	A	342	LEU
1	A	343	ARG
1	A	361	VAL
1	A	367	ARG
1	A	376	ARG
1	A	398	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	412	LEU
1	A	430	LYS
1	A	438	VAL
1	A	444	TYR
1	A	445	ASP
1	A	446	TYR
1	A	457	MET
1	A	463	ARG
1	A	466	ARG
1	A	475	LEU
1	A	480	ARG
1	A	489	LEU
1	A	512	VAL
1	A	524	ARG
1	A	528	SER
1	A	531	ARG
1	A	551	LEU
1	A	558	THR
1	A	560	MET
1	A	569	PHE
1	A	574	MET
1	A	576	LEU
1	A	581	GLN
1	A	585	GLN
1	A	587	LEU
1	A	591	LYS
1	A	592	ARG
1	A	597	VAL
1	A	598	ILE
1	A	599	GLU
1	A	600	TRP
1	A	613	ASN
1	A	619	LEU
1	A	623	LYS
1	A	624	ARG
1	A	625	LYS
1	A	626	MET
1	A	642	ARG
1	A	643	HIS
1	A	644	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	133	HIS
1	A	148	HIS
1	A	317	HIS
1	A	338	ASN
1	A	414	ASN
1	A	471	ASN
1	A	581	GLN
1	A	582	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 carbohydrates 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	$\#\|Z\| > 2$
2	GP3	A	1645	-	44,56,56	1.72	6 (13%)	51,88,88	2.17	15 (29%)
3	GUN	A	1647	-	9,12,12	1.72	2 (22%)	8,17,17	3.56	6 (75%)
3	GUN	A	1646	-	9,12,12	1.87	2 (22%)	8,17,17	3.38	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	GP3	A	1645	-	-	10/24/64/64	0/6/6/6
3	GUN	A	1647	-	-	-	0/2/2/2
3	GUN	A	1646	-	-	-	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1645	GP3	C6A-N1A	5.29	1.42	1.33
2	A	1645	GP3	C6B-N1B	5.06	1.41	1.33
3	A	1646	GUN	C6-C5	4.79	1.49	1.41
3	A	1647	GUN	C6-C5	4.48	1.49	1.41
2	A	1645	GP3	O4E-C1E	4.00	1.46	1.41
2	A	1645	GP3	C2A-N1A	3.81	1.42	1.35
2	A	1645	GP3	C2B-N1B	3.46	1.41	1.35
2	A	1645	GP3	O4D-C1D	3.34	1.45	1.41
3	A	1646	GUN	C5-C4	2.48	1.47	1.40
3	A	1647	GUN	C5-C4	2.07	1.46	1.40

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1645	GP3	C2A-N3A-C4A	5.83	122.01	115.36
3	A	1647	GUN	C6-C5-C4	-5.71	115.34	120.80
2	A	1645	GP3	C2B-N3B-C4B	5.71	121.88	115.36
2	A	1645	GP3	N3A-C2A-N1A	-5.66	119.68	127.22
2	A	1645	GP3	N3B-C2B-N1B	-5.53	119.85	127.22
3	A	1646	GUN	C6-C5-C4	-4.78	116.24	120.80
3	A	1646	GUN	C5-C6-N1	-4.43	117.37	123.43
3	A	1646	GUN	C6-N1-C2	4.36	122.86	115.93
3	A	1647	GUN	C6-N1-C2	4.24	122.67	115.93
3	A	1646	GUN	C4-C5-N7	-3.96	105.27	109.40
3	A	1647	GUN	C5-C6-N1	-3.82	118.20	123.43
3	A	1647	GUN	C2-N3-C4	3.82	119.72	115.36
2	A	1645	GP3	C5A-C6A-N1A	-3.53	118.60	123.43
2	A	1645	GP3	O4E-C1E-C2E	-3.34	102.05	106.93
3	A	1647	GUN	N3-C2-N1	-3.26	122.88	127.22
2	A	1645	GP3	C5B-C6B-N1B	-3.21	119.04	123.43
3	A	1647	GUN	C4-C5-N7	-3.13	106.14	109.40
2	A	1645	GP3	PB-O3A-PA	-2.94	122.74	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1645	GP3	N2B-C2B-N1B	2.67	121.41	117.25
3	A	1646	GUN	N3-C2-N1	-2.63	123.71	127.22
3	A	1646	GUN	C2-N3-C4	2.61	118.34	115.36
2	A	1645	GP3	C6A-N1A-C2A	2.33	119.64	115.93
2	A	1645	GP3	C3D-C2D-C1D	2.25	104.37	100.98
2	A	1645	GP3	N2A-C2A-N1A	2.16	120.62	117.25
2	A	1645	GP3	O2B-PB-O1B	2.12	122.70	112.24
2	A	1645	GP3	C1D-N9A-C4A	2.08	130.30	126.64
2	A	1645	GP3	C6B-N1B-C2B	2.01	119.13	115.93

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1645	GP3	C5D-O5D-PA-O1A
2	A	1645	GP3	C5E-O5E-PG-O2G
2	A	1645	GP3	O4E-C4E-C5E-O5E
2	A	1645	GP3	C3E-C4E-C5E-O5E
2	A	1645	GP3	PB-O3A-PA-O5D
2	A	1645	GP3	C5D-O5D-PA-O3A
2	A	1645	GP3	C5E-O5E-PG-O3B
2	A	1645	GP3	C4E-C5E-O5E-PG
2	A	1645	GP3	C5D-O5D-PA-O2A
2	A	1645	GP3	C5E-O5E-PG-O1G

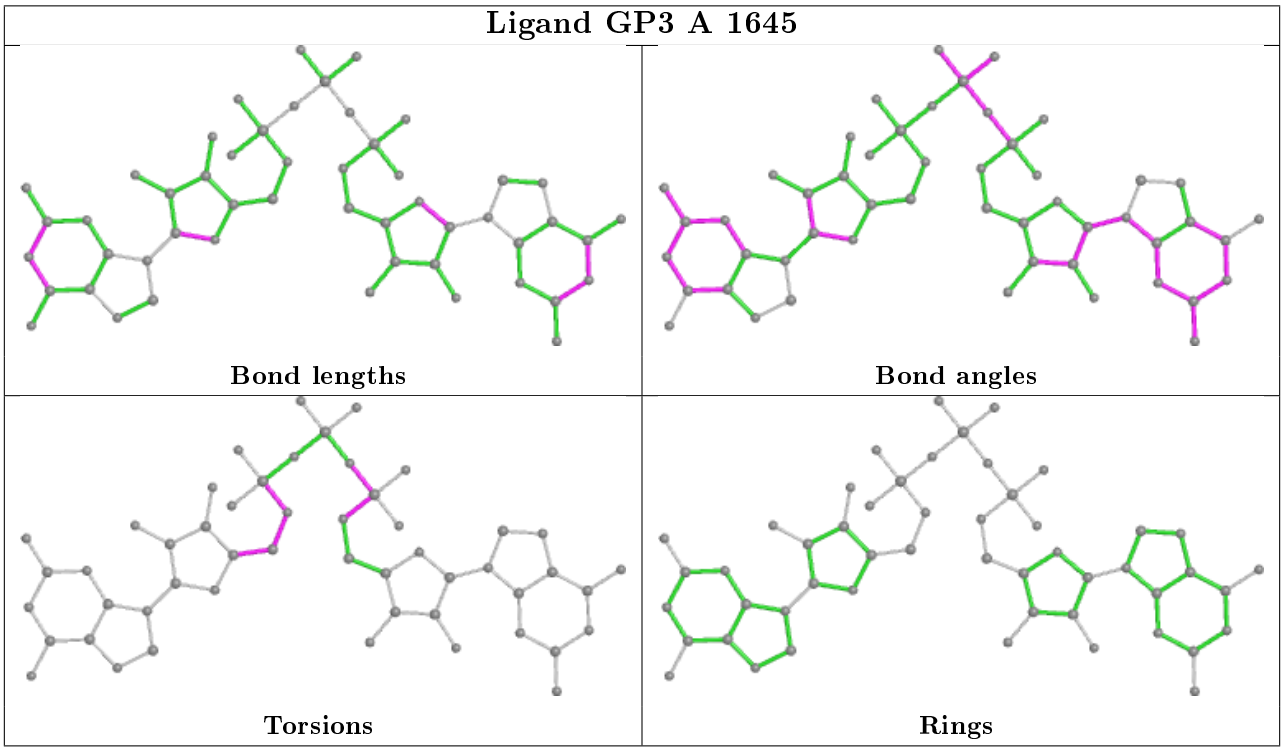
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1645	GP3	1	0
3	A	1647	GUN	1	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.



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, 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%)	-0.13	14 (2%) 60 59	72, 87, 96, 103	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	399	LEU	4.3
1	A	338	ASN	3.3
1	A	168	THR	3.2
1	A	253	ASN	3.1
1	A	314	ASP	3.0
1	A	169	ARG	2.9
1	A	268	SER	2.8
1	A	579	SER	2.6
1	A	162	GLU	2.3
1	A	398	LEU	2.3
1	A	315	GLU	2.3
1	A	265	ASP	2.3
1	A	469	ASP	2.2
1	A	303	ALA	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

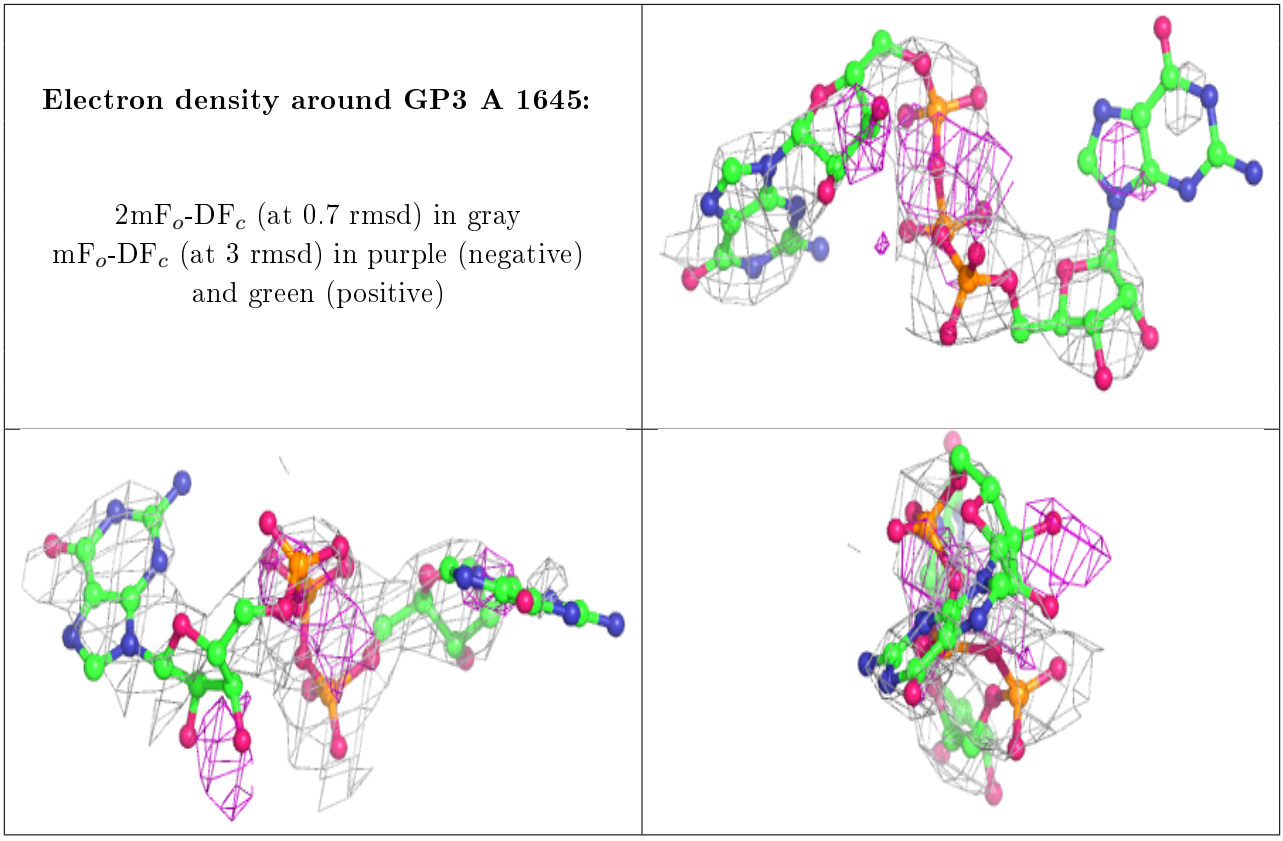
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	GUN	A	1646	11/11	0.62	0.87	184,184,185,185	0
2	GP3	A	1645	51/51	0.75	0.55	179,180,187,188	0
3	GUN	A	1647	11/11	0.89	0.44	133,134,134,134	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 GP3 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

There are no such residues in this entry.