Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 11:11 pm BST

PDB ID	:	2JHC
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

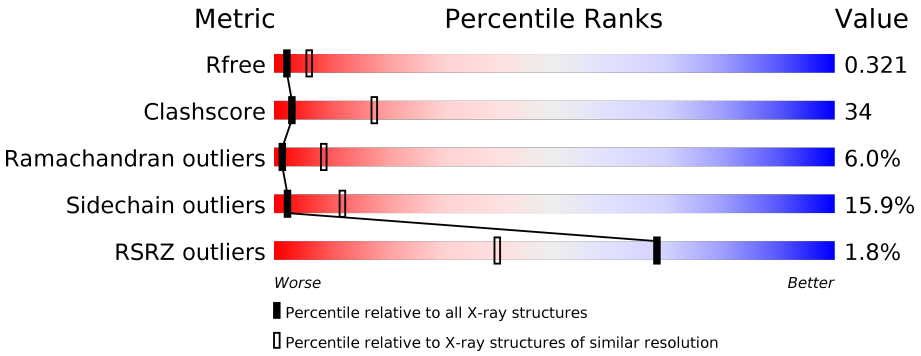
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 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% 41% 41% 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	GUN	A	1645	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5062 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.

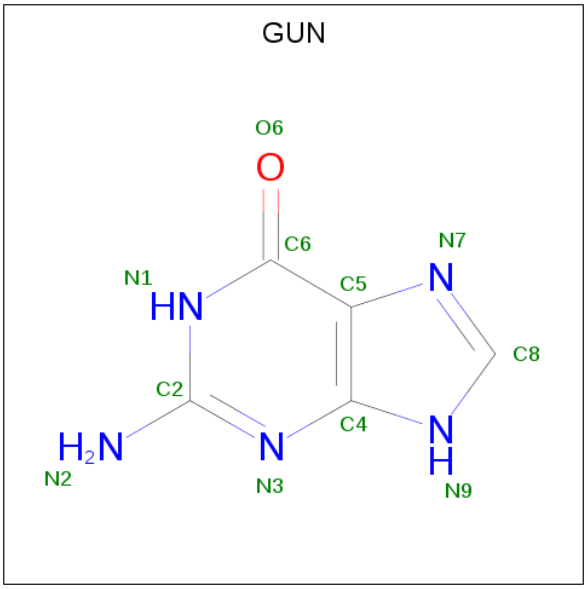
- Molecule 1 is a protein called VP4 CORE PROTEIN.

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



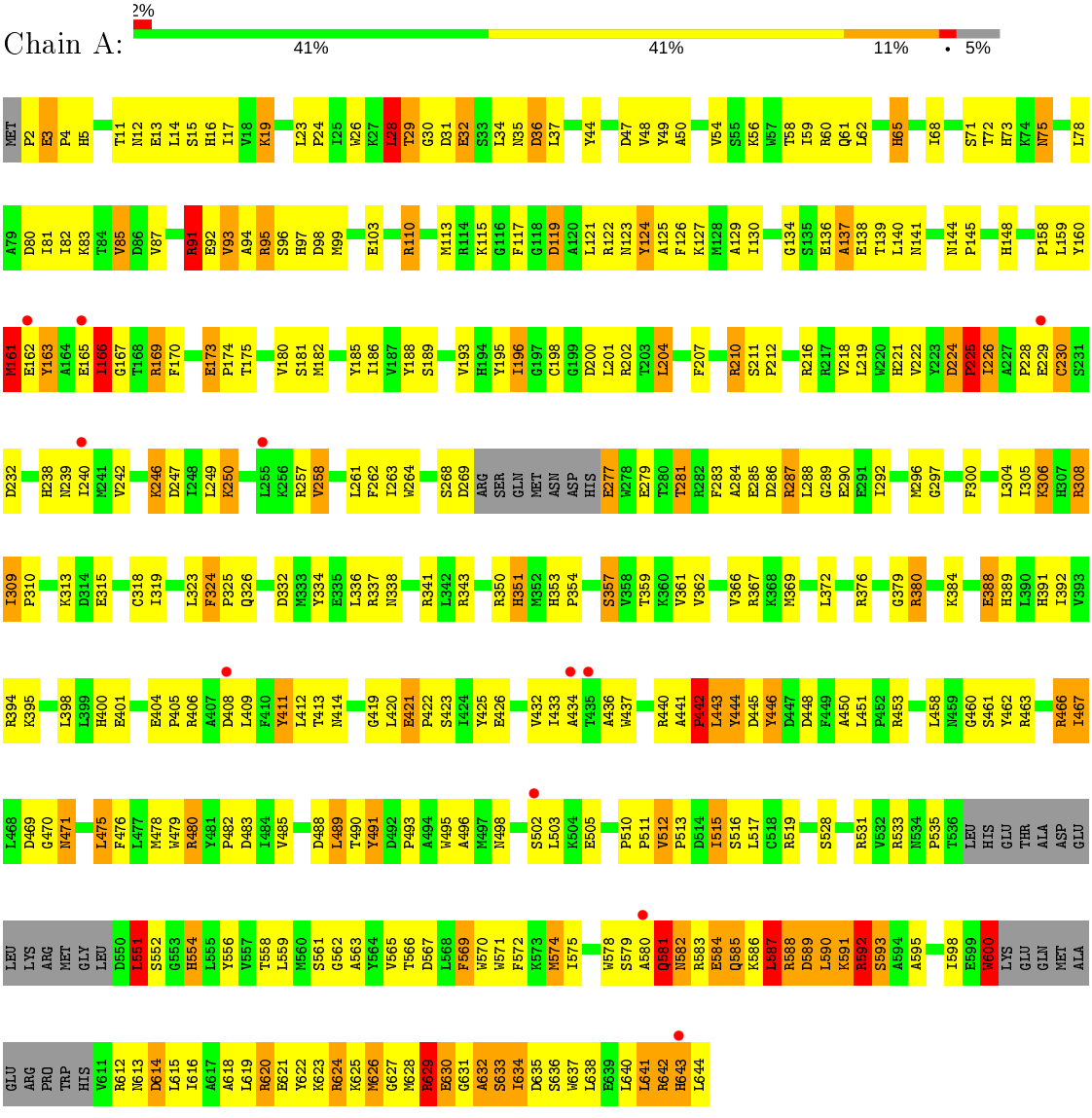
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	5	5	1		
2	A	1	Total	C	N	O	0	0
			11	5	5	1		

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:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	75.24Å 75.24Å 421.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 3.00 19.89 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.00-3.00) 100.0 (19.89-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.254 , 0.333 0.248 , 0.321	Depositor DCC
R_{free} test set	733 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	101.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 57.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5062	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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

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	1.19	44/5167 (0.9%)	0.98	16/6981 (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	5

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	600	TRP	C-O	29.45	1.79	1.23
1	A	92	GLU	CD-OE2	18.16	1.45	1.25
1	A	225	PRO	C-N	17.86	1.75	1.34
1	A	592	ARG	CZ-NH1	16.40	1.54	1.33
1	A	250	LYS	CE-NZ	14.56	1.85	1.49
1	A	173	GLU	CD-OE1	12.95	1.39	1.25
1	A	98	ASP	CG-OD2	12.83	1.54	1.25
1	A	226	ILE	C-O	10.84	1.44	1.23
1	A	35	ASN	CG-OD1	10.61	1.47	1.24
1	A	269	ASP	C-O	10.51	1.43	1.23
1	A	173	GLU	CD-OE2	10.38	1.37	1.25
1	A	279	GLU	CG-CD	10.23	1.67	1.51
1	A	279	GLU	CB-CG	9.81	1.70	1.52
1	A	246	LYS	CE-NZ	9.48	1.72	1.49
1	A	279	GLU	CD-OE1	8.95	1.35	1.25
1	A	202	ARG	CZ-NH1	8.82	1.44	1.33
1	A	165	GLU	CD-OE2	8.75	1.35	1.25
1	A	380	ARG	NE-CZ	8.48	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	587	LEU	CG-CD2	8.47	1.83	1.51
1	A	279	GLU	CD-OE2	8.46	1.34	1.25
1	A	285	GLU	CD-OE2	8.46	1.34	1.25
1	A	277	GLU	CD-OE2	8.45	1.34	1.25
1	A	229	GLU	CD-OE1	8.16	1.34	1.25
1	A	35	ASN	CG-ND2	7.96	1.52	1.32
1	A	239	ASN	CG-ND2	7.73	1.52	1.32
1	A	281	THR	CB-OG1	7.33	1.57	1.43
1	A	380	ARG	CZ-NH1	7.32	1.42	1.33
1	A	584	GLU	CD-OE1	7.17	1.33	1.25
1	A	592	ARG	NE-CZ	6.89	1.42	1.33
1	A	250	LYS	CD-CE	6.41	1.67	1.51
1	A	589	ASP	CG-OD1	5.98	1.39	1.25
1	A	584	GLU	CD-OE2	5.91	1.32	1.25
1	A	226	ILE	C-N	5.89	1.47	1.34
1	A	202	ARG	NE-CZ	5.83	1.40	1.33
1	A	277	GLU	CD-OE1	5.78	1.32	1.25
1	A	239	ASN	C-N	5.67	1.47	1.34
1	A	229	GLU	CD-OE2	5.46	1.31	1.25
1	A	268	SER	CB-OG	5.42	1.49	1.42
1	A	582	ASN	CG-ND2	5.36	1.46	1.32
1	A	91	ARG	CZ-NH1	5.24	1.39	1.33
1	A	246	LYS	CD-CE	5.18	1.64	1.51
1	A	224	ASP	C-O	5.09	1.33	1.23
1	A	165	GLU	CD-OE1	5.06	1.31	1.25
1	A	589	ASP	CG-OD2	5.05	1.36	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	592	ARG	NE-CZ-NH1	17.17	128.88	120.30
1	A	592	ARG	NE-CZ-NH2	-13.06	113.77	120.30
1	A	380	ARG	NE-CZ-NH2	-11.72	114.44	120.30
1	A	600	TRP	CA-C-O	-9.23	100.72	120.10
1	A	202	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	A	250	LYS	CD-CE-NZ	-8.83	91.40	111.70
1	A	269	ASP	CB-CG-OD1	-8.45	110.70	118.30
1	A	202	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	589	ASP	CB-CG-OD1	-7.31	111.72	118.30
1	A	380	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	91	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	246	LYS	CD-CE-NZ	-5.55	98.93	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	35	ASN	CB-CG-OD1	-5.50	110.59	121.60
1	A	581	GLN	N-CA-C	5.42	125.62	111.00
1	A	442	PRO	N-CA-C	5.14	125.47	112.10
1	A	224	ASP	O-C-N	5.13	130.85	121.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	LEU	Peptide
1	A	442	PRO	Peptide
1	A	443	LEU	Peptide
1	A	483	ASP	Peptide
1	A	587	LEU	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	4984	337	0
2	A	22	0	10	3	0
All	All	5062	0	4994	337	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 34.

All (337) 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:587:LEU:CG	1:A:587:LEU:CD2	1.83	1.56
1:A:246:LYS:CE	1:A:246:LYS:NZ	1.72	1.50
1:A:632:ALA:HB3	1:A:633:SER:CB	1.48	1.41
1:A:225:PRO:C	1:A:226:ILE:N	1.75	1.40
1:A:250:LYS:CE	1:A:250:LYS:NZ	1.85	1.36
1:A:632:ALA:CB	1:A:633:SER:HB2	1.60	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:ASN:O	1:A:586:LYS:HG2	1.38	1.23
1:A:600:TRP:C	1:A:600:TRP:O	1.79	1.20
1:A:441:ALA:HB1	1:A:442:PRO:HD3	1.31	1.10
1:A:623:LYS:HD3	1:A:634:ILE:HG21	1.32	1.10
1:A:2:PRO:HB3	1:A:440:ARG:HB2	1.29	1.05
1:A:28:LEU:HA	1:A:29:THR:HG22	1.33	1.05
1:A:591:LYS:N	1:A:592:ARG:HB3	1.72	1.02
1:A:460:GLY:HA3	1:A:467:ILE:HD13	1.41	1.01
1:A:95:ARG:N	1:A:97:HIS:H	1.57	1.00
1:A:633:SER:H	1:A:635:ASP:N	1.57	1.00
1:A:94:ALA:HB3	1:A:95:ARG:CB	1.92	0.98
1:A:632:ALA:HB3	1:A:633:SER:HB3	1.49	0.95
1:A:3:GLU:H	1:A:4:PRO:HD2	1.29	0.94
1:A:3:GLU:H	1:A:4:PRO:CD	1.81	0.93
1:A:580:ALA:HA	1:A:581:GLN:O	1.69	0.91
1:A:210:ARG:HG3	1:A:210:ARG:HH11	1.36	0.91
1:A:631:GLY:O	1:A:633:SER:HB3	1.70	0.90
1:A:632:ALA:HB3	1:A:633:SER:HB2	0.89	0.89
1:A:634:ILE:HG22	1:A:635:ASP:N	1.88	0.88
1:A:94:ALA:HB3	1:A:95:ARG:HB2	1.55	0.88
1:A:632:ALA:CB	1:A:633:SER:CB	2.32	0.87
1:A:309:ILE:HG12	1:A:366:VAL:HG11	1.57	0.86
1:A:91:ARG:HH11	1:A:91:ARG:HB2	1.40	0.86
1:A:336:LEU:HD11	1:A:366:VAL:HG13	1.58	0.86
1:A:95:ARG:H	1:A:96:SER:HB2	1.40	0.85
1:A:633:SER:H	1:A:635:ASP:H	1.21	0.84
1:A:634:ILE:HG22	1:A:635:ASP:H	1.42	0.83
1:A:95:ARG:H	1:A:96:SER:CB	1.91	0.83
1:A:32:GLU:HG2	1:A:37:LEU:HD23	1.60	0.83
1:A:630:GLU:HB3	1:A:631:GLY:CA	2.07	0.83
1:A:124:TYR:O	1:A:127:LYS:HB2	1.79	0.82
1:A:261:LEU:HD12	1:A:262:PHE:H	1.44	0.81
1:A:441:ALA:HB1	1:A:442:PRO:CD	2.09	0.80
1:A:28:LEU:HA	1:A:29:THR:CG2	2.12	0.80
1:A:95:ARG:N	1:A:96:SER:HB2	1.96	0.79
1:A:567:ASP:OD2	1:A:570:TRP:HB3	1.83	0.78
1:A:2:PRO:CG	1:A:453:ARG:HH12	1.96	0.78
1:A:44:TYR:CG	1:A:48:VAL:HG11	2.19	0.78
1:A:257:ARG:O	1:A:258:VAL:HG13	1.84	0.77
1:A:591:LYS:HG3	1:A:592:ARG:HB2	1.67	0.77
1:A:16:HIS:NE2	1:A:97:HIS:CD2	2.52	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:PRO:HG3	1:A:453:ARG:HH12	1.50	0.77
1:A:16:HIS:NE2	1:A:97:HIS:HD2	1.83	0.76
1:A:32:GLU:HG2	1:A:37:LEU:CD2	2.17	0.74
1:A:210:ARG:HG3	1:A:210:ARG:NH1	1.97	0.74
1:A:444:TYR:N	1:A:444:TYR:CD2	2.56	0.74
1:A:28:LEU:CA	1:A:29:THR:HG22	2.16	0.74
1:A:495:TRP:HE1	2:A:1646:GUN:HN21	1.34	0.74
1:A:58:THR:OG1	1:A:61:GLN:HG3	1.87	0.73
1:A:309:ILE:HD13	1:A:366:VAL:HG12	1.70	0.73
1:A:250:LYS:CD	1:A:250:LYS:NZ	2.52	0.72
1:A:59:ILE:HG23	1:A:60:ARG:N	2.04	0.72
1:A:95:ARG:H	1:A:96:SER:CA	2.03	0.72
1:A:95:ARG:N	1:A:97:HIS:N	2.36	0.71
1:A:261:LEU:HD12	1:A:262:PHE:N	2.06	0.71
1:A:637:TRP:O	1:A:641:LEU:HD22	1.89	0.71
1:A:94:ALA:CB	1:A:95:ARG:HB2	2.21	0.71
1:A:495:TRP:HA	1:A:498:ASN:HD22	1.56	0.70
1:A:2:PRO:HG3	1:A:453:ARG:HH22	1.57	0.70
1:A:425:TYR:OH	1:A:451:LEU:HD22	1.92	0.70
1:A:581:GLN:H	1:A:581:GLN:NE2	1.89	0.70
1:A:94:ALA:H	1:A:95:ARG:HB2	1.57	0.70
1:A:630:GLU:CB	1:A:631:GLY:HA2	2.22	0.69
1:A:122:ARG:HH22	2:A:1646:GUN:HN9	1.38	0.69
1:A:246:LYS:CD	1:A:246:LYS:NZ	2.55	0.69
1:A:75:ASN:HB2	1:A:83:LYS:O	1.93	0.68
1:A:94:ALA:HB3	1:A:95:ARG:CG	2.24	0.68
1:A:323:LEU:HD23	1:A:338:ASN:HA	1.75	0.68
1:A:633:SER:N	1:A:635:ASP:N	2.37	0.68
1:A:336:LEU:CD1	1:A:366:VAL:HG13	2.24	0.68
1:A:59:ILE:HG23	1:A:60:ARG:H	1.59	0.68
1:A:210:ARG:CG	1:A:210:ARG:HH11	2.08	0.67
1:A:436:ALA:HB1	1:A:451:LEU:HD12	1.77	0.67
1:A:29:THR:O	1:A:31:ASP:N	2.25	0.66
1:A:444:TYR:C	1:A:446:TYR:H	1.98	0.66
1:A:230:CYS:SG	1:A:232:ASP:HB2	2.35	0.66
1:A:453:ARG:HD3	1:A:565:VAL:HG23	1.78	0.66
1:A:630:GLU:HB3	1:A:631:GLY:HA2	1.78	0.66
1:A:559:LEU:HB3	1:A:622:TYR:CE1	2.31	0.66
1:A:93:VAL:HG12	1:A:93:VAL:O	1.97	0.65
1:A:144:ASN:H	1:A:148:HIS:HD2	1.43	0.65
1:A:633:SER:N	1:A:635:ASP:H	1.93	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:ILE:CG2	1:A:635:ASP:N	2.60	0.65
1:A:574:MET:O	1:A:578:TRP:HB3	1.96	0.65
1:A:437:TRP:O	1:A:450:ALA:HA	1.97	0.65
1:A:95:ARG:H	1:A:97:HIS:H	1.42	0.64
1:A:551:LEU:HD21	1:A:575:ILE:HD12	1.79	0.64
1:A:630:GLU:CB	1:A:631:GLY:CA	2.76	0.64
1:A:94:ALA:HB3	1:A:95:ARG:HG3	1.80	0.64
1:A:200:ASP:O	1:A:201:LEU:HB2	1.98	0.63
1:A:408:ASP:HB2	1:A:434:ALA:HB2	1.79	0.63
1:A:144:ASN:H	1:A:148:HIS:CD2	2.17	0.63
1:A:94:ALA:HB3	1:A:95:ARG:CA	2.27	0.63
1:A:286:ASP:OD1	1:A:308:ARG:NH1	2.32	0.62
1:A:517:LEU:HD12	1:A:566:THR:OG1	1.99	0.62
1:A:623:LYS:HB3	1:A:634:ILE:HD13	1.80	0.62
1:A:480:ARG:O	1:A:482:PRO:HD3	2.00	0.62
1:A:99:MET:O	1:A:103:GLU:HG3	1.98	0.62
1:A:632:ALA:HB1	1:A:633:SER:HB2	1.76	0.61
1:A:323:LEU:HD21	1:A:338:ASN:HB2	1.83	0.61
1:A:34:LEU:HD11	1:A:598:ILE:HG23	1.81	0.61
1:A:59:ILE:O	1:A:62:LEU:N	2.34	0.61
1:A:426:GLU:OE2	1:A:426:GLU:HA	2.01	0.61
1:A:122:ARG:NH2	2:A:1646:GUN:N9	2.48	0.61
1:A:587:LEU:CD2	1:A:587:LEU:CD1	2.79	0.61
1:A:65:HIS:HE2	1:A:598:ILE:HG21	1.65	0.60
1:A:571:TRP:O	1:A:574:MET:HG3	2.00	0.60
1:A:11:THR:HG23	1:A:71:SER:HB2	1.82	0.60
1:A:95:ARG:H	1:A:97:HIS:N	1.98	0.60
1:A:515:ILE:O	1:A:516:SER:C	2.40	0.60
1:A:554:HIS:C	1:A:554:HIS:ND1	2.54	0.60
1:A:591:LYS:H	1:A:592:ARG:HB3	1.63	0.60
1:A:122:ARG:HG2	1:A:126:PHE:CE1	2.37	0.59
1:A:453:ARG:HD2	1:A:562:GLY:O	2.03	0.59
1:A:305:ILE:HG22	1:A:306:LYS:O	2.03	0.59
1:A:94:ALA:N	1:A:95:ARG:HB2	2.17	0.59
1:A:3:GLU:N	1:A:4:PRO:CD	2.51	0.59
1:A:510:PRO:O	1:A:512:VAL:HG12	2.02	0.59
1:A:2:PRO:HG3	1:A:453:ARG:NH1	2.17	0.58
1:A:598:ILE:HG22	1:A:598:ILE:O	2.03	0.58
1:A:591:LYS:CA	1:A:592:ARG:HB3	2.32	0.58
1:A:574:MET:C	1:A:574:MET:SD	2.82	0.58
1:A:158:PRO:O	1:A:159:LEU:HD23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:CYS:SG	1:A:222:VAL:HB	2.43	0.58
1:A:341:ARG:HD2	1:A:350:ARG:HB2	1.86	0.58
1:A:513:PRO:HB3	1:A:574:MET:HE3	1.86	0.58
1:A:309:ILE:CG1	1:A:366:VAL:HG11	2.29	0.57
1:A:166:ILE:HG22	1:A:167:GLY:HA2	1.86	0.57
1:A:441:ALA:CB	1:A:442:PRO:HD3	2.17	0.57
1:A:470:GLY:HA3	1:A:496:ALA:O	2.04	0.57
1:A:309:ILE:HD13	1:A:366:VAL:CG1	2.34	0.57
1:A:2:PRO:CD	1:A:453:ARG:HH12	2.17	0.57
1:A:122:ARG:HG2	1:A:126:PHE:HE1	1.70	0.56
1:A:201:LEU:HD12	1:A:228:PRO:HD2	1.87	0.56
1:A:286:ASP:O	1:A:290:GLU:HG3	2.05	0.56
1:A:552:SER:CB	1:A:614:ASP:HB3	2.35	0.56
1:A:517:LEU:HD11	1:A:571:TRP:HB2	1.87	0.56
1:A:310:PRO:O	1:A:367:ARG:NH2	2.34	0.56
1:A:587:LEU:H	1:A:588:ARG:HB3	1.69	0.56
1:A:225:PRO:CA	1:A:226:ILE:N	2.65	0.56
1:A:589:ASP:HA	1:A:592:ARG:HG2	1.87	0.56
1:A:341:ARG:NH1	1:A:351:HIS:HA	2.21	0.56
1:A:288:LEU:O	1:A:292:ILE:HG13	2.05	0.55
1:A:635:ASP:HA	1:A:638:LEU:HD12	1.87	0.55
1:A:471:ASN:O	1:A:475:LEU:HD22	2.05	0.55
1:A:589:ASP:O	1:A:593:SER:OG	2.25	0.55
1:A:394:ARG:HG3	1:A:394:ARG:HH11	1.71	0.55
1:A:13:GLU:O	1:A:16:HIS:CE1	2.60	0.55
1:A:406:ARG:NH2	1:A:408:ASP:OD1	2.39	0.55
1:A:409:LEU:HD21	1:A:433:ILE:HG12	1.88	0.55
1:A:196:ILE:HG12	1:A:263:ILE:O	2.07	0.54
1:A:630:GLU:HB3	1:A:631:GLY:HA3	1.89	0.54
1:A:59:ILE:CG2	1:A:60:ARG:N	2.70	0.54
1:A:68:ILE:CD1	1:A:110:ARG:HH11	2.20	0.54
1:A:319:ILE:HA	1:A:357:SER:O	2.06	0.54
1:A:441:ALA:HB3	1:A:443:LEU:HD12	1.88	0.54
1:A:318:CYS:SG	1:A:359:THR:HB	2.48	0.54
1:A:580:ALA:CA	1:A:581:GLN:O	2.49	0.54
1:A:2:PRO:HG3	1:A:453:ARG:NH2	2.21	0.54
1:A:309:ILE:CD1	1:A:366:VAL:CG1	2.85	0.54
1:A:59:ILE:CG2	1:A:60:ARG:H	2.20	0.54
1:A:138:GLU:HG2	1:A:139:THR:N	2.24	0.54
1:A:75:ASN:HA	1:A:85:VAL:HG23	1.89	0.54
1:A:478:MET:HG2	1:A:485:VAL:HG12	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PRO:C	1:A:226:ILE:CA	2.73	0.53
1:A:290:GLU:HG2	1:A:305:ILE:HG21	1.90	0.53
1:A:625:LYS:C	1:A:626:MET:HG2	2.29	0.53
1:A:162:GLU:N	1:A:163:TYR:CB	2.72	0.53
1:A:140:LEU:HD21	1:A:392:ILE:HG13	1.91	0.53
1:A:218:VAL:CG1	1:A:219:LEU:N	2.72	0.53
1:A:16:HIS:HD1	1:A:16:HIS:H	1.56	0.53
1:A:512:VAL:HG21	1:A:595:ALA:CB	2.40	0.52
1:A:631:GLY:O	1:A:633:SER:CB	2.51	0.52
1:A:34:LEU:CD1	1:A:598:ILE:HG23	2.39	0.52
1:A:633:SER:H	1:A:634:ILE:C	2.09	0.52
1:A:623:LYS:HB3	1:A:634:ILE:CD1	2.39	0.52
1:A:91:ARG:CB	1:A:91:ARG:HH11	2.17	0.52
1:A:632:ALA:CA	1:A:633:SER:CB	2.88	0.52
1:A:283:PHE:CE1	1:A:310:PRO:HG3	2.45	0.52
1:A:615:LEU:O	1:A:618:ALA:HB3	2.10	0.52
1:A:634:ILE:O	1:A:635:ASP:C	2.49	0.51
1:A:173:GLU:HB3	1:A:174:PRO:HD2	1.92	0.51
1:A:444:TYR:C	1:A:446:TYR:N	2.63	0.51
1:A:619:LEU:O	1:A:622:TYR:HB3	2.09	0.51
1:A:264:TRP:CE3	1:A:289:GLY:HA2	2.45	0.51
1:A:460:GLY:CA	1:A:467:ILE:HD13	2.27	0.51
1:A:11:THR:CG2	1:A:71:SER:HB2	2.40	0.51
1:A:136:GLU:O	1:A:139:THR:N	2.44	0.50
1:A:23:LEU:HD12	1:A:49:TYR:HE2	1.74	0.50
1:A:324:PHE:HB2	1:A:325:PRO:CD	2.42	0.50
1:A:600:TRP:CA	1:A:600:TRP:O	2.58	0.50
1:A:13:GLU:OE1	1:A:13:GLU:N	2.43	0.50
1:A:224:ASP:C	1:A:226:ILE:N	2.65	0.50
1:A:469:ASP:HB3	1:A:565:VAL:HB	1.92	0.50
1:A:513:PRO:HB3	1:A:574:MET:CE	2.42	0.50
1:A:600:TRP:CE3	1:A:600:TRP:HA	2.46	0.50
1:A:75:ASN:CB	1:A:83:LYS:O	2.58	0.50
1:A:218:VAL:HG13	1:A:219:LEU:N	2.27	0.50
1:A:622:TYR:CD2	1:A:622:TYR:C	2.85	0.50
1:A:388:GLU:HB3	1:A:392:ILE:HD12	1.94	0.49
1:A:332:ASP:O	1:A:334:TYR:HD1	1.94	0.49
1:A:622:TYR:O	1:A:626:MET:HG3	2.12	0.49
1:A:94:ALA:C	1:A:97:HIS:H	2.15	0.49
1:A:582:ASN:O	1:A:586:LYS:CG	2.32	0.49
1:A:591:LYS:HG3	1:A:592:ARG:CB	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LEU:O	1:A:423:SER:OG	2.30	0.49
1:A:569:PHE:O	1:A:572:PHE:HB2	2.12	0.49
1:A:94:ALA:CA	1:A:95:ARG:HB2	2.42	0.49
1:A:134:GLY:HA3	1:A:411:TYR:CG	2.48	0.48
1:A:620:ARG:O	1:A:621:GLU:C	2.51	0.48
1:A:587:LEU:CD2	1:A:587:LEU:CB	2.82	0.48
1:A:185:TYR:OH	1:A:304:LEU:HD21	2.14	0.48
1:A:517:LEU:HD22	1:A:570:TRP:CE2	2.49	0.48
1:A:262:PHE:HB2	1:A:300:PHE:CE2	2.49	0.47
1:A:182:MET:CE	1:A:337:ARG:HH11	2.27	0.47
1:A:68:ILE:HD11	1:A:110:ARG:HH11	1.79	0.47
1:A:441:ALA:O	1:A:443:LEU:HB2	2.14	0.47
1:A:26:TRP:HB3	1:A:50:ALA:HB2	1.97	0.47
1:A:592:ARG:HG3	1:A:593:SER:N	2.29	0.47
1:A:186:ILE:HD13	1:A:304:LEU:HD22	1.94	0.47
1:A:323:LEU:CD2	1:A:338:ASN:HB2	2.44	0.47
1:A:488:ASP:O	1:A:489:LEU:C	2.53	0.47
1:A:633:SER:HA	1:A:636:SER:H	1.78	0.47
1:A:462:TYR:O	1:A:463:ARG:C	2.53	0.47
1:A:588:ARG:O	1:A:590:LEU:N	2.48	0.47
1:A:326:GLN:OE1	1:A:337:ARG:HG3	2.15	0.47
1:A:441:ALA:CB	1:A:442:PRO:CD	2.82	0.47
1:A:505:GLU:HA	1:A:505:GLU:OE1	2.14	0.47
1:A:476:PHE:HB2	1:A:516:SER:HB2	1.97	0.47
1:A:113:MET:HG2	1:A:490:THR:HG22	1.96	0.47
1:A:623:LYS:HD3	1:A:634:ILE:CG2	2.24	0.46
1:A:404:GLU:HB3	1:A:405:PRO:HD2	1.98	0.46
1:A:495:TRP:HA	1:A:498:ASN:ND2	2.28	0.46
1:A:264:TRP:CD2	1:A:289:GLY:HA3	2.51	0.46
1:A:304:LEU:HA	1:A:304:LEU:HD12	1.81	0.46
1:A:552:SER:HB2	1:A:614:ASP:HB3	1.96	0.46
1:A:249:LEU:HD13	1:A:296:MET:HE2	1.98	0.46
1:A:5:HIS:HB2	1:A:47:ASP:HA	1.97	0.46
1:A:640:LEU:O	1:A:644:LEU:HA	2.15	0.46
1:A:136:GLU:O	1:A:137:ALA:C	2.54	0.46
1:A:584:GLU:O	1:A:587:LEU:HD12	2.15	0.46
1:A:24:PRO:HB2	1:A:48:VAL:HG12	1.97	0.46
1:A:2:PRO:HD3	1:A:440:ARG:H	1.81	0.46
1:A:350:ARG:NH2	1:A:391:HIS:ND1	2.64	0.45
1:A:432:VAL:O	1:A:503:LEU:HA	2.16	0.45
1:A:578:TRP:CE3	1:A:579:SER:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:TYR:CD2	1:A:189:SER:N	2.84	0.45
1:A:58:THR:HA	1:A:80:ASP:HB2	1.98	0.45
1:A:17:ILE:HD11	1:A:97:HIS:CD2	2.52	0.45
1:A:32:GLU:HG3	1:A:36:ASP:HB3	1.98	0.45
1:A:388:GLU:O	1:A:389:HIS:C	2.55	0.45
1:A:433:ILE:HA	1:A:502:SER:O	2.17	0.45
1:A:441:ALA:C	1:A:443:LEU:HB2	2.37	0.45
1:A:91:ARG:HB3	1:A:95:ARG:HH21	1.82	0.45
1:A:323:LEU:HD23	1:A:323:LEU:HA	1.81	0.45
1:A:138:GLU:O	1:A:141:ASN:HB2	2.17	0.45
1:A:287:ARG:HA	1:A:287:ARG:HD3	1.80	0.45
1:A:162:GLU:HB3	1:A:163:TYR:CB	2.47	0.44
1:A:3:GLU:HB2	1:A:4:PRO:HD3	2.00	0.44
1:A:221:HIS:ND1	1:A:238:HIS:NE2	2.64	0.44
1:A:124:TYR:CD2	1:A:124:TYR:C	2.90	0.44
1:A:17:ILE:HG12	1:A:97:HIS:HB3	1.99	0.44
1:A:242:VAL:HG22	1:A:247:ASP:HB2	1.99	0.44
1:A:262:PHE:HB2	1:A:300:PHE:CD2	2.53	0.44
1:A:408:ASP:HB2	1:A:434:ALA:CB	2.47	0.44
1:A:466:ARG:HA	1:A:466:ARG:CZ	2.47	0.44
1:A:58:THR:O	1:A:61:GLN:HB2	2.16	0.44
1:A:515:ILE:C	1:A:517:LEU:N	2.71	0.44
1:A:515:ILE:HD11	1:A:598:ILE:CG1	2.48	0.44
1:A:395:LYS:HG2	1:A:400:HIS:CD2	2.53	0.44
1:A:515:ILE:O	1:A:517:LEU:N	2.51	0.44
1:A:421:GLU:O	1:A:422:PRO:C	2.56	0.43
1:A:379:GLY:O	1:A:380:ARG:C	2.57	0.43
1:A:414:ASN:HD22	1:A:414:ASN:N	2.15	0.43
1:A:419:GLY:C	1:A:421:GLU:H	2.21	0.43
1:A:587:LEU:HA	1:A:590:LEU:HB2	2.00	0.43
1:A:162:GLU:CA	1:A:163:TYR:CB	2.96	0.43
1:A:204:LEU:O	1:A:207:PHE:HB3	2.18	0.43
1:A:119:ASP:O	1:A:123:ASN:HB2	2.19	0.43
1:A:531:ARG:O	1:A:535:PRO:HB3	2.19	0.43
1:A:453:ARG:HB2	1:A:562:GLY:HA2	2.01	0.43
1:A:570:TRP:CD1	1:A:570:TRP:C	2.91	0.43
1:A:58:THR:HB	1:A:80:ASP:OD2	2.18	0.43
1:A:125:ALA:C	1:A:127:LYS:H	2.20	0.43
1:A:68:ILE:CD1	1:A:110:ARG:NH1	2.82	0.43
1:A:193:VAL:HG22	1:A:261:LEU:HB3	2.00	0.43
1:A:23:LEU:HD12	1:A:49:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:PRO:CG	1:A:453:ARG:HH22	2.28	0.42
1:A:613:ASN:HA	1:A:616:ILE:HG13	2.01	0.42
1:A:633:SER:H	1:A:634:ILE:CA	2.32	0.42
1:A:216:ARG:C	1:A:218:VAL:H	2.22	0.42
1:A:394:ARG:NH1	1:A:394:ARG:HG3	2.34	0.42
1:A:479:TRP:NE1	1:A:593:SER:O	2.45	0.42
1:A:353:HIS:HA	1:A:354:PRO:HD2	1.83	0.42
1:A:414:ASN:ND2	1:A:448:ASP:OD2	2.53	0.42
1:A:44:TYR:CD2	1:A:48:VAL:HG11	2.54	0.42
1:A:581:GLN:H	1:A:581:GLN:HE21	1.63	0.42
1:A:586:LYS:O	1:A:587:LEU:HB3	2.20	0.42
1:A:629:ARG:O	1:A:630:GLU:CB	2.67	0.42
1:A:166:ILE:HD13	1:A:369:MET:HG3	2.02	0.42
1:A:627:GLY:O	1:A:629:ARG:N	2.48	0.42
1:A:585:GLN:HA	1:A:588:ARG:HD2	2.02	0.42
1:A:264:TRP:CD2	1:A:289:GLY:CA	3.02	0.42
1:A:412:LEU:HA	1:A:412:LEU:HD12	1.90	0.41
1:A:480:ARG:C	1:A:482:PRO:HD3	2.40	0.41
1:A:13:GLU:O	1:A:16:HIS:HE1	2.01	0.41
1:A:59:ILE:HG22	1:A:80:ASP:OD2	2.20	0.41
1:A:140:LEU:HD21	1:A:392:ILE:CG1	2.50	0.41
1:A:290:GLU:CG	1:A:305:ILE:HG21	2.51	0.41
1:A:26:TRP:O	1:A:50:ALA:HA	2.21	0.41
1:A:71:SER:OG	1:A:72:THR:N	2.53	0.41
1:A:638:LEU:C	1:A:640:LEU:H	2.23	0.41
1:A:642:ARG:O	1:A:643:HIS:HB2	2.19	0.41
1:A:2:PRO:CG	1:A:453:ARG:NH1	2.74	0.41
1:A:73:HIS:O	1:A:85:VAL:HG21	2.20	0.41
1:A:324:PHE:CB	1:A:325:PRO:CD	2.98	0.41
1:A:117:PHE:CZ	1:A:121:LEU:HD11	2.56	0.41
1:A:161:MET:O	1:A:162:GLU:C	2.59	0.41
1:A:384:LYS:O	1:A:388:GLU:HG3	2.20	0.41
1:A:491:TYR:O	1:A:493:PRO:HD3	2.19	0.41
1:A:629:ARG:O	1:A:630:GLU:HB2	2.21	0.41
1:A:160:TYR:HB2	1:A:369:MET:CE	2.51	0.41
1:A:624:ARG:O	1:A:624:ARG:NE	2.53	0.41
1:A:326:GLN:OE1	1:A:337:ARG:CG	2.69	0.41
1:A:83:LYS:HD2	1:A:488:ASP:OD1	2.21	0.41
1:A:129:ALA:C	1:A:130:ILE:HD12	2.41	0.40
1:A:633:SER:O	1:A:637:TRP:CD1	2.74	0.40
1:A:144:ASN:HA	1:A:145:PRO:HD3	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ARG:HG3	1:A:170:PHE:N	2.36	0.40
1:A:212:PRO:O	1:A:216:ARG:NH1	2.54	0.40
1:A:561:SER:C	1:A:563:ALA:H	2.25	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%)	476 (79%)	93 (15%)	36 (6%)	1 9

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	30	GLY
1	A	163	TYR
1	A	445	ASP
1	A	581	GLN
1	A	587	LEU
1	A	592	ARG
1	A	630	GLU
1	A	632	ALA
1	A	633	SER
1	A	643	HIS
1	A	15	SER
1	A	19	LYS
1	A	95	ARG
1	A	489	LEU
1	A	634	ILE
1	A	3	GLU
1	A	32	GLU

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Mol	Chain	Res	Type
1	A	137	ALA
1	A	284	ALA
1	A	629	ARG
1	A	240	ILE
1	A	388	GLU
1	A	551	LEU
1	A	351	HIS
1	A	411	TYR
1	A	588	ARG
1	A	620	ARG
1	A	81	ILE
1	A	161	MET
1	A	225	PRO
1	A	85	VAL
1	A	93	VAL
1	A	166	ILE
1	A	511	PRO
1	A	297	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	542/571 (95%)	456 (84%)	86 (16%)	2 12

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	14	LEU
1	A	19	LYS
1	A	28	LEU
1	A	36	ASP
1	A	54	VAL
1	A	56	LYS
1	A	65	HIS

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Mol	Chain	Res	Type
1	A	75	ASN
1	A	78	LEU
1	A	82	ILE
1	A	87	VAL
1	A	91	ARG
1	A	110	ARG
1	A	115	LYS
1	A	119	ASP
1	A	124	TYR
1	A	161	MET
1	A	166	ILE
1	A	169	ARG
1	A	175	THR
1	A	180	VAL
1	A	181	SER
1	A	195	TYR
1	A	196	ILE
1	A	204	LEU
1	A	210	ARG
1	A	211	SER
1	A	230	CYS
1	A	258	VAL
1	A	277	GLU
1	A	281	THR
1	A	287	ARG
1	A	306	LYS
1	A	308	ARG
1	A	309	ILE
1	A	313	LYS
1	A	315	GLU
1	A	324	PHE
1	A	343	ARG
1	A	357	SER
1	A	361	VAL
1	A	362	VAL
1	A	372	LEU
1	A	376	ARG
1	A	398	LEU
1	A	401	GLU
1	A	413	THR
1	A	421	GLU
1	A	444	TYR

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Mol	Chain	Res	Type
1	A	446	TYR
1	A	458	LEU
1	A	461	SER
1	A	466	ARG
1	A	467	ILE
1	A	471	ASN
1	A	475	LEU
1	A	480	ARG
1	A	491	TYR
1	A	512	VAL
1	A	515	ILE
1	A	519	ARG
1	A	528	SER
1	A	533	ARG
1	A	551	LEU
1	A	554	HIS
1	A	556	TYR
1	A	558	THR
1	A	569	PHE
1	A	574	MET
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	593	SER
1	A	600	TRP
1	A	612	ARG
1	A	614	ASP
1	A	624	ARG
1	A	626	MET
1	A	628	MET
1	A	629	ARG
1	A	641	LEU
1	A	642	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	97	HIS

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Mol	Chain	Res	Type
1	A	104	ASN
1	A	148	HIS
1	A	338	ASN
1	A	400	HIS
1	A	414	ASN
1	A	471	ASN
1	A	498	ASN
1	A	581	GLN
1	A	585	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	GUN	A	1645	-	9,12,12	1.91	2 (22%)	8,17,17	3.52	6 (75%)
2	GUN	A	1646	-	9,12,12	1.53	1 (11%)	8,17,17	3.70	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	GUN	A	1645	-	-	-	0/2/2/2
2	GUN	A	1646	-	-	-	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1645	GUN	C6-C5	4.96	1.49	1.41
2	A	1646	GUN	C6-C5	3.86	1.48	1.41
2	A	1645	GUN	C5-C4	2.47	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1646	GUN	C6-C5-C4	-6.12	114.96	120.80
2	A	1645	GUN	C5-C6-N1	-4.73	116.96	123.43
2	A	1645	GUN	C6-C5-C4	-4.62	116.39	120.80
2	A	1646	GUN	C6-N1-C2	4.59	123.22	115.93
2	A	1645	GUN	C6-N1-C2	4.55	123.17	115.93
2	A	1645	GUN	C4-C5-N7	-4.45	104.76	109.40
2	A	1646	GUN	N3-C2-N1	-4.09	121.76	127.22
2	A	1646	GUN	C2-N3-C4	3.87	119.78	115.36
2	A	1646	GUN	C5-C6-N1	-3.43	118.74	123.43
2	A	1645	GUN	C2-N3-C4	2.79	118.55	115.36
2	A	1645	GUN	N3-C2-N1	-2.57	123.79	127.22
2	A	1646	GUN	C4-C5-N7	-2.38	106.92	109.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1646	GUN	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	225:PRO	C	226:ILE	N	1.75

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%)	-0.39	11 (1%) 68 40	41, 54, 63, 73	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	580	ALA	3.2
1	A	434	ALA	2.7
1	A	162	GLU	2.5
1	A	502	SER	2.4
1	A	255	LEU	2.4
1	A	240	ILE	2.3
1	A	165	GLU	2.2
1	A	229	GLU	2.2
1	A	408	ASP	2.1
1	A	435	THR	2.1
1	A	643	HIS	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 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
2	GUN	A	1645	11/11	0.75	0.43	140,141,141,141	0
2	GUN	A	1646	11/11	0.94	0.26	133,133,134,134	0

6.5 Other polymers (i)

There are no such residues in this entry.