



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:22 AM UTC

PDB ID : 3VR1 / pdb_00003vr1
Title : Crystal structure analysis of the translation factor RF3
Authors : Kihira, K.; Shomura, Y.; Shibata, N.; Kitamura, M.; Higuchi, Y.
Deposited on : 2012-04-03
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

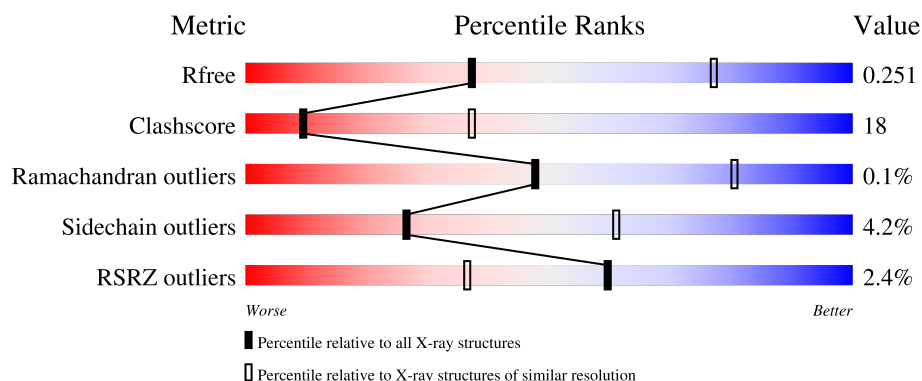
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

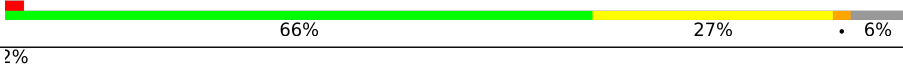
The reported resolution of this entry is 3.00 Å.

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	548	 2% 66% 28% • 6%
1	B	548	 2% 66% 27% • 6%
1	C	548	 2% 66% 25% • 6%
1	D	548	 3% 65% 27% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16396 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 Peptide chain release factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4063	2571	716	753	23			
1	B	516	Total	C	N	O	S	0	0	0
			4063	2571	716	753	23			
1	C	516	Total	C	N	O	S	0	0	0
			4063	2571	716	753	23			
1	D	516	Total	C	N	O	S	0	0	0
			4063	2571	716	753	23			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP B8DIL5
A	-17	SER	-	expression tag	UNP B8DIL5
A	-16	SER	-	expression tag	UNP B8DIL5
A	-15	HIS	-	expression tag	UNP B8DIL5
A	-14	HIS	-	expression tag	UNP B8DIL5
A	-13	HIS	-	expression tag	UNP B8DIL5
A	-12	HIS	-	expression tag	UNP B8DIL5
A	-11	HIS	-	expression tag	UNP B8DIL5
A	-10	HIS	-	expression tag	UNP B8DIL5
A	-9	SER	-	expression tag	UNP B8DIL5
A	-8	SER	-	expression tag	UNP B8DIL5
A	-7	GLY	-	expression tag	UNP B8DIL5
A	-6	LEU	-	expression tag	UNP B8DIL5
A	-5	VAL	-	expression tag	UNP B8DIL5
A	-4	PRO	-	expression tag	UNP B8DIL5
A	-3	ARG	-	expression tag	UNP B8DIL5
A	-2	GLY	-	expression tag	UNP B8DIL5
A	-1	SER	-	expression tag	UNP B8DIL5
A	0	HIS	-	expression tag	UNP B8DIL5
B	-18	GLY	-	expression tag	UNP B8DIL5
B	-17	SER	-	expression tag	UNP B8DIL5

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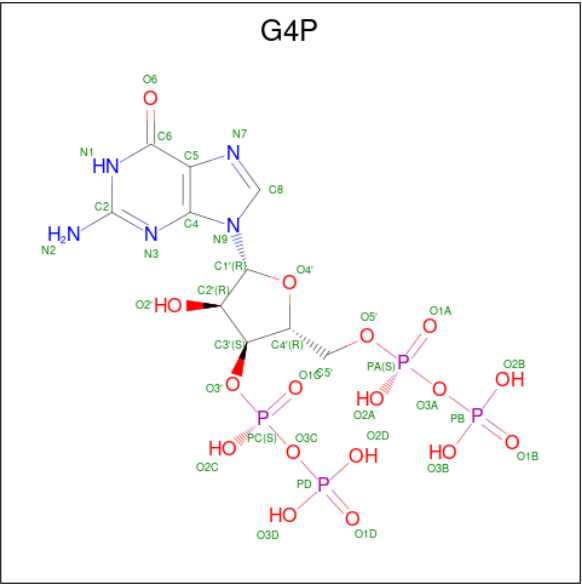
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP B8DIL5
B	-15	HIS	-	expression tag	UNP B8DIL5
B	-14	HIS	-	expression tag	UNP B8DIL5
B	-13	HIS	-	expression tag	UNP B8DIL5
B	-12	HIS	-	expression tag	UNP B8DIL5
B	-11	HIS	-	expression tag	UNP B8DIL5
B	-10	HIS	-	expression tag	UNP B8DIL5
B	-9	SER	-	expression tag	UNP B8DIL5
B	-8	SER	-	expression tag	UNP B8DIL5
B	-7	GLY	-	expression tag	UNP B8DIL5
B	-6	LEU	-	expression tag	UNP B8DIL5
B	-5	VAL	-	expression tag	UNP B8DIL5
B	-4	PRO	-	expression tag	UNP B8DIL5
B	-3	ARG	-	expression tag	UNP B8DIL5
B	-2	GLY	-	expression tag	UNP B8DIL5
B	-1	SER	-	expression tag	UNP B8DIL5
B	0	HIS	-	expression tag	UNP B8DIL5
C	-18	GLY	-	expression tag	UNP B8DIL5
C	-17	SER	-	expression tag	UNP B8DIL5
C	-16	SER	-	expression tag	UNP B8DIL5
C	-15	HIS	-	expression tag	UNP B8DIL5
C	-14	HIS	-	expression tag	UNP B8DIL5
C	-13	HIS	-	expression tag	UNP B8DIL5
C	-12	HIS	-	expression tag	UNP B8DIL5
C	-11	HIS	-	expression tag	UNP B8DIL5
C	-10	HIS	-	expression tag	UNP B8DIL5
C	-9	SER	-	expression tag	UNP B8DIL5
C	-8	SER	-	expression tag	UNP B8DIL5
C	-7	GLY	-	expression tag	UNP B8DIL5
C	-6	LEU	-	expression tag	UNP B8DIL5
C	-5	VAL	-	expression tag	UNP B8DIL5
C	-4	PRO	-	expression tag	UNP B8DIL5
C	-3	ARG	-	expression tag	UNP B8DIL5
C	-2	GLY	-	expression tag	UNP B8DIL5
C	-1	SER	-	expression tag	UNP B8DIL5
C	0	HIS	-	expression tag	UNP B8DIL5
D	-18	GLY	-	expression tag	UNP B8DIL5
D	-17	SER	-	expression tag	UNP B8DIL5
D	-16	SER	-	expression tag	UNP B8DIL5
D	-15	HIS	-	expression tag	UNP B8DIL5
D	-14	HIS	-	expression tag	UNP B8DIL5
D	-13	HIS	-	expression tag	UNP B8DIL5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP B8DIL5
D	-11	HIS	-	expression tag	UNP B8DIL5
D	-10	HIS	-	expression tag	UNP B8DIL5
D	-9	SER	-	expression tag	UNP B8DIL5
D	-8	SER	-	expression tag	UNP B8DIL5
D	-7	GLY	-	expression tag	UNP B8DIL5
D	-6	LEU	-	expression tag	UNP B8DIL5
D	-5	VAL	-	expression tag	UNP B8DIL5
D	-4	PRO	-	expression tag	UNP B8DIL5
D	-3	ARG	-	expression tag	UNP B8DIL5
D	-2	GLY	-	expression tag	UNP B8DIL5
D	-1	SER	-	expression tag	UNP B8DIL5
D	0	HIS	-	expression tag	UNP B8DIL5

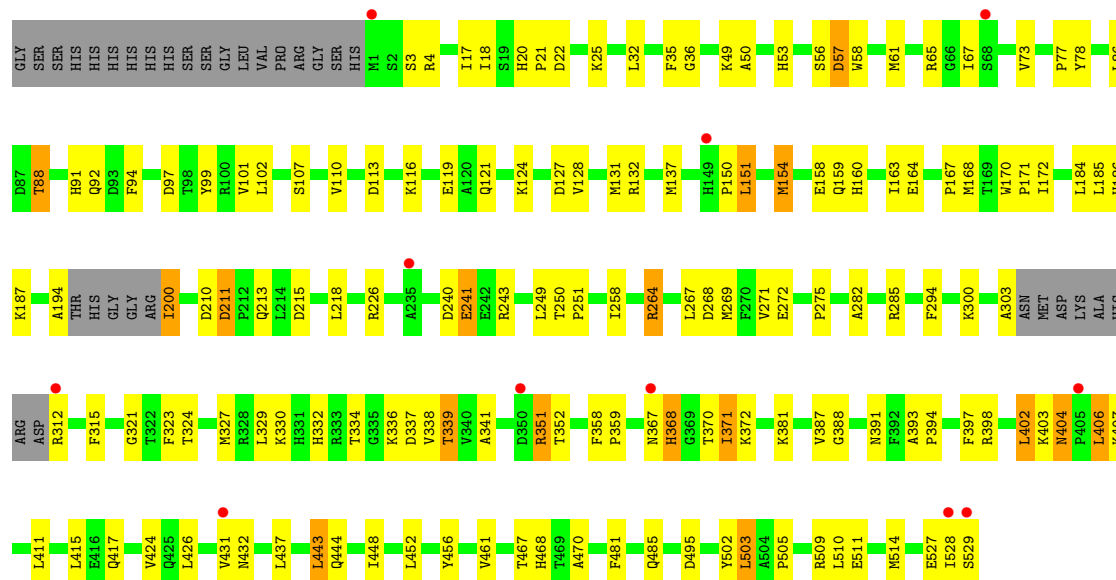
- Molecule 2 is GUANOSINE-5',3'-TETRAPHOSPHATE (CCD ID: G4P) (formula: $C_{10}H_{17}N_5O_{17}P_4$).



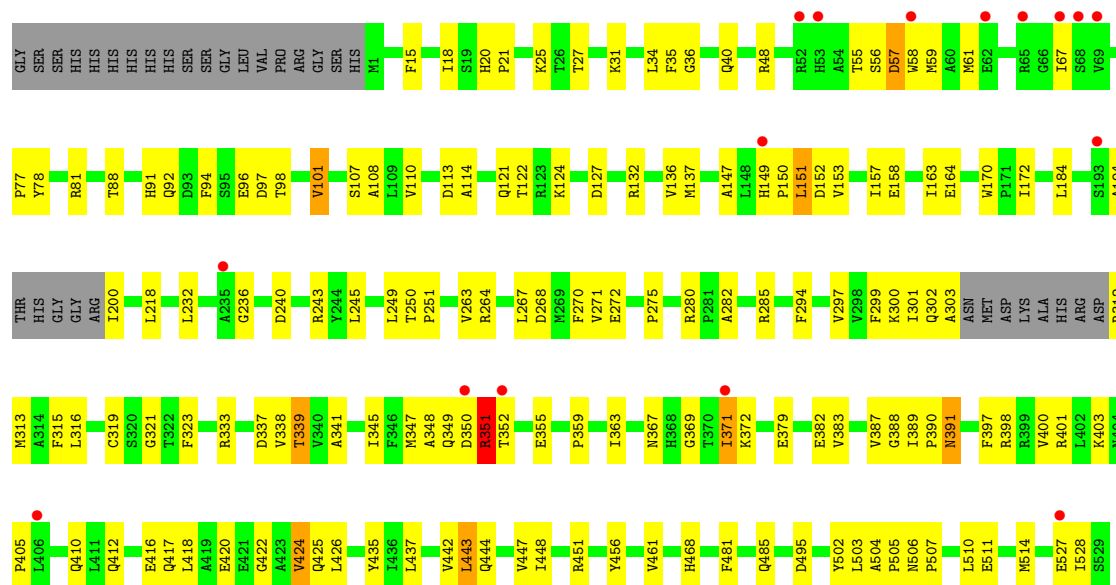
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 36	C 10	N 5	O 17	P 4	0	0
2	B	1	Total 36	C 10	N 5	O 17	P 4	0	0
2	C	1	Total 36	C 10	N 5	O 17	P 4	0	0
2	D	1	Total 36	C 10	N 5	O 17	P 4	0	0



• Molecule 1: Peptide chain release factor 3



• Molecule 1: Peptide chain release factor 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.20Å 83.46Å 114.25Å 72.98° 74.18° 89.78°	Depositor
Resolution (Å)	41.60 – 3.00 41.60 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (41.60-3.00) 96.5 (41.60-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.218 , 0.259 0.214 , 0.251	Depositor DCC
R_{free} test set	2755 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16396	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G4P

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	0.72	0/4146	1.00	8/5602 (0.1%)
1	B	0.73	1/4146 (0.0%)	1.00	10/5602 (0.2%)
1	C	0.74	0/4146	1.00	5/5602 (0.1%)
1	D	0.75	0/4146	1.02	6/5602 (0.1%)
All	All	0.73	1/16584 (0.0%)	1.00	29/22408 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	252	VAL	CA-CB	5.09	1.60	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	HIS	CB-CA-C	-7.55	107.87	116.63
1	D	91	HIS	CB-CA-C	-7.55	107.87	116.63
1	B	91	HIS	CB-CA-C	-7.52	107.90	116.63
1	C	91	HIS	CB-CA-C	-7.21	108.25	116.54
1	D	351	ARG	N-CA-C	6.70	120.41	109.76
1	D	313	MET	N-CA-C	6.35	119.93	108.69
1	C	332	HIS	N-CA-C	6.14	118.77	111.71
1	B	467	THR	N-CA-C	6.10	119.19	110.10
1	B	276	GLY	N-CA-C	-5.89	104.86	112.10
1	A	467	THR	N-CA-C	5.49	118.19	109.96
1	B	432	ASN	N-CA-C	5.47	116.58	108.86
1	B	211	ASP	CA-C-N	5.47	125.29	119.28
1	B	211	ASP	C-N-CA	5.47	125.29	119.28
1	D	388	GLY	N-CA-C	5.46	121.19	114.69
1	A	404	ASN	CA-C-N	5.43	125.10	119.56
1	A	404	ASN	C-N-CA	5.43	125.10	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	101	VAL	N-CA-C	-5.41	105.10	110.62
1	A	120	ALA	N-CA-C	5.39	116.84	111.07
1	C	211	ASP	CA-C-N	5.39	125.21	119.28
1	C	211	ASP	C-N-CA	5.39	125.21	119.28
1	C	467	THR	N-CA-C	5.36	118.08	110.10
1	A	20	HIS	N-CA-C	-5.32	103.23	110.36
1	B	332	HIS	N-CA-C	5.25	117.00	111.28
1	B	161	LEU	N-CA-C	-5.20	106.94	113.28
1	A	332	HIS	N-CA-C	5.18	117.01	111.36
1	D	263	VAL	N-CA-C	5.12	115.85	110.62
1	B	32	LEU	N-CA-C	-5.06	105.77	111.28
1	A	473	VAL	N-CA-C	5.04	115.57	108.36
1	B	159	GLN	N-CA-C	5.01	116.43	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4063	0	4036	141	0
1	B	4063	0	4036	149	0
1	C	4063	0	4036	181	0
1	D	4063	0	4036	153	0
2	A	36	0	11	1	0
2	B	36	0	11	0	0
2	C	36	0	11	2	0
2	D	36	0	11	0	0
All	All	16396	0	16188	584	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 18.

All (584) 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:C:200:ILE:CG2	1:C:264:ARG:NH2	1.88	1.36
1:A:200:ILE:HB	1:A:264:ARG:NH2	1.44	1.30
1:C:200:ILE:HG22	1:C:264:ARG:NH2	1.46	1.23
1:D:200:ILE:CD1	1:D:264:ARG:HH21	1.52	1.19
1:A:200:ILE:CB	1:A:264:ARG:NH2	2.12	1.11
1:D:200:ILE:HD12	1:D:264:ARG:HH21	0.99	1.11
1:C:194:ALA:HB2	1:D:194:ALA:HB3	1.32	1.08
1:C:200:ILE:HG22	1:C:264:ARG:HH22	0.96	1.07
1:B:351:ARG:HH11	1:B:351:ARG:HB3	0.95	1.06
1:C:200:ILE:HG21	1:C:264:ARG:HH21	0.94	1.06
1:B:52:ARG:HG3	1:B:52:ARG:HH11	1.10	1.06
1:C:200:ILE:HG21	1:C:264:ARG:NH2	1.61	1.04
1:A:92:GLN:O	1:A:443:LEU:HD22	1.56	1.04
1:C:200:ILE:CG2	1:C:264:ARG:HH21	1.58	1.01
1:B:347:MET:SD	1:B:351:ARG:NH1	2.33	1.01
1:B:351:ARG:HB3	1:B:351:ARG:NH1	1.76	1.00
1:A:347:MET:SD	1:A:351:ARG:NH1	2.32	1.00
1:D:200:ILE:HD12	1:D:264:ARG:NH2	1.78	0.99
1:D:200:ILE:CB	1:D:264:ARG:NH2	2.26	0.98
1:D:200:ILE:CD1	1:D:264:ARG:NH2	2.28	0.97
1:A:200:ILE:CD1	1:A:264:ARG:HH21	1.78	0.97
1:D:200:ILE:HB	1:D:264:ARG:NH2	1.81	0.96
1:A:61:MET:HE2	1:B:67:ILE:HD11	1.50	0.94
1:B:50:ALA:HA	1:B:53:HIS:HE1	1.33	0.94
1:C:406:LEU:HD13	1:C:406:LEU:O	1.68	0.94
1:C:368:HIS:HB2	1:C:370:THR:HG23	1.49	0.94
1:D:124:LYS:O	1:D:127:ASP:HB2	1.68	0.93
1:D:200:ILE:HB	1:D:264:ARG:HH22	1.30	0.93
1:A:67:ILE:HD11	1:B:61:MET:HE2	1.49	0.93
1:C:194:ALA:CB	1:D:194:ALA:HB3	1.99	0.91
1:C:200:ILE:CG2	1:C:264:ARG:HH22	1.68	0.90
1:B:50:ALA:HA	1:B:53:HIS:CE1	2.06	0.90
1:A:200:ILE:HG22	1:A:201:GLN:H	1.35	0.89
1:D:347:MET:HE2	1:D:351:ARG:NH2	1.86	0.89
1:B:63:ARG:HH11	1:B:63:ARG:HG2	1.39	0.88
1:A:200:ILE:HD12	1:A:264:ARG:HH21	1.38	0.88
1:A:200:ILE:HB	1:A:264:ARG:HH22	1.14	0.88
1:D:426:LEU:HD11	1:D:435:TYR:HD1	1.39	0.87
1:C:404:ASN:CG	1:C:406:LEU:HD11	2.00	0.87
1:A:200:ILE:HB	1:A:264:ARG:HH21	1.37	0.86
1:C:402:LEU:HD12	1:C:403:LYS:N	1.91	0.86
1:D:200:ILE:HG21	1:D:264:ARG:NH2	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:MET:HB2	1:D:351:ARG:HE	1.38	0.86
1:B:94:PHE:O	1:B:443:LEU:HD11	1.75	0.85
1:C:371:ILE:HG22	1:C:372:LYS:H	1.40	0.85
1:D:200:ILE:CG2	1:D:264:ARG:NH2	2.40	0.84
1:A:200:ILE:CB	1:A:264:ARG:HH21	1.89	0.83
1:C:371:ILE:HG22	1:C:372:LYS:N	1.92	0.83
1:D:200:ILE:CB	1:D:264:ARG:HH22	1.88	0.83
1:C:404:ASN:OD1	1:C:406:LEU:HD11	1.78	0.82
1:B:52:ARG:HG3	1:B:52:ARG:NH1	1.86	0.82
1:B:347:MET:HB2	1:B:351:ARG:CZ	2.10	0.82
1:A:35:PHE:CZ	1:A:200:ILE:CD1	2.63	0.82
1:D:347:MET:HB2	1:D:351:ARG:NE	1.93	0.82
1:A:78:TYR:HD2	1:A:271:VAL:HG11	1.45	0.82
1:C:67:ILE:HD11	1:D:61:MET:HE2	1.61	0.81
1:A:426:LEU:HD11	1:A:435:TYR:HD1	1.44	0.81
1:A:35:PHE:HZ	1:A:200:ILE:CD1	1.93	0.81
1:B:367:ASN:HB3	1:B:371:ILE:HD11	1.63	0.80
1:C:404:ASN:HB2	1:C:406:LEU:CD1	2.11	0.80
1:B:347:MET:HB2	1:B:351:ARG:NH1	1.97	0.80
1:C:404:ASN:C	1:C:406:LEU:HD12	2.07	0.79
1:A:35:PHE:CZ	1:A:200:ILE:HD11	2.18	0.79
1:B:202:SER:HB2	1:D:352:THR:HG21	1.63	0.79
1:B:351:ARG:HH11	1:B:351:ARG:CB	1.86	0.79
1:A:200:ILE:CG2	1:A:264:ARG:NH2	2.46	0.79
1:D:57:ASP:O	1:D:61:MET:HG2	1.83	0.78
1:C:371:ILE:N	1:C:371:ILE:HD12	1.98	0.78
1:C:50:ALA:HA	1:C:53:HIS:CE1	2.20	0.77
1:D:94:PHE:O	1:D:443:LEU:HD11	1.85	0.76
1:C:97:ASP:O	1:C:101:VAL:HG23	1.86	0.76
1:C:268:ASP:O	1:C:272:GLU:HG3	1.84	0.76
1:C:57:ASP:O	1:C:61:MET:HG2	1.86	0.75
1:D:200:ILE:CG2	1:D:264:ARG:HH22	2.00	0.74
1:D:417:GLN:HG2	1:D:456:TYR:OH	1.87	0.74
1:A:61:MET:HE3	1:B:61:MET:HB3	1.70	0.73
1:C:406:LEU:O	1:C:406:LEU:CD1	2.35	0.73
1:A:367:ASN:HB3	1:A:371:ILE:HD11	1.70	0.73
1:A:200:ILE:CG2	1:A:201:GLN:H	2.02	0.73
1:B:97:ASP:O	1:B:101:VAL:HG23	1.87	0.73
1:D:78:TYR:HD2	1:D:271:VAL:HG11	1.51	0.73
1:A:200:ILE:CB	1:A:264:ARG:HH22	1.89	0.73
1:A:200:ILE:HG22	1:A:201:GLN:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:PRO:HB2	1:C:170:TRP:CZ2	2.23	0.73
1:D:200:ILE:CG1	1:D:264:ARG:HH21	2.02	0.73
1:D:426:LEU:HD11	1:D:435:TYR:CD1	2.23	0.72
1:A:417:GLN:HG2	1:A:456:TYR:OH	1.90	0.72
1:C:35:PHE:HE2	1:C:264:ARG:HE	1.38	0.72
1:B:202:SER:HB2	1:D:352:THR:CG2	2.19	0.72
1:C:404:ASN:CB	1:C:406:LEU:HD11	2.19	0.71
1:C:426:LEU:O	1:C:495:ASP:HA	1.90	0.71
1:C:404:ASN:O	1:C:406:LEU:HD12	1.90	0.71
1:B:57:ASP:O	1:B:61:MET:HG2	1.91	0.71
1:B:63:ARG:HG2	1:B:63:ARG:NH1	1.99	0.71
1:C:61:MET:HE2	1:D:67:ILE:HD11	1.72	0.71
1:B:18:ILE:HD11	1:B:110:VAL:HG22	1.73	0.71
1:B:158:GLU:HG2	1:B:163:ILE:O	1.90	0.70
1:C:194:ALA:CB	1:D:194:ALA:CB	2.68	0.70
1:A:481:PHE:O	1:A:485:GLN:HG3	1.91	0.70
1:C:368:HIS:O	1:C:371:ILE:CD1	2.39	0.70
1:D:481:PHE:O	1:D:485:GLN:HG3	1.92	0.70
1:C:78:TYR:HD2	1:C:271:VAL:HG11	1.56	0.70
1:C:368:HIS:HB2	1:C:370:THR:CG2	2.22	0.70
1:C:61:MET:HB3	1:D:61:MET:HE3	1.74	0.70
1:D:349:GLN:O	1:D:350:ASP:HB2	1.90	0.69
1:B:20:HIS:CD2	1:B:21:PRO:HD2	2.27	0.69
1:C:403:LYS:C	1:C:404:ASN:HD22	2.00	0.69
1:C:20:HIS:CD2	1:C:21:PRO:HD2	2.28	0.68
1:C:351:ARG:HG2	1:C:352:THR:N	2.08	0.68
1:C:172:ILE:HG21	1:C:218:LEU:HD22	1.74	0.68
1:A:61:MET:CE	1:B:61:MET:HB3	2.24	0.68
1:D:97:ASP:O	1:D:101:VAL:HG23	1.92	0.68
1:A:57:ASP:O	1:A:61:MET:HG2	1.93	0.68
1:A:153:VAL:O	1:A:157:ILE:HG13	1.93	0.68
1:B:347:MET:CB	1:B:351:ARG:NH1	2.57	0.68
1:B:150:PRO:HB2	1:B:170:TRP:CZ2	2.28	0.67
1:D:371:ILE:HG22	1:D:372:LYS:N	2.09	0.67
1:B:200:ILE:HG22	1:B:201:GLN:N	2.09	0.67
1:B:371:ILE:HG22	1:B:372:LYS:N	2.10	0.67
1:C:404:ASN:CB	1:C:406:LEU:CD1	2.72	0.67
1:A:124:LYS:O	1:A:127:ASP:HB2	1.95	0.67
1:D:107:SER:HB3	1:D:275:PRO:HD2	1.76	0.67
1:C:371:ILE:HD12	1:C:371:ILE:H	1.58	0.66
1:B:282:ALA:HB3	1:B:285:ARG:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LYS:HA	1:B:52:ARG:NH1	2.11	0.66
1:A:35:PHE:HZ	1:A:200:ILE:HD11	1.58	0.66
1:A:35:PHE:HE2	1:A:264:ARG:HE	1.44	0.66
1:D:312:ARG:HD2	1:D:369:GLY:H	1.61	0.66
1:C:444:GLN:O	1:C:448:ILE:HG12	1.96	0.65
1:C:370:THR:H	1:C:371:ILE:HD12	1.61	0.65
1:A:20:HIS:HA	1:A:121:GLN:HB2	1.78	0.65
1:C:397:PHE:O	1:C:398:ARG:HG2	1.97	0.65
1:A:426:LEU:HD11	1:A:435:TYR:CD1	2.29	0.65
1:B:313:MET:HE3	1:B:315:PHE:CE1	2.32	0.65
1:C:406:LEU:HD12	1:C:406:LEU:N	2.12	0.65
1:D:412:GLN:HG2	1:D:416:GLU:OE2	1.97	0.65
1:A:339:THR:HG23	1:A:341:ALA:H	1.62	0.65
1:A:347:MET:CG	1:A:351:ARG:HH12	2.09	0.65
1:C:116:LYS:HD3	1:C:119:GLU:OE2	1.96	0.65
1:C:282:ALA:HB3	1:C:285:ARG:O	1.97	0.64
1:A:61:MET:HB3	1:B:61:MET:HE3	1.80	0.64
1:A:502:TYR:HE2	1:A:504:ALA:HB2	1.61	0.64
1:D:78:TYR:CE2	1:D:267:LEU:HG	2.31	0.64
1:C:20:HIS:HA	1:C:121:GLN:HB2	1.79	0.64
1:D:268:ASP:O	1:D:272:GLU:HG3	1.97	0.64
1:A:150:PRO:HB2	1:A:170:TRP:CZ2	2.33	0.64
1:D:232:LEU:O	1:D:236:GLY:HA3	1.98	0.64
1:B:347:MET:CG	1:B:351:ARG:HH22	2.11	0.64
1:C:137:MET:HA	1:C:251:PRO:HD2	1.80	0.64
1:A:200:ILE:CG1	1:A:264:ARG:HH21	2.11	0.64
1:C:18:ILE:HD11	1:C:110:VAL:HG22	1.80	0.63
1:D:137:MET:HA	1:D:251:PRO:HD2	1.80	0.63
1:B:232:LEU:O	1:B:236:GLY:HA3	1.98	0.63
1:B:402:LEU:CD2	1:B:408:ALA:HA	2.29	0.63
1:C:249:LEU:HD23	1:C:250:THR:N	2.14	0.63
1:A:200:ILE:CD1	1:A:264:ARG:NH2	2.56	0.63
1:C:371:ILE:CG2	1:C:372:LYS:H	2.10	0.62
1:C:371:ILE:CG2	1:C:372:LYS:N	2.62	0.62
1:D:387:VAL:HB	1:D:527:GLU:OE2	1.98	0.62
1:B:347:MET:SD	1:B:351:ARG:NH2	2.72	0.62
1:B:172:ILE:HG21	1:B:218:LEU:HD22	1.82	0.61
1:C:61:MET:HE3	1:D:61:MET:HB3	1.82	0.61
1:C:403:LYS:HB3	1:C:404:ASN:ND2	2.15	0.61
1:D:96:GLU:OE1	1:D:391:ASN:ND2	2.32	0.61
1:C:158:GLU:HG2	1:C:163:ILE:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:ALA:O	1:D:351:ARG:HG2	2.00	0.61
1:C:61:MET:CE	1:D:61:MET:HB3	2.31	0.60
1:C:404:ASN:OD1	1:C:406:LEU:HD21	2.02	0.60
1:A:316:LEU:HD23	1:A:363:ILE:HD11	1.84	0.60
1:C:94:PHE:O	1:C:443:LEU:HD11	2.02	0.60
1:C:132:ARG:HG2	1:C:132:ARG:HH11	1.66	0.60
1:D:303:ALA:HB2	1:D:312:ARG:HH12	1.66	0.60
1:B:200:ILE:CG2	1:B:201:GLN:N	2.64	0.60
1:D:35:PHE:HE2	1:D:264:ARG:HE	1.49	0.60
1:D:348:ALA:HB3	1:D:351:ARG:HD3	1.82	0.60
1:B:417:GLN:HG2	1:B:456:TYR:OH	2.02	0.59
1:C:387:VAL:HB	1:C:527:GLU:OE2	2.02	0.59
1:A:424:VAL:HG22	1:A:425:GLN:N	2.16	0.59
1:A:61:MET:HE2	1:B:67:ILE:CD1	2.29	0.59
1:A:468:HIS:HB2	1:A:505:PRO:O	2.02	0.59
1:C:58:TRP:HA	1:C:61:MET:HG3	1.85	0.59
1:A:35:PHE:HE2	1:A:264:ARG:NE	2.00	0.59
1:D:282:ALA:HB3	1:D:285:ARG:O	2.02	0.59
1:B:347:MET:HG3	1:B:351:ARG:HH22	1.68	0.59
1:B:347:MET:CG	1:B:351:ARG:NH2	2.65	0.59
1:C:67:ILE:HD11	1:D:61:MET:CE	2.33	0.59
1:D:170:TRP:CE3	1:D:232:LEU:HD11	2.37	0.59
1:A:240:ASP:CG	1:A:243:ARG:HG3	2.28	0.59
1:B:35:PHE:HE2	1:B:264:ARG:HE	1.50	0.58
1:B:430:LEU:HD12	1:B:492:LEU:HB2	1.85	0.58
1:D:424:VAL:HG22	1:D:425:GLN:N	2.18	0.58
1:A:444:GLN:O	1:A:448:ILE:HG12	2.03	0.58
1:B:240:ASP:CG	1:B:243:ARG:HG3	2.28	0.58
1:A:137:MET:HA	1:A:251:PRO:HD2	1.85	0.58
1:B:347:MET:SD	1:B:351:ARG:CZ	2.91	0.58
1:D:339:THR:HG23	1:D:341:ALA:H	1.68	0.58
1:A:200:ILE:HG21	1:A:264:ARG:NH2	2.18	0.58
1:D:347:MET:HE2	1:D:351:ARG:CZ	2.34	0.58
1:B:402:LEU:HG	1:B:404:ASN:O	2.03	0.58
1:C:150:PRO:HG3	1:C:171:PRO:HG2	1.86	0.58
1:A:94:PHE:O	1:A:443:LEU:HD11	2.05	0.57
1:B:200:ILE:O	1:B:201:GLN:HG2	2.04	0.57
1:D:20:HIS:CG	1:D:21:PRO:HD2	2.39	0.57
1:D:200:ILE:CG1	1:D:264:ARG:NH2	2.65	0.57
1:B:52:ARG:NH1	1:B:52:ARG:CG	2.64	0.57
1:B:339:THR:HG23	1:B:341:ALA:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:ILE:HG22	1:D:372:LYS:H	1.68	0.57
1:A:509:ARG:NH1	1:C:164:GLU:OE2	2.37	0.57
1:B:63:ARG:HH11	1:B:63:ARG:CG	2.13	0.57
1:C:406:LEU:HD13	1:C:406:LEU:C	2.30	0.57
1:C:194:ALA:HB1	1:D:194:ALA:CB	2.34	0.57
1:D:92:GLN:O	1:D:443:LEU:HD13	2.04	0.57
1:C:397:PHE:C	1:C:398:ARG:HG2	2.31	0.56
1:A:17:ILE:HG21	1:A:25:LYS:HG3	1.87	0.56
1:C:402:LEU:HD12	1:C:402:LEU:C	2.30	0.56
1:D:35:PHE:CZ	1:D:200:ILE:HD11	2.40	0.56
1:A:36:GLY:O	1:A:77:PRO:HD2	2.06	0.56
1:C:211:ASP:OD1	1:C:213:GLN:HB2	2.05	0.56
1:C:240:ASP:CG	1:C:243:ARG:HG3	2.31	0.56
1:C:403:LYS:C	1:C:404:ASN:ND2	2.64	0.56
1:C:92:GLN:O	1:C:443:LEU:HD22	2.06	0.56
1:A:249:LEU:HD23	1:A:250:THR:N	2.21	0.56
1:B:347:MET:HG3	1:B:351:ARG:NH2	2.21	0.56
1:B:406:LEU:H	1:B:406:LEU:CD2	2.19	0.55
1:C:327:MET:HE2	1:C:329:LEU:HD21	1.88	0.55
1:C:36:GLY:O	1:C:77:PRO:HD2	2.06	0.55
1:C:57:ASP:O	1:C:61:MET:CG	2.55	0.55
1:A:14:THR:OG1	1:A:84:ASN:HB2	2.05	0.55
1:B:20:HIS:CG	1:B:21:PRO:HD2	2.42	0.55
1:B:78:TYR:CE2	1:B:267:LEU:HG	2.41	0.55
1:A:94:PHE:O	1:A:443:LEU:HD21	2.07	0.55
1:D:150:PRO:HB2	1:D:170:TRP:CZ2	2.41	0.55
1:C:402:LEU:HD12	1:C:404:ASN:H	1.71	0.55
1:C:61:MET:HB3	1:D:61:MET:CE	2.38	0.54
1:A:333:ARG:HG2	1:A:333:ARG:HH21	1.72	0.54
1:C:327:MET:HE2	1:C:329:LEU:CD2	2.37	0.54
1:D:367:ASN:HB3	1:D:371:ILE:HD11	1.89	0.54
1:C:303:ALA:HB2	1:C:312:ARG:HH12	1.72	0.54
1:C:424:VAL:HB	1:C:448:ILE:HD11	1.90	0.54
1:C:67:ILE:CD1	1:D:61:MET:HE2	2.36	0.54
1:C:168:MET:HE2	1:C:269:MET:CE	2.38	0.54
1:A:14:THR:HG22	1:A:105:VAL:HA	1.89	0.54
1:A:245:LEU:CD2	1:A:275:PRO:HG3	2.38	0.54
1:B:444:GLN:O	1:B:448:ILE:HG12	2.08	0.54
1:D:345:ILE:HD12	1:D:355:GLU:HG2	1.89	0.54
1:B:20:HIS:HA	1:B:121:GLN:HB2	1.89	0.53
1:B:406:LEU:O	1:B:407:LYS:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:LEU:HD23	1:B:443:LEU:H	1.73	0.53
1:B:507:PRO:O	1:B:510:LEU:HB3	2.08	0.53
1:C:371:ILE:N	1:C:371:ILE:CD1	2.71	0.53
1:C:404:ASN:ND2	1:C:404:ASN:N	2.57	0.53
1:B:200:ILE:HG23	1:B:264:ARG:HH22	1.73	0.53
1:C:406:LEU:CD1	1:C:406:LEU:C	2.82	0.53
1:A:116:LYS:HD3	1:A:119:GLU:OE2	2.08	0.53
1:C:154:MET:HE1	1:C:167:PRO:HD3	1.91	0.53
1:B:49:LYS:HA	1:B:52:ARG:HH12	1.72	0.53
1:D:36:GLY:O	1:D:77:PRO:HD2	2.09	0.53
1:C:21:PRO:O	1:C:22:ASP:HB2	2.08	0.53
1:C:154:MET:HE2	1:C:170:TRP:CZ3	2.44	0.53
1:C:194:ALA:HB2	1:D:194:ALA:CB	2.20	0.53
1:B:116:LYS:HD2	1:B:119:GLU:OE2	2.09	0.52
1:C:94:PHE:O	1:C:443:LEU:HD21	2.09	0.52
1:C:402:LEU:HG	1:C:404:ASN:O	2.09	0.52
1:A:67:ILE:CD1	1:B:61:MET:HE2	2.33	0.52
1:C:25:LYS:NZ	1:C:88:THR:O	2.42	0.52
1:C:78:TYR:CE2	1:C:267:LEU:HG	2.44	0.52
1:C:154:MET:HE2	1:C:170:TRP:HZ3	1.74	0.52
1:D:20:HIS:CD2	1:D:21:PRO:HD2	2.45	0.52
1:D:502:TYR:HE2	1:D:504:ALA:HB2	1.73	0.52
1:D:56:SER:HA	1:D:59:MET:HE2	1.91	0.52
1:B:107:SER:HA	1:B:134:THR:CG2	2.39	0.52
1:C:406:LEU:HD22	1:C:407:LYS:HE3	1.90	0.52
1:C:132:ARG:HG2	1:C:132:ARG:NH1	2.23	0.52
1:C:258:ILE:HB	2:C:601:G4P:C5	2.40	0.52
1:D:20:HIS:HA	1:D:121:GLN:HB2	1.90	0.52
1:B:371:ILE:CG2	1:B:372:LYS:N	2.74	0.51
1:B:397:PHE:C	1:B:398:ARG:HG2	2.36	0.51
1:C:18:ILE:CD1	1:C:110:VAL:HG22	2.40	0.51
1:B:92:GLN:HA	1:B:92:GLN:OE1	2.10	0.51
1:C:334:THR:HB	1:C:336:LYS:HG2	1.92	0.51
1:B:468:HIS:HB2	1:B:505:PRO:O	2.11	0.51
1:A:492:LEU:HD23	1:A:502:TYR:HA	1.92	0.51
1:B:170:TRP:CE3	1:B:232:LEU:HD11	2.46	0.51
1:C:367:ASN:HB3	1:C:371:ILE:HD11	1.92	0.51
1:D:410:GLN:NE2	1:D:456:TYR:O	2.44	0.51
1:D:280:ARG:HD3	1:D:319:CYS:SG	2.50	0.51
1:B:78:TYR:HD2	1:B:271:VAL:HG11	1.76	0.51
1:D:401:ARG:HB3	1:D:461:VAL:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:LEU:HD22	1:B:406:LEU:N	2.26	0.51
1:A:78:TYR:CE2	1:A:267:LEU:HG	2.46	0.50
1:A:371:ILE:HG22	1:A:372:LYS:N	2.25	0.50
1:B:35:PHE:HE2	1:B:264:ARG:NE	2.09	0.50
1:B:338:VAL:HG12	1:B:339:THR:N	2.25	0.50
1:D:57:ASP:O	1:D:61:MET:CG	2.56	0.50
1:D:92:GLN:O	1:D:443:LEU:HD22	2.11	0.50
1:A:426:LEU:O	1:A:495:ASP:HA	2.11	0.50
1:C:368:HIS:O	1:C:370:THR:N	2.40	0.50
1:B:132:ARG:HH11	1:B:132:ARG:HG2	1.77	0.50
1:A:351:ARG:HH11	1:A:351:ARG:HB3	1.77	0.50
1:D:48:ARG:HD2	1:D:67:ILE:HG22	1.93	0.50
1:A:164:GLU:HG2	1:C:509:ARG:NH2	2.27	0.50
1:C:294:PHE:HA	1:C:321:GLY:HA3	1.93	0.50
1:C:58:TRP:CZ2	1:D:67:ILE:HG21	2.47	0.50
1:B:296:GLY:HA3	1:B:316:LEU:HD21	1.93	0.50
1:C:240:ASP:OD1	1:C:243:ARG:HG3	2.11	0.50
1:A:445:PHE:HB3	1:A:462:TYR:CE1	2.47	0.49
1:B:426:LEU:HD11	1:B:435:TYR:HD1	1.77	0.49
1:C:53:HIS:O	1:D:40:GLN:HA	2.12	0.49
1:A:508:TRP:HZ3	1:C:164:GLU:HG3	1.77	0.49
1:D:88:THR:HB	1:D:98:THR:HG23	1.94	0.49
1:D:232:LEU:O	1:D:236:GLY:CA	2.60	0.49
1:A:200:ILE:HD12	1:A:264:ARG:NH2	2.18	0.49
1:B:3:SER:O	1:B:4:ARG:C	2.55	0.49
1:D:297:VAL:C	1:D:316:LEU:HD12	2.38	0.49
1:B:382:GLU:HG2	1:B:383:VAL:N	2.27	0.49
1:A:168:MET:HE1	1:A:239:PHE:HB3	1.94	0.49
1:D:172:ILE:HG21	1:D:218:LEU:HD22	1.95	0.49
1:D:426:LEU:O	1:D:495:ASP:HA	2.13	0.49
1:A:61:MET:CE	1:B:67:ILE:HD11	2.32	0.49
1:B:313:MET:HE3	1:B:315:PHE:CZ	2.47	0.49
1:A:430:LEU:HD12	1:A:492:LEU:HB2	1.95	0.48
1:C:358:PHE:HB3	1:C:359:PRO:HD2	1.95	0.48
1:C:215:ASP:CG	1:C:226:ARG:HH22	2.20	0.48
1:C:404:ASN:HB2	1:C:406:LEU:HD12	1.94	0.48
1:A:507:PRO:O	1:A:510:LEU:HB3	2.13	0.48
1:B:21:PRO:O	1:B:22:ASP:HB2	2.13	0.48
1:D:321:GLY:O	1:D:359:PRO:HD3	2.12	0.48
1:B:73:VAL:HG22	1:B:86:LEU:HD22	1.95	0.48
1:A:21:PRO:HD3	1:A:121:GLN:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ILE:HD11	1:B:371:ILE:HG22	1.95	0.48
1:C:194:ALA:HB1	1:D:194:ALA:HB2	1.94	0.48
1:C:368:HIS:O	1:C:371:ILE:HD11	2.12	0.48
1:C:404:ASN:HB2	1:C:406:LEU:HG	1.95	0.48
1:D:240:ASP:CG	1:D:243:ARG:HG3	2.38	0.48
1:A:48:ARG:HD2	1:A:67:ILE:HG22	1.96	0.48
1:A:113:ASP:C	1:A:113:ASP:OD1	2.54	0.48
1:A:200:ILE:CG2	1:A:264:ARG:HH22	2.22	0.48
1:B:202:SER:CB	1:D:352:THR:HG21	2.38	0.48
1:B:249:LEU:HD23	1:B:250:THR:N	2.28	0.48
1:D:25:LYS:NZ	1:D:88:THR:O	2.46	0.48
1:D:55:THR:O	1:D:59:MET:HG3	2.14	0.48
1:D:158:GLU:HG2	1:D:163:ILE:O	2.14	0.48
1:D:367:ASN:CB	1:D:371:ILE:HD11	2.43	0.48
1:A:401:ARG:HB3	1:A:461:VAL:HG23	1.95	0.48
1:B:240:ASP:HB3	1:B:243:ARG:HG3	1.94	0.48
1:C:78:TYR:CD2	1:C:271:VAL:HG11	2.44	0.48
1:C:468:HIS:HB2	1:C:505:PRO:O	2.14	0.47
1:A:78:TYR:CD2	1:A:271:VAL:HG11	2.37	0.47
1:D:333:ARG:HG2	1:D:333:ARG:HH21	1.79	0.47
1:B:347:MET:CB	1:B:351:ARG:CZ	2.88	0.47
1:C:397:PHE:HA	1:C:437:LEU:O	2.13	0.47
1:B:280:ARG:HH21	1:B:389:ILE:HD11	1.78	0.47
1:C:388:GLY:N	1:C:527:GLU:OE2	2.48	0.47
1:D:400:VAL:HG23	1:D:437:LEU:HG	1.96	0.47
1:A:55:THR:O	1:A:59:MET:HG3	2.13	0.47
1:B:185:LEU:HA	1:B:185:LEU:HD23	1.58	0.47
1:C:20:HIS:CG	1:C:21:PRO:HD2	2.50	0.47
1:D:468:HIS:HB2	1:D:505:PRO:O	2.14	0.47
1:A:20:HIS:CD2	1:A:119:GLU:CD	2.93	0.47
1:A:67:ILE:HD13	1:B:58:TRP:CZ2	2.50	0.47
1:C:107:SER:HB3	1:C:275:PRO:HD2	1.97	0.47
1:C:351:ARG:CG	1:C:352:THR:N	2.77	0.47
1:A:20:HIS:CG	1:A:21:PRO:HD2	2.50	0.46
1:A:329:LEU:HD12	1:A:340:VAL:HG11	1.96	0.46
1:B:151:LEU:HD23	1:B:151:LEU:HA	1.72	0.46
1:C:402:LEU:CD1	1:C:404:ASN:H	2.28	0.46
1:C:151:LEU:HD23	1:C:151:LEU:HA	1.66	0.46
1:C:327:MET:CE	1:C:329:LEU:HD21	2.45	0.46
1:C:338:VAL:HG12	1:C:339:THR:N	2.30	0.46
1:D:35:PHE:HZ	1:D:200:ILE:HD11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LEU:O	1:A:236:GLY:HA3	2.15	0.46
1:A:268:ASP:O	1:A:272:GLU:HG3	2.15	0.46
1:B:5:LEU:O	1:B:6:GLU:C	2.55	0.46
1:B:406:LEU:CD2	1:B:406:LEU:N	2.78	0.46
1:D:316:LEU:HD23	1:D:363:ILE:HD11	1.96	0.46
1:A:58:TRP:CZ2	1:B:67:ILE:HG21	2.50	0.46
1:A:502:TYR:CE2	1:A:504:ALA:HB2	2.47	0.46
1:C:17:ILE:HG21	1:C:25:LYS:HG3	1.97	0.46
1:C:58:TRP:HE1	1:D:67:ILE:HG23	1.81	0.46
1:C:73:VAL:HG13	1:C:86:LEU:CD2	2.46	0.46
1:C:404:ASN:HB2	1:C:406:LEU:CG	2.44	0.46
1:D:27:THR:O	1:D:31:LYS:HG2	2.15	0.46
1:A:410:GLN:NE2	1:A:456:TYR:O	2.49	0.46
1:C:49:LYS:O	1:C:53:HIS:CE1	2.69	0.46
1:C:258:ILE:HB	2:C:601:G4P:C6	2.46	0.46
1:D:347:MET:CB	1:D:351:ARG:HE	2.20	0.46
1:A:25:LYS:NZ	1:A:88:THR:O	2.49	0.46
1:B:443:LEU:H	1:B:443:LEU:CD2	2.25	0.46
1:C:358:PHE:HB3	1:C:359:PRO:CD	2.45	0.46
1:A:138:THR:HG21	1:A:157:ILE:HD13	1.98	0.46
1:C:249:LEU:HD23	1:C:249:LEU:C	2.41	0.46
1:D:149:HIS:ND1	1:D:150:PRO:HD2	2.30	0.46
1:D:349:GLN:O	1:D:350:ASP:CB	2.62	0.46
1:A:108:ALA:O	1:A:136:VAL:HA	2.16	0.46
1:A:154:MET:HE2	1:A:170:TRP:HZ3	1.81	0.46
1:A:424:VAL:CG2	1:A:425:GLN:N	2.79	0.46
1:B:316:LEU:HD23	1:B:363:ILE:HD11	1.98	0.46
1:C:339:THR:HG23	1:C:341:ALA:H	1.80	0.46
1:D:447:VAL:O	1:D:451:ARG:HG3	2.16	0.46
1:A:27:THR:O	1:A:31:LYS:HG2	2.16	0.45
1:B:124:LYS:O	1:B:127:ASP:HB2	2.15	0.45
1:B:410:GLN:NE2	1:B:456:TYR:O	2.50	0.45
1:D:443:LEU:HD23	1:D:443:LEU:H	1.81	0.45
1:D:506:ASN:HB2	1:D:507:PRO:HD2	1.99	0.45
1:B:137:MET:HA	1:B:251:PRO:HD2	1.97	0.45
1:D:18:ILE:O	1:D:18:ILE:HG13	2.16	0.45
1:A:97:ASP:O	1:A:101:VAL:HG23	2.17	0.45
1:C:159:GLN:HG2	1:C:160:HIS:CD2	2.51	0.45
1:D:294:PHE:HB3	1:D:379:GLU:HB2	1.98	0.45
1:A:257:ALA:O	1:A:258:ILE:C	2.59	0.45
1:C:371:ILE:CD1	1:C:371:ILE:H	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:PHE:CD2	1:D:270:PHE:CZ	3.04	0.45
1:B:58:TRP:O	1:B:61:MET:N	2.47	0.45
1:D:113:ASP:OD1	1:D:113:ASP:C	2.59	0.45
1:C:61:MET:CE	1:D:67:ILE:HD11	2.42	0.45
1:C:99:TYR:O	1:C:102:LEU:HB2	2.16	0.45
1:B:21:PRO:HD3	1:B:121:GLN:HG3	1.98	0.45
1:B:25:LYS:NZ	1:B:88:THR:O	2.50	0.45
1:D:510:LEU:HG	1:D:514:MET:HE2	1.98	0.45
1:B:268:ASP:O	1:B:272:GLU:HG3	2.17	0.45
1:D:299:PHE:CD1	1:D:300:LYS:HB2	2.52	0.45
1:B:315:PHE:CD1	1:B:315:PHE:N	2.85	0.44
1:B:424:VAL:HG22	1:B:425:GLN:N	2.32	0.44
1:C:65:ARG:NH1	1:C:303:ALA:O	2.50	0.44
1:C:303:ALA:HB2	1:C:312:ARG:NH1	2.32	0.44
1:D:511:GLU:HA	1:D:514:MET:HB2	1.98	0.44
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.76	0.44
1:C:330:LYS:HE3	1:C:381:LYS:HG2	1.98	0.44
1:D:81:ARG:HD3	1:D:271:VAL:HB	1.99	0.44
1:A:303:ALA:HB2	1:A:312:ARG:HH12	1.81	0.44
1:B:343:ALA:HA	1:B:366:PRO:HD3	2.00	0.44
1:C:58:TRP:HZ2	1:D:67:ILE:HG21	1.81	0.44
1:C:61:MET:HE2	1:D:67:ILE:CD1	2.45	0.44
1:C:102:LEU:HD23	1:C:102:LEU:HA	1.80	0.44
1:C:294:PHE:CE1	1:C:323:PHE:HB2	2.52	0.44
1:A:159:GLN:HG2	1:A:160:HIS:CE1	2.52	0.44
1:B:347:MET:CG	1:B:351:ARG:NH1	2.80	0.44
1:C:185:LEU:HD23	1:C:185:LEU:HA	1.60	0.44
1:D:389:ILE:HA	1:D:390:PRO:HD3	1.88	0.44
1:D:397:PHE:O	1:D:398:ARG:HG2	2.17	0.44
1:B:28:LEU:CD1	1:B:263:VAL:HG22	2.47	0.44
1:B:48:ARG:HD2	1:B:67:ILE:HG22	1.99	0.44
1:C:67:ILE:HG21	1:D:58:TRP:CZ2	2.51	0.44
1:A:323:PHE:C	1:A:323:PHE:CD2	2.95	0.44
1:A:334:THR:HB	1:A:336:LYS:HG2	1.99	0.44
1:B:150:PRO:HG3	1:B:171:PRO:HG2	2.00	0.44
1:C:32:LEU:HD22	1:C:267:LEU:HD13	1.99	0.44
1:C:300:LYS:HB3	1:C:315:PHE:HB2	2.00	0.44
1:D:301:ILE:HG22	1:D:302:GLN:N	2.32	0.44
1:C:338:VAL:CG1	1:C:339:THR:N	2.81	0.44
1:D:108:ALA:HB3	1:D:136:VAL:HG12	2.00	0.44
1:A:170:TRP:CE3	1:A:232:LEU:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ASP:O	1:C:211:ASP:C	2.61	0.43
1:C:431:VAL:HG23	1:C:432:ASN:HD22	1.83	0.43
1:A:401:ARG:HD3	1:A:401:ARG:HA	1.77	0.43
1:B:154:MET:HE2	1:B:170:TRP:HZ3	1.82	0.43
1:B:159:GLN:HG2	1:B:160:HIS:CD2	2.53	0.43
1:D:18:ILE:HD11	1:D:110:VAL:HG22	2.00	0.43
1:C:168:MET:CE	1:C:269:MET:CE	2.97	0.43
1:A:107:SER:HB3	1:A:275:PRO:HD2	2.01	0.43
1:A:412:GLN:O	1:A:416:GLU:HG3	2.18	0.43
1:D:149:HIS:O	1:D:152:ASP:N	2.51	0.43
1:A:172:ILE:HG21	1:A:218:LEU:HD22	2.00	0.43
1:B:287:VAL:HG21	1:B:384:LEU:HD21	2.00	0.43
1:A:280:ARG:HG3	1:A:281:PRO:HD2	2.00	0.43
1:A:479:LYS:HD3	1:A:479:LYS:HA	1.87	0.43
1:C:168:MET:CE	1:C:269:MET:HE1	2.48	0.43
1:C:417:GLN:HG2	1:C:456:TYR:OH	2.19	0.43
1:D:323:PHE:CD2	1:D:323:PHE:C	2.97	0.43
1:C:3:SER:O	1:C:4:ARG:C	2.61	0.43
1:C:402:LEU:HB2	1:C:411:LEU:HD22	2.01	0.43
1:C:511:GLU:HA	1:C:514:MET:HB2	2.00	0.43
1:D:418:LEU:O	1:D:422:GLY:N	2.50	0.43
1:A:333:ARG:HH21	1:A:333:ARG:CG	2.32	0.43
1:B:116:LYS:CD	1:B:119:GLU:OE2	2.67	0.43
1:B:294:PHE:CE1	1:B:323:PHE:HB2	2.54	0.43
1:B:348:ALA:O	1:B:351:ARG:HD2	2.19	0.43
1:D:149:HIS:O	1:D:150:PRO:C	2.62	0.43
1:D:424:VAL:CG2	1:D:425:GLN:N	2.82	0.43
1:A:274:ALA:HA	1:A:275:PRO:HD3	1.93	0.42
1:D:132:ARG:HH11	1:D:132:ARG:HG2	1.84	0.42
1:A:35:PHE:CZ	1:A:200:ILE:HD12	2.52	0.42
1:B:149:HIS:ND1	1:B:150:PRO:HD2	2.34	0.42
1:A:154:MET:HE2	1:A:170:TRP:CZ3	2.55	0.42
1:A:282:ALA:HB3	1:A:285:ARG:O	2.19	0.42
1:A:402:LEU:HD22	1:A:411:LEU:HD22	2.01	0.42
1:C:404:ASN:O	1:C:406:LEU:CD1	2.61	0.42
1:D:153:VAL:O	1:D:157:ILE:HG13	2.18	0.42
1:A:157:ILE:HG23	1:A:161:LEU:HD12	2.01	0.42
1:B:57:ASP:O	1:B:61:MET:CG	2.65	0.42
1:C:294:PHE:CD2	1:C:294:PHE:C	2.97	0.42
1:C:368:HIS:O	1:C:371:ILE:HD12	2.17	0.42
1:D:35:PHE:HZ	1:D:200:ILE:CD1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:TYR:CE2	1:D:504:ALA:HB2	2.55	0.42
1:A:158:GLU:HG2	1:A:163:ILE:O	2.19	0.42
1:B:107:SER:HA	1:B:134:THR:HG23	2.01	0.42
1:B:426:LEU:O	1:B:495:ASP:HA	2.20	0.42
1:C:128:VAL:O	1:C:131:MET:HG2	2.19	0.42
1:D:338:VAL:HG12	1:D:339:THR:N	2.33	0.42
1:D:371:ILE:CG2	1:D:372:LYS:N	2.79	0.42
1:D:397:PHE:C	1:D:398:ARG:HG2	2.44	0.42
1:D:412:GLN:CG	1:D:416:GLU:OE2	2.66	0.42
1:A:127:ASP:HA	1:A:130:ARG:NH1	2.35	0.42
1:A:347:MET:HG3	1:A:351:ARG:NH1	2.34	0.42
1:A:403:LYS:O	1:A:405:PRO:HD3	2.19	0.42
1:A:472:TRP:CE2	1:A:526:ARG:HG2	2.55	0.42
1:B:15:PHE:CG	1:B:270:PHE:CZ	3.07	0.42
1:B:506:ASN:HB2	1:B:507:PRO:HD2	2.02	0.42
1:D:35:PHE:CZ	1:D:200:ILE:CD1	3.01	0.42
1:D:250:THR:HA	1:D:251:PRO:HD3	1.85	0.42
1:A:506:ASN:HB2	1:A:507:PRO:HD2	2.01	0.42
1:B:154:MET:HE1	1:B:167:PRO:HD3	2.02	0.42
1:B:402:LEU:HD21	1:B:408:ALA:HA	1.99	0.42
1:B:132:ARG:HG2	1:B:132:ARG:NH1	2.34	0.42
1:B:294:PHE:HA	1:B:321:GLY:HA3	2.02	0.42
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.80	0.42
1:A:325:ARG:O	1:A:340:VAL:HG23	2.19	0.42
1:B:325:ARG:HH11	1:B:325:ARG:HG2	1.85	0.42
1:B:346:PHE:C	1:B:347:MET:CG	2.93	0.42
1:B:417:GLN:CG	1:B:456:TYR:OH	2.67	0.42
1:B:269:MET:HE2	1:B:269:MET:HB2	1.89	0.41
1:C:20:HIS:CD2	1:C:21:PRO:CD	3.02	0.41
1:C:510:LEU:HG	1:C:514:MET:HG3	2.01	0.41
1:D:58:TRP:HA	1:D:61:MET:HG3	2.02	0.41
1:A:426:LEU:CD1	1:A:435:TYR:HD1	2.24	0.41
1:B:20:HIS:CG	1:B:21:PRO:CD	3.03	0.41
1:B:108:ALA:O	1:B:136:VAL:HA	2.20	0.41
1:B:299:PHE:CD1	1:B:300:LYS:HB2	2.54	0.41
1:C:186:HIS:O	1:C:187:LYS:C	2.63	0.41
1:C:481:PHE:O	1:C:485:GLN:HG3	2.19	0.41
1:D:444:GLN:O	1:D:448:ILE:HG12	2.21	0.41
1:A:266:MET:HE3	1:A:266:MET:HB3	1.97	0.41
1:B:405:PRO:O	1:B:408:ALA:HB2	2.20	0.41
1:C:324:THR:O	1:C:327:MET:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:PHE:N	1:A:315:PHE:CD1	2.87	0.41
1:B:240:ASP:CB	1:B:243:ARG:HG3	2.49	0.41
1:B:351:ARG:NH1	1:B:351:ARG:CB	2.63	0.41
1:C:393:ALA:HA	1:C:394:PRO:HD3	1.93	0.41
1:C:426:LEU:HD13	1:C:437:LEU:HD23	2.02	0.41
1:D:108:ALA:O	1:D:136:VAL:HA	2.21	0.41
1:D:200:ILE:HD12	1:D:264:ARG:CZ	2.42	0.41
1:C:240:ASP:O	1:C:241:GLU:C	2.62	0.41
1:C:406:LEU:CD1	1:C:406:LEU:N	2.81	0.41
1:D:249:LEU:HD23	1:D:250:THR:N	2.36	0.41
1:B:209:ALA:O	1:B:226:ARG:HD3	2.20	0.41
1:C:113:ASP:C	1:C:113:ASP:OD1	2.64	0.41
1:C:502:TYR:CD2	1:C:502:TYR:C	2.99	0.41
1:A:92:GLN:O	1:A:443:LEU:CD2	2.46	0.41
1:A:170:TRP:CG	1:A:171:PRO:HD2	2.55	0.41
1:A:347:MET:HG3	1:A:351:ARG:HH12	1.86	0.41
1:D:245:LEU:CD2	1:D:275:PRO:HG3	2.51	0.41
1:A:509:ARG:NE	1:C:158:GLU:OE1	2.52	0.41
1:B:124:LYS:NZ	1:B:395:GLU:OE1	2.52	0.41
1:B:232:LEU:O	1:B:236:GLY:CA	2.68	0.41
1:C:20:HIS:CG	1:C:21:PRO:CD	3.04	0.41
1:C:78:TYR:HD2	1:C:271:VAL:CG1	2.28	0.41
1:C:184:LEU:HD12	1:C:184:LEU:H	1.85	0.41
1:C:415:LEU:HD21	1:C:452:LEU:HD11	2.03	0.41
1:D:34:LEU:HD23	1:D:34:LEU:HA	1.88	0.41
1:D:151:LEU:HD23	1:D:151:LEU:HA	1.50	0.41
1:D:184:LEU:HD12	1:D:184:LEU:H	1.86	0.41
1:A:347:MET:CG	1:A:351:ARG:NH1	2.77	0.41
1:B:353:GLY:O	1:B:354:VAL:C	2.64	0.41
1:C:124:LYS:O	1:C:127:ASP:HB2	2.21	0.41
1:B:52:ARG:HH11	1:B:52:ARG:CG	1.98	0.40
1:A:67:ILE:HG21	1:B:58:TRP:CZ2	2.57	0.40
1:A:258:ILE:HB	2:A:601:G4P:C5	2.52	0.40
1:A:372:LYS:N	1:A:375:ASP:OD2	2.45	0.40
1:B:338:VAL:CG1	1:B:339:THR:N	2.84	0.40
1:C:470:ALA:CB	1:C:503:LEU:HD12	2.51	0.40
1:D:114:ALA:HB1	1:D:147:ALA:HB1	2.03	0.40
1:D:333:ARG:HH21	1:D:333:ARG:CG	2.34	0.40
1:A:61:MET:HB3	1:B:61:MET:CE	2.50	0.40
1:A:336:LYS:HA	1:A:336:LYS:HD3	1.93	0.40
1:B:18:ILE:O	1:B:18:ILE:HG13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:PHE:O	1:B:359:PRO:C	2.64	0.40
1:D:245:LEU:HD23	1:D:245:LEU:HA	1.92	0.40
1:A:249:LEU:HD23	1:A:249:LEU:C	2.46	0.40
1:A:325:ARG:HD3	1:A:341:ALA:O	2.22	0.40
1:B:52:ARG:HG2	1:B:62:GLU:OE1	2.22	0.40
1:D:315:PHE:CD1	1:D:315:PHE:N	2.89	0.40
1:A:299:PHE:CD1	1:A:300:LYS:HB2	2.56	0.40
1:D:35:PHE:HE2	1:D:264:ARG:NE	2.18	0.40
1:D:403:LYS:O	1:D:405:PRO:HD3	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	510/548 (93%)	498 (98%)	11 (2%)	1 (0%)	43	76
1	B	510/548 (93%)	494 (97%)	15 (3%)	1 (0%)	43	76
1	C	510/548 (93%)	485 (95%)	25 (5%)	0	100	100
1	D	510/548 (93%)	494 (97%)	15 (3%)	1 (0%)	43	76
All	All	2040/2192 (93%)	1971 (97%)	66 (3%)	3 (0%)	48	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	424	VAL
1	A	390	PRO
1	B	390	PRO

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	427/453 (94%)	410 (96%)	17 (4%)	28	62
1	B	427/453 (94%)	410 (96%)	17 (4%)	28	62
1	C	427/453 (94%)	405 (95%)	22 (5%)	21	55
1	D	427/453 (94%)	411 (96%)	16 (4%)	30	64
All	All	1708/1812 (94%)	1636 (96%)	72 (4%)	26	61

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
1	A	122	THR
1	A	176	SER
1	A	220	ASP
1	A	249	LEU
1	A	317	ARG
1	A	322	THR
1	A	337	ASP
1	A	339	THR
1	A	351	ARG
1	A	383	VAL
1	A	391	ASN
1	A	442	VAL
1	A	443	LEU
1	A	466	SER
1	A	503	LEU
1	A	528	ILE
1	B	30	GLU
1	B	52	ARG
1	B	57	ASP
1	B	63	ARG
1	B	151	LEU
1	B	176	SER
1	B	264	ARG

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Mol	Chain	Res	Type
1	B	322	THR
1	B	337	ASP
1	B	339	THR
1	B	351	ARG
1	B	382	GLU
1	B	406	LEU
1	B	443	LEU
1	B	466	SER
1	B	503	LEU
1	B	528	ILE
1	C	56	SER
1	C	57	ASP
1	C	88	THR
1	C	151	LEU
1	C	154	MET
1	C	200	ILE
1	C	241	GLU
1	C	264	ARG
1	C	337	ASP
1	C	339	THR
1	C	351	ARG
1	C	368	HIS
1	C	371	ILE
1	C	391	ASN
1	C	402	LEU
1	C	404	ASN
1	C	406	LEU
1	C	443	LEU
1	C	461	VAL
1	C	503	LEU
1	C	528	ILE
1	C	529	SER
1	D	57	ASP
1	D	122	THR
1	D	151	LEU
1	D	164	GLU
1	D	337	ASP
1	D	339	THR
1	D	351	ARG
1	D	371	ILE
1	D	382	GLU
1	D	383	VAL

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Mol	Chain	Res	Type
1	D	391	ASN
1	D	420	GLU
1	D	442	VAL
1	D	443	LEU
1	D	503	LEU
1	D	528	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	A	188	GLN
1	A	367	ASN
1	B	367	ASN
1	B	396	HIS
1	B	444	GLN
1	C	221	GLN
1	C	396	HIS
1	C	444	GLN
1	D	162	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	G4P	D	601	-	36,38,38	0.97	2 (5%)	56,61,61	1.66	13 (23%)
2	G4P	C	601	-	36,38,38	0.96	1 (2%)	56,61,61	1.73	12 (21%)
2	G4P	A	601	-	36,38,38	1.07	4 (11%)	56,61,61	1.60	13 (23%)
2	G4P	B	601	-	36,38,38	1.02	2 (5%)	56,61,61	1.67	10 (17%)

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	G4P	D	601	-	-	3/27/43/43	0/3/3/3
2	G4P	C	601	-	-	4/27/43/43	0/3/3/3
2	G4P	A	601	-	-	3/27/43/43	0/3/3/3
2	G4P	B	601	-	-	6/27/43/43	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	G4P	C5-N7	-2.76	1.33	1.39
2	C	601	G4P	C5-N7	-2.53	1.34	1.39
2	D	601	G4P	C5-N7	-2.41	1.34	1.39
2	D	601	G4P	C4-N9	-2.32	1.32	1.38
2	A	601	G4P	PC-O3C	2.25	1.61	1.59
2	A	601	G4P	C4-N9	-2.24	1.32	1.38
2	A	601	G4P	C5-N7	-2.13	1.34	1.39
2	A	601	G4P	PA-O3A	2.03	1.61	1.59
2	B	601	G4P	C4-N9	-2.00	1.33	1.38

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	G4P	C5-C4-N3	-5.69	119.33	128.39
2	B	601	G4P	C5-C4-N3	-5.54	119.58	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	G4P	C5-C4-N3	-5.06	120.34	128.39
2	D	601	G4P	C2-N3-C4	4.87	120.69	112.30
2	D	601	G4P	C5-C4-N3	-4.74	120.84	128.39
2	A	601	G4P	C2-N3-C4	4.73	120.45	112.30
2	B	601	G4P	C2-N3-C4	4.45	119.97	112.30
2	C	601	G4P	C2-N3-C4	4.39	119.86	112.30
2	C	601	G4P	N9-C4-N3	3.51	132.98	125.95
2	B	601	G4P	N9-C8-N7	-3.28	107.33	113.40
2	C	601	G4P	C2-N1-C6	-3.26	119.20	125.11
2	C	601	G4P	N9-C8-N7	-3.22	107.42	113.40
2	B	601	G4P	C2-N1-C6	-3.15	119.39	125.11
2	C	601	G4P	O4'-C1'-N9	3.13	115.45	108.36
2	D	601	G4P	N9-C8-N7	-3.05	107.75	113.40
2	B	601	G4P	N9-C4-N3	2.91	131.77	125.95
2	B	601	G4P	C8-N7-C5	2.86	109.36	104.26
2	C	601	G4P	C8-N7-C5	2.83	109.30	104.26
2	B	601	G4P	C4-C5-N7	-2.77	106.29	110.67
2	B	601	G4P	O3D-PD-O2D	2.75	118.12	107.80
2	D	601	G4P	O6-C6-C5	-2.75	119.28	126.53
2	D	601	G4P	N2-C2-N1	2.71	122.49	116.76
2	C	601	G4P	O6-C6-C5	-2.68	119.45	126.53
2	D	601	G4P	N9-C4-N3	2.66	131.27	125.95
2	A	601	G4P	N9-C4-N3	2.63	131.21	125.95
2	A	601	G4P	C4-C5-N7	-2.56	106.61	110.67
2	A	601	G4P	C2-N1-C6	-2.53	120.53	125.11
2	A	601	G4P	N9-C8-N7	-2.51	108.75	113.40
2	C	601	G4P	C4-C5-N7	-2.51	106.70	110.67
2	D	601	G4P	C4-C5-N7	-2.33	106.97	110.67
2	B	601	G4P	O3B-PB-O2B	2.30	116.44	107.80
2	C	601	G4P	C5-C6-N1	2.29	119.08	113.25
2	D	601	G4P	O3B-PB-O2B	2.25	116.24	107.80
2	D	601	G4P	C8-N7-C5	2.25	108.27	104.26
2	A	601	G4P	C6-C5-N7	2.21	134.31	130.29
2	B	601	G4P	C5-C6-N1	2.19	118.84	113.25
2	D	601	G4P	O3D-PD-O2D	2.17	115.94	107.80
2	D	601	G4P	O3'-C3'-C2'	-2.17	103.89	111.68
2	A	601	G4P	O3D-PD-O2D	2.17	115.93	107.80
2	A	601	G4P	C5-C6-N1	2.14	118.70	113.25
2	C	601	G4P	O3C-PD-O1D	-2.12	99.87	111.04
2	A	601	G4P	C8-N7-C5	2.08	107.97	104.26
2	C	601	G4P	C2'-C1'-N9	-2.06	107.51	113.25
2	A	601	G4P	O3C-PD-O1D	-2.04	100.31	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	G4P	C2-N1-C6	-2.04	121.42	125.11
2	A	601	G4P	N2-C2-N1	2.03	121.05	116.76
2	D	601	G4P	N1-C2-N3	-2.03	119.60	123.32
2	A	601	G4P	O6-C6-C5	-2.01	121.23	126.53

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	G4P	PC-O3C-PD-O2D
2	A	601	G4P	PC-O3C-PD-O3D
2	B	601	G4P	C3'-O3'-PC-O2C
2	B	601	G4P	C3'-O3'-PC-O3C
2	B	601	G4P	PD-O3C-PC-O3'
2	C	601	G4P	PA-O3A-PB-O2B
2	C	601	G4P	PA-O3A-PB-O3B
2	C	601	G4P	PC-O3C-PD-O2D
2	C	601	G4P	PC-O3C-PD-O3D
2	D	601	G4P	PC-O3C-PD-O3D
2	B	601	G4P	PC-O3C-PD-O1D
2	B	601	G4P	PC-O3C-PD-O2D
2	D	601	G4P	PC-O3C-PD-O2D
2	D	601	G4P	PC-O3C-PD-O1D
2	B	601	G4P	C3'-O3'-PC-O1C
2	A	601	G4P	PC-O3C-PD-O1D

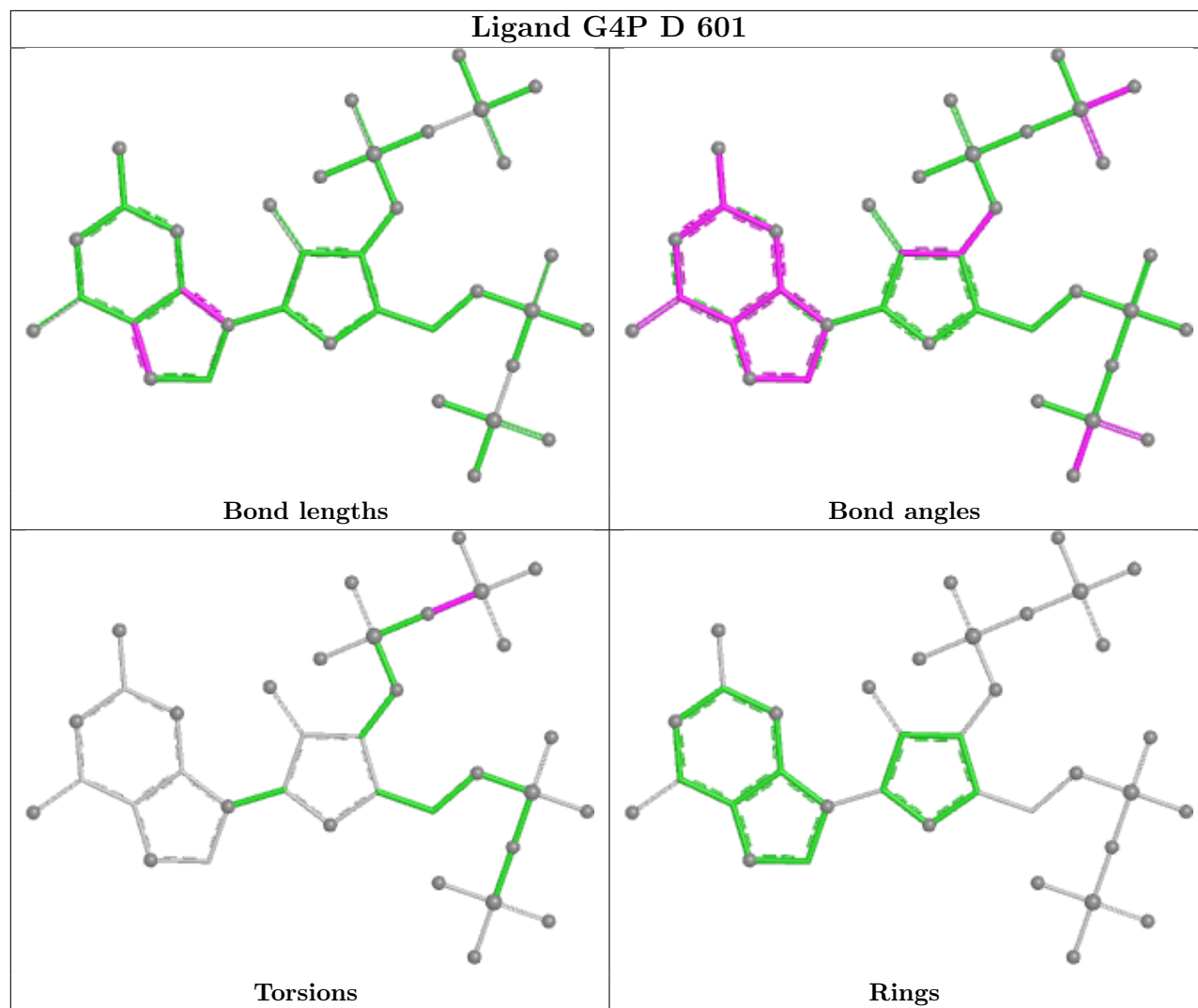
There are no ring outliers.

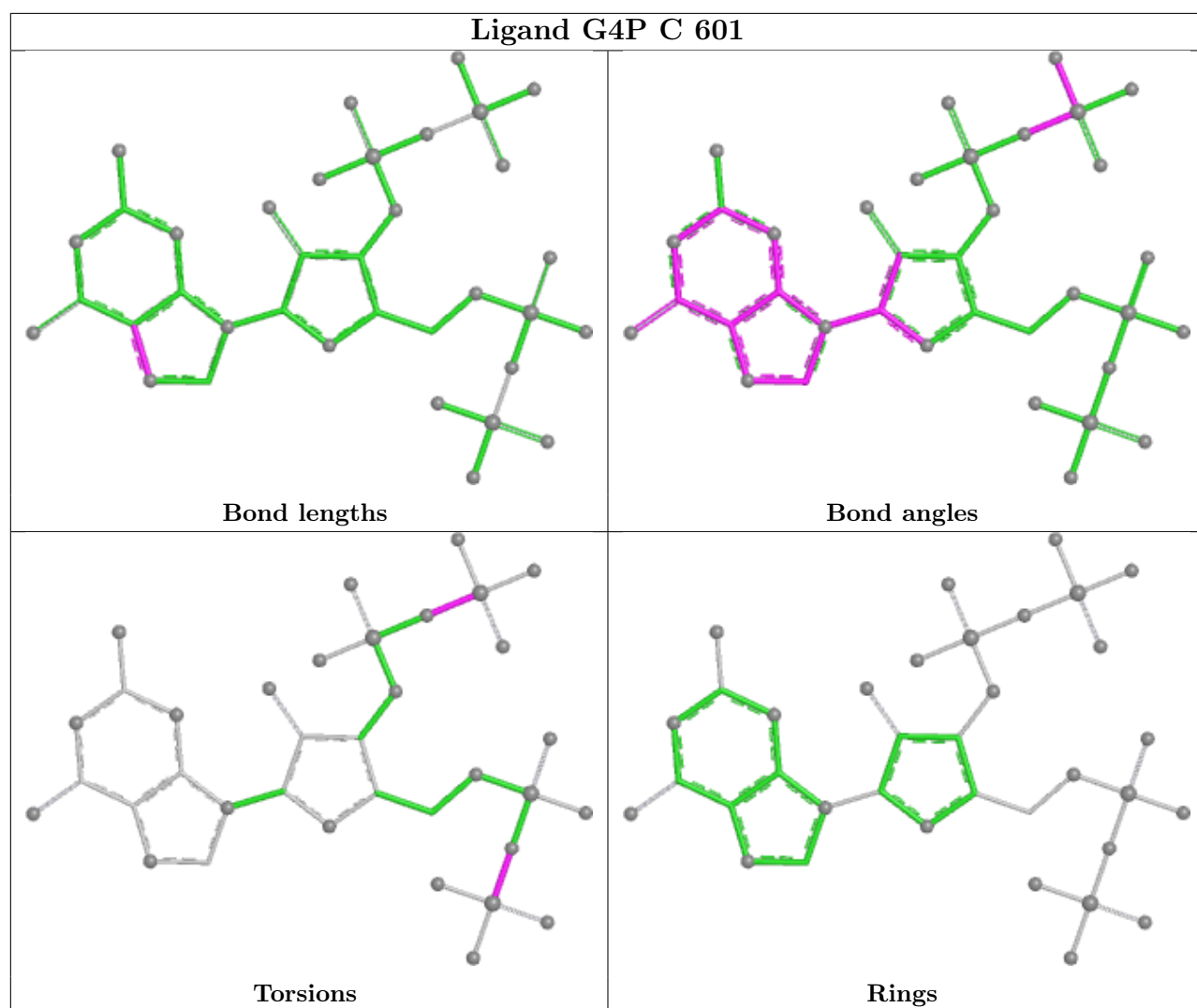
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	G4P	2	0
2	A	601	G4P	1	0

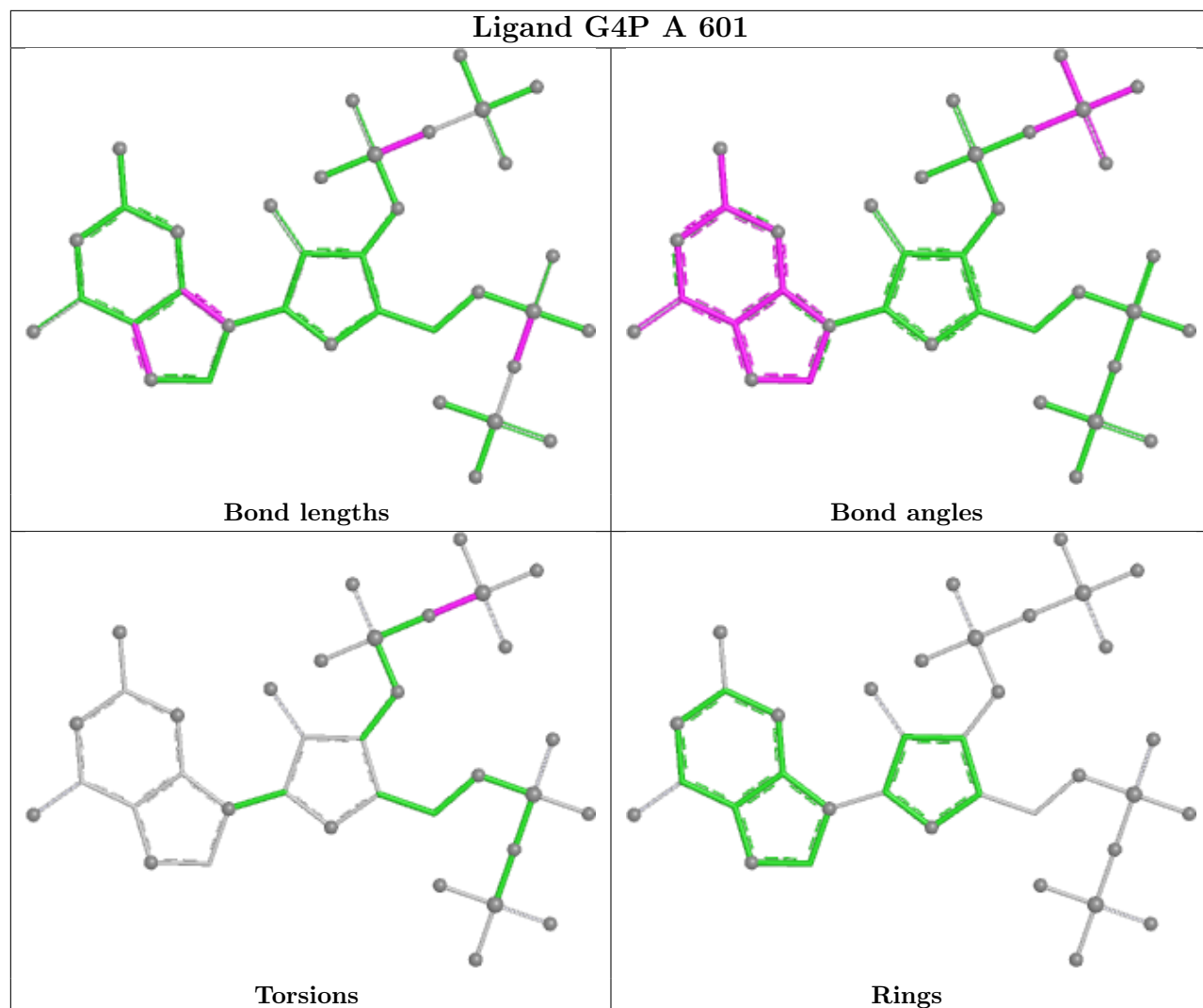
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

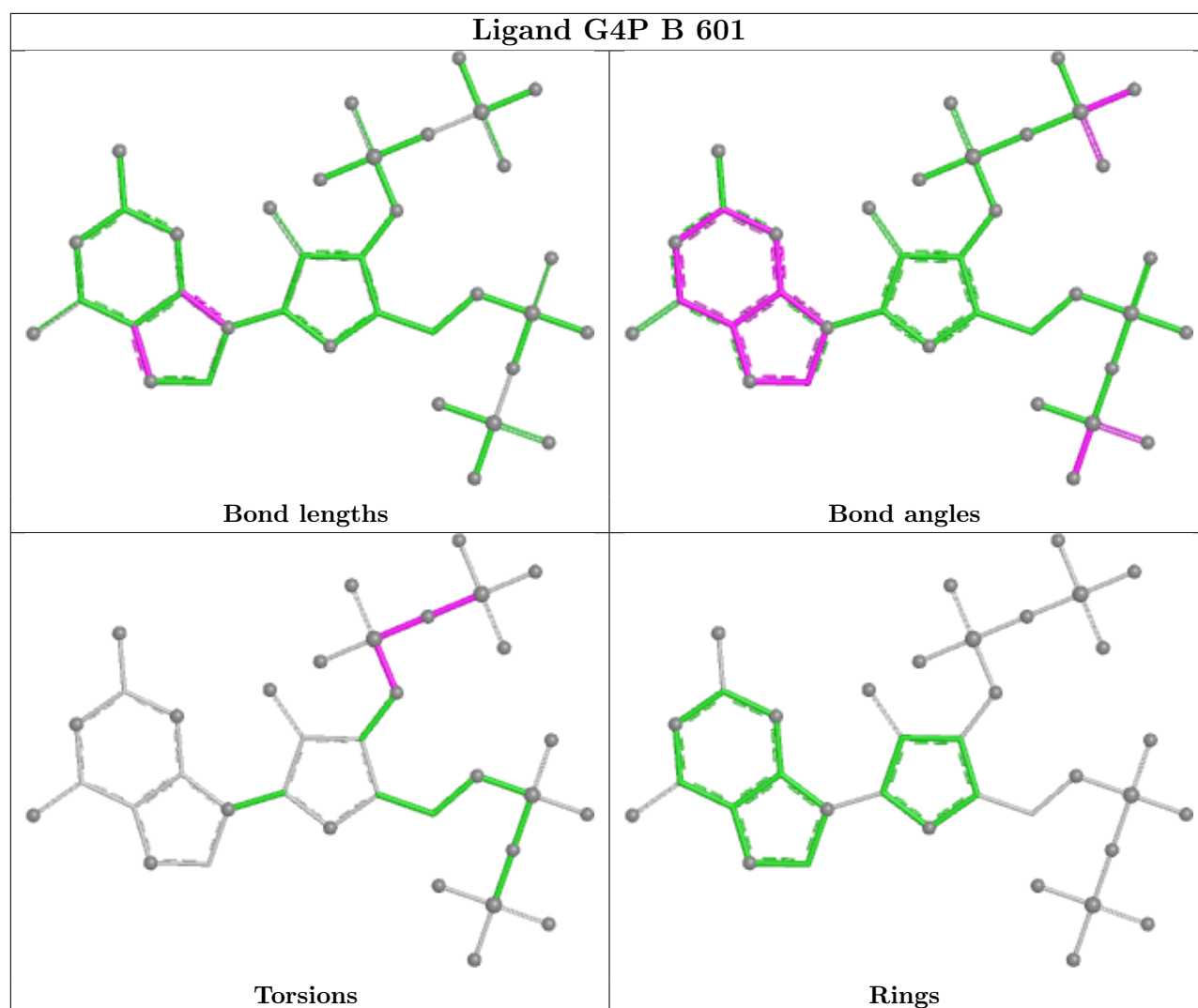
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





Ligand G4P A 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	516/548 (94%)	-0.10	13 (2%) 58 35	13, 43, 103, 171	0
1	B	516/548 (94%)	-0.03	10 (1%) 66 43	11, 48, 114, 172	0
1	C	516/548 (94%)	-0.10	11 (2%) 63 40	11, 48, 116, 167	0
1	D	516/548 (94%)	-0.06	16 (3%) 51 30	15, 43, 110, 183	0
All	All	2064/2192 (94%)	-0.07	50 (2%) 59 36	11, 45, 112, 183	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	350	ASP	4.4
1	B	350	ASP	4.2
1	A	350	ASP	4.0
1	A	53	HIS	3.9
1	C	235	ALA	3.9
1	D	352	THR	3.9
1	D	68	SER	3.7
1	C	68	SER	3.6
1	C	149	HIS	3.4
1	D	53	HIS	3.2
1	D	193	SER	3.1
1	C	529	SER	3.1
1	A	528	ILE	3.1
1	C	350	ASP	3.0
1	B	312	ARG	2.9
1	D	149	HIS	2.9
1	D	69	VAL	2.8
1	D	527	GLU	2.7
1	A	235	ALA	2.7
1	B	528	ILE	2.7
1	B	149	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	393	ALA	2.6
1	C	528	ILE	2.6
1	A	406	LEU	2.5
1	A	352	THR	2.5
1	D	235	ALA	2.4
1	D	406	LEU	2.4
1	A	69	VAL	2.4
1	A	404	ASN	2.3
1	D	62	GLU	2.3
1	A	527	GLU	2.3
1	A	483	ASP	2.3
1	B	200	ILE	2.3
1	C	431	VAL	2.3
1	B	405	PRO	2.2
1	C	312	ARG	2.2
1	B	498	GLY	2.2
1	C	1	MET	2.2
1	D	52	ARG	2.1
1	C	405	PRO	2.1
1	C	367	ASN	2.1
1	B	407	LYS	2.1
1	B	235	ALA	2.1
1	D	58	TRP	2.1
1	D	371	ILE	2.1
1	A	403	LYS	2.0
1	D	67	ILE	2.0
1	A	194	ALA	2.0
1	A	52	ARG	2.0
1	D	65	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

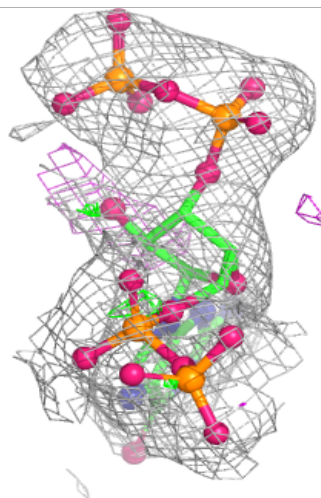
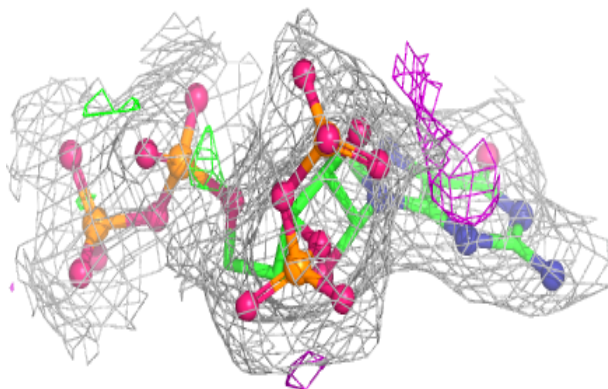
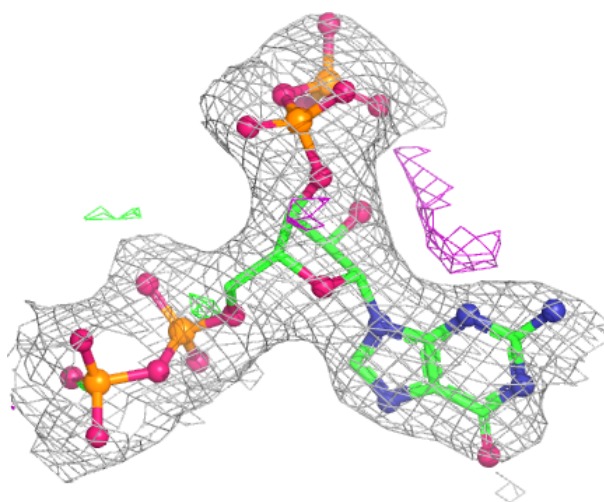
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	G4P	D	601	36/36	0.93	0.11	42,56,80,82	0
2	G4P	C	601	36/36	0.94	0.09	41,51,78,78	0
2	G4P	B	601	36/36	0.94	0.10	41,49,84,85	0
2	G4P	A	601	36/36	0.95	0.09	42,50,72,73	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.

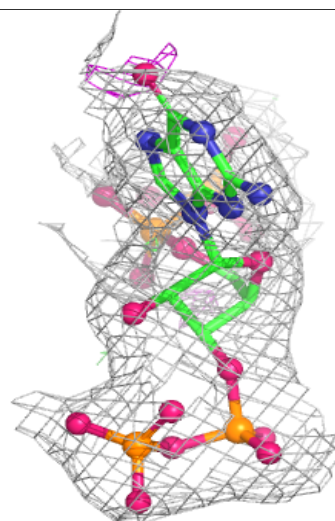
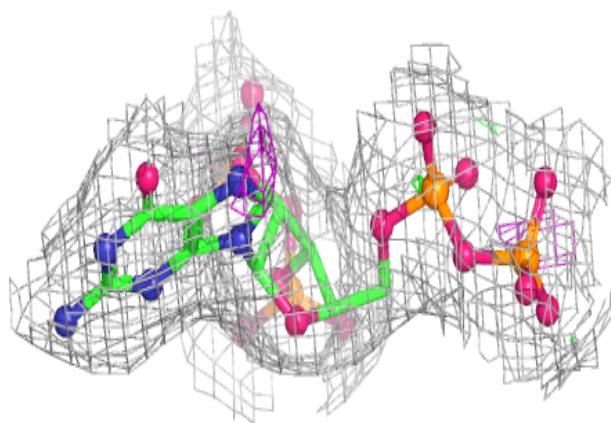
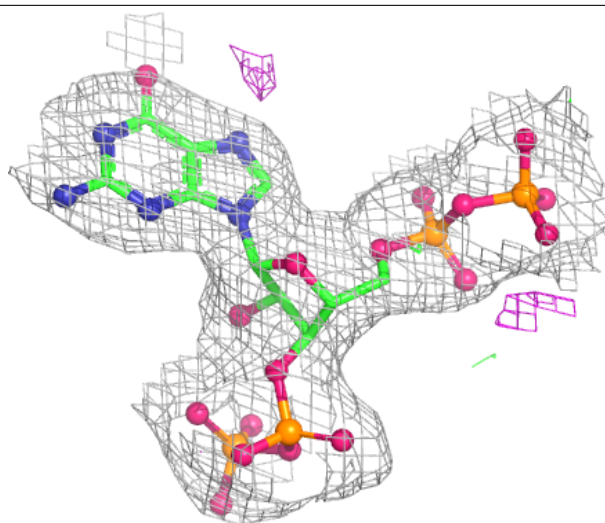
Electron density around G4P D 601:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



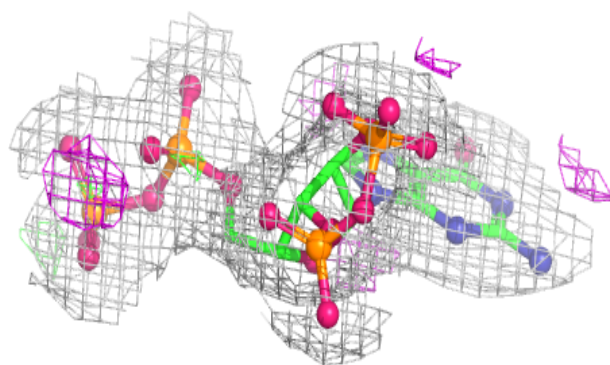
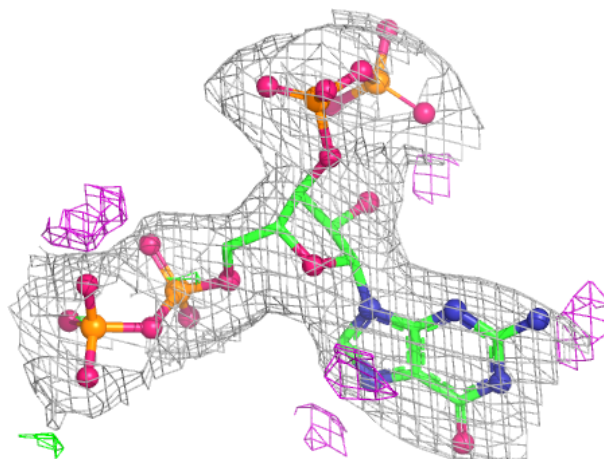
Electron density around G4P C 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



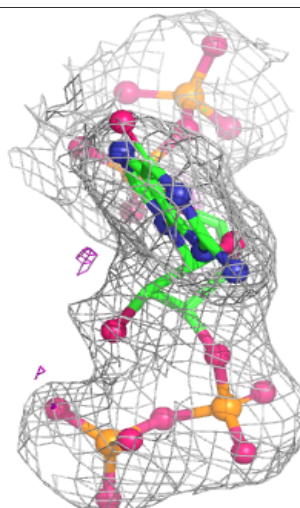
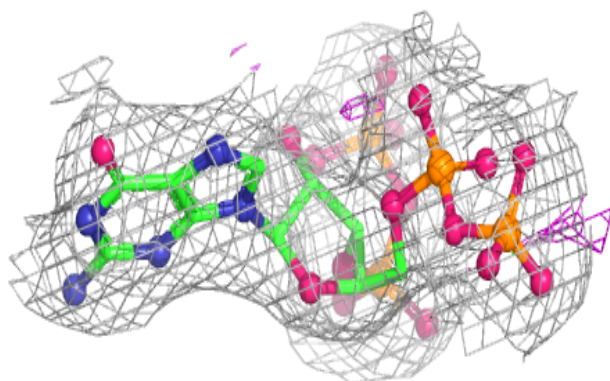
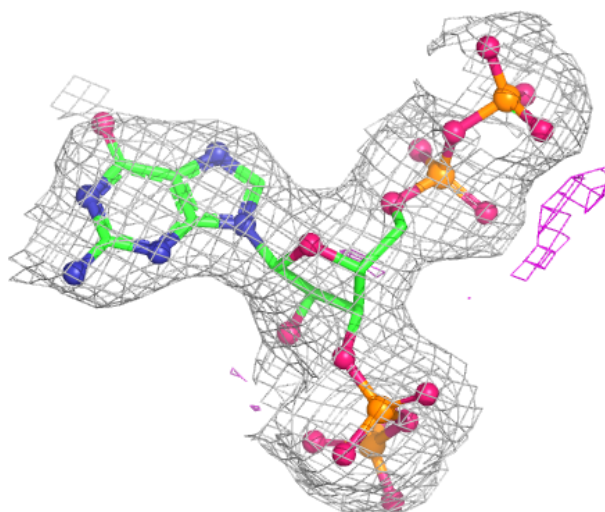
Electron density around G4P B 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around G4P A 601:

$2mF_o-DF_c$ (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.