



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:52 PM UTC

PDB ID : 5X21 / pdb_00005x21
Title : Crystal structure of Thermus thermophilus transcription initiation complex with GpA and pseudouridimycin (PUM)
Authors : Zhang, Y.; Ebright, R.
Deposited on : 2017-01-29
Resolution : 3.32 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

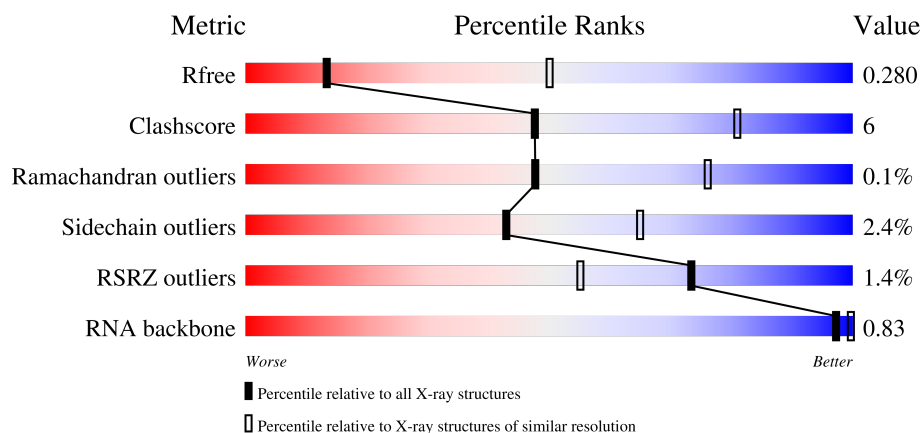
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 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.



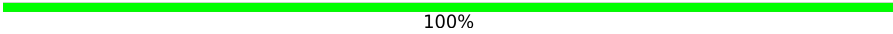
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)
RNA backbone	3983	1067 (3.64-3.00)

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	315	
1	B	315	
2	C	1119	
3	D	1524	

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Mol	Chain	Length	Quality of chain
4	E	99	 80% 14% 5%
5	F	443	 2% 70% 7% 22%
6	G	21	 76% 14% 10%
7	H	27	 74% 26%
8	I	2	 100%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 28731 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1496	Total	C	N	O	S	0	0	0
			11800	7479	2078	2207	36			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			758	483	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	UNP Q72L95
F	-18	GLY	-	expression tag	UNP Q72L95
F	-17	SER	-	expression tag	UNP Q72L95
F	-16	SER	-	expression tag	UNP Q72L95
F	-15	HIS	-	expression tag	UNP Q72L95
F	-14	HIS	-	expression tag	UNP Q72L95
F	-13	HIS	-	expression tag	UNP Q72L95
F	-12	HIS	-	expression tag	UNP Q72L95
F	-11	HIS	-	expression tag	UNP Q72L95
F	-10	HIS	-	expression tag	UNP Q72L95
F	-9	SER	-	expression tag	UNP Q72L95
F	-8	SER	-	expression tag	UNP Q72L95
F	-7	GLY	-	expression tag	UNP Q72L95
F	-6	LEU	-	expression tag	UNP Q72L95
F	-5	VAL	-	expression tag	UNP Q72L95
F	-4	PRO	-	expression tag	UNP Q72L95
F	-3	ARG	-	expression tag	UNP Q72L95
F	-2	GLY	-	expression tag	UNP Q72L95
F	-1	SER	-	expression tag	UNP Q72L95
F	0	HIS	-	expression tag	UNP Q72L95

- Molecule 6 is a DNA chain called promoter DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	19	Total	C	N	O	P	0	0	0
			385	184	71	112	18			

- Molecule 7 is a DNA chain called promoter DNA nontemplate strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	27	Total	C	N	O	P	0	0	0
			560	266	109	159	26			

- Molecule 8 is a RNA chain called RNA (5'-R(*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	2	Total	C	N	O	P	0	0	0
			42	20	10	11	1			

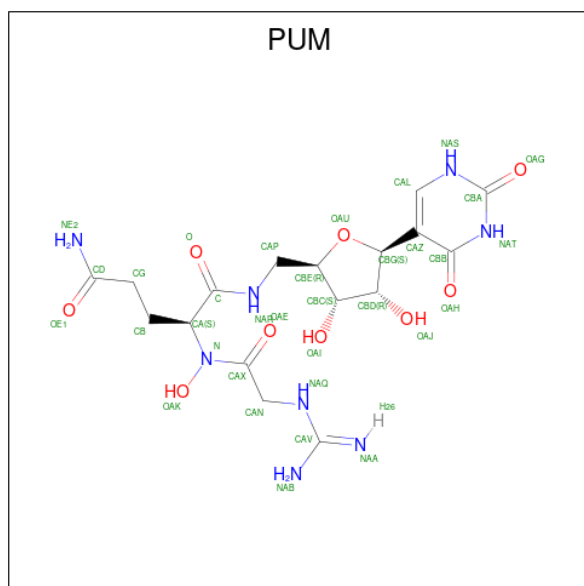
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Mg 1 1	0	0
9	C	1	Total Mg 1 1	0	0
9	D	2	Total Mg 2 2	0	0
9	F	1	Total Mg 1 1	0	0
9	H	1	Total Mg 1 1	0	0

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	2	Total Zn 2 2	0	0

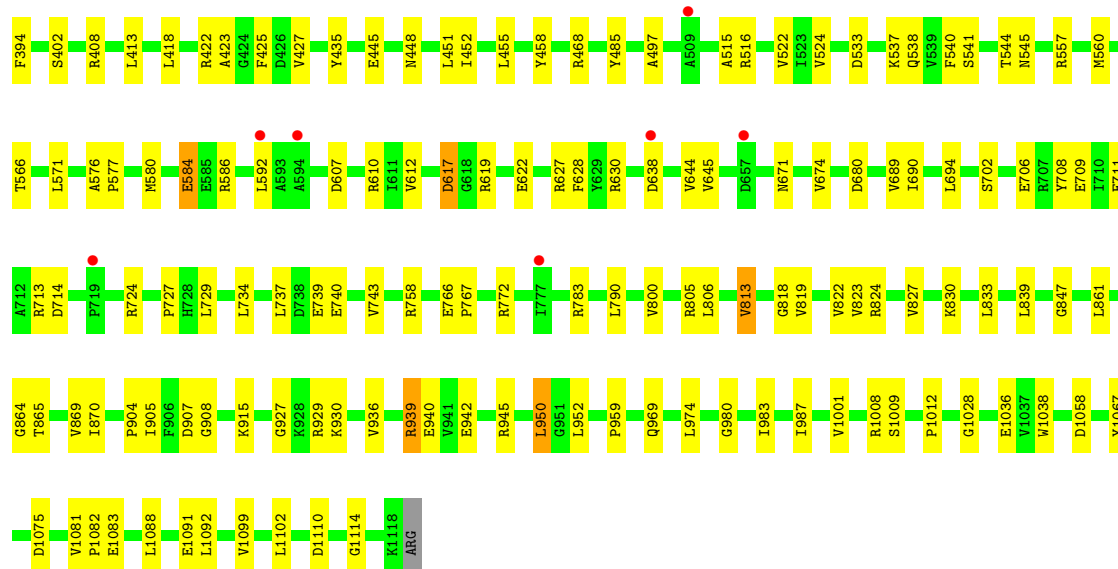
- Molecule 11 is (1S)-1,4-anhydro-5-[(N-carbamimidoylglycyl-N 2 -hydroxy-L-glutaminy]amino]-5-deoxy-1-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl)-D-ribose (CCD ID: PUM) (formula: C₁₇H₂₆N₈O₉).



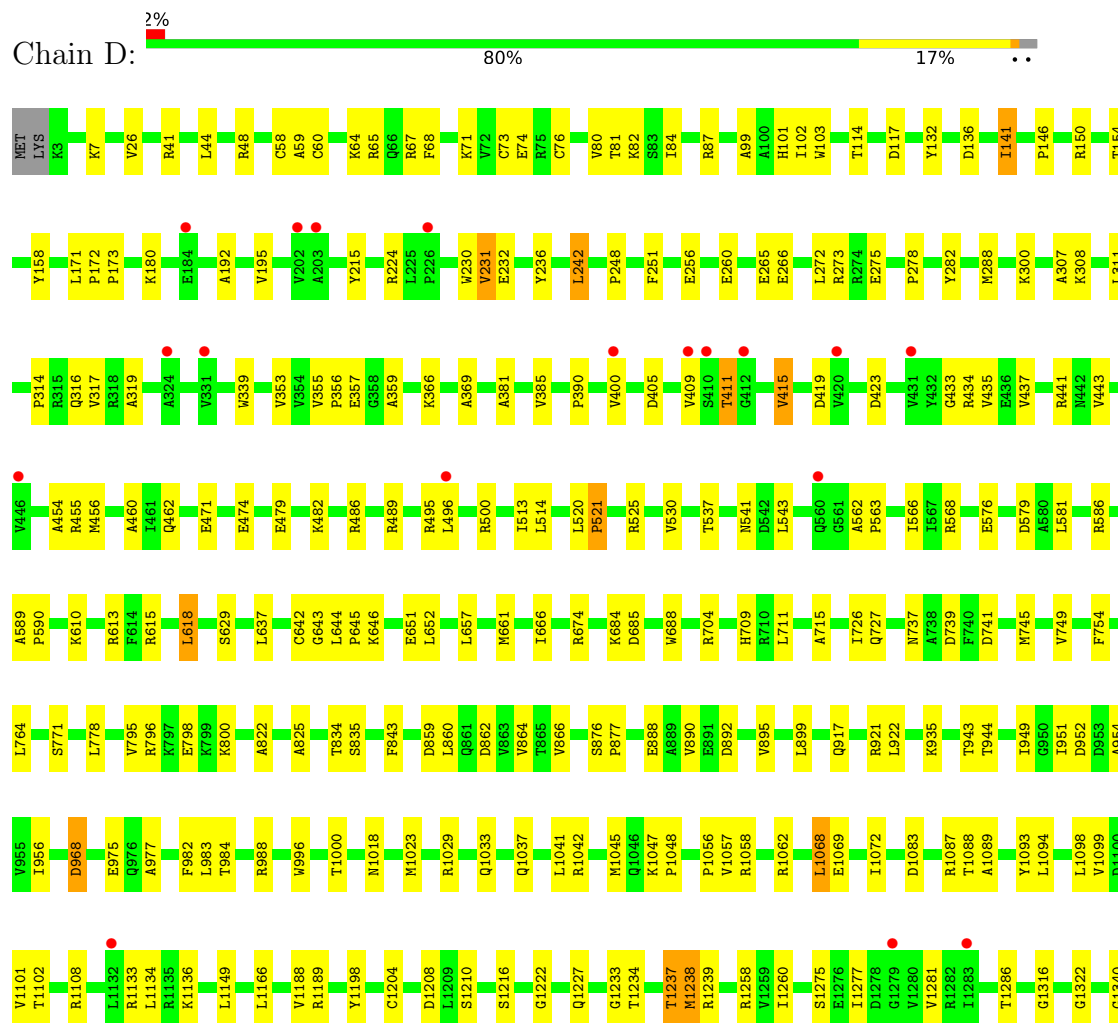
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	I	1	Total C N O 34 17 8 9	0	0

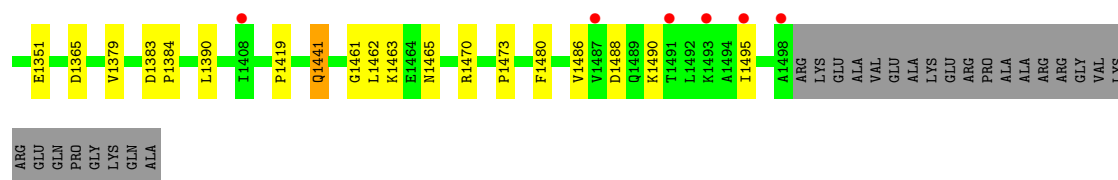
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	4	Total 4	O 4	0	0
12	B	3	Total 3	O 3	0	0
12	C	10	Total 10	O 10	0	0
12	D	11	Total 11	O 11	0	0
12	E	3	Total 3	O 3	0	0
12	F	2	Total 2	O 2	0	0
12	H	2	Total 2	O 2	0	0



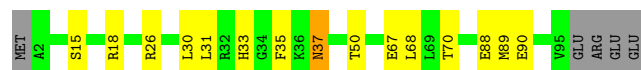
• Molecule 3: DNA-directed RNA polymerase subunit beta'





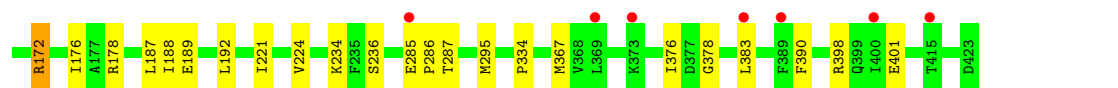
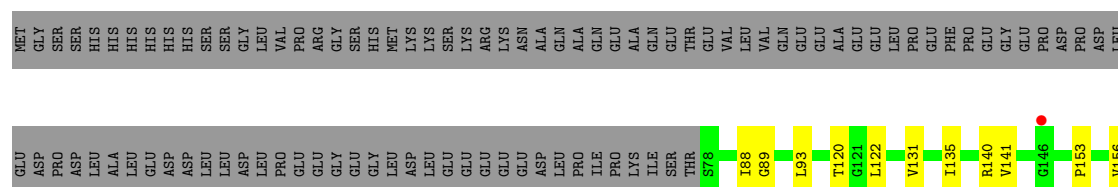
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 80% 14% 5%



- Molecule 5: RNA polymerase sigma factor SigA

Chain F: 2% 70% 7% 22%



- Molecule 6: promoter DNA template strand

Chain G: 76% 14% 10%



- Molecule 7: promoter DNA nontemplate strand

Chain H: 74% 26%



- Molecule 8: RNA (5'-R(*GP*A)-3')

Chain I: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.79Å 103.09Å 296.23Å 90.00° 98.71° 90.00°	Depositor
Resolution (Å)	39.67 – 3.32 39.67 – 3.32	Depositor EDS
% Data completeness (in resolution range)	85.1 (39.67-3.32) 85.0 (39.67-3.32)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.232 , 0.280 0.234 , 0.280	Depositor DCC
R_{free} test set	1565 reflections (1.86%)	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 21.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	28731	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: ZN, PUM, MG

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	0.26	0/1814	0.76	2/2466 (0.1%)
1	B	0.26	0/1782	0.77	0/2424
2	C	0.27	0/8937	0.74	1/12087 (0.0%)
3	D	0.26	0/12009	0.73	10/16240 (0.1%)
4	E	0.26	0/772	0.71	0/1040
5	F	0.26	0/2852	0.71	0/3837
6	G	0.18	0/431	0.33	0/663
7	H	0.17	0/630	0.38	0/973
8	I	0.04	0/47	0.13	0/72
All	All	0.26	0/29274	0.72	13/39802 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	433	GLY	N-CA-C	5.76	118.35	110.69
3	D	136	ASP	CA-C-N	5.48	125.13	119.05
3	D	136	ASP	C-N-CA	5.48	125.13	119.05
3	D	1018	ASN	CA-C-N	5.46	126.66	119.84
3	D	1018	ASN	C-N-CA	5.46	126.66	119.84
3	D	1340	GLY	CA-C-N	5.39	125.04	119.05
3	D	1340	GLY	C-N-CA	5.39	125.04	119.05
1	A	172	SER	CA-C-N	5.19	124.80	119.56
1	A	172	SER	C-N-CA	5.19	124.80	119.56
3	D	275	GLU	CB-CA-C	-5.18	110.58	116.54
3	D	521	PRO	CA-C-N	5.06	124.67	119.05
3	D	521	PRO	C-N-CA	5.06	124.67	119.05
2	C	980	GLY	N-CA-C	-5.03	107.71	114.25

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	1782	0	1834	27	0
1	B	1750	0	1797	18	0
2	C	8770	0	8874	110	0
3	D	11800	0	12024	161	0
4	E	758	0	770	9	0
5	F	2807	0	2882	20	0
6	G	385	0	215	2	0
7	H	560	0	305	7	0
8	I	42	0	23	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
9	D	2	0	0	0	0
9	F	1	0	0	0	0
9	H	1	0	0	0	0
10	D	2	0	0	0	0
11	I	34	0	0	1	0
12	A	4	0	0	1	0
12	B	3	0	0	0	0
12	C	10	0	0	0	0
12	D	11	0	0	0	0
12	E	3	0	0	0	0
12	F	2	0	0	0	0
12	H	2	0	0	0	0
All	All	28731	0	28724	318	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 6.

All (318) 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)
2:C:628:PHE:H	2:C:638:ASP:HB3	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.70	0.74
3:D:60:CYS:SG	3:D:76:CYS:HB3	2.28	0.74
3:D:117:ASP:HB3	3:D:150:ARG:HH22	1.53	0.71
2:C:422:ARG:HH22	7:H:13:DT:H5'	1.56	0.69
3:D:411:THR:HB	3:D:437:VAL:H	1.58	0.69
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.75	0.69
2:C:537:LYS:HA	2:C:905:ILE:HD11	1.76	0.67
3:D:73:CYS:HB3	3:D:76:CYS:SG	2.34	0.67
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.28	0.67
2:C:806:LEU:HB3	2:C:813:VAL:HG21	1.76	0.66
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.77	0.66
3:D:1281:VAL:HB	3:D:1316:GLY:H	1.60	0.66
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.77	0.65
3:D:73:CYS:CB	3:D:76:CYS:SG	2.82	0.65
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.79	0.65
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.31	0.64
3:D:685:ASP:HA	3:D:688:TRP:HD1	1.63	0.64
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.80	0.63
2:C:144:PRO:HB2	2:C:273:GLY:HA3	1.80	0.63
3:D:256:GLU:HG3	3:D:300:LYS:HG3	1.80	0.63
3:D:1083:ASP:OD2	3:D:1087:ARG:NH1	2.32	0.63
2:C:402:SER:HA	2:C:566:THR:HG23	1.81	0.62
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.82	0.62
3:D:562:ALA:H	5:F:140:ARG:HH12	1.45	0.62
2:C:1083:GLU:OE2	3:D:87:ARG:NH2	2.32	0.61
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.66	0.60
3:D:1234:THR:HG22	3:D:1238:MET:HE2	1.82	0.60
2:C:674:VAL:HG23	2:C:869:VAL:HB	1.84	0.59
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.84	0.59
2:C:331:ARG:NH2	7:H:14:DG:O6	2.35	0.59
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.84	0.59
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.85	0.59
1:A:62:LEU:HD23	1:A:163:ASN:HD21	1.68	0.59
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.85	0.58
3:D:400:VAL:HG13	3:D:443:VAL:HG21	1.84	0.58
3:D:1486:VAL:HG11	4:E:26:ARG:HB2	1.84	0.58
3:D:968:ASP:OD2	3:D:1058:ARG:NH2	2.36	0.58
3:D:711:LEU:HD22	3:D:778:LEU:HD23	1.84	0.58
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.68	0.58
2:C:243:ARG:NH2	7:H:9:DG:O6	2.31	0.58
2:C:516:ARG:HD3	3:D:1068:LEU:HD11	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:231:VAL:O	3:D:236:TYR:OH	2.23	0.57
1:A:99:LEU:HB2	1:A:142:VAL:HG13	1.86	0.57
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.85	0.57
3:D:951:ILE:O	3:D:1062:ARG:NE	2.34	0.57
2:C:283:ILE:HD13	2:C:305:PRO:HG2	1.88	0.56
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.86	0.56
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.87	0.56
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.87	0.56
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.39	0.56
3:D:500:ARG:HH12	3:D:1390:LEU:HD21	1.69	0.56
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.86	0.56
2:C:223:ASP:OD1	2:C:225:SER:OG	2.23	0.56
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.39	0.56
3:D:949:ILE:HD11	3:D:1023:MET:HE1	1.88	0.56
2:C:124:ASP:OD1	2:C:124:ASP:N	2.37	0.55
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.88	0.55
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.39	0.55
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.88	0.55
1:B:27:PRO:HG3	1:B:186:LEU:HD12	1.88	0.55
2:C:497:ALA:HA	2:C:515:ALA:HA	1.89	0.55
3:D:132:TYR:OH	3:D:568:ARG:NH2	2.40	0.55
3:D:796:ARG:NH1	3:D:862:ASP:OD2	2.40	0.54
2:C:15:LEU:O	2:C:586:ARG:NH2	2.33	0.54
2:C:767:PRO:HG2	2:C:772:ARG:HD3	1.90	0.54
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.40	0.54
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.41	0.54
5:F:187:LEU:HD23	5:F:224:VAL:HG13	1.88	0.54
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.40	0.54
3:D:563:PRO:HB3	5:F:189:GLU:HG3	1.90	0.54
3:D:657:LEU:HG	3:D:661:MET:HE2	1.89	0.54
3:D:890:VAL:HG23	3:D:892:ASP:H	1.72	0.53
5:F:188:ILE:HG12	5:F:224:VAL:HG21	1.90	0.53
2:C:458:TYR:HD1	2:C:538:GLN:HB3	1.74	0.53
3:D:954:ALA:HB3	3:D:1062:ARG:HD2	1.90	0.53
2:C:259:GLY:HA2	2:C:263:ASP:HB2	1.90	0.53
3:D:65:ARG:HB3	3:D:67:ARG:HG3	1.91	0.53
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.91	0.53
2:C:714:ASP:N	2:C:818:GLY:O	2.36	0.53
2:C:1075:ASP:OD1	2:C:1075:ASP:N	2.41	0.53
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.90	0.52
2:C:708:TYR:HB3	2:C:790:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.32	0.52
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.91	0.52
3:D:637:LEU:O	3:D:935:LYS:NZ	2.43	0.52
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.45	0.52
2:C:541:SER:O	2:C:545:ASN:ND2	2.27	0.52
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.91	0.52
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.92	0.51
3:D:1047:LYS:HD2	3:D:1048:PRO:HD2	1.93	0.51
1:A:188:GLN:HG3	1:A:189:ARG:HG3	1.92	0.51
3:D:771:SER:HB2	3:D:778:LEU:HD13	1.93	0.51
2:C:1058:ASP:OD1	2:C:1083:GLU:N	2.43	0.51
2:C:724:ARG:NH2	2:C:734:LEU:O	2.44	0.51
3:D:71:LYS:NZ	3:D:74:GLU:OE2	2.40	0.51
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.93	0.51
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.92	0.51
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.92	0.50
2:C:724:ARG:HD2	2:C:739:GLU:HA	1.92	0.50
3:D:1133:ARG:HH12	3:D:1136:LYS:HE3	1.76	0.50
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.93	0.50
2:C:17:PRO:HB2	2:C:20:GLU:HB3	1.93	0.50
3:D:26:VAL:HG11	3:D:44:LEU:HD23	1.93	0.50
3:D:834:THR:OG1	3:D:835:SER:N	2.43	0.50
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.94	0.50
3:D:520:LEU:O	3:D:525:ARG:NE	2.45	0.50
1:A:219:ARG:HG3	1:B:219:ARG:HG3	1.94	0.49
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.93	0.49
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.92	0.49
3:D:479:GLU:HA	3:D:482:LYS:HD3	1.94	0.49
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.94	0.49
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.93	0.49
3:D:975:GLU:OE2	3:D:988:ARG:NH2	2.45	0.49
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.95	0.49
7:H:16:DC:H2"	7:H:17:DA:C8	2.47	0.49
2:C:468:ARG:HB3	2:C:485:TYR:HB3	1.95	0.49
3:D:943:THR:HG23	3:D:944:THR:HG23	1.93	0.49
3:D:1093:TYR:OH	3:D:1441:GLN:OE1	2.28	0.49
2:C:1012:PRO:HB3	5:F:334:PRO:HB3	1.95	0.49
3:D:224:ARG:H	3:D:251:PHE:HE1	1.61	0.49
3:D:537:THR:OG1	3:D:541:ASN:ND2	2.42	0.49
3:D:704:ARG:HB2	3:D:745:MET:HE3	1.95	0.49
4:E:37:ASN:OD1	4:E:37:ASN:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LEU:O	1:A:146:ARG:NH1	2.46	0.49
1:A:50:GLY:HA3	1:A:173:PRO:HD3	1.95	0.48
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.95	0.48
2:C:927:GLY:HA2	2:C:930:LYS:HE3	1.95	0.48
2:C:950:LEU:HB3	2:C:952:LEU:HG	1.95	0.48
1:A:25:LEU:HD23	1:A:28:LEU:HD11	1.94	0.48
3:D:1216:SER:HB3	4:E:15:SER:HB2	1.95	0.48
1:A:133:GLU:HG3	2:C:645:VAL:HG21	1.94	0.48
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.95	0.48
3:D:610:LYS:HA	3:D:615:ARG:HD3	1.95	0.48
1:A:133:GLU:HG2	1:A:134:GLU:H	1.79	0.48
2:C:929:ARG:NH2	2:C:940:GLU:OE2	2.46	0.48
3:D:434:ARG:NH2	5:F:135:ILE:O	2.46	0.48
3:D:265:GLU:OE2	3:D:316:GLN:NE2	2.43	0.48
1:B:13:VAL:HG22	1:B:23:PHE:HD1	1.77	0.48
3:D:737:ASN:OD1	3:D:1239:ARG:NH1	2.47	0.48
3:D:1088:THR:HG22	3:D:1237:THR:HB	1.96	0.47
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.96	0.47
2:C:861:LEU:HD12	2:C:865:THR:HB	1.95	0.47
2:C:123:GLU:HB2	2:C:592:LEU:HD11	1.95	0.47
2:C:1067:TYR:OH	3:D:674:ARG:NH1	2.47	0.47
3:D:739:ASP:OD1	3:D:739:ASP:N	2.42	0.47
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.95	0.47
2:C:194:VAL:HG12	2:C:226:VAL:HG11	1.96	0.47
2:C:709:GLU:HG3	2:C:824:ARG:HG2	1.95	0.47
3:D:353:VAL:HG12	3:D:355:VAL:H	1.79	0.47
1:A:54:THR:HB	1:A:158:ILE:HD12	1.97	0.47
2:C:690:ILE:HB	2:C:694:LEU:HD12	1.97	0.47
3:D:41:ARG:HG3	3:D:48:ARG:HE	1.80	0.47
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.95	0.47
3:D:486:ARG:HD3	3:D:489:ARG:HH22	1.79	0.47
2:C:448:ASN:HB3	2:C:452:ILE:HG12	1.97	0.47
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.97	0.47
2:C:1009:SER:HB3	3:D:651:GLU:O	2.15	0.47
3:D:272:LEU:HD22	3:D:282:TYR:HE2	1.79	0.47
2:C:627:ARG:HD3	2:C:638:ASP:HB2	1.97	0.46
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.97	0.46
3:D:1000:THR:HA	3:D:1041:LEU:HD11	1.97	0.46
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.96	0.46
2:C:1091:GLU:OE2	3:D:613:ARG:NH2	2.48	0.46
3:D:1133:ARG:NH2	3:D:1134:LEU:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.98	0.46
2:C:952:LEU:O	2:C:969:GLN:NE2	2.48	0.46
2:C:1008:ARG:HH11	2:C:1028:GLY:HA2	1.81	0.46
3:D:737:ASN:ND2	11:I:101:PUM:OAI	2.49	0.46
3:D:1208:ASP:OD1	3:D:1210:SER:OG	2.29	0.46
4:E:33:HIS:HD2	4:E:89:MET:HE2	1.80	0.46
5:F:236:SER:OG	7:H:5:DA:OP2	2.26	0.46
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.98	0.46
3:D:59:ALA:HB3	3:D:76:CYS:HB2	1.97	0.46
4:E:67:GLU:O	4:E:70:THR:OG1	2.27	0.46
2:C:680:ASP:H	3:D:943:THR:HB	1.80	0.46
3:D:1094:LEU:O	3:D:1098:LEU:HG	2.16	0.46
2:C:904:PRO:HB2	2:C:907:ASP:HB3	1.98	0.46
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.97	0.46
2:C:557:ARG:HA	2:C:560:MET:HG3	1.98	0.46
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.97	0.46
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.96	0.46
2:C:35:PRO:HG2	2:C:38:LYS:HB2	1.98	0.46
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.50	0.46
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.97	0.46
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.98	0.46
2:C:1038:TRP:HB3	3:D:1227:GLN:HE21	1.81	0.46
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.98	0.46
5:F:89:GLY:HA3	7:H:7:DG:C6	2.52	0.45
1:B:41:ARG:HA	1:B:177:VAL:HG11	1.98	0.45
1:B:124:ASN:OD1	1:B:124:ASN:N	2.49	0.45
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.98	0.45
3:D:895:VAL:HG11	3:D:922:LEU:HD21	1.98	0.45
1:A:161:ARG:C	1:A:163:ASN:H	2.25	0.45
3:D:1383:ASP:HA	3:D:1384:PRO:HD3	1.83	0.45
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.98	0.45
3:D:589:ALA:HA	3:D:590:PRO:HD3	1.84	0.45
3:D:1045:MET:HB2	3:D:1072:ILE:HG22	1.98	0.45
3:D:172:PRO:HA	3:D:173:PRO:HD3	1.87	0.45
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.99	0.45
1:A:206:THR:HB	1:A:209:GLU:HG3	1.99	0.45
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.99	0.45
1:A:53:VAL:HG22	1:A:144:VAL:HG22	1.99	0.45
2:C:76:PRO:HA	2:C:77:PRO:HD3	1.89	0.45
3:D:405:ASP:HB3	3:D:423:ASP:HA	1.98	0.45
1:B:138:LEU:HD11	1:B:140:MET:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:939:ARG:H	2:C:939:ARG:HG2	1.53	0.45
3:D:652:LEU:HB3	3:D:749:VAL:HG21	1.98	0.44
1:B:51:THR:OG1	1:B:87:VAL:O	2.26	0.44
2:C:800:VAL:HG22	2:C:827:VAL:HG22	1.98	0.44
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.99	0.44
5:F:172:ARG:O	5:F:176:ILE:HG12	2.17	0.44
3:D:215:TYR:HE1	3:D:381:ALA:H	1.66	0.44
3:D:456:MET:HE1	3:D:568:ARG:NE	2.33	0.44
3:D:58:CYS:HB2	3:D:76:CYS:SG	2.58	0.44
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.99	0.44
3:D:520:LEU:HA	3:D:521:PRO:HD2	1.82	0.44
1:A:178:ALA:HB2	2:C:864:GLY:HA3	2.00	0.44
1:B:177:VAL:HG13	1:B:197:LEU:HD11	1.99	0.44
2:C:408:ARG:NH1	2:C:455:LEU:O	2.50	0.43
2:C:711:GLU:O	2:C:758:ARG:NH1	2.51	0.43
2:C:76:PRO:HG3	2:C:120:LEU:HD12	1.99	0.43
2:C:580:MET:SD	2:C:584:GLU:HG3	2.58	0.43
2:C:847:GLY:HA2	3:D:741:ASP:HA	2.01	0.43
3:D:171:LEU:HD22	3:D:390:PRO:HG2	2.01	0.43
3:D:798:GLU:OE2	3:D:822:ALA:HB1	2.18	0.43
6:G:6:DA:H1'	6:G:7:DT:H5'	1.99	0.43
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.75	0.43
2:C:1081:VAL:HA	2:C:1082:PRO:HD3	1.90	0.43
3:D:629:SER:HB3	3:D:726:ILE:HG13	2.00	0.43
3:D:685:ASP:HA	3:D:688:TRP:CD1	2.49	0.43
2:C:689:VAL:HB	2:C:870:ILE:HB	2.00	0.43
3:D:409:VAL:HG21	3:D:435:VAL:HG21	2.01	0.43
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.84	0.43
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.99	0.43
1:B:29:GLU:HB3	1:B:32:PHE:CD1	2.53	0.43
3:D:1490:LYS:HB2	3:D:1490:LYS:HE3	1.83	0.43
1:B:115:LEU:HA	1:B:116:PRO:HD3	1.89	0.43
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.89	0.43
3:D:141:ILE:HA	3:D:146:PRO:HA	2.01	0.43
3:D:1275:SER:O	3:D:1322:GLY:N	2.42	0.43
5:F:367:MET:HB3	5:F:390:PHE:HZ	1.82	0.43
1:A:124:ASN:OD1	1:A:124:ASN:N	2.51	0.43
1:B:150:TYR:CE1	1:B:170:VAL:HG22	2.54	0.43
2:C:729:LEU:HD23	2:C:729:LEU:HA	1.87	0.43
3:D:860:LEU:HD23	3:D:877:PRO:HB2	2.01	0.43
3:D:1462:LEU:HD23	3:D:1473:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:205:GLU:O	2:C:209:ARG:HG2	2.19	0.42
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.33	0.42
2:C:905:ILE:C	2:C:907:ASP:H	2.27	0.42
3:D:366:LYS:HD3	3:D:369:ALA:HB2	2.00	0.42
3:D:455:ARG:HB2	3:D:460:ALA:HB2	2.00	0.42
3:D:1233:GLY:O	3:D:1237:THR:OG1	2.37	0.42
2:C:612:VAL:HG22	2:C:622:GLU:HG3	2.00	0.42
5:F:383:LEU:HD13	5:F:398:ARG:HB2	2.01	0.42
3:D:82:LYS:HB2	3:D:84:ILE:HG22	2.00	0.42
3:D:462:GLN:HB2	3:D:513:ILE:HG21	2.01	0.42
3:D:1149:LEU:HD21	3:D:1166:LEU:HD11	2.01	0.42
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	2.02	0.42
2:C:540:PHE:HB3	2:C:544:THR:HB	2.01	0.42
2:C:737:LEU:HA	2:C:743:VAL:HA	2.01	0.42
3:D:248:PRO:HG3	3:D:308:LYS:HG3	2.02	0.42
3:D:956:ILE:HD11	3:D:1062:ARG:HD3	2.02	0.42
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.37	0.42
2:C:1088:LEU:HD22	3:D:618:LEU:HD21	2.01	0.42
3:D:171:LEU:HA	3:D:172:PRO:HD3	1.95	0.42
3:D:843:PHE:HD1	3:D:866:VAL:HG22	1.84	0.42
2:C:805:ARG:HG3	2:C:823:VAL:HG22	2.02	0.42
3:D:415:VAL:HG13	3:D:419:ASP:HB2	2.01	0.42
3:D:1094:LEU:HD22	3:D:1260:ILE:HG12	2.01	0.42
2:C:270:GLY:O	2:C:274:ARG:N	2.49	0.41
2:C:630:ARG:HE	2:C:706:GLU:HA	1.84	0.41
3:D:99:ALA:O	3:D:514:LEU:N	2.45	0.41
1:A:163:ASN:ND2	12:A:2101:HOH:O	2.53	0.41
3:D:441:ARG:HB2	3:D:443:VAL:HG12	2.02	0.41
5:F:93:LEU:HD23	5:F:93:LEU:HA	1.89	0.41
2:C:218:VAL:O	2:C:222:MET:HG2	2.21	0.41
3:D:230:TRP:CZ2	3:D:232:GLU:HG2	2.55	0.41
3:D:1365:ASP:OD2	3:D:1365:ASP:N	2.53	0.41
5:F:376:ILE:C	5:F:378:GLY:H	2.28	0.41
2:C:160:ALA:HB3	2:C:174:LEU:HB2	2.02	0.41
2:C:418:LEU:HD11	7:H:14:DG:C8	2.55	0.41
2:C:833:LEU:HD21	2:C:839:LEU:HD11	2.03	0.41
2:C:1036:GLU:OE2	2:C:1036:GLU:N	2.49	0.41
3:D:1102:THR:O	3:D:1222:GLY:HA3	2.20	0.41
3:D:1463:LYS:HB3	3:D:1463:LYS:HE2	1.82	0.41
1:B:175:ARG:N	1:B:200:TRP:O	2.39	0.41
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1089:ALA:HA	6:G:14:DA:C8	2.55	0.41
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.71	0.41
3:D:1033:GLN:O	3:D:1037:GLN:HG3	2.19	0.41
3:D:102:ILE:HD12	3:D:579:ASP:HB3	2.03	0.41
3:D:314:PRO:HB2	3:D:317:VAL:HG12	2.02	0.41
3:D:1057:VAL:HG13	3:D:1069:GLU:HB3	2.01	0.41
3:D:796:ARG:NH2	3:D:859:ASP:OD2	2.40	0.41
3:D:899:LEU:HD21	3:D:921:ARG:HG3	2.03	0.41
1:A:31:GLY:N	1:A:193:ASP:OD2	2.49	0.41
2:C:278:GLU:HG2	2:C:284:ARG:HA	2.03	0.41
2:C:571:LEU:HD23	2:C:702:SER:HB3	2.02	0.41
2:C:727:PRO:HB3	2:C:783:ARG:HG3	2.03	0.41
3:D:566:ILE:HD11	5:F:192:LEU:HD21	2.02	0.41
3:D:661:MET:HG2	3:D:666:ILE:HD12	2.02	0.41
1:A:48:ILE:HA	1:A:49:PRO:HD3	1.89	0.40
2:C:942:GLU:HG3	2:C:945:ARG:HH21	1.85	0.40
3:D:180:LYS:NZ	3:D:357:GLU:OE1	2.54	0.40
3:D:288:MET:HG3	3:D:307:ALA:HB2	2.03	0.40
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.75	0.40
2:C:713:ARG:HA	2:C:819:VAL:HA	2.03	0.40
2:C:904:PRO:HD2	2:C:908:GLY:HA2	2.03	0.40
2:C:343:GLN:HG3	2:C:385:PHE:HB2	2.04	0.40
2:C:576:ALA:O	2:C:671:ASN:ND2	2.50	0.40
2:C:766:GLU:HG3	3:D:64:LYS:HB3	2.03	0.40
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.57	0.40
3:D:684:LYS:HB3	3:D:684:LYS:HE2	1.86	0.40
3:D:795:VAL:HG12	3:D:876:SER:HB3	2.04	0.40
4:E:30:LEU:HB3	4:E:35:PHE:CD2	2.56	0.40
3:D:101:HIS:CE1	3:D:103:TRP:HB2	2.57	0.40
3:D:977:ALA:O	3:D:982:PHE:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/315 (71%)	218 (97%)	5 (2%)	1 (0%)	30	60
1	B	220/315 (70%)	215 (98%)	5 (2%)	0	100	100
2	C	1107/1119 (99%)	1069 (97%)	37 (3%)	1 (0%)	48	76
3	D	1494/1524 (98%)	1455 (97%)	38 (2%)	1 (0%)	48	76
4	E	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
5	F	344/443 (78%)	340 (99%)	4 (1%)	0	100	100
All	All	3481/3815 (91%)	3388 (97%)	90 (3%)	3 (0%)	48	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ILE
2	C	423	ALA
3	D	530	VAL

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	199/273 (73%)	195 (98%)	4 (2%)	48	67
1	B	195/273 (71%)	192 (98%)	3 (2%)	57	71
2	C	936/941 (100%)	911 (97%)	25 (3%)	39	63
3	D	1258/1279 (98%)	1230 (98%)	28 (2%)	45	66
4	E	82/88 (93%)	78 (95%)	4 (5%)	22	51
5	F	301/387 (78%)	294 (98%)	7 (2%)	44	66
All	All	2971/3241 (92%)	2900 (98%)	71 (2%)	43	65

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	67	THR
1	A	80	LEU
1	A	142	VAL
1	B	38	ASN
1	B	94	LEU
1	B	190	THR
2	C	11	GLU
2	C	42	VAL
2	C	103	LYS
2	C	168	ARG
2	C	177	GLU
2	C	218	VAL
2	C	269	LEU
2	C	274	ARG
2	C	285	LEU
2	C	342	ASP
2	C	394	PHE
2	C	425	PHE
2	C	427	VAL
2	C	445	GLU
2	C	522	VAL
2	C	524	VAL
2	C	584	GLU
2	C	617	ASP
2	C	644	VAL
2	C	813	VAL
2	C	830	LYS
2	C	939	ARG
2	C	950	LEU
2	C	974	LEU
2	C	1001	VAL
3	D	68	PHE
3	D	80	VAL
3	D	81	THR
3	D	141	ILE
3	D	154	THR
3	D	231	VAL
3	D	242	LEU
3	D	411	THR
3	D	415	VAL
3	D	471	GLU
3	D	576	GLU

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Mol	Chain	Res	Type
3	D	586	ARG
3	D	618	LEU
3	D	646	LYS
3	D	709	HIS
3	D	754	PHE
3	D	864	VAL
3	D	968	ASP
3	D	983	LEU
3	D	984	THR
3	D	1029	ARG
3	D	1068	LEU
3	D	1188	VAL
3	D	1237	THR
3	D	1238	MET
3	D	1277	ILE
3	D	1286	THR
3	D	1441	GLN
4	E	31	LEU
4	E	37	ASN
4	E	50	THR
4	E	90	GLU
5	F	88	ILE
5	F	141	VAL
5	F	172	ARG
5	F	234	LYS
5	F	287	THR
5	F	295	MET
5	F	401	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	B	63	HIS
1	B	128	HIS
1	B	212	ASN
2	C	41	ASN
2	C	187	ASN
2	C	556	ASN
2	C	575	GLN
2	C	1026	GLN
3	D	386	HIS

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Mol	Chain	Res	Type
3	D	703	ASN
3	D	724	GLN
3	D	727	GLN
3	D	748	HIS
3	D	816	HIS
3	D	1018	ASN
3	D	1031	ASN
3	D	1172	HIS
3	D	1195	GLN
3	D	1202	GLN
3	D	1235	GLN
3	D	1254	GLN
3	D	1353	GLN
3	D	1359	GLN
4	E	33	HIS
5	F	245	GLN
5	F	279	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/2 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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](#)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
11	PUM	I	101	-	35,35,35	2.30	8 (22%)	39,49,49	1.71	6 (15%)

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
11	PUM	I	101	-	-	8/31/47/47	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	101	PUM	OAK-N	-7.01	1.31	1.40
11	I	101	PUM	CBA-NAS	5.86	1.44	1.36
11	I	101	PUM	CAL-NAS	5.84	1.45	1.36
11	I	101	PUM	CBD-CBG	-3.91	1.48	1.53
11	I	101	PUM	CBA-NAT	3.37	1.43	1.37
11	I	101	PUM	CAL-CAZ	3.35	1.39	1.35
11	I	101	PUM	CBC-CBD	-2.82	1.45	1.53
11	I	101	PUM	OAI-CBC	-2.10	1.37	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	101	PUM	CBB-NAT-CBA	-4.46	120.23	126.37
11	I	101	PUM	NAS-CBA-NAT	4.36	119.76	115.17
11	I	101	PUM	OAU-CBG-CBD	3.94	110.60	105.15
11	I	101	PUM	CAL-NAS-CBA	-2.84	120.06	122.69
11	I	101	PUM	OAG-CBA-NAS	-2.63	120.07	122.79
11	I	101	PUM	OAU-CBE-CBC	2.15	109.43	105.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

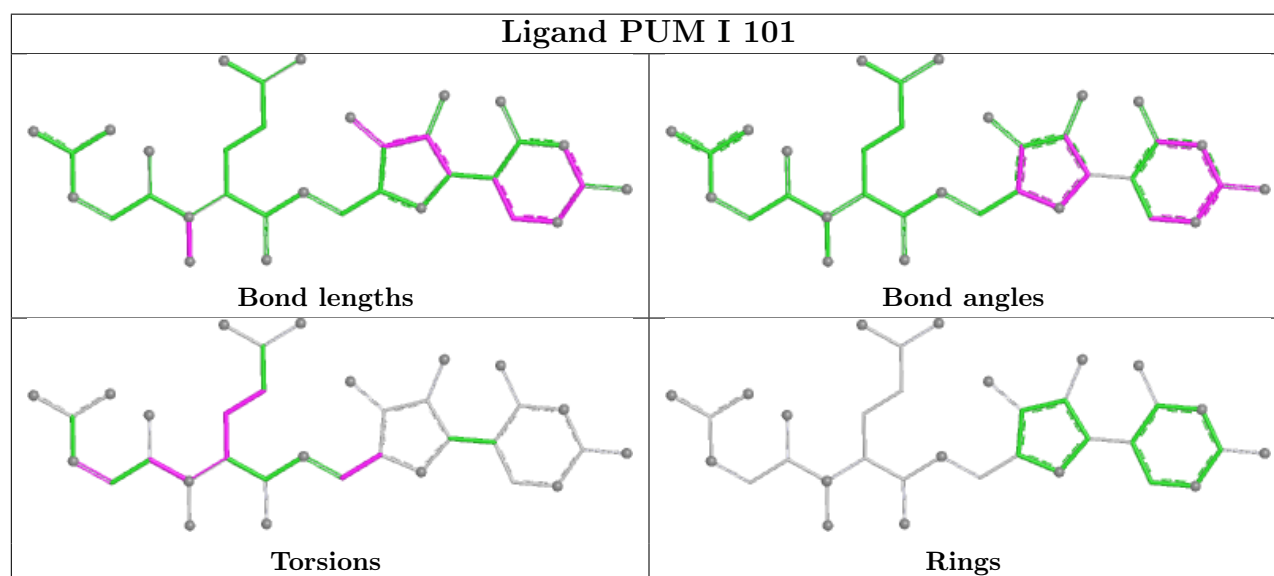
Mol	Chain	Res	Type	Atoms
11	I	101	PUM	C-CA-CB-CG
11	I	101	PUM	N-CA-CB-CG
11	I	101	PUM	C-CA-N-OAK
11	I	101	PUM	CB-CA-N-OAK
11	I	101	PUM	CA-CB-CG-CD
11	I	101	PUM	NAR-CAP-CBE-OAU
11	I	101	PUM	OAE-CAX-N-OAK
11	I	101	PUM	CAX-CAN-NAQ-CAV

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	I	101	PUM	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.



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	226/315 (71%)	0.38	3 (1%) 75 57	34, 60, 83, 99	0
1	B	222/315 (70%)	0.34	2 (0%) 81 66	33, 70, 100, 122	0
2	C	1111/1119 (99%)	0.18	13 (1%) 76 58	15, 55, 109, 132	0
3	D	1496/1524 (98%)	0.21	24 (1%) 70 52	14, 52, 110, 144	1 (0%)
4	E	94/99 (94%)	0.32	0 100 100	35, 68, 101, 107	0
5	F	346/443 (78%)	0.34	8 (2%) 61 42	22, 60, 126, 140	0
6	G	19/21 (90%)	0.32	0 100 100	20, 48, 153, 153	0
7	H	27/27 (100%)	0.33	0 100 100	49, 67, 141, 158	0
8	I	2/2 (100%)	-0.68	0 100 100	28, 28, 28, 30	0
All	All	3543/3865 (91%)	0.23	50 (1%) 73 55	14, 57, 112, 158	1 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	184	GLU	3.7
1	B	190	THR	3.6
2	C	107	LEU	3.2
3	D	203	ALA	3.1
3	D	1495	ILE	2.9
3	D	431	VAL	2.9
3	D	420	VAL	2.9
3	D	1132	LEU	2.8
1	A	162	ILE	2.8
3	D	1279	GLY	2.7
5	F	369	LEU	2.7
3	D	1408	ILE	2.6
3	D	410	SER	2.6
3	D	331	VAL	2.6
1	A	97	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	638	ASP	2.5
1	A	55	SER	2.5
3	D	1487	VAL	2.5
2	C	272	ALA	2.5
5	F	389	PHE	2.5
3	D	1491	THR	2.4
5	F	383	LEU	2.4
5	F	285	GLU	2.4
2	C	509	ALA	2.4
3	D	560	GLN	2.4
5	F	373	LYS	2.3
3	D	324	ALA	2.3
2	C	594	ALA	2.3
3	D	409	VAL	2.3
3	D	446	VAL	2.3
3	D	412	GLY	2.2
3	D	1493	LYS	2.2
2	C	211	LEU	2.2
3	D	202	VAL	2.2
2	C	369	PRO	2.2
5	F	415	THR	2.2
2	C	777	ILE	2.2
2	C	592	LEU	2.2
2	C	231	PRO	2.1
2	C	719	PRO	2.1
3	D	400	VAL	2.1
3	D	496	LEU	2.1
3	D	1498	ALA	2.1
5	F	400	ILE	2.1
2	C	657	ASP	2.1
5	F	146	GLY	2.1
1	B	100	LEU	2.0
3	D	1283	ILE	2.0
3	D	226	PRO	2.0
2	C	174	LEU	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

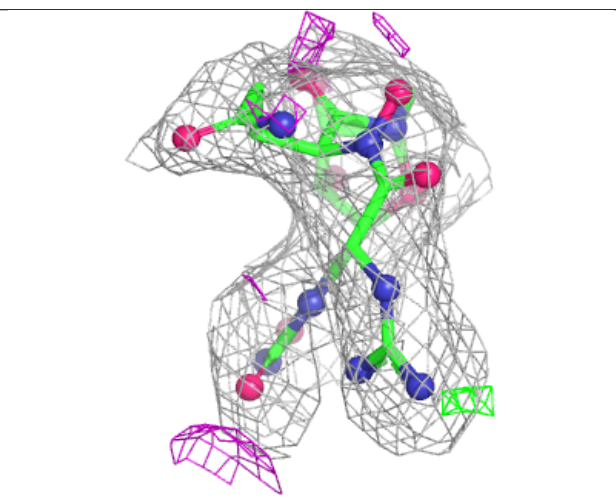
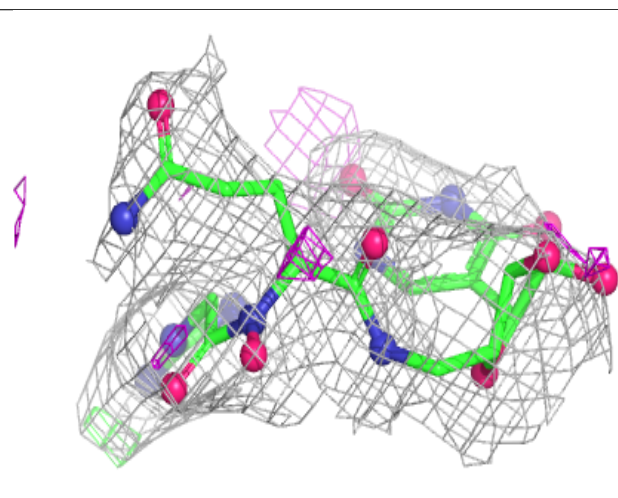
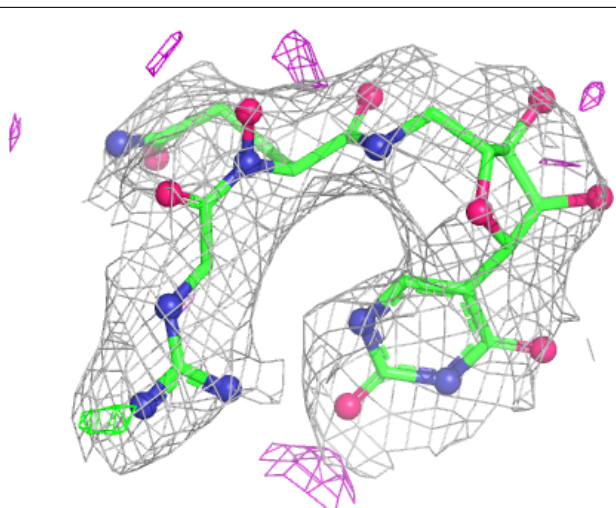
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
9	MG	A	2001	1/1	0.78	0.17	43,43,43,43	0
9	MG	D	1601	1/1	0.83	0.24	39,39,39,39	0
9	MG	H	2001	1/1	0.84	0.30	50,50,50,50	0
11	PUM	I	101	34/34	0.90	0.12	20,27,36,40	0
9	MG	C	2000	1/1	0.93	0.13	31,31,31,31	0
9	MG	F	2001	1/1	0.93	0.09	45,45,45,45	0
9	MG	D	1604	1/1	0.97	0.06	21,21,21,21	0
10	ZN	D	1603	1/1	0.99	0.02	80,80,80,80	0
10	ZN	D	1602	1/1	1.00	0.01	36,36,36,36	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 PUM I 101:

$2mF_o-DF_c$ (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.