



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 03:55 AM EDT

PDB ID : 7KEE / pdb_00007kee
Title : RNA polymerase II elongation complex with unnatural base dTPT3, rNaMTP bound to E-site
Authors : Oh, J.; Wang, D.
Deposited on : 2020-10-10
Resolution : 3.45 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

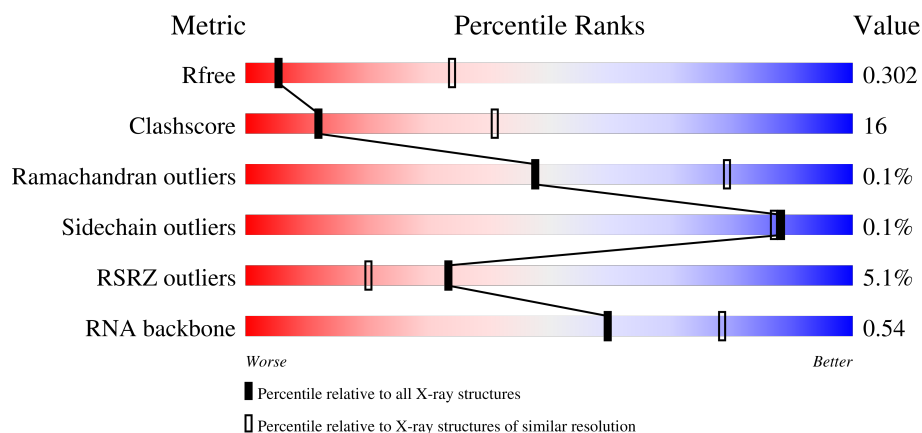
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)
RNA backbone	3983	1186 (3.92-3.00)

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	1733	4% 51% 29% 20%
2	B	1224	6% 57% 33% 10%
3	C	318	2% 60% 23% 16%
4	E	215	7% 71% 29%

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	10	
12	T	29	
13	N	16	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 29039 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1390	Total	C	N	O	S	0	0	0
			10898	6875	1903	2059	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 11 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	10	Total	C	N	O	P	0	0	0
			216	98	45	64	9			

- Molecule 12 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	24	Total	C	N	O	P	0	0	0
			490	235	87	142	24	2		

- Molecule 13 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	11	Total	C	N	O	P	0	0	0
			222	107	34	70	11			

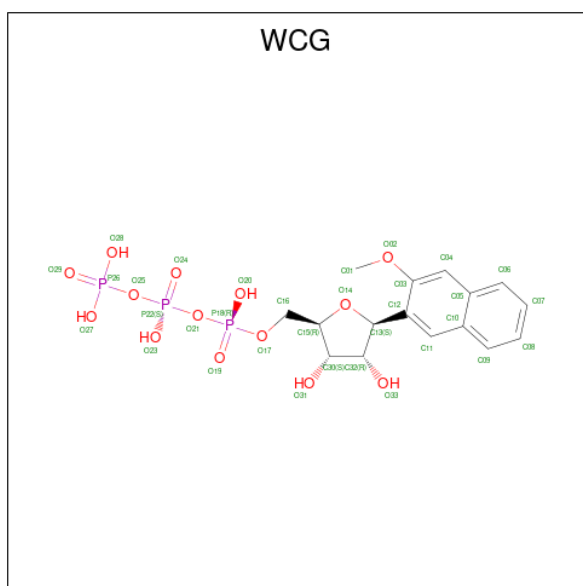
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	2	Total Zn 2 2	0	0
14	B	1	Total Zn 1 1	0	0
14	C	1	Total Zn 1 1	0	0
14	I	2	Total Zn 2 2	0	0
14	J	1	Total Zn 1 1	0	0
14	L	1	Total Zn 1 1	0	0

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total Mg 1 1	0	0

- Molecule 16 is (1S)-1,4-anhydro-5-O-[(R)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}phosphoryl]-1-(3-methoxynaphthalen-2-yl)-D-ribitol (CCD ID: WCG) (formula: C₁₆H₂₁O₁₄P₃) (labeled as "Ligand of Interest" by depositor).

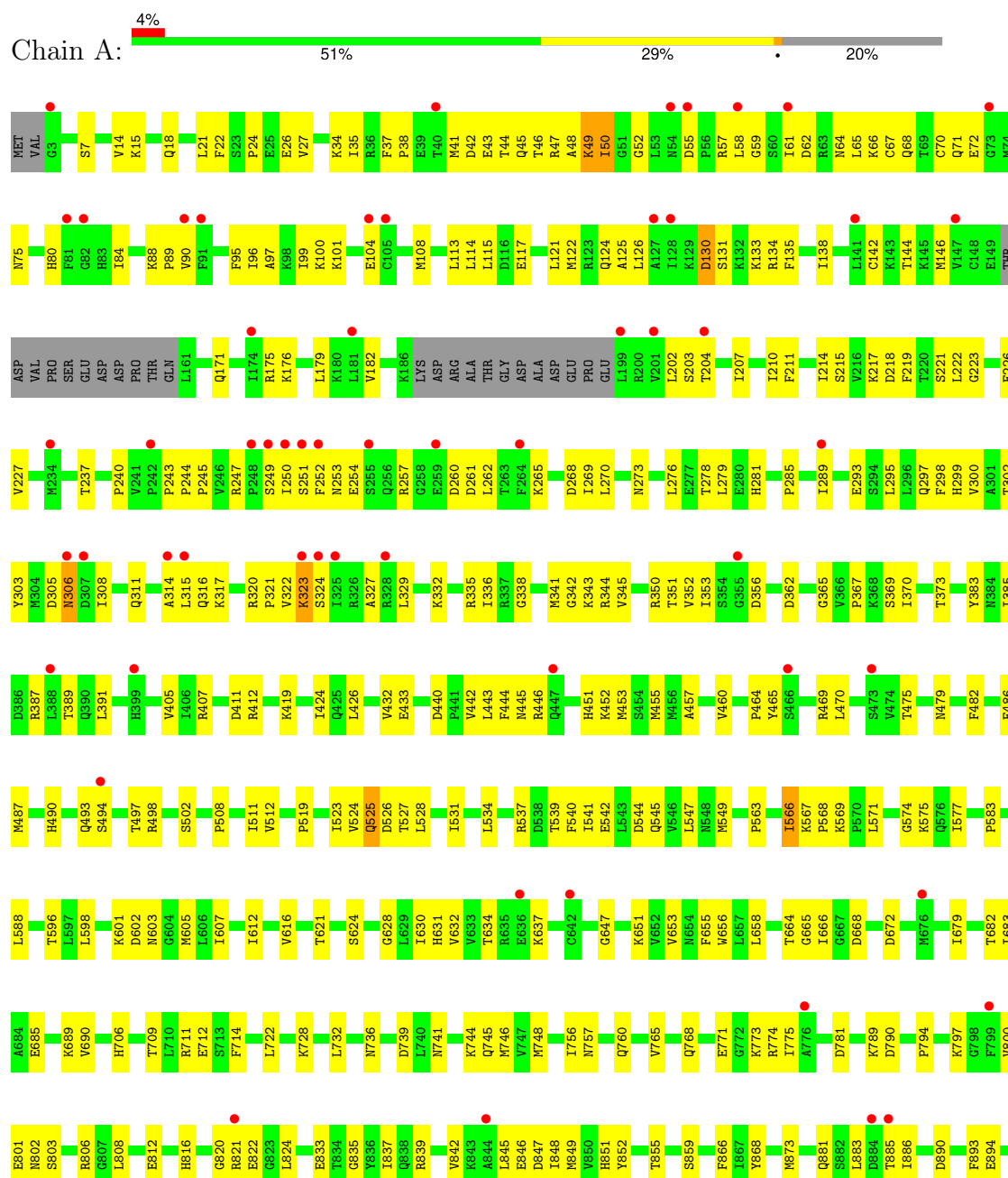


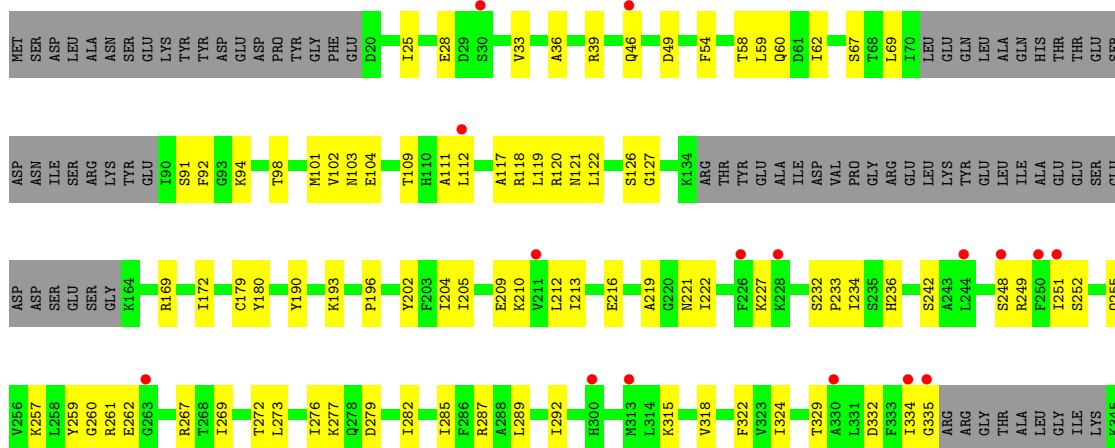
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	B	1	Total	C	O	P	0	0
			33	16	14	3		

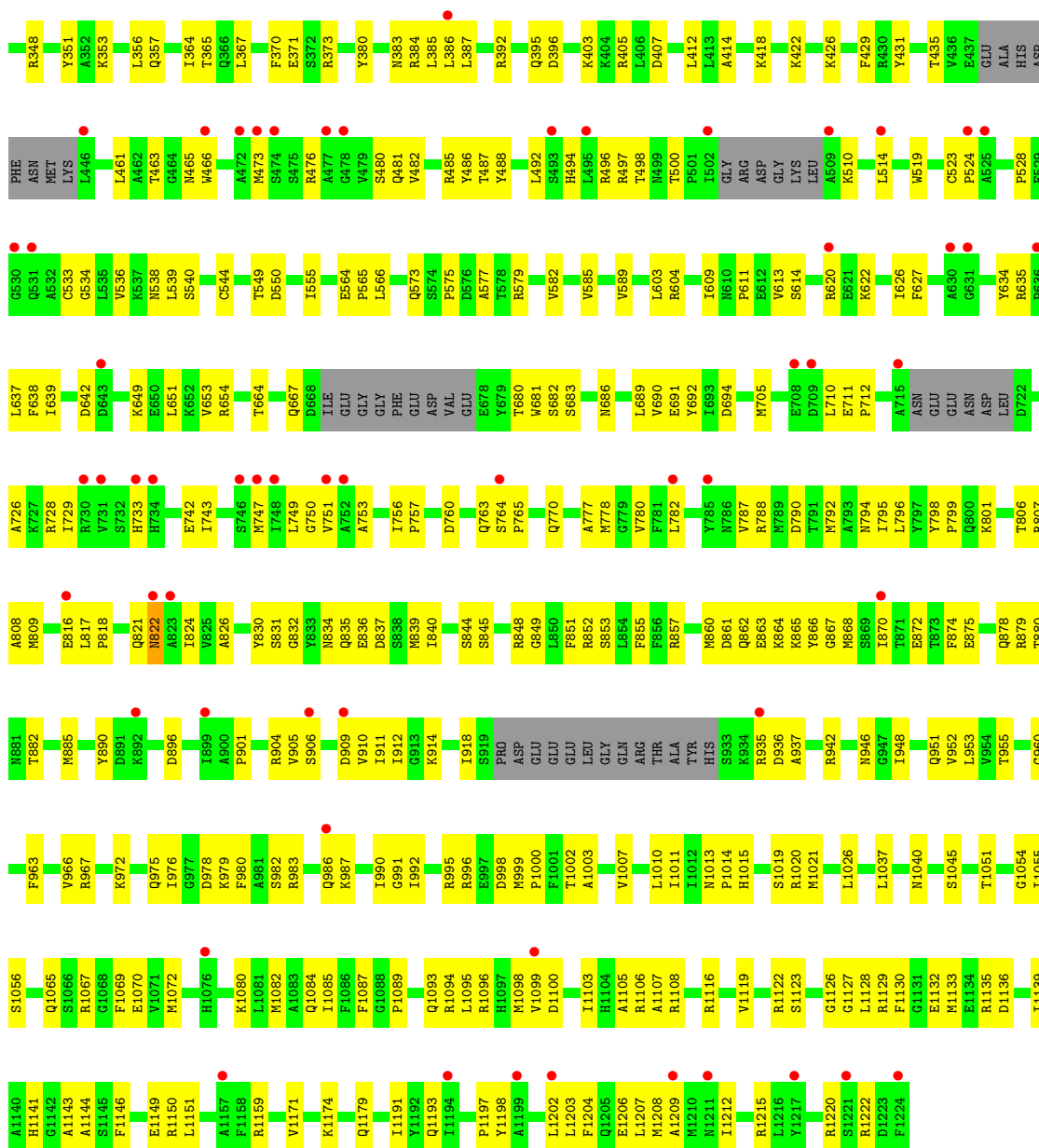
3 Residue-property plots

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

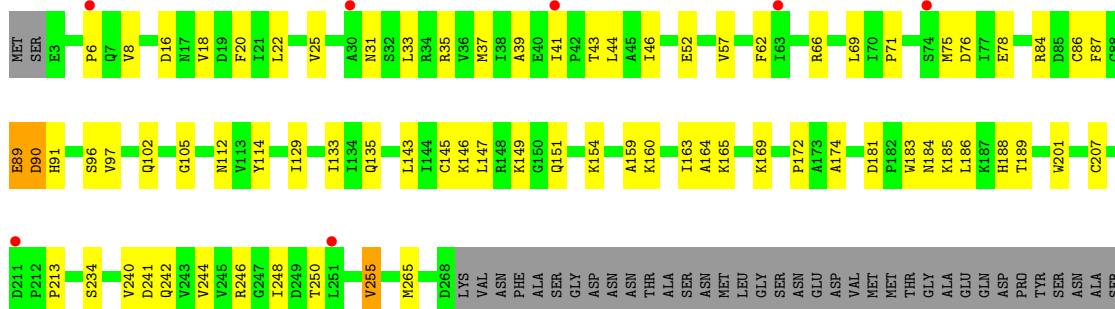
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1







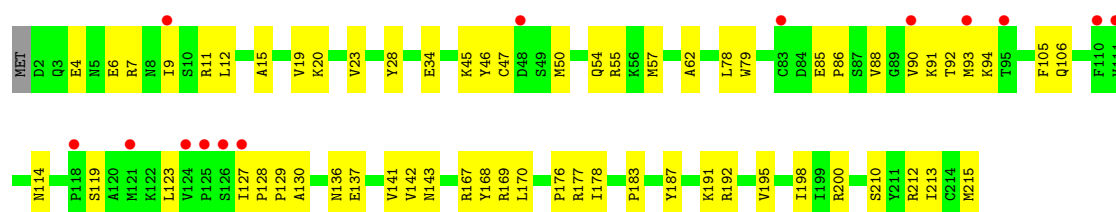
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



GLN
MET
GLY
ASN
THR
GLY
SER
GLY
TYR
ASP
ASN
ALA
TRP

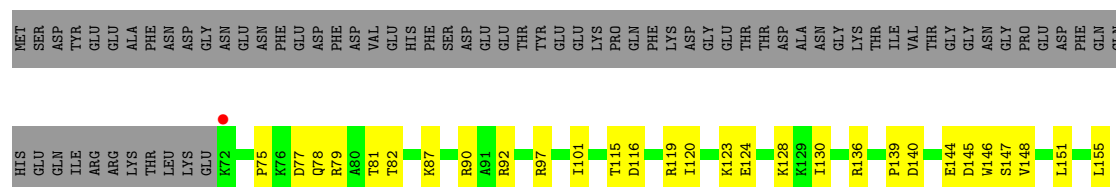
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 7% 71% 29%



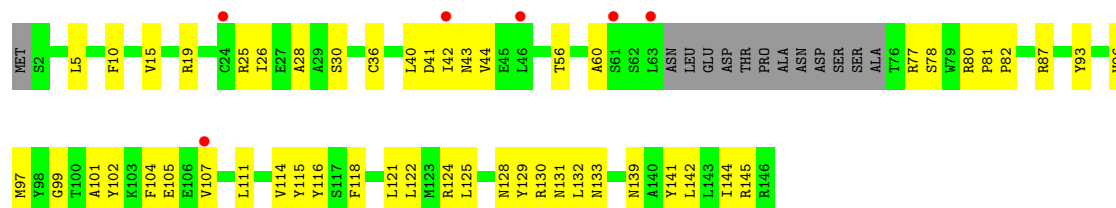
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: % 35% 19% 46%



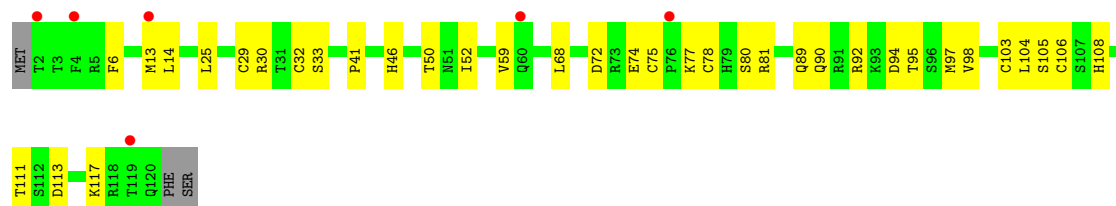
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 4% 56% 35% 9%



- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I: 5% 68% 30% 7%

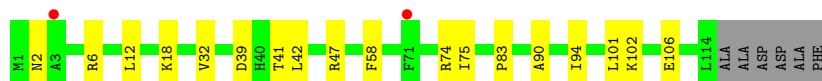
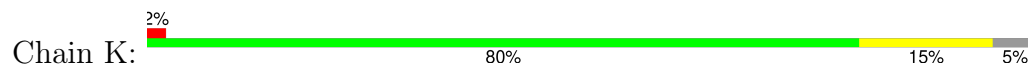


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

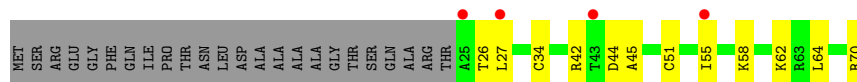
Chain J: 6% 46% 47% 7%



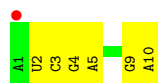
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



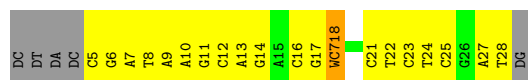
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 11: RNA



- Molecule 12: Template strand DNA



- Molecule 13: Non-template DNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.54Å 222.74Å 194.66Å 90.00° 101.90° 90.00°	Depositor
Resolution (Å)	49.15 – 3.45 49.15 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.15-3.45) 99.8 (49.15-3.45)	Depositor EDS
R_{merge}	0.66	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.259 , 0.302 0.260 , 0.302	Depositor DCC
R_{free} test set	2000 reflections (2.08%)	wwPDB-VP
Wilson B-factor (Å ²)	78.1	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	29039	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: WCG, MG, ZN, WC7

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	3/11091 (0.0%)	0.62	13/15000 (0.1%)
2	B	0.27	3/8963 (0.0%)	0.59	6/12086 (0.0%)
3	C	0.20	0/2133	0.47	0/2891
4	E	0.19	0/1788	0.44	0/2406
5	F	0.20	0/691	0.41	0/933
6	H	0.20	0/1086	0.47	0/1470
7	I	0.18	0/989	0.40	0/1331
8	J	0.27	0/541	0.45	0/727
9	K	0.20	0/937	0.38	0/1265
10	L	0.15	0/365	0.42	0/485
11	R	0.26	0/243	0.39	0/378
12	T	0.32	0/524	0.60	0/803
13	N	0.29	0/246	0.64	0/377
All	All	0.25	6/29597 (0.0%)	0.56	19/40152 (0.0%)

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	8
3	C	0	1
4	E	0	1
All	All	0	10

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	822	ASN	CG-OD1	-9.62	1.05	1.23
2	B	822	ASN	CG-ND2	8.73	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	306	ASN	CG-OD1	-7.98	1.08	1.23
1	A	306	ASN	CG-ND2	6.48	1.46	1.33
2	B	822	ASN	CB-CG	-6.40	1.36	1.52
1	A	306	ASN	C-N	5.45	1.42	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	822	ASN	CB-CG-OD1	29.55	179.91	120.80
2	B	822	ASN	OD1-CG-ND2	-25.14	97.47	122.60
1	A	306	ASN	CB-CG-OD1	24.43	169.65	120.80
1	A	306	ASN	CB-CG-ND2	-24.26	80.01	116.40
2	B	822	ASN	CB-CG-ND2	-22.62	82.47	116.40
1	A	306	ASN	OD1-CG-ND2	-21.79	100.81	122.60
1	A	306	ASN	CB-CA-C	-15.38	85.93	110.08
1	A	306	ASN	N-CA-C	-12.08	96.86	112.93
1	A	306	ASN	N-CA-CB	9.54	126.93	110.34
2	B	822	ASN	CB-CA-C	6.88	123.07	112.00
1	A	524	VAL	CA-C-N	6.40	133.76	121.54
1	A	524	VAL	C-N-CA	6.40	133.76	121.54
1	A	306	ASN	O-C-N	-5.69	114.30	122.03
2	B	822	ASN	N-CA-CB	5.65	119.14	110.60
1	A	525	GLN	N-CA-C	5.41	122.32	110.80
1	A	61	ILE	CA-C-N	-5.39	113.69	122.65
1	A	61	ILE	C-N-CA	-5.39	113.69	122.65
1	A	323	LYS	CA-CB-CG	-5.26	103.58	114.10
2	B	822	ASN	CA-C-O	5.25	129.20	122.64

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1106	ASN	Peptide
1	A	1187	GLN	Peptide
1	A	1188	GLN	Peptide
1	A	1220	PHE	Peptide
1	A	130	ASP	Peptide
1	A	1402	PHE	Peptide
1	A	49	LYS	Peptide
1	A	566	ILE	Peptide
3	C	89	GLU	Peptide
4	E	47	CYS	Peptide

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	10898	0	10959	415	0
2	B	8792	0	8824	334	0
3	C	2095	0	2051	61	0
4	E	1752	0	1776	45	0
5	F	679	0	701	21	0
6	H	1068	0	1040	38	0
7	I	971	0	932	27	0
8	J	532	0	542	35	0
9	K	919	0	929	15	0
10	L	363	0	388	11	0
11	R	216	0	109	5	0
12	T	490	0	259	23	0
13	N	222	0	127	0	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
16	B	33	0	0	2	0
All	All	29039	0	28637	907	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 16.

All (907) 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:821:ARG:NH2	2:B:524:PRO:O	1.80	1.13
1:A:821:ARG:HH21	2:B:514:LEU:HD13	1.23	1.04
1:A:525:GLN:O	2:B:1015:HIS:NE2	1.90	1.02
1:A:821:ARG:NH2	2:B:514:LEU:HD13	1.76	1.01
2:B:67:SER:HB2	2:B:92:PHE:HB2	1.49	0.94
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:ARG:HH22	2:B:524:PRO:C	1.87	0.82
1:A:131:SER:HB3	1:A:223:GLY:HA2	1.62	0.82
1:A:455:MET:HE1	2:B:1130:PHE:HE1	1.44	0.81
2:B:496:ARG:NH2	2:B:540:SER:O	2.12	0.81
3:C:89:GLU:HG2	3:C:90:ASP:H	1.44	0.81
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.65	0.79
12:T:8:DT:H2'	12:T:9:DA:C8	2.18	0.78
1:A:179:LEU:HB2	1:A:297:GLN:HE22	1.48	0.78
1:A:317:LYS:HD3	12:T:28:DT:H2''	1.65	0.78
1:A:1363:VAL:HB	1:A:1368:MET:HE2	1.65	0.78
1:A:709:THR:HG22	1:A:711:ARG:H	1.46	0.78
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.65	0.76
1:A:59:GLY:HA2	1:A:67:CYS:HA	1.66	0.75
6:H:41:ASP:OD2	6:H:122:LEU:N	2.18	0.75
12:T:16:DC:H2''	12:T:17:DG:H5''	1.68	0.75
1:A:956:LEU:HD13	1:A:1021:LEU:HD22	1.68	0.75
4:E:62:ALA:HB3	4:E:78:LEU:HB3	1.69	0.75
4:E:192:ARG:NH1	4:E:215:MET:O	2.20	0.74
2:B:287:ARG:NH1	2:B:292:ILE:O	2.20	0.74
1:A:545:GLN:HG2	1:A:549:MET:HE3	1.70	0.74
1:A:821:ARG:CZ	2:B:524:PRO:O	2.35	0.73
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.70	0.73
1:A:35:ILE:HG12	1:A:84:ILE:HG12	1.67	0.73
3:C:43:THR:HG22	3:C:44:LEU:H	1.54	0.73
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.71	0.72
2:B:778:MET:HG2	2:B:794:ASN:HB3	1.71	0.72
2:B:273:LEU:HD11	2:B:285:ILE:HD11	1.71	0.72
1:A:821:ARG:NH1	2:B:524:PRO:O	2.22	0.72
1:A:1364:ASN:HD21	1:A:1366:ARG:HH21	1.37	0.72
12:T:13:DA:H2'	12:T:14:DG:H8	1.51	0.72
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.72	0.71
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.24	0.71
1:A:883:LEU:H	1:A:952:ALA:HB1	1.56	0.71
1:A:49:LYS:O	1:A:50:ILE:HG13	1.90	0.70
1:A:350:ARG:NH2	1:A:486:GLU:OE2	2.25	0.70
6:H:96:VAL:HA	6:H:142:LEU:O	1.92	0.70
6:H:97:MET:HE3	6:H:118:PHE:HD1	1.56	0.70
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.73	0.70
1:A:1146:VAL:HG13	1:A:1197:LEU:HD22	1.74	0.69
1:A:542:GLU:OE1	1:A:569:LYS:NZ	2.26	0.69
1:A:218:ASP:OD1	1:A:219:PHE:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:LEU:HD11	1:A:1032:LEU:HD21	1.73	0.68
5:F:75:PRO:HG2	5:F:78:GLN:HB2	1.75	0.68
1:A:247:ARG:HD2	1:A:262:LEU:HD22	1.73	0.68
2:B:232:SER:O	2:B:261:ARG:NH2	2.27	0.68
2:B:473:MET:SD	2:B:473:MET:N	2.66	0.68
2:B:486:TYR:OH	2:B:778:MET:HG3	1.94	0.68
2:B:952:VAL:HG22	2:B:966:VAL:HG22	1.75	0.68
1:A:350:ARG:HD3	2:B:1128:LEU:HD11	1.75	0.68
3:C:255:VAL:HG12	9:K:42:LEU:HD11	1.76	0.68
1:A:868:TYR:HE1	1:A:1064:VAL:HG21	1.56	0.68
4:E:127:ILE:HG13	4:E:129:PRO:HD2	1.77	0.67
1:A:122:MET:HG3	1:A:126:LEU:HB2	1.77	0.67
2:B:54:PHE:HA	2:B:58:THR:HB	1.76	0.67
2:B:101:MET:HG2	2:B:111:ALA:HA	1.75	0.67
6:H:40:LEU:HD21	6:H:42:ILE:HD12	1.75	0.67
1:A:57:ARG:HA	1:A:68:GLN:HB2	1.76	0.67
2:B:875:GLU:HB3	10:L:42:ARG:HH22	1.59	0.67
3:C:84:ARG:HH22	3:C:163:ILE:HD11	1.58	0.67
1:A:276:LEU:HD11	1:A:293:GLU:HG2	1.74	0.67
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.77	0.67
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.77	0.67
2:B:1094:ARG:HH22	2:B:1098:MET:HE1	1.59	0.66
7:I:80:SER:OG	7:I:103:CYS:SG	2.53	0.66
1:A:526:ASP:HB2	2:B:835:GLN:HE21	1.59	0.66
1:A:526:ASP:HB2	2:B:835:GLN:NE2	2.11	0.66
2:B:792:MET:HE1	2:B:1096:ARG:HH21	1.58	0.66
2:B:1019:SER:OG	16:B:2101:WCG:O33	2.12	0.66
2:B:1072:MET:HG3	2:B:1085:ILE:HB	1.77	0.66
4:E:88:VAL:HG23	4:E:92:THR:HB	1.77	0.66
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.76	0.65
1:A:125:ALA:HB1	1:A:138:ILE:HG22	1.79	0.65
2:B:1082:MET:HA	3:C:189:THR:HA	1.78	0.65
2:B:837:ASP:OD2	2:B:1020:ARG:NH1	2.29	0.65
8:J:7:CYS:HB2	8:J:49:MET:HG3	1.79	0.65
1:A:251:SER:OG	1:A:253:ASN:O	2.15	0.65
1:A:260:ASP:OD1	1:A:261:ASP:N	2.30	0.65
12:T:7:DA:H2'	12:T:8:DT:C6	2.32	0.65
4:E:11:ARG:HH21	4:E:141:VAL:HG21	1.62	0.64
2:B:901:PRO:HG3	2:B:951:GLN:HA	1.78	0.64
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.25	0.64
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:VAL:HA	1:A:1327:ILE:HG13	1.78	0.64
1:A:114:LEU:HD12	1:A:142:CYS:HB3	1.80	0.64
1:A:469:ARG:NH2	2:B:991:GLY:O	2.28	0.64
1:A:302:THR:HA	1:A:305:ASP:O	1.98	0.63
4:E:93:MET:HG3	4:E:123:LEU:HD13	1.79	0.63
1:A:146:MET:SD	1:A:171:GLN:NE2	2.71	0.63
1:A:265:LYS:HB2	1:A:323:LYS:HD3	1.81	0.63
2:B:979:LYS:NZ	11:R:10:A:OP1	2.31	0.63
2:B:1222:ARG:H	2:B:1222:ARG:HD2	1.64	0.63
1:A:1144:LYS:NZ	1:A:1269:GLU:OE2	2.32	0.63
1:A:452:LYS:HB2	2:B:1141:HIS:CD2	2.34	0.63
7:I:50:THR:HG22	7:I:52:ILE:H	1.63	0.63
1:A:108:MET:SD	1:A:108:MET:N	2.71	0.63
2:B:492:LEU:HD22	2:B:751:VAL:HG21	1.79	0.63
2:B:872:GLU:OE1	2:B:914:LYS:NZ	2.32	0.63
3:C:35:ARG:NH1	9:K:39:ASP:OD2	2.29	0.62
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.29	0.62
1:A:839:ARG:NH1	2:B:1132:GLU:OE2	2.31	0.62
2:B:205:ILE:HD12	2:B:461:LEU:HB3	1.80	0.62
1:A:821:ARG:HH21	2:B:514:LEU:CD1	2.07	0.62
1:A:1212:VAL:O	1:A:1216:ILE:HG13	1.99	0.62
6:H:105:GLU:OE1	6:H:124:ARG:NH2	2.33	0.62
1:A:278:THR:O	1:A:281:HIS:ND1	2.32	0.62
1:A:335:ARG:NH1	2:B:1206:GLU:OE2	2.32	0.62
2:B:996:ARG:NH1	3:C:174:ALA:O	2.32	0.62
1:A:898:ARG:O	1:A:898:ARG:NH1	2.28	0.62
2:B:465:ASN:HA	2:B:476:ARG:HA	1.81	0.62
8:J:12:LYS:NZ	8:J:40:GLY:O	2.33	0.62
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.82	0.61
2:B:975:GLN:NE2	2:B:1100:ASP:OD2	2.32	0.61
2:B:603:LEU:HB3	2:B:609:ILE:HG13	1.81	0.61
1:A:215:SER:N	1:A:218:ASP:OD2	2.33	0.61
1:A:833:GLU:O	1:A:837:ILE:HG12	2.01	0.61
1:A:849:MET:HE3	1:A:1061:GLY:HA2	1.83	0.61
1:A:890:ASP:OD1	1:A:940:ARG:NH1	2.34	0.61
1:A:1143:LEU:H	1:A:1271:ILE:HD13	1.66	0.61
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.83	0.61
2:B:806:THR:HG22	2:B:808:ALA:H	1.66	0.61
1:A:789:LYS:HG3	7:I:68:LEU:HD23	1.82	0.61
1:A:1029:ARG:NH1	1:A:1033:GLN:OE1	2.33	0.61
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.82	0.61
3:C:46:ILE:HA	3:C:159:ALA:HA	1.83	0.61
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.36	0.61
1:A:96:ILE:HA	1:A:99:ILE:HD12	1.83	0.61
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.81	0.61
4:E:136:ASN:OD1	4:E:137:GLU:N	2.33	0.61
1:A:567:LYS:CB	6:H:96:VAL:H	2.14	0.60
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.65	0.60
1:A:588:LEU:HB3	1:A:607:ILE:HB	1.82	0.60
1:A:848:ILE:HD13	1:A:1370:LEU:HD11	1.83	0.60
6:H:101:ALA:HB2	6:H:116:TYR:HE2	1.65	0.60
1:A:113:LEU:HD12	1:A:113:LEU:H	1.67	0.60
1:A:1170:ILE:O	1:A:1173:HIS:ND1	2.30	0.60
4:E:169:ARG:HB3	5:F:140:ASP:HB3	1.83	0.60
1:A:254:GLU:HG3	2:B:918:ILE:HG12	1.84	0.60
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.83	0.60
6:H:128:ASN:O	6:H:131:ASN:ND2	2.32	0.60
12:T:5:DC:H1'	12:T:6:DG:N7	2.17	0.60
1:A:405:VAL:HG22	1:A:432:VAL:HG22	1.84	0.59
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.65	0.59
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.66	0.59
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.83	0.59
9:K:12:LEU:HD21	9:K:18:LYS:HG2	1.84	0.59
1:A:490:HIS:HB3	2:B:1150:ARG:NH1	2.16	0.59
3:C:75:MET:O	3:C:246:ARG:NH2	2.36	0.59
1:A:897:TYR:HE1	1:A:1030:ARG:HG3	1.68	0.59
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.84	0.59
1:A:739:ASP:O	1:A:745:GLN:NE2	2.34	0.59
1:A:672:ASP:OD1	1:A:736:ASN:ND2	2.33	0.59
2:B:848:ARG:NH1	8:J:8:PHE:O	2.35	0.59
2:B:1020:ARG:NH2	16:B:2101:WCG:O19	2.34	0.58
3:C:20:PHE:HE1	3:C:22:LEU:HB2	1.68	0.58
6:H:60:ALA:O	6:H:141:TYR:HB2	2.02	0.58
1:A:757:ASN:HD22	2:B:1021:MET:HE2	1.69	0.58
1:A:1281:ARG:HG2	1:A:1309:ASP:HB2	1.86	0.58
3:C:89:GLU:HG2	3:C:90:ASP:N	2.11	0.58
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.85	0.58
1:A:1113:THR:O	1:A:1330:ASN:ND2	2.33	0.58
6:H:43:ASN:OD1	6:H:44:VAL:N	2.37	0.58
3:C:78:GLU:OE1	3:C:246:ARG:NH1	2.36	0.58
1:A:709:THR:HG23	7:I:94:ASP:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:90:ARG:HD2	5:F:155:LEU:HD12	1.85	0.58
1:A:130:ASP:O	1:A:133:LYS:HG2	2.04	0.58
2:B:497:ARG:HG3	2:B:538:ASN:HD21	1.69	0.58
4:E:6:GLU:HA	4:E:9:ILE:HD12	1.85	0.58
1:A:219:PHE:HA	1:A:222:LEU:HD23	1.86	0.57
1:A:1066:VAL:O	1:A:1070:GLN:HG3	2.03	0.57
1:A:412:ARG:NH2	1:A:433:GLU:OE2	2.36	0.57
1:A:1434:ALA:O	1:A:1436:ILE:N	2.37	0.57
2:B:839:MET:HE2	2:B:1010:LEU:HD22	1.86	0.57
1:A:722:LEU:HD11	1:A:794:PRO:HB3	1.87	0.57
2:B:232:SER:OG	2:B:234:ILE:O	2.23	0.57
4:E:90:VAL:HG22	4:E:119:SER:HB2	1.86	0.57
1:A:226:GLU:HG3	1:A:227:VAL:HG23	1.87	0.57
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.87	0.57
9:K:75:ILE:HD12	9:K:83:PRO:HB2	1.87	0.57
1:A:859:SER:O	1:A:1422:ARG:NH1	2.36	0.57
2:B:463:THR:O	2:B:480:SER:OG	2.22	0.57
1:A:134:ARG:NE	1:A:221:SER:O	2.22	0.57
2:B:1135:ARG:NH2	2:B:1136:ASP:OD1	2.38	0.57
8:J:45:CYS:O	8:J:48:ARG:NH1	2.38	0.57
1:A:781:ASP:HB2	1:A:789:LYS:HD2	1.86	0.57
1:A:1002:GLY:O	1:A:1008:GLN:NE2	2.38	0.57
4:E:198:ILE:HB	4:E:210:SER:HB3	1.86	0.57
5:F:79:ARG:NH1	5:F:145:ASP:O	2.38	0.57
9:K:102:LYS:O	9:K:106:GLU:HG3	2.04	0.57
1:A:523:ILE:HG22	1:A:528:LEU:HB2	1.87	0.57
12:T:9:DA:H2"	12:T:10:DA:C8	2.39	0.57
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.37	0.56
2:B:848:ARG:HD2	8:J:8:PHE:HA	1.86	0.56
2:B:906:SER:N	2:B:909:ASP:OD2	2.26	0.56
2:B:485:ARG:HG2	2:B:485:ARG:HH11	1.70	0.56
1:A:446:ARG:NH1	1:A:479:ASN:O	2.37	0.56
1:A:601:LYS:HG3	1:A:603:ASN:HB2	1.87	0.56
1:A:898:ARG:HH12	1:A:1029:ARG:CZ	2.19	0.56
3:C:31:ASN:O	3:C:35:ARG:HG3	2.05	0.56
4:E:85:GLU:HB3	4:E:86:PRO:HD2	1.86	0.56
4:E:143:ASN:ND2	4:E:187:TYR:OH	2.37	0.56
7:I:32:CYS:SG	7:I:33:SER:N	2.79	0.56
2:B:28:GLU:OE2	2:B:807:ARG:NH1	2.39	0.56
3:C:241:ASP:OD1	3:C:242:GLN:N	2.37	0.56
1:A:90:VAL:HG11	1:A:297:GLN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:486:TYR:CZ	2:B:1096:ARG:HB3	2.41	0.56
1:A:490:HIS:HB3	2:B:1150:ARG:HH12	1.71	0.56
3:C:112:ASN:ND2	8:J:19:GLU:OE1	2.39	0.56
5:F:82:THR:O	5:F:136:ARG:NH1	2.36	0.56
1:A:252:PHE:HB3	2:B:865:LYS:HZ2	1.71	0.56
2:B:999:MET:SD	2:B:1011:ILE:HD11	2.46	0.56
1:A:1155:ASP:HB3	1:A:1241:ARG:HH12	1.71	0.56
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.06	0.55
2:B:431:TYR:O	2:B:435:THR:OG1	2.24	0.55
2:B:682:SER:O	2:B:686:ASN:ND2	2.39	0.55
1:A:848:ILE:HB	1:A:1065:GLY:HA3	1.88	0.55
2:B:255:GLN:H	2:B:272:THR:HG22	1.71	0.55
1:A:315:LEU:H	1:A:321:PRO:HD2	1.70	0.55
1:A:596:THR:OG1	1:A:598:LEU:O	2.24	0.55
4:E:54:GLN:HG3	4:E:57:MET:HE2	1.87	0.55
7:I:98:VAL:HG11	7:I:113:ASP:HB2	1.87	0.55
1:A:690:VAL:HG11	1:A:794:PRO:HD3	1.87	0.55
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.89	0.55
2:B:864:LYS:NZ	2:B:960:GLY:O	2.31	0.55
2:B:414:ALA:O	2:B:418:LYS:HG2	2.07	0.55
6:H:130:ARG:HB3	6:H:133:ASN:HD21	1.72	0.55
1:A:315:LEU:HB3	1:A:321:PRO:HG2	1.88	0.55
1:A:465:TYR:H	9:K:2:ASN:HB3	1.72	0.55
1:A:1035:TYR:HB3	1:A:1037:LEU:HD23	1.87	0.55
1:A:1348:LEU:HD21	1:A:1375:MET:HE2	1.89	0.55
3:C:6:PRO:HB2	9:K:101:LEU:HB2	1.88	0.55
1:A:46:THR:HG22	1:A:47:ARG:H	1.72	0.55
1:A:303:TYR:HA	1:A:323:LYS:NZ	2.22	0.55
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	1.89	0.55
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.39	0.55
1:A:338:GLY:O	2:B:1129:ARG:NH2	2.40	0.54
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.72	0.54
6:H:80:ARG:HD2	6:H:81:PRO:HD2	1.90	0.54
1:A:343:LYS:NZ	2:B:1151:LEU:O	2.40	0.54
2:B:364:ILE:HD13	2:B:585:VAL:HG13	1.89	0.54
2:B:866:TYR:HB3	2:B:870:ILE:HD11	1.88	0.54
2:B:878:GLN:NE2	2:B:880:THR:O	2.39	0.54
1:A:664:THR:HB	2:B:1014:PRO:HB3	1.88	0.54
2:B:1123:SER:OG	12:T:23:DC:OP2	2.26	0.54
6:H:104:PHE:HD2	6:H:114:VAL:HA	1.72	0.54
1:A:512:VAL:HA	1:A:519:PRO:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:705:MET:H	2:B:710:LEU:HD12	1.73	0.54
2:B:878:GLN:O	2:B:882:THR:OG1	2.25	0.54
2:B:975:GLN:O	2:B:990:ILE:HD12	2.07	0.54
10:L:44:ASP:OD1	10:L:45:ALA:N	2.37	0.54
12:T:13:DA:H2'	12:T:14:DG:C8	2.39	0.54
2:B:862:GLN:HB3	2:B:963:PHE:HB2	1.90	0.54
1:A:774:ARG:HD2	1:A:797:LYS:HB3	1.89	0.54
1:A:881:GLN:HG3	1:A:956:LEU:HD12	1.88	0.54
1:A:1364:ASN:OD1	1:A:1366:ARG:NE	2.41	0.54
4:E:12:LEU:O	4:E:15:ALA:HB3	2.08	0.54
4:E:191:LYS:HG3	4:E:192:ARG:H	1.72	0.54
2:B:209:GLU:CD	2:B:485:ARG:HE	2.16	0.54
2:B:249:ARG:HG3	2:B:251:ILE:HG12	1.90	0.54
4:E:106:GLN:O	4:E:130:ALA:HA	2.08	0.54
10:L:26:THR:HG22	10:L:27:LEU:H	1.72	0.54
1:A:175:ARG:NH1	1:A:176:LYS:O	2.41	0.54
1:A:452:LYS:HE3	1:A:453:MET:HE1	1.89	0.54
2:B:664:THR:HA	2:B:667:GLN:HE22	1.72	0.54
6:H:99:GLY:HA3	6:H:118:PHE:HD2	1.73	0.54
1:A:265:LYS:HB3	1:A:323:LYS:HZ3	1.71	0.53
8:J:21:TYR:HA	8:J:24:LEU:HD12	1.91	0.53
1:A:666:ILE:HB	2:B:1026:LEU:HB3	1.88	0.53
3:C:246:ARG:O	3:C:250:THR:OG1	2.26	0.53
1:A:771:GLU:H	1:A:822:GLU:CD	2.17	0.53
1:A:1384:VAL:HA	1:A:1389:PHE:HD2	1.73	0.53
3:C:52:GLU:HA	10:L:64:LEU:HD13	1.91	0.53
1:A:65:LEU:O	1:A:66:LYS:HE2	2.09	0.53
1:A:1142:THR:OG1	1:A:1145:SER:OG	2.23	0.53
1:A:356:ASP:HB2	1:A:469:ARG:HD3	1.90	0.53
1:A:605:MET:HG3	1:A:621:THR:HG21	1.90	0.53
2:B:753:ALA:HA	2:B:756:ILE:HD12	1.90	0.53
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.42	0.53
1:A:345:VAL:HG21	2:B:1150:ARG:HH21	1.73	0.53
1:A:781:ASP:O	1:A:790:ASP:N	2.35	0.53
2:B:69:LEU:HD11	2:B:429:PHE:HD1	1.74	0.53
2:B:845:SER:HB2	8:J:8:PHE:HB3	1.91	0.53
1:A:1005:GLU:HG2	1:A:1009:ASN:ND2	2.24	0.53
2:B:118:ARG:HD2	2:B:204:ILE:HG12	1.90	0.53
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.91	0.53
2:B:1056:SER:OG	2:B:1067:ARG:NH1	2.41	0.53
6:H:10:PHE:HB3	6:H:28:ALA:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:129:TYR:HD2	6:H:130:ARG:HG2	1.73	0.53
1:A:18:GLN:NE2	1:A:1417:GLU:O	2.41	0.53
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.23	0.53
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.44	0.53
2:B:1171:VAL:HG11	2:B:1191:ILE:HG21	1.90	0.53
5:F:77:ASP:OD1	5:F:78:GLN:N	2.38	0.53
12:T:9:DA:H2''	12:T:10:DA:H8	1.73	0.53
6:H:87:ARG:HA	6:H:87:ARG:HE	1.74	0.53
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.42	0.52
2:B:236:HIS:HB3	2:B:385:LEU:HD11	1.91	0.52
12:T:21:DC:H2'	12:T:22:DT:C6	2.44	0.52
1:A:1384:VAL:HA	1:A:1389:PHE:CD2	2.44	0.52
1:A:135:PHE:HA	1:A:138:ILE:HG12	1.91	0.52
2:B:67:SER:O	2:B:67:SER:OG	2.26	0.52
1:A:14:VAL:HB	1:A:1432:GLN:HE22	1.74	0.52
1:A:89:PRO:HB3	1:A:237:THR:HA	1.92	0.52
1:A:744:LYS:HE3	1:A:748:MET:HE1	1.92	0.52
1:A:800:VAL:HG13	1:A:812:GLU:HB3	1.91	0.52
2:B:604:ARG:NH2	2:B:691:GLU:OE1	2.43	0.52
2:B:726:ALA:HB1	2:B:1051:THR:OG1	2.09	0.52
2:B:896:ASP:OD2	10:L:58:LYS:NZ	2.39	0.52
1:A:1118:VAL:HG22	1:A:1327:ILE:HD11	1.92	0.52
1:A:1438:THR:HG22	5:F:92:ARG:HD2	1.92	0.52
6:H:132:LEU:HD12	6:H:132:LEU:H	1.75	0.52
1:A:22:PHE:HZ	2:B:1208:MET:HE3	1.74	0.52
1:A:265:LYS:HD2	1:A:268:ASP:OD2	2.10	0.52
1:A:541:ILE:HG22	1:A:545:GLN:HB3	1.91	0.52
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.45	0.52
1:A:1116:LEU:HD22	1:A:1316:VAL:HG11	1.90	0.52
7:I:74:GLU:HG2	7:I:81:ARG:HD2	1.91	0.52
2:B:261:ARG:HG3	2:B:262:GLU:H	1.74	0.51
3:C:114:TYR:HA	3:C:143:LEU:HA	1.91	0.51
4:E:4:GLU:HA	4:E:7:ARG:HD3	1.92	0.51
6:H:93:TYR:CD2	6:H:145:ARG:HB3	2.44	0.51
1:A:1067:LEU:O	1:A:1071:SER:OG	2.25	0.51
2:B:242:SER:OG	2:B:252:SER:OG	2.08	0.51
2:B:778:MET:HE1	2:B:853:SER:HB3	1.92	0.51
2:B:1070:GLU:OE2	8:J:44:TYR:OH	2.23	0.51
1:A:70:CYS:O	1:A:71:GLN:HG2	2.10	0.51
1:A:252:PHE:HB3	2:B:865:LYS:NZ	2.25	0.51
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:549:THR:HG22	2:B:550:ASP:H	1.74	0.51
2:B:918:ILE:HG21	2:B:935:ARG:HD3	1.92	0.51
4:E:50:MET:HG2	4:E:54:GLN:HE22	1.74	0.51
2:B:367:LEU:HD11	2:B:370:PHE:CD2	2.46	0.51
1:A:324:SER:O	1:A:327:ALA:N	2.42	0.51
1:A:915:SER:HB2	1:A:918:GLU:HB3	1.93	0.51
2:B:757:PRO:HG3	2:B:983:ARG:NH2	2.25	0.51
1:A:845:LEU:HD21	1:A:1371:LEU:HD23	1.93	0.51
2:B:778:MET:CE	2:B:853:SER:HB3	2.41	0.51
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	1.93	0.51
1:A:41:MET:HE1	1:A:257:ARG:HD3	1.93	0.51
1:A:353:ILE:HG13	1:A:482:PHE:HD2	1.76	0.51
1:A:527:THR:O	1:A:531:ILE:HG13	2.11	0.51
1:A:899:VAL:HG21	1:A:929:LEU:HD22	1.90	0.51
2:B:33:VAL:HG11	2:B:638:PHE:HE2	1.76	0.51
2:B:67:SER:O	2:B:91:SER:OG	2.29	0.51
1:A:1295:THR:OG1	1:A:1297:GLU:OE1	2.29	0.51
2:B:486:TYR:OH	2:B:1096:ARG:HB3	2.10	0.51
2:B:637:LEU:HA	2:B:743:ILE:HG13	1.93	0.51
8:J:5:VAL:HA	8:J:15:GLY:HA3	1.93	0.51
1:A:849:MET:HB2	1:A:1063:MET:SD	2.51	0.50
1:A:1100:ARG:NH1	1:A:1103:GLU:OE1	2.44	0.50
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.47	0.50
1:A:311:GLN:OE1	1:A:311:GLN:N	2.29	0.50
1:A:344:ARG:NH1	12:T:21:DC:OP1	2.44	0.50
1:A:1293:SER:HB3	1:A:1297:GLU:HG2	1.93	0.50
4:E:86:PRO:HB2	4:E:114:ASN:HB2	1.92	0.50
2:B:62:ILE:HD12	2:B:418:LYS:HE3	1.94	0.50
2:B:555:ILE:HD11	2:B:582:VAL:HG11	1.94	0.50
1:A:370:ILE:HG23	2:B:1105:ALA:HB2	1.93	0.50
1:A:583:PRO:HB2	1:A:637:LYS:HE3	1.94	0.50
1:A:26:GLU:OE1	2:B:1215:ARG:NH2	2.45	0.50
1:A:62:ASP:OD1	1:A:66:LYS:HE3	2.11	0.50
1:A:575:LYS:NZ	1:A:602:ASP:OD2	2.45	0.50
1:A:665:GLY:N	1:A:668:ASP:OD2	2.45	0.50
2:B:46:GLN:OE1	2:B:544:CYS:HA	2.11	0.50
2:B:1037:LEU:O	8:J:47:ARG:NH1	2.44	0.50
1:A:265:LYS:CB	1:A:323:LYS:HZ3	2.25	0.50
1:A:497:THR:HG21	2:B:1149:GLU:OE1	2.11	0.50
2:B:788:ARG:O	2:B:967:ARG:NH1	2.45	0.50
1:A:900:ASP:HB3	1:A:906:HIS:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:GLU:O	3:C:90:ASP:O	2.30	0.49
2:B:353:LYS:HE3	2:B:357:GLN:HB2	1.94	0.49
1:A:1115:SER:N	1:A:1330:ASN:OD1	2.45	0.49
2:B:577:ALA:HB1	2:B:589:VAL:HB	1.94	0.49
1:A:75:ASN:OD1	2:B:1116:ARG:NH1	2.40	0.49
1:A:493:GLN:N	2:B:1149:GLU:OE1	2.45	0.49
1:A:847:ASP:HB3	1:A:1424:VAL:HG23	1.94	0.49
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	1.92	0.49
8:J:57:ILE:HA	8:J:60:PHE:HD2	1.77	0.49
12:T:27:DA:H4'	12:T:28:DT:OP1	2.11	0.49
1:A:244:PRO:N	1:A:245:PRO:HD2	2.27	0.49
2:B:711:GLU:N	2:B:712:PRO:HD3	2.27	0.49
2:B:972:LYS:HD3	2:B:1098:MET:HE2	1.93	0.49
2:B:1099:VAL:HG12	2:B:1103:ILE:CD1	2.42	0.49
5:F:128:LYS:NZ	5:F:148:VAL:O	2.42	0.49
2:B:879:ARG:HA	2:B:885:MET:HE2	1.94	0.49
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.48	0.49
1:A:445:ASN:OD1	1:A:446:ARG:N	2.45	0.49
1:A:886:ILE:HD11	1:A:943:LEU:HB2	1.94	0.49
1:A:956:LEU:HD21	1:A:1017:LEU:HD12	1.95	0.49
2:B:212:LEU:HD21	2:B:466:TRP:CZ2	2.48	0.49
2:B:519:TRP:CD1	2:B:635:ARG:HH12	2.31	0.49
3:C:186:LEU:HB3	3:C:188:HIS:ND1	2.27	0.49
7:I:75:CYS:SG	7:I:108:HIS:ND1	2.79	0.49
12:T:24:DT:H1'	12:T:25:DC:H5'	1.95	0.49
1:A:265:LYS:NZ	1:A:323:LYS:HZ3	2.10	0.49
1:A:387:ARG:O	1:A:391:LEU:HG	2.13	0.49
1:A:820:GLY:O	1:A:824:LEU:HG	2.13	0.49
4:E:177:ARG:NE	4:E:215:MET:SD	2.85	0.49
1:A:682:THR:O	1:A:685:GLU:HG2	2.13	0.48
2:B:227:LYS:HB3	2:B:395:GLN:OE1	2.12	0.48
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.95	0.48
2:B:126:SER:HB2	2:B:172:ILE:HD11	1.94	0.48
1:A:15:LYS:HB3	2:B:1220:ARG:HG3	1.95	0.48
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.13	0.48
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.95	0.48
2:B:780:VAL:HA	2:B:795:ILE:HD13	1.95	0.48
8:J:38:ARG:HH11	8:J:38:ARG:HB2	1.77	0.48
12:T:13:DA:C4	12:T:14:DG:C8	3.01	0.48
1:A:383:TYR:HB2	5:F:115:THR:HB	1.95	0.48
1:A:848:ILE:HG21	1:A:1370:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1282:VAL:HG23	1:A:1308:THR:HG22	1.95	0.48
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.96	0.48
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.79	0.48
4:E:20:LYS:NZ	4:E:34:GLU:OE1	2.40	0.48
1:A:320:ARG:N	1:A:321:PRO:HD3	2.28	0.48
1:A:440:ASP:O	1:A:460:VAL:HG23	2.13	0.48
1:A:444:PHE:CE2	1:A:470:LEU:HD21	2.48	0.48
1:A:1117:THR:HB	1:A:1328:TYR:HB3	1.95	0.48
1:A:1134:ILE:HD13	1:A:1322:ILE:HG22	1.95	0.48
2:B:498:THR:O	2:B:536:VAL:HA	2.12	0.48
2:B:680:THR:O	2:B:683:SER:OG	2.32	0.48
2:B:976:ILE:O	2:B:990:ILE:HB	2.14	0.48
4:E:195:VAL:HG22	4:E:213:ILE:HG13	1.94	0.48
1:A:121:LEU:HA	1:A:124:GLN:HE22	1.78	0.48
1:A:315:LEU:HD12	1:A:316:GLN:H	1.79	0.48
1:A:756:ILE:O	1:A:760:GLN:HG3	2.13	0.48
1:A:842:VAL:O	1:A:846:GLU:HB3	2.14	0.48
1:A:1409:LEU:HD22	2:B:1207:LEU:HD11	1.95	0.48
1:A:305:ASP:OD1	1:A:306:ASN:N	2.46	0.48
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.96	0.48
1:A:534:LEU:HA	1:A:539:THR:HG21	1.96	0.48
1:A:943:LEU:HD11	1:A:1020:CYS:HB3	1.96	0.48
1:A:1003:LYS:HE3	5:F:78:GLN:HA	1.96	0.48
1:A:1345:ARG:NE	1:A:1373:ASP:OD1	2.45	0.48
2:B:879:ARG:HG2	2:B:885:MET:HE2	1.95	0.48
1:A:547:LEU:HB3	9:K:58:PHE:HE1	1.78	0.48
2:B:642:ASP:HA	2:B:649:LYS:HA	1.96	0.48
6:H:77:ARG:HG2	6:H:78:SER:N	2.29	0.48
1:A:443:LEU:HB3	1:A:490:HIS:HB2	1.95	0.47
2:B:60:GLN:HE22	2:B:94:LYS:HA	1.78	0.47
1:A:269:ILE:HD11	1:A:299:HIS:O	2.14	0.47
1:A:336:ILE:HD11	2:B:1203:LEU:HD13	1.96	0.47
1:A:658:LEU:HG	2:B:831:SER:H	1.79	0.47
2:B:904:ARG:HA	2:B:948:ILE:HG22	1.95	0.47
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.96	0.47
1:A:367:PRO:HD2	1:A:370:ILE:HD12	1.96	0.47
8:J:9:SER:HB3	8:J:45:CYS:SG	2.54	0.47
2:B:809:MET:HE1	2:B:983:ARG:HH12	1.79	0.47
3:C:242:GLN:HB3	3:C:246:ARG:HE	1.79	0.47
10:L:34:CYS:SG	10:L:51:CYS:HB2	2.55	0.47
1:A:214:ILE:HG12	1:A:218:ASP:OD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1138:ILE:HD11	1:A:1282:VAL:HG21	1.96	0.47
2:B:481:GLN:OE1	2:B:494:HIS:NE2	2.35	0.47
5:F:81:THR:OG1	5:F:144:GLU:OE2	2.24	0.47
6:H:102:TYR:CZ	6:H:115:TYR:HB3	2.50	0.47
1:A:1377:THR:HB	4:E:176:PRO:HB3	1.97	0.47
2:B:315:LYS:HD3	7:I:13:MET:HE1	1.97	0.47
2:B:528:PRO:HD3	2:B:536:VAL:O	2.15	0.47
2:B:874:PHE:CD2	2:B:914:LYS:HB3	2.50	0.47
6:H:30:SER:HB3	6:H:36:CYS:HB3	1.96	0.47
1:A:37:PHE:HB2	1:A:38:PRO:HD2	1.97	0.47
1:A:897:TYR:CE1	1:A:1030:ARG:HG3	2.49	0.47
2:B:486:TYR:HE2	2:B:777:ALA:C	2.23	0.47
2:B:533:CYS:SG	2:B:534:GLY:N	2.88	0.47
6:H:139:ASN:N	6:H:139:ASN:OD1	2.48	0.47
1:A:1287:TYR:OH	1:A:1307:GLU:OE1	2.33	0.47
2:B:277:LYS:HZ2	2:B:335:GLY:H	1.62	0.47
2:B:383:ASN:O	2:B:387:LEU:HB2	2.15	0.47
3:C:33:LEU:O	3:C:37:MET:HG3	2.15	0.47
3:C:91:HIS:HB2	3:C:96:SER:OG	2.15	0.47
2:B:496:ARG:HB3	2:B:539:LEU:HB2	1.95	0.46
2:B:861:ASP:OD1	2:B:862:GLN:N	2.46	0.46
4:E:55:ARG:H	4:E:55:ARG:HD2	1.79	0.46
1:A:114:LEU:HB2	1:A:115:LEU:HD12	1.97	0.46
2:B:380:TYR:HE1	2:B:579:ARG:HE	1.64	0.46
7:I:111:THR:HG22	7:I:113:ASP:H	1.80	0.46
1:A:630:ILE:HD12	1:A:630:ILE:H	1.79	0.46
2:B:620:ARG:NE	7:I:89:GLN:OE1	2.48	0.46
6:H:25:ARG:HA	6:H:41:ASP:HA	1.97	0.46
1:A:90:VAL:HB	1:A:297:GLN:HG3	1.96	0.46
1:A:655:PHE:HA	1:A:658:LEU:HD13	1.97	0.46
1:A:942:PHE:HD2	1:A:943:LEU:HD23	1.80	0.46
1:A:1005:GLU:HG2	1:A:1009:ASN:HD21	1.80	0.46
2:B:497:ARG:HA	2:B:538:ASN:HD22	1.79	0.46
2:B:878:GLN:HG3	2:B:880:THR:H	1.81	0.46
3:C:16:ASP:OD1	3:C:135:GLN:NE2	2.40	0.46
3:C:69:LEU:O	8:J:6:ARG:NH2	2.38	0.46
3:C:147:LEU:HD22	3:C:151:GLN:HB3	1.97	0.46
4:E:50:MET:HG2	4:E:54:GLN:NE2	2.28	0.46
6:H:93:TYR:HD2	6:H:145:ARG:HB3	1.79	0.46
1:A:508:PRO:HA	1:A:511:ILE:HG13	1.98	0.46
1:A:540:PHE:HB3	1:A:571:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:851:HIS:ND1	5:F:139:PRO:HG3	2.30	0.46
8:J:45:CYS:O	8:J:48:ARG:HG3	2.16	0.46
11:R:2:U:H2'	11:R:3:C:C6	2.51	0.46
1:A:37:PHE:CE2	1:A:52:GLY:HA3	2.51	0.46
1:A:38:PRO:HD3	1:A:270:LEU:HD22	1.98	0.46
1:A:628:GLY:O	1:A:632:VAL:HG23	2.15	0.46
2:B:852:ARG:NH2	10:L:70:ARG:O	2.44	0.46
2:B:853:SER:OG	2:B:972:LYS:HB2	2.16	0.46
7:I:92:ARG:O	7:I:95:THR:OG1	2.23	0.46
1:A:709:THR:HB	1:A:712:GLU:H	1.80	0.46
1:A:1371:LEU:O	1:A:1374:VAL:HG12	2.16	0.46
2:B:978:ASP:OD2	2:B:1094:ARG:NH2	2.48	0.46
3:C:8:VAL:HG22	3:C:22:LEU:HD23	1.98	0.46
3:C:20:PHE:CE1	3:C:22:LEU:HB2	2.50	0.46
3:C:145:CYS:SG	3:C:146:LYS:N	2.88	0.46
4:E:46:TYR:CD1	4:E:57:MET:HB3	2.50	0.46
7:I:29:CYS:SG	7:I:30:ARG:N	2.88	0.46
8:J:24:LEU:HD11	8:J:39:LEU:HD21	1.97	0.46
12:T:11:DG:H2'	12:T:12:DC:C5	2.51	0.46
1:A:519:PRO:O	1:A:624:SER:OG	2.33	0.46
2:B:202:TYR:CD1	2:B:209:GLU:HB3	2.51	0.46
1:A:300:VAL:O	1:A:303:TYR:HB3	2.15	0.46
1:A:329:LEU:HD12	1:A:1406:VAL:HG12	1.97	0.46
1:A:736:ASN:ND2	1:A:736:ASN:O	2.49	0.46
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.97	0.46
2:B:622:LYS:HE2	7:I:59:VAL:HG21	1.97	0.46
2:B:979:LYS:HE2	2:B:1095:LEU:HD12	1.98	0.46
7:I:78:CYS:HG	7:I:105:SER:HG	1.64	0.46
9:K:90:ALA:O	9:K:94:ILE:HG13	2.16	0.46
1:A:343:LYS:HE3	2:B:1151:LEU:HD12	1.96	0.46
1:A:1094:VAL:HG12	1:A:1113:THR:HG21	1.97	0.46
2:B:121:ASN:HD21	2:B:860:MET:HE2	1.81	0.46
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.51	0.46
4:E:93:MET:SD	4:E:123:LEU:HD22	2.56	0.46
6:H:114:VAL:HG22	6:H:125:LEU:HB3	1.98	0.46
1:A:531:ILE:HG13	1:A:653:VAL:HG11	1.98	0.45
1:A:873:MET:HE3	1:A:957:PRO:HG2	1.98	0.45
2:B:798:TYR:CD2	8:J:4:PRO:HG3	2.50	0.45
1:A:479:ASN:O	1:A:479:ASN:ND2	2.49	0.45
1:A:908:LEU:HD23	1:A:1029:ARG:NH2	2.32	0.45
1:A:913:LEU:HD12	1:A:914:GLU:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1433:MET:HG2	2:B:1144:ALA:HB1	1.98	0.45
2:B:103:ASN:HD22	2:B:109:THR:HB	1.81	0.45
2:B:219:ALA:HB2	2:B:405:ARG:HE	1.81	0.45
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.98	0.45
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.51	0.45
2:B:995:ARG:HE	9:K:6:ARG:HH12	1.65	0.45
2:B:1051:THR:HG23	2:B:1054:GLY:H	1.81	0.45
1:A:24:PRO:HA	1:A:27:VAL:HG12	1.98	0.45
1:A:1215:ARG:HD2	1:A:1215:ARG:HA	1.74	0.45
2:B:98:THR:HB	2:B:127:GLY:H	1.82	0.45
6:H:81:PRO:CB	6:H:82:PRO:HD2	2.46	0.45
1:A:108:MET:HE3	1:A:210:ILE:HD13	1.98	0.45
1:A:341:MET:HB3	2:B:1132:GLU:HB3	1.97	0.45
1:A:1355:VAL:O	1:A:1358:SER:OG	2.35	0.45
2:B:324:ILE:HD12	2:B:329:THR:HB	1.99	0.45
11:R:9:G:C2	12:T:21:DC:C2	3.05	0.45
2:B:119:LEU:HD12	10:L:55:ILE:HD11	1.98	0.45
2:B:179:CYS:SG	2:B:180:TYR:N	2.89	0.45
2:B:260:GLY:O	2:B:267:ARG:NH2	2.40	0.45
2:B:749:LEU:HB3	2:B:753:ALA:HB3	1.97	0.45
2:B:792:MET:SD	2:B:857:ARG:NH1	2.90	0.45
2:B:816:GLU:HB3	2:B:817:LEU:HD12	1.98	0.45
3:C:62:PHE:O	3:C:66:ARG:HG3	2.16	0.45
4:E:91:LYS:HA	4:E:94:LYS:HD3	1.99	0.45
12:T:5:DC:H1'	12:T:6:DG:C8	2.51	0.45
1:A:323:LYS:H	1:A:323:LYS:HG3	1.19	0.45
1:A:689:LYS:HE3	1:A:689:LYS:HB2	1.78	0.45
1:A:808:LEU:O	2:B:728:ARG:NH1	2.50	0.45
1:A:1079:MET:HE2	1:A:1079:MET:HB3	1.90	0.45
1:A:1435:PRO:C	1:A:1436:ILE:HD12	2.42	0.45
2:B:277:LYS:NZ	2:B:335:GLY:H	2.14	0.45
8:J:7:CYS:SG	8:J:10:CYS:N	2.89	0.45
1:A:7:SER:OG	2:B:1159:ARG:NH2	2.49	0.45
1:A:217:LYS:HA	1:A:217:LYS:HD2	1.74	0.45
1:A:494:SER:O	1:A:498:ARG:HG2	2.17	0.45
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.15	0.45
1:A:1341:ILE:O	1:A:1344:GLY:N	2.50	0.45
7:I:72:ASP:O	7:I:81:ARG:NH1	2.50	0.45
8:J:18:TRP:O	8:J:21:TYR:HB3	2.16	0.45
1:A:1342:GLU:OE1	4:E:200:ARG:NH1	2.50	0.45
2:B:1065:GLN:HB3	2:B:1069:PHE:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1202:LEU:HD23	2:B:1202:LEU:HA	1.83	0.45
3:C:184:ASN:HD21	3:C:189:THR:H	1.64	0.45
6:H:15:VAL:HA	6:H:26:ILE:HD12	1.99	0.45
1:A:728:LYS:HB2	1:A:728:LYS:HE3	1.80	0.45
1:A:803:SER:H	1:A:806:ARG:HB2	1.82	0.45
2:B:119:LEU:HB3	2:B:953:LEU:HD21	1.99	0.45
2:B:276:ILE:HD12	2:B:276:ILE:HA	1.82	0.45
2:B:287:ARG:HD2	2:B:324:ILE:HG22	1.98	0.45
2:B:604:ARG:NH1	2:B:613:VAL:O	2.50	0.45
2:B:844:SER:O	2:B:848:ARG:HG3	2.17	0.45
2:B:1174:LYS:HG3	2:B:1179:GLN:HB3	1.99	0.45
1:A:765:VAL:HG12	1:A:802:ASN:O	2.17	0.44
1:A:816:HIS:CE1	2:B:764:SER:H	2.35	0.44
1:A:845:LEU:CD2	1:A:1374:VAL:HG11	2.47	0.44
4:E:128:PRO:HB2	4:E:129:PRO:HD3	1.98	0.44
5:F:147:SER:O	5:F:151:LEU:HD12	2.17	0.44
1:A:207:ILE:HG22	1:A:211:PHE:CE2	2.52	0.44
1:A:537:ARG:NH2	6:H:25:ARG:HH12	2.14	0.44
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.97	0.44
1:A:894:GLU:O	1:A:898:ARG:HG2	2.17	0.44
2:B:221:ASN:OD1	2:B:242:SER:HA	2.17	0.44
1:A:835:GLY:HA3	12:T:18:WC7:O4'	2.17	0.44
1:A:998:LEU:HD13	1:A:1001:ARG:NH1	2.33	0.44
1:A:249:SER:O	1:A:250:ILE:HD13	2.16	0.44
1:A:1158:PRO:O	1:A:1170:ILE:HG21	2.17	0.44
2:B:102:VAL:HG12	2:B:112:LEU:HB2	2.00	0.44
2:B:710:LEU:HD22	2:B:733:HIS:CD2	2.53	0.44
8:J:46:CYS:O	8:J:49:MET:N	2.49	0.44
1:A:265:LYS:HA	1:A:268:ASP:HB2	1.98	0.44
2:B:651:LEU:HD13	2:B:653:VAL:O	2.17	0.44
9:K:42:LEU:HA	9:K:42:LEU:HD12	1.77	0.44
1:A:1159:ARG:H	1:A:1159:ARG:HG2	1.56	0.44
2:B:219:ALA:HA	2:B:405:ARG:HG2	2.00	0.44
2:B:364:ILE:O	2:B:365:THR:HG23	2.17	0.44
2:B:801:LYS:O	8:J:52:THR:HB	2.18	0.44
2:B:936:ASP:OD1	2:B:937:ALA:N	2.50	0.44
1:A:444:PHE:HE2	1:A:470:LEU:HD21	1.82	0.44
1:A:544:ASP:HB2	9:K:47:ARG:NH2	2.33	0.44
1:A:771:GLU:N	1:A:822:GLU:OE2	2.37	0.44
1:A:943:LEU:HD21	1:A:1020:CYS:SG	2.58	0.44
2:B:39:ARG:NH2	2:B:664:THR:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:ARG:NH2	2:B:664:THR:OG1	2.50	0.44
2:B:289:LEU:HD21	2:B:356:LEU:HD12	2.00	0.44
2:B:634:TYR:HA	2:B:694:ASP:HA	1.99	0.44
2:B:760:ASP:OD1	2:B:760:ASP:N	2.50	0.44
2:B:792:MET:HE3	2:B:855:PHE:HE1	1.83	0.44
3:C:86:CYS:SG	3:C:87:PHE:N	2.91	0.44
4:E:79:TRP:HE3	4:E:105:PHE:HE2	1.65	0.44
1:A:100:LYS:O	1:A:104:GLU:HG2	2.18	0.44
1:A:954:TRP:HE3	1:A:955:PRO:HD2	1.83	0.44
2:B:407:ASP:HB3	2:B:412:LEU:CD2	2.48	0.44
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.52	0.44
7:I:30:ARG:HA	7:I:30:ARG:HD3	1.69	0.44
8:J:1:MET:HA	8:J:56:LEU:HB2	2.00	0.44
8:J:7:CYS:CB	8:J:49:MET:HG3	2.47	0.44
1:A:21:LEU:HD11	1:A:95:PHE:CE1	2.52	0.44
1:A:146:MET:HA	1:A:171:GLN:HE22	1.82	0.44
1:A:351:THR:OG1	1:A:352:VAL:N	2.51	0.44
1:A:706:HIS:CD2	1:A:1135:ARG:HE	2.36	0.44
1:A:977:LYS:NZ	1:A:978:PRO:O	2.44	0.44
2:B:392:ARG:HA	7:I:90:GLN:HA	1.98	0.44
2:B:824:ILE:HA	2:B:1089:PRO:HA	1.99	0.44
2:B:867:GLY:O	2:B:868:MET:HG2	2.18	0.44
5:F:81:THR:HB	5:F:136:ARG:HH11	1.82	0.44
1:A:66:LYS:HD3	1:A:66:LYS:HA	1.48	0.43
1:A:90:VAL:CG1	1:A:297:GLN:HB2	2.48	0.43
1:A:144:THR:O	1:A:144:THR:OG1	2.33	0.43
2:B:242:SER:OG	2:B:252:SER:O	2.36	0.43
2:B:946:ASN:OD1	2:B:946:ASN:N	2.51	0.43
2:B:1116:ARG:HB2	2:B:1198:TYR:CD1	2.53	0.43
1:A:64:ASN:O	1:A:65:LEU:HD22	2.18	0.43
1:A:240:PRO:HG2	2:B:1209:ALA:HA	2.00	0.43
1:A:1062:GLU:OE2	5:F:87:LYS:NZ	2.50	0.43
2:B:332:ASP:OD1	2:B:348:ARG:NE	2.51	0.43
2:B:1159:ARG:NH1	2:B:1193:GLN:OE1	2.51	0.43
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.99	0.43
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.99	0.43
2:B:849:GLY:HA2	2:B:852:ARG:HG3	2.00	0.43
3:C:76:ASP:C	3:C:129:ILE:HD11	2.43	0.43
1:A:362:ASP:OD2	1:A:362:ASP:N	2.43	0.43
2:B:540:SER:OG	2:B:747:MET:O	2.36	0.43
2:B:982:SER:OG	2:B:983:ARG:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:57:ILE:HA	8:J:60:PHE:HB2	1.99	0.43
1:A:43:GLU:HG3	1:A:44:THR:H	1.83	0.43
1:A:1166:ASP:OD2	1:A:1239:ARG:NE	2.47	0.43
3:C:234:SER:HB3	3:C:240:VAL:HG13	2.00	0.43
1:A:308:ILE:HD11	1:A:311:GLN:OE1	2.18	0.43
1:A:419:LYS:HE2	1:A:419:LYS:HB3	1.59	0.43
1:A:773:LYS:HD2	1:A:774:ARG:H	1.84	0.43
2:B:287:ARG:NE	2:B:324:ILE:O	2.52	0.43
3:C:185:LYS:HG2	3:C:213:PRO:HG3	2.00	0.43
8:J:64:ASN:N	8:J:65:PRO:HD2	2.34	0.43
1:A:574:GLY:HA2	1:A:577:ILE:HD11	2.00	0.43
1:A:602:ASP:O	1:A:616:VAL:HG22	2.18	0.43
1:A:956:LEU:HA	1:A:957:PRO:HD3	1.81	0.43
1:A:1191:TRP:HH2	7:I:25:LEU:HD13	1.84	0.43
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	2.00	0.43
2:B:49:ASP:OD1	2:B:49:ASP:N	2.51	0.43
10:L:27:LEU:HD12	10:L:27:LEU:O	2.18	0.43
1:A:775:ILE:HG22	1:A:797:LYS:HA	2.01	0.43
1:A:1116:LEU:HD12	1:A:1310:GLY:O	2.19	0.43
1:A:1424:VAL:HG11	2:B:1139:ILE:CD1	2.48	0.43
2:B:635:ARG:HE	2:B:635:ARG:HB3	1.60	0.43
2:B:857:ARG:NH2	2:B:942:ARG:HH12	2.17	0.43
2:B:216:GLU:OE1	2:B:500:THR:OG1	2.32	0.43
2:B:248:SER:OG	2:B:418:LYS:NZ	2.24	0.43
2:B:510:LYS:HD2	2:B:510:LYS:HA	1.90	0.43
3:C:186:LEU:HD23	3:C:188:HIS:CE1	2.54	0.43
4:E:45:LYS:HA	4:E:45:LYS:HD3	1.63	0.43
7:I:117:LYS:HB3	7:I:117:LYS:HE3	1.86	0.43
8:J:25:LEU:HD21	8:J:32:GLU:HA	2.01	0.43
1:A:442:VAL:O	1:A:457:ALA:HA	2.19	0.43
1:A:765:VAL:HG13	1:A:800:VAL:HB	2.00	0.43
2:B:384:ARG:NH2	2:B:396:ASP:OD1	2.52	0.43
2:B:523:CYS:SG	2:B:750:GLY:N	2.85	0.43
2:B:1080:LYS:NZ	3:C:181:ASP:O	2.52	0.43
2:B:1204:PHE:O	2:B:1208:MET:HG3	2.18	0.43
4:E:168:TYR:HB3	4:E:170:LEU:HG	2.00	0.43
5:F:116:ASP:O	5:F:120:ILE:HG13	2.19	0.43
7:I:6:PHE:HA	7:I:14:LEU:HG	2.01	0.43
1:A:42:ASP:OD1	1:A:43:GLU:N	2.52	0.42
1:A:475:THR:HG21	2:B:836:GLU:HG3	2.00	0.42
1:A:512:VAL:HG21	1:A:631:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:VAL:HG11	7:I:41:PRO:HG3	2.00	0.42
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.51	0.42
2:B:289:LEU:HD22	2:B:371:GLU:HB2	2.01	0.42
2:B:322:PHE:HD1	2:B:322:PHE:O	2.02	0.42
5:F:124:GLU:HB3	5:F:130:ILE:HG12	2.01	0.42
6:H:97:MET:HE1	6:H:121:LEU:HG	2.01	0.42
1:A:265:LYS:NZ	1:A:323:LYS:NZ	2.66	0.42
1:A:269:ILE:HD12	1:A:299:HIS:HB3	2.01	0.42
1:A:342:GLY:C	2:B:1129:ARG:HH21	2.27	0.42
1:A:885:THR:HG22	1:A:893:PHE:HE1	1.84	0.42
1:A:1220:PHE:HE1	1:A:1267:MET:HG3	1.83	0.42
2:B:257:LYS:HE2	2:B:257:LYS:HB3	1.86	0.42
2:B:778:MET:CG	2:B:794:ASN:HB3	2.45	0.42
1:A:321:PRO:O	1:A:322:VAL:HG13	2.19	0.42
1:A:981:LEU:HD12	1:A:981:LEU:O	2.19	0.42
1:A:1373:ASP:O	1:A:1376:THR:N	2.51	0.42
2:B:62:ILE:HD12	2:B:418:LYS:CE	2.49	0.42
2:B:422:LYS:O	2:B:426:LYS:HG2	2.18	0.42
2:B:611:PRO:O	2:B:692:TYR:HB2	2.20	0.42
2:B:770:GLN:HG2	2:B:983:ARG:O	2.18	0.42
12:T:6:DG:C4	12:T:7:DA:C8	3.08	0.42
1:A:42:ASP:HB3	1:A:45:GLN:H	1.84	0.42
1:A:48:ALA:HB1	1:A:55:ASP:OD1	2.19	0.42
1:A:273:ASN:O	1:A:273:ASN:ND2	2.38	0.42
1:A:369:SER:O	1:A:373:THR:OG1	2.35	0.42
1:A:647:GLY:O	1:A:651:LYS:HG3	2.20	0.42
1:A:806:ARG:NH2	2:B:729:ILE:HD11	2.33	0.42
1:A:908:LEU:HD23	1:A:1029:ARG:HH21	1.84	0.42
2:B:103:ASN:CG	2:B:169:ARG:HH22	2.27	0.42
2:B:497:ARG:HA	2:B:538:ASN:ND2	2.34	0.42
3:C:39:ALA:O	3:C:165:LYS:HG3	2.19	0.42
11:R:2:U:H2'	11:R:3:C:H6	1.83	0.42
1:A:21:LEU:HD23	1:A:21:LEU:HA	1.84	0.42
1:A:407:ARG:HD3	1:A:411:ASP:HB2	2.00	0.42
1:A:941:LYS:HA	1:A:941:LYS:HD2	1.87	0.42
2:B:806:THR:HG23	2:B:1045:SER:HA	2.01	0.42
3:C:234:SER:HB3	3:C:240:VAL:CG1	2.49	0.42
2:B:213:ILE:HD12	2:B:213:ILE:HA	1.92	0.42
8:J:57:ILE:O	8:J:61:LEU:HG	2.20	0.42
1:A:279:LEU:HD13	1:A:279:LEU:HA	1.85	0.42
1:A:567:LYS:CB	1:A:568:PRO:CD	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ARG:HH11	7:I:97:MET:HG3	1.84	0.42
1:A:1410:PHE:CD1	2:B:1212:ILE:HD11	2.55	0.42
2:B:982:SER:HB3	2:B:986:GLN:HB2	2.02	0.42
2:B:1037:LEU:HD23	8:J:44:TYR:HB3	2.01	0.42
6:H:5:LEU:HG	6:H:133:ASN:HB2	2.01	0.42
7:I:103:CYS:SG	7:I:104:LEU:N	2.92	0.42
1:A:332:LYS:H	1:A:332:LYS:HG2	1.65	0.42
1:A:426:LEU:HD23	1:A:426:LEU:HA	1.92	0.42
1:A:446:ARG:HB2	1:A:487:MET:SD	2.59	0.42
1:A:534:LEU:O	1:A:574:GLY:HA3	2.19	0.42
1:A:939:ASP:O	1:A:943:LEU:HG	2.20	0.42
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.19	0.42
1:A:1163:ILE:HG21	1:A:1194:ARG:NH1	2.34	0.42
2:B:104:GLU:OE1	2:B:120:ARG:NH1	2.47	0.42
2:B:1133:MET:HE3	2:B:1133:MET:HB3	1.77	0.42
3:C:71:PRO:HG2	3:C:133:ILE:HG22	2.01	0.42
6:H:25:ARG:HH11	6:H:25:ARG:HB2	1.83	0.42
1:A:88:LYS:HE3	1:A:88:LYS:HB3	1.86	0.42
1:A:285:PRO:O	1:A:289:ILE:HG12	2.19	0.42
1:A:525:GLN:O	2:B:1015:HIS:CD2	2.69	0.42
1:A:760:GLN:OE1	1:A:765:VAL:HG23	2.20	0.42
1:A:959:ASN:O	1:A:963:ILE:HG12	2.19	0.42
1:A:1418:LEU:HD23	1:A:1418:LEU:HA	1.88	0.42
2:B:573:GLN:C	2:B:575:PRO:HD3	2.45	0.42
2:B:826:ALA:HB2	2:B:1087:PHE:CE1	2.55	0.42
2:B:987:LYS:H	2:B:987:LYS:HG2	1.59	0.42
2:B:1098:MET:HE3	2:B:1098:MET:HB3	1.90	0.42
4:E:167:ARG:HA	4:E:167:ARG:HD3	1.87	0.42
8:J:32:GLU:CD	8:J:32:GLU:H	2.28	0.42
1:A:70:CYS:SG	1:A:80:HIS:NE2	2.87	0.42
1:A:343:LYS:NZ	2:B:1197:PRO:HB3	2.34	0.42
1:A:362:ASP:HB3	1:A:508:PRO:HD3	2.02	0.42
1:A:567:LYS:HA	6:H:96:VAL:HG12	2.02	0.42
1:A:575:LYS:HB3	1:A:612:ILE:HB	2.02	0.42
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.60	0.42
2:B:821:GLN:HB2	2:B:851:PHE:CE2	2.55	0.42
2:B:832:GLY:O	2:B:835:GLN:HG3	2.20	0.42
1:A:38:PRO:CA	1:A:270:LEU:HD13	2.50	0.41
1:A:343:LYS:HZ1	2:B:1197:PRO:HB3	1.85	0.41
1:A:385:ILE:O	1:A:389:THR:OG1	2.31	0.41
1:A:855:THR:HG23	1:A:866:PHE:HA	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1072:ILE:HD11	1:A:1368:MET:HG2	2.02	0.41
2:B:777:ALA:HB1	2:B:1093:GLN:HB3	2.02	0.41
2:B:1106:ARG:HG2	2:B:1107:ALA:N	2.35	0.41
1:A:630:ILE:O	1:A:634:THR:OG1	2.27	0.41
1:A:679:ILE:HG22	1:A:732:LEU:HD23	2.02	0.41
1:A:741:ASN:O	1:A:745:GLN:HG3	2.19	0.41
1:A:773:LYS:HD2	1:A:774:ARG:N	2.36	0.41
1:A:1271:ILE:H	1:A:1271:ILE:HG13	1.63	0.41
2:B:257:LYS:HG3	2:B:259:TYR:HE1	1.85	0.41
2:B:276:ILE:HD11	2:B:334:ILE:HG23	2.02	0.41
2:B:318:VAL:O	2:B:322:PHE:N	2.53	0.41
2:B:792:MET:HE1	2:B:1096:ARG:NH2	2.31	0.41
3:C:242:GLN:HB3	3:C:246:ARG:NE	2.35	0.41
4:E:177:ARG:HE	4:E:215:MET:CG	2.33	0.41
9:K:58:PHE:HE2	9:K:74:ARG:HE	1.66	0.41
1:A:182:VAL:HG12	1:A:202:LEU:HB3	2.03	0.41
1:A:706:HIS:CD2	1:A:1135:ARG:HH21	2.37	0.41
2:B:60:GLN:NE2	2:B:94:LYS:HA	2.35	0.41
2:B:614:SER:OG	2:B:627:PHE:HB2	2.20	0.41
2:B:816:GLU:C	2:B:818:PRO:HD3	2.45	0.41
2:B:1002:THR:OG1	2:B:1003:ALA:N	2.54	0.41
3:C:105:GLY:O	3:C:149:LYS:HA	2.21	0.41
11:R:3:C:H2'	11:R:4:G:C8	2.56	0.41
12:T:22:DT:H2'	12:T:23:DC:H6	1.85	0.41
1:A:1004:ASN:OD1	4:E:167:ARG:HD2	2.21	0.41
2:B:890:TYR:CE2	2:B:910:VAL:HG11	2.55	0.41
2:B:1000:PRO:HB2	2:B:1072:MET:HE3	2.02	0.41
2:B:1051:THR:O	2:B:1055:ILE:HG12	2.21	0.41
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.56	0.41
2:B:222:ILE:HD13	2:B:403:LYS:HG2	2.01	0.41
2:B:955:THR:OG1	10:L:55:ILE:HA	2.20	0.41
3:C:44:LEU:HD12	3:C:160:LYS:C	2.45	0.41
5:F:119:ARG:HE	5:F:119:ARG:HB3	1.65	0.41
1:A:464:PRO:HB2	1:A:465:TYR:CD1	2.55	0.41
1:A:1278:ASN:HB2	1:A:1312:ASN:HB2	2.03	0.41
2:B:210:LYS:HD2	2:B:482:VAL:HG12	2.03	0.41
2:B:654:ARG:HA	2:B:654:ARG:HD3	1.71	0.41
2:B:1143:ALA:HB1	2:B:1146:PHE:HB3	2.03	0.41
3:C:43:THR:HG22	3:C:44:LEU:N	2.28	0.41
1:A:70:CYS:O	1:A:72:GLU:HG2	2.20	0.41
1:A:299:HIS:HA	1:A:302:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:HIS:CD2	1:A:453:MET:HG2	2.55	0.41
1:A:714:PHE:CD2	7:I:97:MET:HE1	2.55	0.41
2:B:193:LYS:HB3	2:B:787:VAL:HG11	2.02	0.41
2:B:348:ARG:O	2:B:351:TYR:HB3	2.20	0.41
2:B:579:ARG:H	2:B:579:ARG:HG2	1.68	0.41
3:C:265:MET:O	3:C:265:MET:HG3	2.20	0.41
12:T:12:DC:H2"	12:T:13:DA:C8	2.56	0.41
1:A:34:LYS:CD	1:A:34:LYS:H	2.33	0.41
1:A:203:SER:OG	1:A:204:THR:N	2.54	0.41
1:A:295:LEU:HA	1:A:298:PHE:HB3	2.03	0.41
1:A:445:ASN:ND2	1:A:455:MET:HE3	2.36	0.41
1:A:739:ASP:OD1	6:H:19:ARG:NH1	2.54	0.41
1:A:1395:GLY:O	1:A:1399:ARG:HD3	2.20	0.41
2:B:54:PHE:O	2:B:59:LEU:HB2	2.20	0.41
2:B:279:ASP:OD1	2:B:279:ASP:N	2.54	0.41
8:J:57:ILE:HA	8:J:60:PHE:CD2	2.56	0.41
9:K:32:VAL:HG12	9:K:74:ARG:HB2	2.03	0.41
1:A:34:LYS:H	1:A:34:LYS:HD2	1.86	0.41
1:A:58:LEU:HD22	1:A:244:PRO:HD2	2.02	0.41
1:A:746:MET:HG2	2:B:1015:HIS:CE1	2.56	0.41
1:A:1155:ASP:O	1:A:1241:ARG:NH1	2.54	0.41
1:A:1163:ILE:HB	1:A:1166:ASP:HB2	2.03	0.41
2:B:412:LEU:HB3	2:B:466:TRP:CH2	2.56	0.41
2:B:579:ARG:HA	2:B:589:VAL:HG12	2.03	0.41
2:B:905:VAL:HG11	2:B:911:ILE:HD11	2.01	0.41
2:B:978:ASP:OD1	2:B:1099:VAL:HG23	2.21	0.41
3:C:69:LEU:HD23	3:C:169:LYS:HB3	2.02	0.41
4:E:23:VAL:HG12	4:E:28:TYR:HB2	2.02	0.41
4:E:50:MET:CG	4:E:54:GLN:HE22	2.33	0.41
4:E:178:ILE:O	4:E:215:MET:N	2.42	0.41
6:H:114:VAL:O	6:H:124:ARG:HA	2.19	0.41
1:A:117:GLU:N	1:A:117:GLU:OE1	2.54	0.41
1:A:314:ALA:HB1	1:A:321:PRO:HD2	2.02	0.41
1:A:1063:MET:HE3	1:A:1063:MET:HB3	1.57	0.41
1:A:1147:THR:HA	1:A:1197:LEU:HD23	2.03	0.41
1:A:1311:VAL:HG21	1:A:1329:THR:HG21	2.03	0.41
2:B:564:GLU:HA	2:B:565:PRO:HD3	1.95	0.41
2:B:863:GLU:HA	2:B:914:LYS:HZ3	1.85	0.41
3:C:22:LEU:HD13	3:C:25:VAL:HG21	2.03	0.41
3:C:66:ARG:NH2	8:J:3:VAL:O	2.50	0.41
5:F:136:ARG:HD2	5:F:146:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:LEU:HD23	1:A:929:LEU:HA	1.90	0.40
2:B:46:GLN:CD	2:B:46:GLN:H	2.29	0.40
8:J:48:ARG:NH1	8:J:49:MET:HG2	2.35	0.40
1:A:666:ILE:HA	2:B:1026:LEU:HD13	2.02	0.40
2:B:487:THR:OG1	2:B:488:TYR:N	2.54	0.40
2:B:747:MET:N	2:B:747:MET:SD	2.95	0.40
2:B:834:ASN:O	2:B:1013:ASN:ND2	2.54	0.40
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.56	0.40
2:B:1106:ARG:HD2	2:B:1127:GLY:HA2	2.04	0.40
3:C:97:VAL:HG21	3:C:129:ILE:HG22	2.03	0.40
3:C:244:VAL:O	3:C:248:ILE:HG13	2.21	0.40
4:E:15:ALA:O	4:E:19:VAL:HG23	2.21	0.40
5:F:97:ARG:O	5:F:101:ILE:HG13	2.21	0.40
6:H:56:THR:O	6:H:144:ILE:HA	2.21	0.40
1:A:21:LEU:HD21	1:A:95:PHE:CZ	2.56	0.40
1:A:97:ALA:O	1:A:101:LYS:HG3	2.21	0.40
1:A:254:GLU:CG	2:B:918:ILE:HG12	2.50	0.40
1:A:563:PRO:HG2	1:A:566:ILE:HG12	2.03	0.40
1:A:852:TYR:HA	1:A:1060:PRO:HB3	2.03	0.40
1:A:1099:PRO:O	1:A:1103:GLU:HG2	2.21	0.40
1:A:1155:ASP:OD2	1:A:1161:THR:OG1	2.28	0.40
2:B:33:VAL:HG11	2:B:638:PHE:CE2	2.55	0.40
2:B:485:ARG:NH1	2:B:782:LEU:HD11	2.36	0.40
12:T:7:DA:H2'	12:T:8:DT:H6	1.85	0.40
1:A:903:ASN:OD1	1:A:904:THR:N	2.55	0.40
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.36	0.40
2:B:282:ILE:H	2:B:282:ILE:HG13	1.68	0.40
2:B:353:LYS:HA	2:B:353:LYS:HD2	1.84	0.40
2:B:792:MET:HE2	2:B:792:MET:HB3	1.89	0.40
2:B:999:MET:HG3	2:B:1000:PRO:HD2	2.03	0.40
5:F:123:LYS:HE3	5:F:123:LYS:HB2	1.84	0.40
7:I:77:LYS:HD2	7:I:106:CYS:SG	2.62	0.40
1:A:412:ARG:HH22	2:B:1108:ARG:CZ	2.34	0.40
1:A:424:ILE:O	1:A:424:ILE:HD12	2.22	0.40
1:A:498:ARG:O	1:A:502:SER:OG	2.35	0.40
1:A:800:VAL:HG11	1:A:808:LEU:HG	2.04	0.40
2:B:269:ILE:HD11	2:B:386:LEU:HD21	2.02	0.40
4:E:19:VAL:O	4:E:23:VAL:HG23	2.21	0.40
6:H:107:VAL:HB	6:H:111:LEU:CB	2.51	0.40
10:L:62:LYS:HD2	10:L:62:LYS:HA	1.92	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	1378/1733 (80%)	1272 (92%)	103 (8%)	3 (0%)	43	74
2	B	1088/1224 (89%)	1011 (93%)	76 (7%)	1 (0%)	48	79
3	C	264/318 (83%)	259 (98%)	4 (2%)	1 (0%)	30	62
4	E	212/215 (99%)	201 (95%)	11 (5%)	0	100	100
5	F	82/155 (53%)	78 (95%)	4 (5%)	0	100	100
6	H	129/146 (88%)	113 (88%)	16 (12%)	0	100	100
7	I	117/122 (96%)	110 (94%)	7 (6%)	0	100	100
8	J	63/70 (90%)	56 (89%)	7 (11%)	0	100	100
9	K	112/120 (93%)	108 (96%)	4 (4%)	0	100	100
10	L	44/70 (63%)	40 (91%)	4 (9%)	0	100	100
All	All	3489/4173 (84%)	3248 (93%)	236 (7%)	5 (0%)	48	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	90	ASP
1	A	50	ILE
1	A	1188	GLN
2	B	1040	ASN
1	A	1107	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	1206/1520 (79%)	1206 (100%)	0	100	100
2	B	960/1061 (90%)	959 (100%)	1 (0%)	88	87
3	C	234/274 (85%)	233 (100%)	1 (0%)	84	81
4	E	196/197 (100%)	196 (100%)	0	100	100
5	F	74/137 (54%)	74 (100%)	0	100	100
6	H	117/128 (91%)	117 (100%)	0	100	100
7	I	113/116 (97%)	113 (100%)	0	100	100
8	J	60/65 (92%)	60 (100%)	0	100	100
9	K	99/102 (97%)	99 (100%)	0	100	100
10	L	40/57 (70%)	40 (100%)	0	100	100
All	All	3099/3657 (85%)	3097 (100%)	2 (0%)	88	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	822	ASN
3	C	255	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	171	GLN
1	A	306	ASN
1	A	427	GLN
1	A	471	ASN
1	A	517	ASN
1	A	717	ASN
1	A	854	ASN
1	A	926	GLN
1	A	966	ASN
1	A	1130	GLN
1	A	1278	ASN
1	A	1378	GLN
2	B	60	GLN
2	B	178	ASN
2	B	383	ASN
2	B	395	GLN

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Mol	Chain	Res	Type
2	B	538	ASN
2	B	686	ASN
2	B	706	GLN
2	B	733	HIS
3	C	214	ASN
4	E	114	ASN
4	E	146	HIS
7	I	22	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	8/10 (80%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	5	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
12	WC7	T	18	12	18,23,24	2.13	5 (27%)	23,33,36	1.92	5 (21%)

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
12	WC7	T	18	12	-	1/7/21/22	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	18	WC7	C3-C4	6.81	1.46	1.38
12	T	18	WC7	C4-S3	-3.22	1.67	1.72
12	T	18	WC7	C5-S1	-2.75	1.59	1.67
12	T	18	WC7	C2-C3	-2.32	1.38	1.43
12	T	18	WC7	C1-C2	2.09	1.39	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	18	WC7	C5-C4-S3	4.50	130.17	123.13
12	T	18	WC7	C8-S3-C4	4.40	95.88	91.38
12	T	18	WC7	C3-C4-S3	-4.08	108.78	111.42
12	T	18	WC7	C3-C4-C5	-3.05	121.05	124.02
12	T	18	WC7	C2-C1-N1	2.37	125.69	121.84

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	T	18	WC7	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	T	18	WC7	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 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
16	WCG	B	2101	-	34,35,35	4.13	18 (52%)	49,54,54	1.87	7 (14%)

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
16	WCG	B	2101	-	-	13/24/40/40	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	2101	WCG	P22-O21	11.15	1.71	1.59
16	B	2101	WCG	O14-C13	-9.10	1.31	1.44
16	B	2101	WCG	C30-C15	-8.83	1.30	1.53
16	B	2101	WCG	O14-C15	8.12	1.63	1.45
16	B	2101	WCG	P18-O21	7.52	1.67	1.59
16	B	2101	WCG	C08-C07	5.08	1.49	1.38
16	B	2101	WCG	O02-C03	4.40	1.44	1.37
16	B	2101	WCG	C04-C03	4.34	1.44	1.36
16	B	2101	WCG	P22-O25	4.01	1.63	1.59
16	B	2101	WCG	C06-C05	3.89	1.50	1.42
16	B	2101	WCG	C12-C13	3.32	1.57	1.51
16	B	2101	WCG	C09-C10	3.30	1.49	1.42
16	B	2101	WCG	O33-C32	-2.86	1.35	1.43
16	B	2101	WCG	C04-C05	-2.82	1.35	1.42
16	B	2101	WCG	C03-C12	-2.65	1.34	1.39
16	B	2101	WCG	O31-C30	2.51	1.49	1.43
16	B	2101	WCG	C10-C05	-2.25	1.37	1.42
16	B	2101	WCG	C11-C12	2.05	1.40	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	2101	WCG	O02-C03-C12	6.44	122.24	115.84
16	B	2101	WCG	O02-C03-C04	-6.01	117.55	125.16
16	B	2101	WCG	C15-O14-C13	-4.95	101.58	109.13
16	B	2101	WCG	C01-O02-C03	-4.38	111.09	117.51
16	B	2101	WCG	O14-C13-C12	3.32	115.35	110.19
16	B	2101	WCG	C03-C12-C13	2.09	123.26	120.29
16	B	2101	WCG	O27-P26-O25	2.08	111.62	104.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	B	2101	WCG	C03-C12-C13-C32
16	B	2101	WCG	C03-C12-C13-O14
16	B	2101	WCG	C11-C12-C13-C32
16	B	2101	WCG	C11-C12-C13-O14
16	B	2101	WCG	C16-O17-P18-O19
16	B	2101	WCG	C16-O17-P18-O20
16	B	2101	WCG	C04-C03-O02-C01
16	B	2101	WCG	C12-C03-O02-C01
16	B	2101	WCG	C30-C15-C16-O17
16	B	2101	WCG	O14-C15-C16-O17
16	B	2101	WCG	C15-C16-O17-P18
16	B	2101	WCG	C16-O17-P18-O21
16	B	2101	WCG	P22-O21-P18-O19

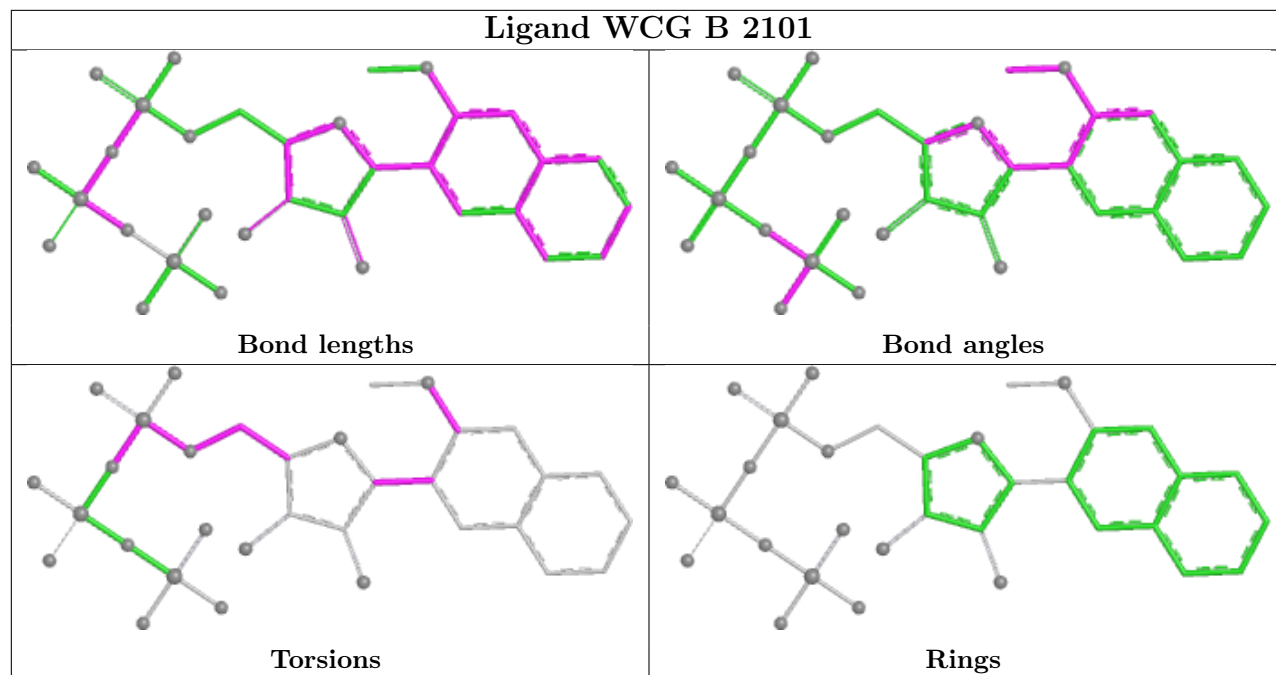
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	2101	WCG	2	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	1390/1733 (80%)	0.59	64 (4%) 37 21	42, 80, 142, 183	0
2	B	1106/1224 (90%)	0.76	74 (6%) 24 16	44, 77, 126, 177	0
3	C	266/318 (83%)	0.48	7 (2%) 57 34	49, 77, 107, 155	0
4	E	214/215 (99%)	0.56	14 (6%) 25 17	58, 97, 152, 170	0
5	F	84/155 (54%)	0.36	1 (1%) 76 53	50, 81, 104, 116	0
6	H	133/146 (91%)	0.63	6 (4%) 38 22	75, 106, 151, 172	0
7	I	119/122 (97%)	0.57	6 (5%) 34 20	62, 87, 114, 149	0
8	J	65/70 (92%)	0.69	4 (6%) 26 17	56, 73, 103, 118	0
9	K	114/120 (95%)	0.39	2 (1%) 67 43	46, 73, 100, 112	0
10	L	46/70 (65%)	1.00	4 (8%) 16 11	58, 114, 151, 177	0
11	R	10/10 (100%)	1.07	1 (10%) 12 9	79, 91, 147, 164	0
12	T	23/29 (79%)	0.76	0 100 100	92, 124, 203, 213	0
13	N	11/16 (68%)	0.86	0 100 100	152, 174, 203, 204	0
All	All	3581/4228 (84%)	0.63	183 (5%) 33 20	42, 81, 140, 213	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	LYS	6.3
10	L	27	LEU	6.1
4	E	83	CYS	5.5
2	B	709	ASP	5.0
2	B	477	ALA	4.9
4	E	121	MET	4.6
1	A	252	PHE	4.5
2	B	816	GLU	4.3
11	R	1	A	4.0

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Mol	Chain	Res	Type	RSRZ
4	E	125	PRO	3.9
1	A	250	ILE	3.9
2	B	870	ILE	3.7
6	H	63	LEU	3.7
4	E	118	PRO	3.7
2	B	472	ALA	3.7
1	A	248	PRO	3.6
1	A	447	GLN	3.4
1	A	127	ALA	3.4
8	J	10	CYS	3.3
10	L	43	THR	3.3
2	B	478	GLY	3.3
2	B	1209	ALA	3.3
1	A	264	PHE	3.2
8	J	9	SER	3.2
1	A	91	PHE	3.1
2	B	822	ASN	3.1
2	B	335	GLY	3.1
1	A	255	SER	3.1
2	B	708	GLU	3.1
7	I	13	MET	3.0
2	B	751	VAL	3.0
4	E	126	SER	3.0
2	B	909	ASP	3.0
1	A	1380	GLY	3.0
1	A	315	LEU	2.9
9	K	3	ALA	2.9
2	B	906	SER	2.9
1	A	307	ASP	2.9
1	A	201	VAL	2.9
2	B	734	HIS	2.9
1	A	776	ALA	2.9
1	A	90	VAL	2.9
1	A	141	LEU	2.8
2	B	530	GLY	2.8
2	B	823	ALA	2.7
2	B	1157	ALA	2.7
1	A	61	ILE	2.7
2	B	248	SER	2.7
2	B	250	PHE	2.7
3	C	30	ALA	2.7
2	B	1202	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	935	ARG	2.7
2	B	446	LEU	2.7
2	B	531	GLN	2.7
1	A	642	CYS	2.7
4	E	93	MET	2.7
2	B	524	PRO	2.7
8	J	5	VAL	2.7
2	B	636	PRO	2.6
2	B	466	TRP	2.6
2	B	1099	VAL	2.6
1	A	964	ILE	2.6
6	H	42	ILE	2.6
9	K	71	PHE	2.6
2	B	211	VAL	2.6
7	I	4	PHE	2.6
1	A	82	GLY	2.6
1	A	355	GLY	2.6
2	B	263	GLY	2.6
2	B	493	SER	2.6
2	B	473	MET	2.6
10	L	25	ALA	2.6
1	A	55	ASP	2.6
1	A	58	LEU	2.6
1	A	251	SER	2.5
2	B	46	GLN	2.5
1	A	388	LEU	2.5
2	B	630	ALA	2.5
2	B	715	ALA	2.5
7	I	2	THR	2.5
2	B	733	HIS	2.5
1	A	199	LEU	2.5
2	B	731	VAL	2.5
2	B	386	LEU	2.5
4	E	90	VAL	2.5
1	A	105	CYS	2.5
4	E	9	ILE	2.5
1	A	676	MET	2.5
1	A	242	PRO	2.5
1	A	314	ALA	2.4
1	A	821	ARG	2.4
1	A	885	THR	2.4
2	B	730	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	251	LEU	2.4
2	B	764	SER	2.4
1	A	399	HIS	2.4
3	C	211	ASP	2.4
1	A	174	ILE	2.3
1	A	289	ILE	2.3
2	B	502	ILE	2.3
3	C	41	ILE	2.3
2	B	1221	SER	2.3
7	I	76	PRO	2.3
3	C	63	ILE	2.3
7	I	119	THR	2.3
1	A	259	GLU	2.3
1	A	249	SER	2.3
1	A	466	SER	2.3
2	B	746	SER	2.3
1	A	958	VAL	2.3
10	L	55	ILE	2.3
2	B	330	ALA	2.3
1	A	234	MET	2.3
4	E	48	ASP	2.3
2	B	748	ILE	2.3
3	C	6	PRO	2.3
2	B	226	PHE	2.3
4	E	110	PHE	2.3
1	A	181	LEU	2.2
1	A	306	ASN	2.2
1	A	104	GLU	2.2
1	A	325	ILE	2.2
2	B	495	LEU	2.2
4	E	95	THR	2.2
2	B	251	ILE	2.2
2	B	334	ILE	2.2
2	B	228	LYS	2.2
1	A	1220	PHE	2.2
1	A	204	THR	2.2
1	A	147	VAL	2.2
2	B	474	SER	2.2
2	B	782	LEU	2.2
1	A	73	GLY	2.2
2	B	1199	ALA	2.2
1	A	40	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	897	TYR	2.2
1	A	128	ILE	2.2
2	B	30	SER	2.2
2	B	514	LEU	2.2
2	B	747	MET	2.2
1	A	844	ALA	2.2
1	A	328	ARG	2.2
2	B	620	ARG	2.2
2	B	643	ASP	2.2
1	A	473	SER	2.1
2	B	300	HIS	2.1
6	H	107	VAL	2.1
7	I	60	GLN	2.1
1	A	1434	ALA	2.1
2	B	509	ALA	2.1
2	B	525	ALA	2.1
2	B	631	GLY	2.1
6	H	61	SER	2.1
2	B	1211	ASN	2.1
2	B	244	LEU	2.1
1	A	799	PHE	2.1
3	C	74	SER	2.1
4	E	124	VAL	2.1
2	B	1217	TYR	2.1
1	A	494	SER	2.1
4	E	111	VAL	2.1
1	A	54	ASN	2.1
5	F	72	LYS	2.1
2	B	1076	HIS	2.1
2	B	986	GLN	2.1
1	A	636	GLU	2.1
2	B	892	LYS	2.0
1	A	324	SER	2.0
1	A	1268	LEU	2.0
6	H	46	LEU	2.0
6	H	24	CYS	2.0
8	J	8	PHE	2.0
2	B	899	ILE	2.0
2	B	1194	ILE	2.0
4	E	127	ILE	2.0
2	B	313	MET	2.0
2	B	752	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	785	TYR	2.0
1	A	884	ASP	2.0
1	A	3	GLY	2.0
1	A	81	PHE	2.0
2	B	1224	PHE	2.0
2	B	112	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
12	WC7	T	18	21/22	0.78	0.21	97,104,113,117	0

6.3 Carbohydrates [i](#)

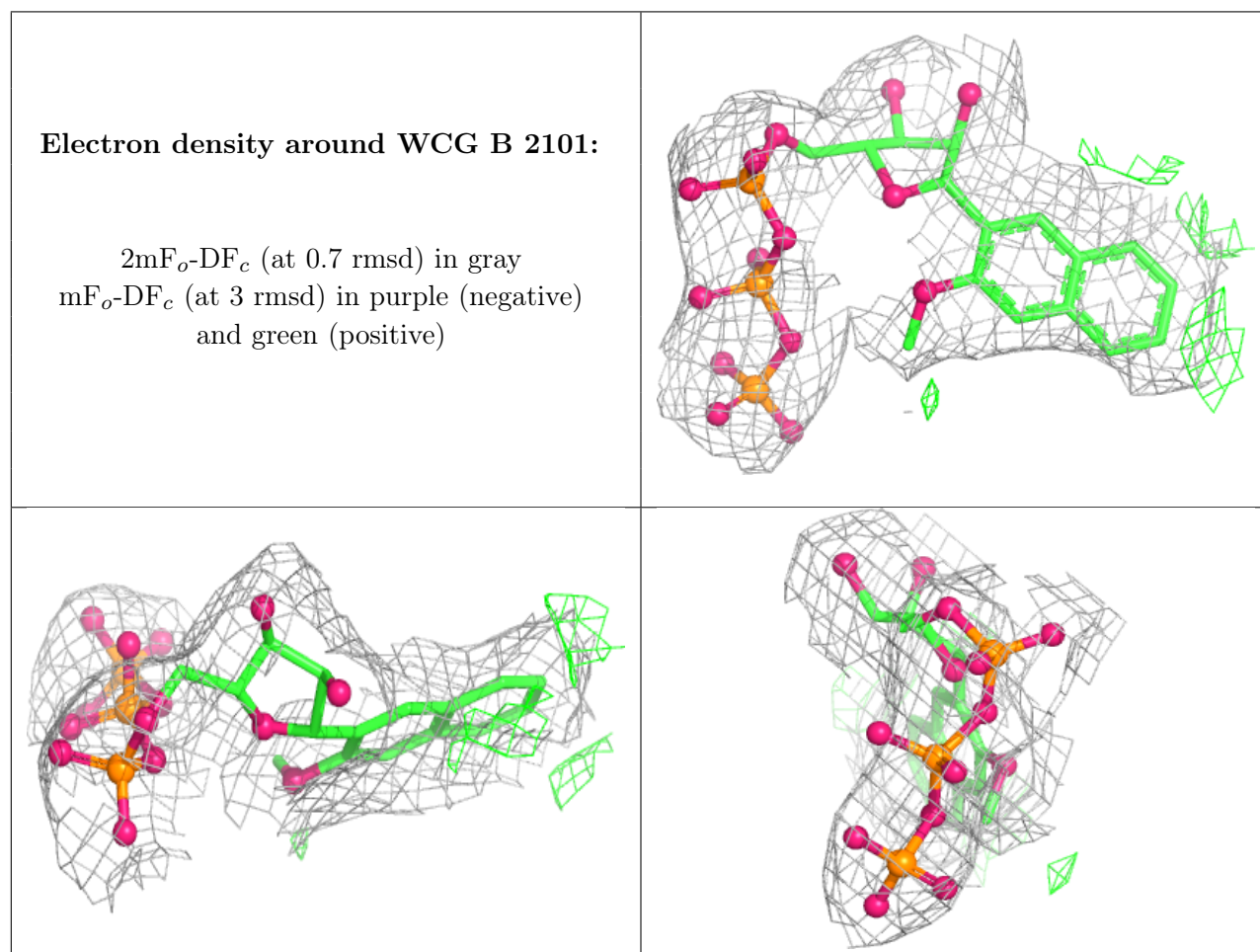
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
16	WCG	B	2101	33/33	0.44	0.15	79,116,204,209	0
14	ZN	A	1801	1/1	0.92	0.11	193,193,193,193	0
14	ZN	C	401	1/1	0.97	0.06	76,76,76,76	0
14	ZN	J	101	1/1	0.97	0.07	70,70,70,70	0
14	ZN	L	101	1/1	0.97	0.04	120,120,120,120	0
15	MG	A	1803	1/1	0.97	0.06	53,53,53,53	0
14	ZN	B	2102	1/1	0.97	0.05	121,121,121,121	0
14	ZN	I	201	1/1	0.98	0.09	71,71,71,71	0
14	ZN	I	202	1/1	0.98	0.05	76,76,76,76	0
14	ZN	A	1802	1/1	0.98	0.04	116,116,116,116	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.