



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2025 – 10:57 AM JST

PDB ID : 9V4M / pdb_00009v4m
Title : Crystal structure of the T.thermophilus transcription initiation complex bound to Ap4G
Authors : Duan, W.; Kaushik, A.; Serganov, A.
Deposited on : 2025-05-24
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

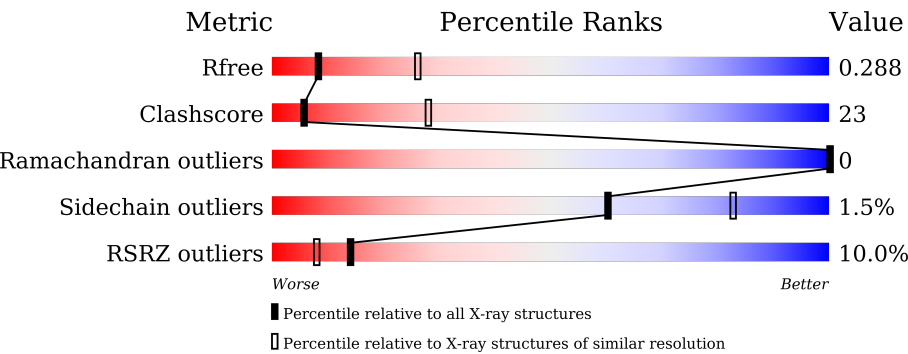
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	<div><div>6%</div><div>35%</div><div>35%</div><div>28%</div></div>
1	B	315	<div><div>44%</div><div>27%</div><div>28%</div></div>
2	C	1119	<div><div>8%</div><div>55%</div><div>44%</div><div></div></div>
3	D	1524	<div><div>10%</div><div>55%</div><div>34%</div><div>11%</div></div>
4	E	99	<div><div>7%</div><div>55%</div><div>40%</div><div>5%</div></div>
5	F	444	<div><div>16%</div><div>39%</div><div>37%</div><div>24%</div></div>

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Mol	Chain	Length	Quality of chain
6	G	22	 <p>9% 32% 36% 32%</p>
7	H	27	 <p>26% 30% 52% 19%</p>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 27396 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	227	Total	C	N	O	S	0	1	0
			1788	1144	311	331	2			
1	B	226	Total	C	N	O	S	0	0	0
			1776	1135	307	332	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1113	Total	C	N	O	S	0	1	0
			8778	5555	1560	1639	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1357	Total	C	N	O	S	0	2	0
			10660	6738	1898	1990	34			

- 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
			753	481	129	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	338	Total	C	N	O	S	0	1	0
			2743	1729	498	512	4			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-20	MET	-	initiating methionine	UNP Q5SKW1
F	-19	GLY	-	expression tag	UNP Q5SKW1
F	-18	SER	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	HIS	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	SER	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	GLY	-	expression tag	UNP Q5SKW1
F	-7	LEU	-	expression tag	UNP Q5SKW1
F	-6	VAL	-	expression tag	UNP Q5SKW1
F	-5	PRO	-	expression tag	UNP Q5SKW1
F	-4	ARG	-	expression tag	UNP Q5SKW1
F	-3	GLY	-	expression tag	UNP Q5SKW1
F	-2	SER	-	expression tag	UNP Q5SKW1
F	-1	HIS	-	expression tag	UNP Q5SKW1
F	0	MET	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	15	Total	C	N	O	P	0	0	0
			301	141	57	88	15			

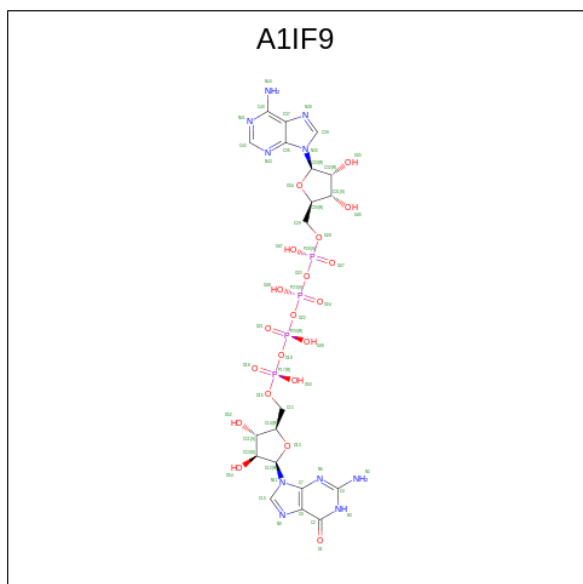
- Molecule 7 is a DNA chain called Non-template DNA Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	22	Total	C	N	O	P	0	0	0
			454	217	86	130	21			

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

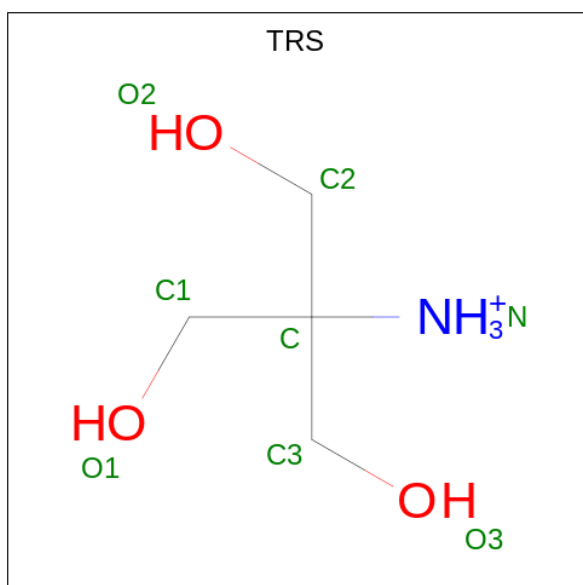
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		
8	D	2	Total	Mg	0	0
			2	2		

- Molecule 9 is [[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [[[(2 {R},3 {S},4 {R},5 {R})-5-(2-azanylidene-1 {H}-purin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl] hydrogen phosphate (CCD ID: A1IF9) (formula: C₂₀H₂₈N₁₀O₂₀P₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	C	1	54	20	10	20	4	0	0

- Molecule 10 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total C N O 8 4 1 3	0	0
10	D	1	Total C N O 8 4 1 3	0	0

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

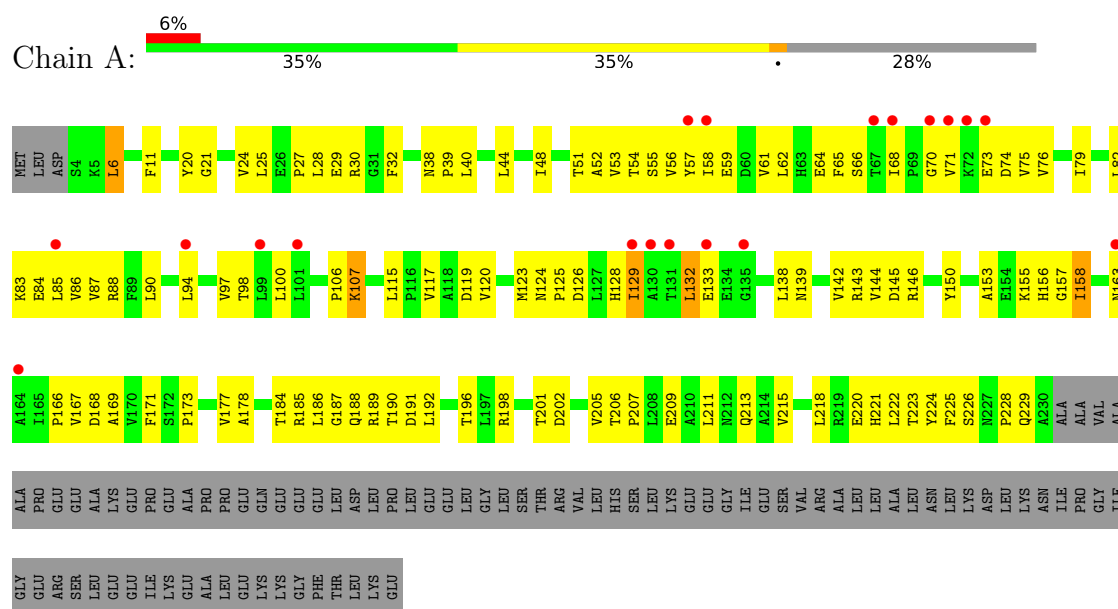
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	3	Total O 3 3	0	0
12	B	4	Total O 4 4	0	0
12	C	19	Total O 19 19	0	0
12	D	27	Total O 27 27	0	0
12	E	3	Total O 3 3	0	0
12	F	6	Total O 6 6	0	0
12	G	4	Total O 4 4	0	0
12	H	1	Total O 1 1	0	0

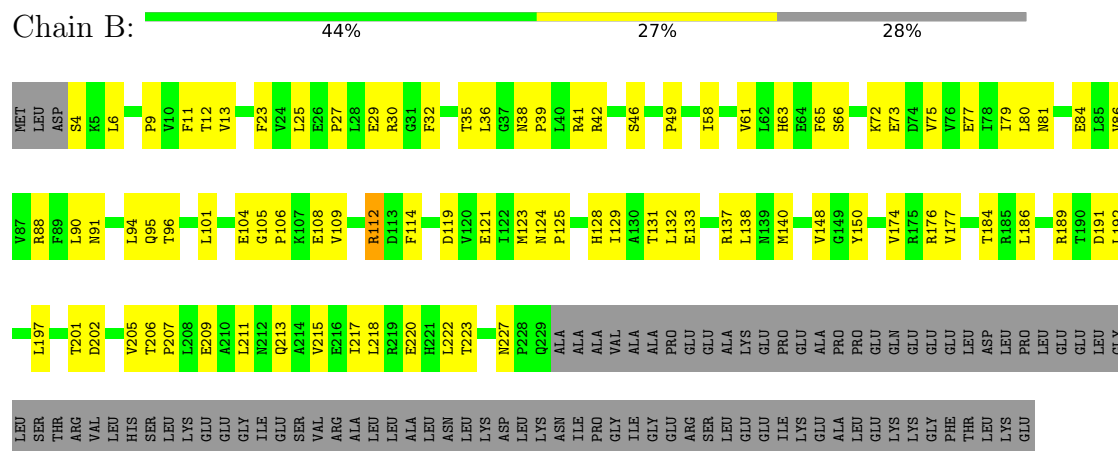
3 Residue-property plots

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 subunit alpha

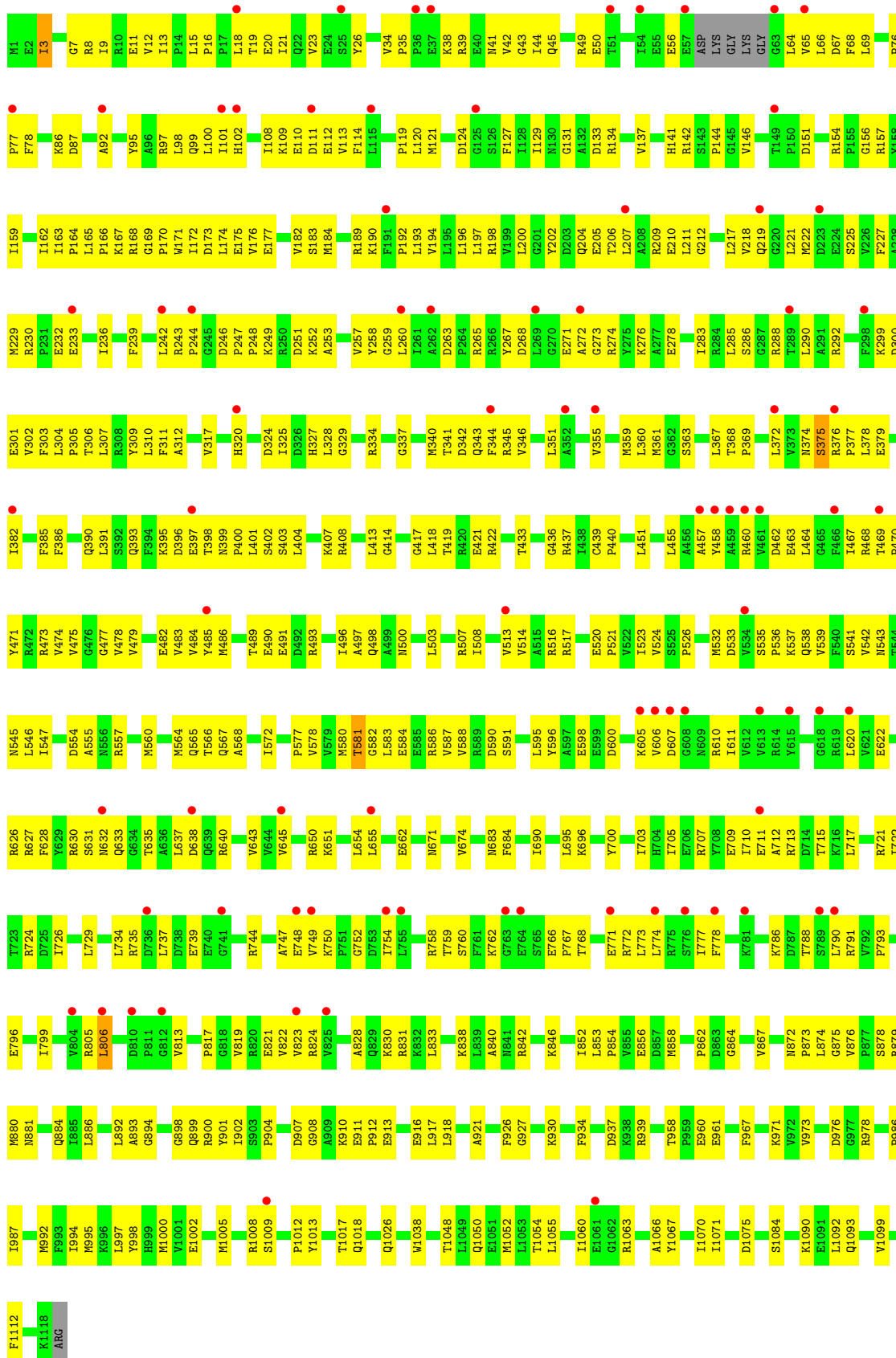


• Molecule 1: DNA-directed RNA polymerase subunit alpha



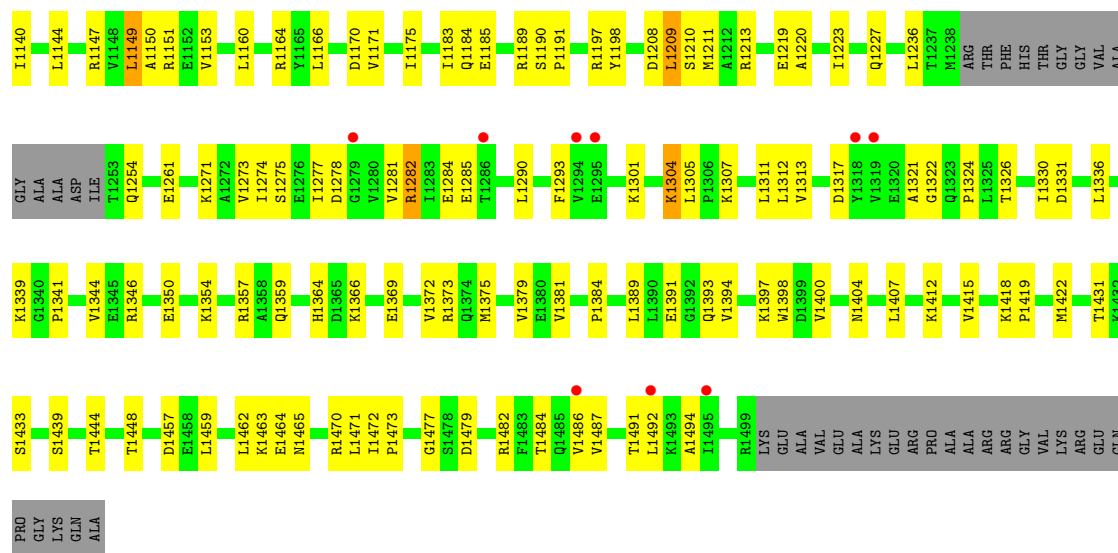
• Molecule 2: DNA-directed RNA polymerase subunit beta



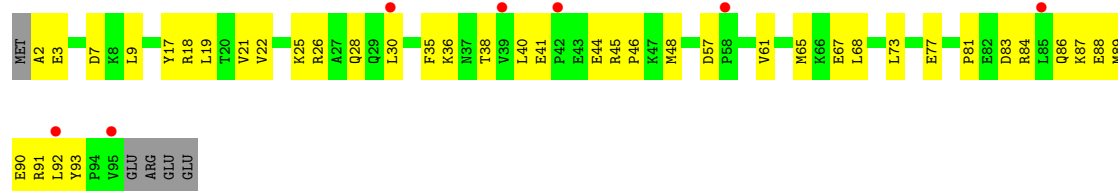


- Molecule 3: DNA-directed RNA polymerase subunit beta'

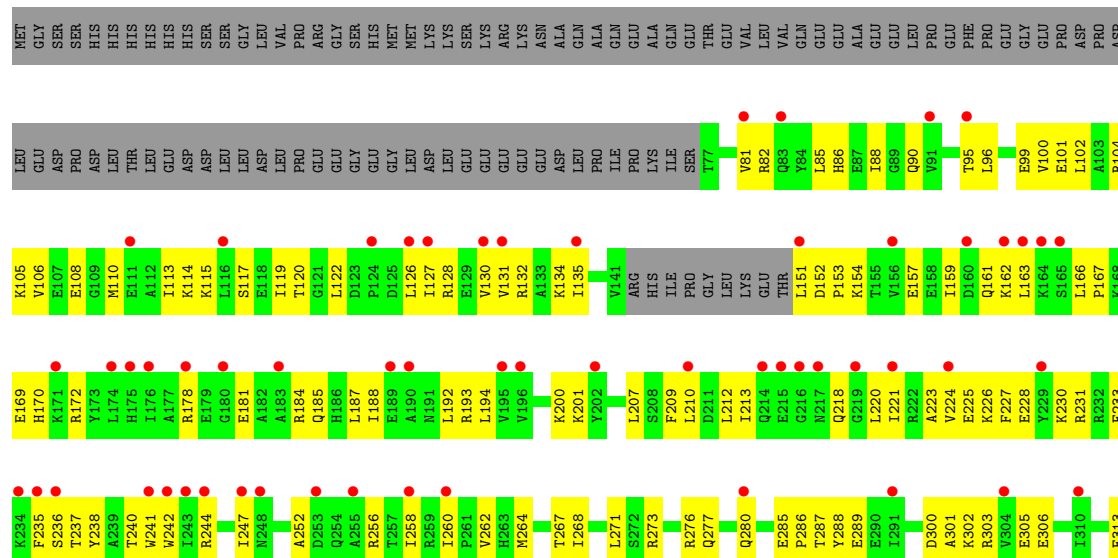


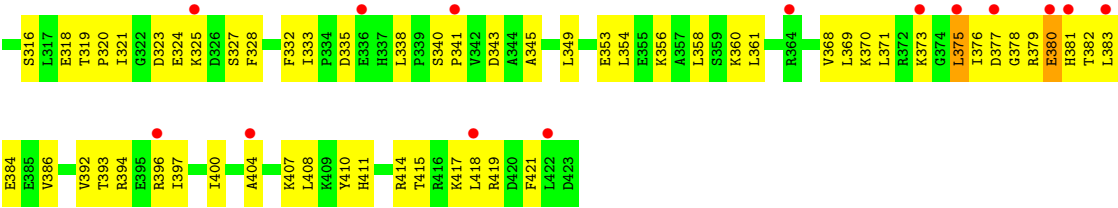


• Molecule 4: DNA-directed RNA polymerase subunit omega

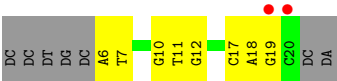


• Molecule 5: RNA polymerase sigma factor SigA

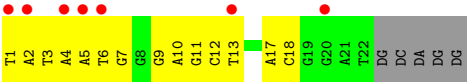




● Molecule 6: Template DNA strand



● Molecule 7: Non-template DNA Strand



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.06Å 103.21Å 296.51Å 90.00° 98.89° 90.00°	Depositor
Resolution (Å)	29.96 – 3.00 29.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	78.4 (29.96-3.00) 78.4 (29.96-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.00Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.279 , 0.288 0.279 , 0.288	Depositor DCC
R_{free} test set	2024 reflections (1.82%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.1	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	0.85	EDS
Total number of atoms	27396	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, ZN, A1IF9, 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	0.47	0/1823	0.72	0/2479
1	B	0.39	0/1808	0.68	0/2459
2	C	0.28	0/8948	0.50	0/12103
3	D	0.28	0/10848	0.48	0/14660
4	E	0.29	0/767	0.55	0/1035
5	F	0.37	0/2788	0.63	0/3749
6	G	0.45	0/337	0.69	0/518
7	H	0.46	0/510	0.72	0/787
All	All	0.32	0/27829	0.55	0/37790

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1788	0	1846	119	0
1	B	1776	0	1823	85	0
2	C	8778	0	8868	468	0
3	D	10660	0	10807	460	0
4	E	753	0	760	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	2743	0	2812	157	0
6	G	301	0	164	8	0
7	H	454	0	250	23	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	D	2	0	0	0	0
9	C	54	0	0	2	0
10	C	8	0	12	0	0
10	D	8	0	12	1	0
11	D	2	0	0	0	0
12	A	3	0	0	0	0
12	B	4	0	0	0	0
12	C	19	0	0	0	0
12	D	27	0	0	0	0
12	E	3	0	0	1	0
12	F	6	0	0	0	0
12	G	4	0	0	0	0
12	H	1	0	0	0	0
All	All	27396	0	27354	1246	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 23.

All (1246) 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:53:VAL:HG11	1:A:82:LEU:CD2	1.77	1.15
1:A:53:VAL:HG11	1:A:82:LEU:HD21	1.29	1.14
2:C:109:LYS:HG2	2:C:368:THR:HG22	1.46	0.97
3:D:45:PHE:HZ	3:D:541:ASN:HD21	1.13	0.94
2:C:458:TYR:HE2	2:C:535:SER:HG	1.15	0.93
2:C:711:GLU:HG2	2:C:822:VAL:HG23	1.51	0.93
2:C:176:VAL:HG22	2:C:182:VAL:HG12	1.51	0.92
2:C:503:LEU:HD11	2:C:532:MET:HE1	1.54	0.90
3:D:112:ILE:HG12	3:D:512:MET:HE3	1.54	0.90
2:C:210:GLU:HG3	2:C:304:LEU:HD11	1.54	0.89
1:B:90:LEU:HD21	1:B:121:GLU:HB2	1.54	0.89
1:A:53:VAL:CG1	1:A:82:LEU:HD21	2.03	0.88
1:A:53:VAL:HG21	1:A:82:LEU:HD23	1.53	0.88
3:D:1486:VAL:HG11	4:E:22:VAL:HG13	1.55	0.87
5:F:386:VAL:HG12	5:F:397:ILE:HD12	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:VAL:HG13	1:B:222:LEU:HD12	1.55	0.86
3:D:135:LEU:HD22	3:D:455:ARG:HH21	1.38	0.85
5:F:193:ARG:HB2	7:H:6:DT:H1'	1.59	0.84
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.60	0.84
2:C:249:LYS:HB2	2:C:252:LYS:HG2	1.60	0.83
2:C:1005:MET:HE2	3:D:648:MET:HG3	1.59	0.83
3:D:45:PHE:HZ	3:D:541:ASN:ND2	1.77	0.83
4:E:9:LEU:HB3	4:E:19:LEU:HD11	1.61	0.82
2:C:674:VAL:HG11	2:C:992:MET:HE3	1.62	0.82
2:C:66:LEU:HD11	2:C:98:LEU:HB3	1.60	0.81
1:B:63:HIS:CD2	1:B:66:SER:HB2	2.15	0.81
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.63	0.80
2:C:129:ILE:HG12	2:C:386:PHE:HB3	1.62	0.80
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.60	0.80
2:C:200:LEU:HD13	2:C:300:ASP:HB2	1.61	0.80
3:D:656:PHE:HB3	3:D:694:VAL:HG21	1.64	0.80
2:C:610:ARG:HD3	2:C:622:GLU:HG3	1.63	0.80
2:C:164:PRO:HD2	2:C:171:TRP:CD1	2.16	0.80
1:A:221:HIS:HB3	1:B:36:LEU:HD21	1.65	0.79
1:A:53:VAL:CG1	1:A:82:LEU:CD2	2.59	0.78
2:C:419:THR:HG22	2:C:422:ARG:HG2	1.64	0.78
2:C:734:LEU:HA	2:C:737:LEU:HD23	1.64	0.78
3:D:407:VAL:HG12	3:D:422:ALA:HB2	1.65	0.78
2:C:156:GLY:C	2:C:157:ARG:HE	1.92	0.78
1:B:112:ARG:HG3	1:B:125:PRO:HB3	1.64	0.78
1:A:53:VAL:HG11	1:A:82:LEU:HD23	1.65	0.78
1:A:225:PHE:HE1	1:B:36:LEU:HD23	1.48	0.78
1:A:100:LEU:HD13	1:A:115:LEU:HG	1.66	0.78
3:D:190:GLU:HA	3:D:196:VAL:HA	1.63	0.78
3:D:586[B]:ARG:HH12	6:G:10:DG:H3'	1.45	0.78
3:D:31:THR:HG22	3:D:45:PHE:HE2	1.47	0.77
1:A:82:LEU:HD11	1:A:142:VAL:HG21	1.65	0.77
2:C:628:PHE:H	2:C:638:ASP:HB3	1.50	0.77
2:C:34:VAL:HG13	2:C:39:ARG:HG2	1.68	0.76
3:D:527:MET:HG3	3:D:537:THR:HB	1.67	0.76
2:C:774:LEU:HD13	5:F:418:LEU:HG	1.67	0.76
1:B:86:VAL:H	1:B:124:ASN:HD21	1.33	0.76
3:D:586[B]:ARG:HH12	6:G:10:DG:C3'	1.99	0.76
5:F:200:LYS:HG3	5:F:201:LYS:HD3	1.65	0.76
3:D:690:ALA:HA	3:D:693:GLU:HG3	1.68	0.75
3:D:401:TYR:CE2	3:D:429:SER:HA	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:191:LEU:HD13	3:D:393:ILE:HB	1.68	0.75
2:C:127:PHE:O	2:C:133:ASP:HA	1.87	0.75
2:C:23:VAL:HA	2:C:121:MET:HE1	1.69	0.75
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.69	0.75
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.67	0.74
3:D:711:LEU:HD12	3:D:778:LEU:HD23	1.67	0.74
3:D:86:ARG:HG3	3:D:522:PRO:HG2	1.68	0.74
1:A:54:THR:HB	1:A:158:ILE:HD13	1.70	0.74
1:A:156:HIS:NE2	1:A:167:VAL:O	2.21	0.74
3:D:573:MET:HE2	5:F:210:LEU:HB3	1.70	0.73
3:D:67:ARG:HH21	5:F:379:ARG:HD3	1.52	0.73
1:A:68:ILE:HG23	1:A:71:VAL:HB	1.71	0.73
2:C:497:ALA:HB3	2:C:532:MET:HG3	1.68	0.73
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.68	0.73
3:D:489:ARG:NH1	3:D:1391:GLU:OE1	2.22	0.73
1:A:71:VAL:HG12	1:A:73:GLU:H	1.52	0.73
1:B:104:GLU:HG2	1:B:137:ARG:HG3	1.70	0.73
2:C:271:GLU:CD	2:C:271:GLU:H	1.96	0.73
3:D:573:MET:CE	5:F:210:LEU:HB3	2.20	0.72
3:D:567:ILE:O	3:D:571:LYS:HG3	1.88	0.72
3:D:1223:ILE:O	3:D:1227:GLN:HG3	1.90	0.72
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.70	0.72
1:B:104:GLU:HA	1:B:137:ARG:HA	1.72	0.72
1:A:225:PHE:CE1	1:B:36:LEU:HD23	2.25	0.71
2:C:3:ILE:HG23	2:C:902:ILE:HD13	1.72	0.71
2:C:97:ARG:NH2	2:C:110:GLU:OE1	2.22	0.71
2:C:1054:THR:OG1	2:C:1055:LEU:N	2.21	0.71
1:A:220:GLU:O	1:A:223:THR:HG22	1.91	0.71
3:D:192:ALA:HB3	3:D:195:VAL:HG22	1.70	0.71
1:B:73:GLU:N	1:B:73:GLU:OE1	2.22	0.71
2:C:312:ALA:HB1	2:C:317:VAL:HG21	1.73	0.71
5:F:360:LYS:HB3	5:F:411:HIS:CD2	2.26	0.71
3:D:1281:VAL:HG12	3:D:1317:ASP:H	1.52	0.70
3:D:169:TYR:OH	3:D:199:LEU:HD22	1.91	0.70
3:D:593:ASN:H	3:D:600:LEU:HD21	1.55	0.70
2:C:748:GLU:HB3	2:C:799:ILE:HD13	1.72	0.70
2:C:752:GLY:HA3	3:D:679:ARG:HA	1.72	0.70
3:D:474:GLU:HG3	3:D:496:LEU:HD21	1.74	0.70
2:C:225:SER:O	2:C:229:MET:HG2	1.90	0.70
3:D:657:LEU:HG	3:D:661:MET:HE2	1.72	0.70
2:C:1075:ASP:OD2	4:E:28:GLN:HG2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:565:GLN:HA	2:C:995:MET:HE1	1.74	0.69
2:C:580:MET:HE2	2:C:902:ILE:HD11	1.74	0.69
3:D:683:ILE:HG21	3:D:688:TRP:CZ2	2.28	0.69
2:C:142:ARG:HD3	2:C:325:ILE:HB	1.75	0.69
3:D:208:PRO:HA	3:D:390:PRO:HA	1.73	0.69
3:D:1282:ARG:HE	3:D:1293:PHE:HB2	1.57	0.69
1:A:53:VAL:HG21	1:A:82:LEU:CD2	2.22	0.69
2:C:64:LEU:HD22	2:C:102:HIS:CD2	2.28	0.69
3:D:1372:VAL:HA	3:D:1375:MET:HG3	1.73	0.69
2:C:206:THR:HA	2:C:209:ARG:HD2	1.75	0.69
3:D:140:ALA:HB1	3:D:161:LEU:HD23	1.73	0.68
5:F:268:ILE:HA	5:F:271:LEU:HD12	1.75	0.68
2:C:462:ASP:OD1	2:C:464:LEU:N	2.26	0.68
2:C:458:TYR:HE2	2:C:535:SER:OG	1.75	0.68
3:D:1046:GLN:HG2	3:D:1052:THR:HG22	1.75	0.68
1:A:82:LEU:HD11	1:A:142:VAL:CG2	2.23	0.68
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.75	0.67
1:A:229:GLN:HB3	1:B:12:THR:HA	1.77	0.67
2:C:709:GLU:HG3	2:C:824:ARG:HG2	1.76	0.67
1:A:79:ILE:HD12	1:A:82:LEU:HB3	1.77	0.67
1:A:211:LEU:O	1:A:215:VAL:HG23	1.93	0.67
2:C:274:ARG:HG2	2:C:278:GLU:OE2	1.94	0.67
2:C:838:LYS:HE3	3:D:741:ASP:O	1.94	0.67
5:F:323:ASP:OD1	5:F:324:GLU:N	2.28	0.67
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.77	0.67
3:D:1197:ARG:HD3	3:D:1198:TYR:CE2	2.28	0.67
2:C:168:ARG:CG	2:C:268:ASP:HB3	2.25	0.67
3:D:408:GLU:OE2	3:D:420:VAL:HG13	1.95	0.67
3:D:435:VAL:HG23	3:D:444:VAL:HG13	1.76	0.67
3:D:896:ALA:O	3:D:900:ILE:HG12	1.95	0.67
5:F:368:VAL:HG21	5:F:400:ILE:HD11	1.76	0.67
2:C:278:GLU:HB2	2:C:283:ILE:O	1.95	0.67
3:D:93:ILE:HB	3:D:517:VAL:HG22	1.77	0.67
2:C:397:GLU:OE2	2:C:632:ASN:N	2.25	0.67
2:C:473:ARG:HD2	2:C:482:GLU:OE2	1.95	0.66
2:C:252:LYS:HD3	2:C:252:LYS:N	2.08	0.66
2:C:778:PHE:CE2	5:F:419:ARG:HB2	2.31	0.66
5:F:361:LEU:HD21	5:F:407:LYS:HB3	1.77	0.66
2:C:351:LEU:HD11	2:C:374:ASN:H	1.60	0.66
4:E:41:GLU:H	4:E:44:GLU:HB2	1.61	0.66
1:A:106:PRO:HA	1:A:133:GLU:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:253:ALA:O	2:C:257:VAL:HG23	1.96	0.65
2:C:596:TYR:CE1	2:C:654:LEU:HD12	2.31	0.65
3:D:1164:ARG:NH1	3:D:1170:ASP:OD1	2.30	0.65
1:A:54:THR:HG21	1:A:145:ASP:HB3	1.77	0.65
2:C:404:LEU:HD22	2:C:542:VAL:HG21	1.78	0.65
2:C:912:PRO:O	2:C:916:GLU:HG3	1.95	0.65
3:D:619:LEU:HD11	3:D:1439:SER:HB2	1.77	0.65
5:F:127:ILE:HA	5:F:130:VAL:HG22	1.77	0.65
2:C:309:TYR:HA	2:C:320:HIS:CE1	2.32	0.65
1:B:6:LEU:HD13	1:B:189:ARG:HH11	1.60	0.65
2:C:15:LEU:HD21	2:C:457:ALA:HB1	1.79	0.65
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.79	0.65
3:D:129:PHE:HD2	3:D:456:MET:HE3	1.62	0.65
1:B:123:MET:C	1:B:125:PRO:HD3	2.22	0.65
5:F:396:ARG:O	5:F:400:ILE:HG23	1.96	0.65
1:B:6:LEU:HD22	1:B:29:GLU:HG2	1.79	0.64
1:A:57:TYR:HE1	1:A:163:ASN:HB2	1.61	0.64
2:C:463:GLU:OE1	2:C:463:GLU:N	2.20	0.64
2:C:584:GLU:O	2:C:588:VAL:HG23	1.97	0.64
3:D:886:VAL:O	3:D:890:VAL:HG22	1.97	0.64
1:A:53:VAL:CG2	1:A:82:LEU:HD23	2.28	0.64
2:C:568:ALA:HB2	2:C:995:MET:HE3	1.80	0.64
3:D:79:GLU:HG2	3:D:80:VAL:H	1.62	0.64
3:D:586[B]:ARG:NH1	6:G:10:DG:H3'	2.12	0.64
3:D:964:LEU:HD11	3:D:1041:LEU:HD12	1.79	0.64
3:D:1183:ILE:HD12	3:D:1184:GLN:H	1.63	0.64
5:F:236:SER:HB2	7:H:5:DA:H2'	1.79	0.64
2:C:596:TYR:HE1	2:C:654:LEU:HD12	1.62	0.64
2:C:168:ARG:HG2	2:C:268:ASP:HB3	1.80	0.63
2:C:768:THR:HG23	2:C:771:GLU:H	1.63	0.63
1:B:80:LEU:HB3	3:D:867:ARG:HH12	1.62	0.63
2:C:398:THR:HG23	2:C:633:GLN:HG2	1.78	0.63
3:D:178:LEU:HD13	3:D:192:ALA:HA	1.78	0.63
2:C:711:GLU:HB2	2:C:713:ARG:CZ	2.29	0.63
3:D:1069:GLU:O	3:D:1072:ILE:HG22	1.99	0.63
5:F:224:VAL:HG22	5:F:235:PHE:CZ	2.33	0.63
5:F:224:VAL:HG22	5:F:235:PHE:HZ	1.61	0.63
1:B:94:LEU:HD11	1:B:96:THR:O	1.98	0.63
1:A:66:SER:HB3	1:A:75:VAL:HG21	1.81	0.63
1:B:72:LYS:HB2	1:B:73:GLU:OE1	1.99	0.63
2:C:351:LEU:HD13	2:C:377:PRO:HG3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:999:THR:O	3:D:1003:VAL:HG12	1.98	0.63
1:A:218:LEU:HD23	1:B:222:LEU:HD11	1.81	0.63
3:D:138:LYS:HG3	3:D:451:ASP:O	1.99	0.63
2:C:375:SER:HB2	2:C:379:GLU:OE2	1.99	0.63
5:F:86:HIS:HA	7:H:7:DG:N2	2.14	0.63
1:B:94:LEU:HD12	1:B:95:GLN:H	1.63	0.62
1:B:58:ILE:O	1:B:61:VAL:HG22	1.99	0.62
3:D:5:VAL:O	3:D:1470:ARG:NH1	2.32	0.62
1:A:222:LEU:HD22	1:B:215:VAL:HG13	1.82	0.62
2:C:206:THR:O	2:C:210:GLU:HG2	1.99	0.62
2:C:402:SER:HA	2:C:566:THR:HG23	1.81	0.62
2:C:471:TYR:CD1	2:C:496:ILE:HG21	2.35	0.62
1:B:75:VAL:O	1:B:79:ILE:HG13	2.00	0.62
2:C:292:ARG:HG3	2:C:299:LYS:HB2	1.81	0.62
3:D:760:ARG:HH21	4:E:3:GLU:CD	2.07	0.62
5:F:152:ASP:OD1	5:F:154:LYS:HG2	1.99	0.62
2:C:9:ILE:HD11	2:C:500:ASN:HA	1.80	0.62
3:D:401:TYR:HE2	3:D:429:SER:HA	1.62	0.62
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.82	0.62
1:A:59:GLU:HB2	1:A:139:ASN:HB3	1.81	0.62
2:C:560:MET:O	2:C:564:MET:HG3	2.00	0.62
3:D:567:ILE:HG22	3:D:571:LYS:HE2	1.82	0.62
2:C:399:ASN:OD1	2:C:401:LEU:N	2.32	0.61
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.82	0.61
3:D:798:GLU:HG2	3:D:824:ASN:HB2	1.82	0.61
2:C:536:PRO:HB3	3:D:1067:VAL:HG21	1.80	0.61
4:E:40:LEU:HD13	4:E:46:PRO:HD3	1.82	0.61
1:A:57:TYR:CE1	1:A:163:ASN:HB2	2.34	0.61
3:D:186:VAL:HA	3:D:200:ASP:HA	1.81	0.61
3:D:45:PHE:CZ	3:D:541:ASN:ND2	2.62	0.61
3:D:1045:MET:HE2	3:D:1073:SER:HA	1.82	0.61
3:D:546:ARG:O	3:D:550:ARG:HG3	2.01	0.61
3:D:486:ARG:HG2	3:D:489:ARG:HH22	1.65	0.61
2:C:236:ILE:HG23	2:C:248:PRO:HB2	1.83	0.61
3:D:1254:GLN:HA	3:D:1254:GLN:NE2	2.16	0.61
1:A:228:PRO:HA	1:B:11:PHE:CD2	2.35	0.61
1:B:101:LEU:HB2	1:B:114:PHE:CD1	2.36	0.61
1:B:213:GLN:O	1:B:217:ILE:HG13	2.01	0.61
3:D:1254:GLN:HA	3:D:1254:GLN:HE21	1.65	0.61
2:C:65:VAL:HB	2:C:101:ILE:HG23	1.83	0.60
2:C:218:VAL:O	2:C:222:MET:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1026:GLN:N	2:C:1026:GLN:OE1	2.34	0.60
3:D:756:GLN:O	3:D:760:ARG:HG3	2.00	0.60
1:A:82:LEU:HD23	1:A:82:LEU:O	2.01	0.60
1:B:58:ILE:HG12	1:B:140:MET:HG2	1.82	0.60
5:F:321:ILE:HG21	5:F:332:PHE:HE2	1.64	0.60
3:D:527:MET:HA	3:D:536:ALA:O	2.01	0.60
2:C:404:LEU:CD2	2:C:542:VAL:HG21	2.32	0.60
3:D:33:ASN:H	3:D:38:LYS:H	1.48	0.60
2:C:840:ALA:HB3	2:C:997:LEU:HD21	1.82	0.60
1:B:94:LEU:HD12	1:B:95:GLN:N	2.17	0.60
2:C:342:ASP:O	2:C:345:ARG:HG3	2.01	0.60
3:D:132:TYR:HE1	3:D:155:ASP:HA	1.66	0.60
3:D:184:GLU:HG3	3:D:202:VAL:HA	1.84	0.60
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.83	0.60
2:C:683:ASN:HB3	2:C:872:ASN:HB2	1.83	0.60
5:F:240:THR:O	5:F:244[B]:ARG:HG2	2.02	0.60
1:A:132:LEU:HD11	1:A:138:LEU:HD22	1.84	0.59
3:D:398:ALA:HB2	3:D:447:VAL:HG22	1.84	0.59
5:F:96:LEU:O	5:F:100:VAL:HG23	2.01	0.59
3:D:1183:ILE:HD11	3:D:1185:GLU:O	2.02	0.59
5:F:227:PHE:CE2	5:F:235:PHE:HA	2.38	0.59
1:A:79:ILE:HG12	1:A:167:VAL:HG12	1.83	0.59
1:B:63:HIS:HD2	1:B:66:SER:HB2	1.63	0.59
2:C:99:GLN:O	2:C:109:LYS:O	2.20	0.59
1:A:51:THR:HG22	1:A:146:ARG:HB3	1.84	0.59
5:F:131:VAL:HG12	5:F:181:GLU:HG3	1.83	0.59
2:C:748:GLU:HB3	2:C:799:ILE:CD1	2.32	0.59
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.38	0.59
5:F:120:THR:HB	5:F:122:LEU:HG	1.84	0.59
3:D:3:LYS:HD2	3:D:4:GLU:OE1	2.02	0.59
4:E:30:LEU:HB3	4:E:35:PHE:CD2	2.37	0.59
5:F:157:GLU:O	5:F:161:GLN:HG2	2.02	0.59
7:H:3:DT:H2'	7:H:4:DA:C8	2.38	0.59
1:A:30:ARG:HD3	1:A:191:ASP:HB3	1.85	0.59
2:C:1060:ILE:HA	2:C:1063:ARG:NE	2.17	0.59
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.37	0.59
3:D:1431:THR:HG23	3:D:1433:SER:H	1.68	0.59
1:B:86:VAL:N	1:B:124:ASN:HD21	1.99	0.59
2:C:174:LEU:HD11	2:C:184:MET:HG3	1.84	0.59
3:D:1171:VAL:O	3:D:1175:ILE:HG13	2.03	0.59
5:F:371:LEU:HG	5:F:376:ILE:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.85	0.58
5:F:117:SER:HB2	5:F:127:ILE:HD11	1.84	0.58
5:F:167:PRO:HG2	5:F:170:HIS:CD2	2.39	0.58
1:A:79:ILE:HD11	1:A:167:VAL:HG11	1.86	0.58
1:A:83:LYS:HE3	1:A:168:ASP:HB2	1.83	0.58
3:D:45:PHE:HB3	3:D:86:ARG:HH12	1.67	0.58
1:B:13:VAL:HG22	1:B:23:PHE:CD1	2.39	0.58
2:C:846:LYS:HG3	3:D:741:ASP:HB2	1.86	0.58
2:C:490:GLU:HG3	2:C:493:ARG:HH11	1.68	0.58
1:B:13:VAL:HG22	1:B:23:PHE:HD1	1.68	0.58
2:C:374:ASN:OD1	5:F:276:ARG:NH1	2.36	0.58
3:D:399:ARG:HB2	3:D:401:TYR:HE1	1.69	0.58
2:C:572:ILE:HG21	2:C:830:LYS:NZ	2.18	0.58
5:F:218:GLN:O	5:F:221:ILE:HG12	2.03	0.58
1:B:86:VAL:HG21	1:B:202:ASP:HB2	1.86	0.57
3:D:1150:ALA:O	3:D:1151:ARG:HD3	2.04	0.57
1:A:6:LEU:HD11	1:A:27:PRO:HG2	1.85	0.57
2:C:217:LEU:HB3	2:C:311:PHE:CD2	2.39	0.57
2:C:872:ASN:OD1	2:C:873:PRO:HD2	2.04	0.57
4:E:18:ARG:O	4:E:21:VAL:HG12	2.04	0.57
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.86	0.57
2:C:440:PRO:HB2	3:D:1074:SER:OG	2.05	0.57
1:A:68:ILE:HG12	1:A:71:VAL:HG21	1.87	0.57
2:C:292:ARG:HD2	2:C:301:GLU:OE2	2.04	0.57
3:D:1028:ALA:O	3:D:1029:ARG:HG2	2.04	0.57
7:H:12:DC:H1'	7:H:13:DT:C6	2.39	0.57
1:A:58:ILE:HB	1:A:61:VAL:HG21	1.84	0.57
1:B:105:GLY:HA3	1:B:133:GLU:O	2.05	0.57
3:D:952:ASP:HA	3:D:1062:ARG:HH12	1.68	0.57
5:F:361:LEU:HG	5:F:408:LEU:HD21	1.86	0.57
7:H:1:DT:H2''	7:H:2:DA:C8	2.39	0.57
2:C:724:ARG:NH2	2:C:734:LEU:O	2.37	0.57
3:D:922:LEU:HB3	3:D:926:LYS:HD2	1.86	0.57
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.05	0.57
3:D:1273:VAL:HG21	3:D:1305:LEU:HD11	1.86	0.57
1:B:123:MET:O	1:B:125:PRO:HD3	2.05	0.57
2:C:259:GLY:HA2	2:C:263:ASP:HB2	1.87	0.57
2:C:360:LEU:HD12	2:C:361:MET:N	2.20	0.57
2:C:300:ASP:OD1	2:C:301:GLU:N	2.38	0.57
4:E:26:ARG:O	4:E:30:LEU:HG	2.04	0.57
1:B:86:VAL:H	1:B:124:ASN:ND2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.85	0.57
2:C:398:THR:HG1	2:C:402:SER:HG	1.52	0.57
2:C:545:ASN:O	2:C:581:THR:HG21	2.05	0.57
2:C:367:LEU:HD13	2:C:372:LEU:HD21	1.86	0.56
2:C:773:LEU:HD21	5:F:358:LEU:HD11	1.87	0.56
2:C:1090:LYS:HE2	2:C:1112:PHE:CE2	2.39	0.56
3:D:134:VAL:HA	3:D:454:ALA:HA	1.87	0.56
7:H:1:DT:H2"	7:H:2:DA:H8	1.70	0.56
2:C:18:LEU:HD13	2:C:404:LEU:HD11	1.86	0.56
3:D:1106:VAL:HG22	3:D:1220:ALA:HA	1.87	0.56
2:C:168:ARG:HG3	2:C:268:ASP:H	1.70	0.56
2:C:259:GLY:C	2:C:260:LEU:HD23	2.29	0.56
2:C:268:ASP:CG	2:C:288:ARG:NH1	2.63	0.56
2:C:762:LYS:HG2	2:C:786:LYS:HB3	1.87	0.56
3:D:400:VAL:HG12	3:D:402:PRO:HD3	1.87	0.56
2:C:233:GLU:N	2:C:233:GLU:OE1	2.39	0.56
2:C:247:PRO:HG3	7:H:7:DG:C6	2.41	0.56
2:C:458:TYR:HD2	2:C:538:GLN:HB3	1.70	0.56
3:D:917:GLN:O	3:D:921:ARG:HG2	2.06	0.56
3:D:978:TYR:HB2	3:D:983:LEU:HD11	1.86	0.56
2:C:12:VAL:HG23	2:C:13:ILE:HG12	1.87	0.56
2:C:345:ARG:HD2	2:C:346:VAL:N	2.20	0.56
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.88	0.56
5:F:102:LEU:O	5:F:106:VAL:HG23	2.06	0.56
2:C:1017:THR:HG22	3:D:613:ARG:NH1	2.20	0.56
3:D:132:TYR:OH	3:D:568:ARG:NH2	2.37	0.56
2:C:157:ARG:HE	2:C:157:ARG:N	2.04	0.56
2:C:247:PRO:O	2:C:249:LYS:N	2.36	0.56
2:C:1009:SER:O	3:D:624:ASP:HB3	2.06	0.56
3:D:361:VAL:O	3:D:382:GLU:HA	2.05	0.56
1:A:87:VAL:HG21	1:A:144:VAL:HG11	1.87	0.56
2:C:50:GLU:O	2:C:265:ARG:NH2	2.39	0.56
2:C:156:GLY:HA3	2:C:157:ARG:HH21	1.71	0.56
2:C:606:VAL:HA	2:C:611:ILE:HG23	1.88	0.56
4:E:89:MET:SD	4:E:93:TYR:HD2	2.29	0.56
1:A:53:VAL:CG1	1:A:82:LEU:HD23	2.34	0.56
2:C:374:ASN:OD1	5:F:276:ARG:HD3	2.06	0.56
2:C:546:LEU:HD11	2:C:587:VAL:HG21	1.88	0.56
3:D:578:VAL:HG12	3:D:582:LEU:HD11	1.87	0.56
5:F:212:LEU:HD22	5:F:247:ILE:HG23	1.88	0.56
2:C:498:GLN:HB2	2:C:514:VAL:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:901:TYR:C	2:C:902:ILE:HD12	2.31	0.55
3:D:166:GLN:HB3	3:D:394:LEU:HD11	1.86	0.55
3:D:556:LYS:HE3	5:F:218:GLN:HG3	1.88	0.55
5:F:110:MET:HE1	5:F:225:GLU:O	2.06	0.55
7:H:9:DG:H2''	7:H:10:DA:OP2	2.06	0.55
1:B:91:ASN:H	1:B:119:ASP:HB3	1.71	0.55
2:C:288:ARG:HH11	2:C:288:ARG:HB2	1.72	0.55
3:D:583:ASP:OD2	3:D:586[A]:ARG:NE	2.38	0.55
3:D:808:THR:HG23	3:D:811:GLU:HG3	1.87	0.55
3:D:951:ILE:O	3:D:1062:ARG:NH1	2.38	0.55
3:D:963:TYR:CE1	3:D:1002:LYS:HD3	2.41	0.55
1:A:97:VAL:HG12	1:A:144:VAL:HB	1.87	0.55
2:C:249:LYS:HD2	2:C:252:LYS:HE2	1.88	0.55
3:D:441:ARG:HB2	3:D:443:VAL:HG22	1.88	0.55
3:D:805:GLU:HG2	3:D:828:LYS:HG3	1.86	0.55
2:C:1038:TRP:HH2	3:D:1096:ARG:HG3	1.71	0.55
5:F:126:LEU:HD11	5:F:159:ILE:HG12	1.88	0.55
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.42	0.55
3:D:1322:GLY:HA3	3:D:1339:LYS:HG3	1.88	0.55
3:D:346:ARG:O	3:D:351:MET:HE1	2.06	0.55
5:F:353:GLU:HA	5:F:356:LYS:HD3	1.87	0.55
1:A:228:PRO:HA	1:B:11:PHE:HD2	1.71	0.55
3:D:1271:LYS:HD3	3:D:1331:ASP:HB2	1.88	0.55
2:C:600:ASP:HA	2:C:650:ARG:HA	1.89	0.55
3:D:123:LEU:HD22	3:D:127:LEU:HD11	1.87	0.55
3:D:853:VAL:HG22	3:D:858:VAL:HG13	1.88	0.55
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.89	0.55
2:C:351:LEU:HD13	2:C:377:PRO:CG	2.37	0.55
2:C:831:ARG:HD2	2:C:1000:MET:HE1	1.89	0.55
3:D:969:ARG:HG2	3:D:969:ARG:HH11	1.72	0.55
1:A:52:ALA:HB3	1:A:171:PHE:CD1	2.42	0.54
2:C:109:LYS:O	2:C:109:LYS:HG3	2.07	0.54
2:C:193:LEU:HG	2:C:197:LEU:HD13	1.89	0.54
2:C:419:THR:N	2:C:422:ARG:HE	2.05	0.54
3:D:34:TYR:HD2	5:F:260:ILE:HG12	1.73	0.54
3:D:116:LEU:HD13	3:D:464:LEU:HD23	1.89	0.54
3:D:844:ALA:O	3:D:867:ARG:HB3	2.07	0.54
3:D:1418:LYS:HG2	3:D:1419:PRO:CD	2.37	0.54
5:F:233:PHE:CD2	7:H:2:DA:H2''	2.42	0.54
2:C:165:LEU:HB3	2:C:168:ARG:HB3	1.89	0.54
2:C:572:ILE:HG21	2:C:830:LYS:HZ3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:799:ILE:N	2:C:828:ALA:O	2.36	0.54
3:D:84:ILE:HG13	3:D:87:ARG:HD3	1.88	0.54
3:D:664:LYS:HD2	3:D:664:LYS:N	2.22	0.54
2:C:154:ARG:NE	2:C:157:ARG:HG3	2.21	0.54
3:D:796:ARG:HH12	3:D:859:ASP:HB2	1.71	0.54
5:F:264:MET:O	5:F:267:THR:OG1	2.25	0.54
3:D:129:PHE:CD2	3:D:456:MET:HE3	2.42	0.54
3:D:413:ASP:O	3:D:435:VAL:HG12	2.07	0.54
1:A:58:ILE:HB	1:A:61:VAL:CG2	2.37	0.54
1:A:85:LEU:HA	1:A:124:ASN:HD21	1.71	0.54
3:D:102:ILE:HD11	3:D:587:ARG:HB2	1.89	0.54
3:D:44:LEU:HB3	3:D:525:ARG:HH22	1.72	0.54
5:F:415:THR:HB	5:F:417:LYS:HE2	1.89	0.54
1:A:68:ILE:HG12	1:A:71:VAL:CG2	2.38	0.54
3:D:359:ALA:H	3:D:385:VAL:HB	1.72	0.54
3:D:1019:PRO:O	3:D:1023:MET:HG3	2.07	0.54
3:D:458:ALA:HB1	3:D:513:ILE:HG23	1.90	0.54
5:F:119:ILE:HG21	5:F:170:HIS:ND1	2.23	0.54
5:F:321:ILE:HD12	5:F:328:PHE:C	2.32	0.54
2:C:163:ILE:HG23	2:C:171:TRP:CE2	2.43	0.54
2:C:360:LEU:HD12	2:C:361:MET:HG2	1.89	0.54
2:C:474:VAL:HG22	2:C:479:VAL:HG22	1.90	0.54
3:D:525:ARG:HH21	3:D:541:ASN:CG	2.15	0.54
3:D:1341:PRO:O	3:D:1344:VAL:HG12	2.08	0.54
5:F:237:THR:HA	7:H:5:DA:N7	2.22	0.54
5:F:166:LEU:HB3	5:F:170:HIS:HB2	1.89	0.53
2:C:69:LEU:HD12	2:C:97:ARG:HB3	1.89	0.53
2:C:207:LEU:HD12	2:C:227:PHE:HZ	1.73	0.53
3:D:543:LEU:HD21	3:D:600:LEU:HD12	1.90	0.53
3:D:601:ARG:HD3	3:D:606:ILE:HG12	1.90	0.53
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.89	0.53
4:E:92:LEU:HD12	4:E:92:LEU:H	1.73	0.53
5:F:407:LYS:HA	5:F:410:TYR:HD2	1.74	0.53
2:C:307:LEU:HG	2:C:311:PHE:CE1	2.44	0.53
2:C:921:ALA:HB3	2:C:967:PHE:HE2	1.74	0.53
3:D:530:VAL:HG22	3:D:534:ARG:O	2.08	0.53
2:C:503:LEU:HD23	2:C:508:ILE:HA	1.90	0.53
2:C:596:TYR:HD1	2:C:654:LEU:HA	1.72	0.53
2:C:710:ILE:HG23	2:C:758:ARG:NH2	2.23	0.53
2:C:99:GLN:O	2:C:100:LEU:HB3	2.09	0.53
3:D:1147:ARG:HH11	3:D:1147:ARG:HG2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:181:GLU:O	5:F:185:GLN:HG2	2.09	0.53
5:F:383:LEU:HD12	5:F:383:LEU:H	1.74	0.53
5:F:392:VAL:HG21	5:F:396:ARG:HH21	1.74	0.53
2:C:1008:ARG:NH2	2:C:1013:TYR:CE1	2.77	0.53
3:D:93:ILE:HB	3:D:517:VAL:CG2	2.38	0.53
3:D:486:ARG:HG2	3:D:489:ARG:NH2	2.24	0.53
3:D:690:ALA:CA	3:D:693:GLU:HG3	2.38	0.53
3:D:1285:GLU:HA	3:D:1290:LEU:HA	1.91	0.53
3:D:1462:LEU:HD23	3:D:1473:PRO:HD2	1.90	0.53
1:A:90[A]:LEU:HG	1:A:119:ASP:HA	1.91	0.53
2:C:766:GLU:OE2	3:D:65:ARG:NH1	2.42	0.53
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.91	0.53
3:D:1130:ARG:HE	3:D:1130:ARG:HA	1.73	0.53
3:D:1486:VAL:CG1	4:E:22:VAL:HG13	2.34	0.53
1:B:4:SER:O	1:B:4:SER:OG	2.27	0.53
3:D:702:LEU:HB3	3:D:745:MET:CE	2.39	0.53
3:D:767:HIS:HA	3:D:924:MET:HE2	1.91	0.53
3:D:1112:CYS:SG	3:D:1114:THR:HG22	2.49	0.53
5:F:114:LYS:HD3	5:F:114:LYS:C	2.34	0.53
2:C:419:THR:H	2:C:422:ARG:HE	1.55	0.52
2:C:1013:TYR:CD2	2:C:1063:ARG:CZ	2.92	0.52
3:D:438:ASP:OD2	3:D:441:ARG:NH1	2.42	0.52
3:D:631:ILE:HG21	3:D:745:MET:HG3	1.91	0.52
5:F:345:ALA:O	5:F:349:LEU:HG	2.09	0.52
1:A:185:ARG:HG3	1:A:189:ARG:O	2.08	0.52
1:A:201:THR:HG22	1:A:202:ASP:H	1.74	0.52
2:C:486:MET:HE2	2:C:490:GLU:HG2	1.90	0.52
2:C:547:ILE:HD13	2:C:842:ARG:O	2.10	0.52
2:C:894:GLY:O	2:C:898:GLY:N	2.41	0.52
3:D:123:LEU:C	3:D:127:LEU:HD12	2.34	0.52
3:D:166:GLN:HG2	3:D:396:VAL:HG23	1.91	0.52
3:D:170:PRO:O	3:D:195:VAL:HG11	2.10	0.52
5:F:99:GLU:OE2	5:F:235:PHE:HB2	2.10	0.52
3:D:206:ARG:HH12	5:F:101:GLU:CD	2.18	0.52
3:D:659:LYS:HE3	3:D:663:GLU:OE2	2.09	0.52
3:D:690:ALA:HA	3:D:693:GLU:CG	2.40	0.52
3:D:775:GLY:HA2	3:D:1209:LEU:HB3	1.91	0.52
2:C:626:ARG:HG3	2:C:626:ARG:HH11	1.74	0.52
1:A:53:VAL:CB	1:A:82:LEU:CD2	2.87	0.52
3:D:828:LYS:HA	3:D:833:GLU:HA	1.91	0.52
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:798:GLU:HB2	3:D:825:ALA:HB2	1.92	0.52
1:A:125:PRO:HD2	1:A:126:ASP:H	1.75	0.52
2:C:189:ARG:NH1	2:C:242:LEU:O	2.42	0.52
2:C:1050:GLN:O	2:C:1054:THR:HG23	2.10	0.52
3:D:686:GLU:H	3:D:686:GLU:CD	2.18	0.52
3:D:1491:THR:HG21	12:E:103:HOH:O	2.08	0.52
2:C:34:VAL:CG1	2:C:39:ARG:HG2	2.36	0.52
2:C:754:ILE:HG13	2:C:791:ARG:HD3	1.90	0.52
3:D:508:ARG:HB3	3:D:510:GLU:CD	2.35	0.52
3:D:1444:THR:O	3:D:1448:THR:HG23	2.09	0.52
4:E:38:THR:HG23	4:E:67:GLU:CD	2.35	0.52
1:A:88:ARG:HD2	1:A:123:MET:SD	2.49	0.52
2:C:239:PHE:CD2	2:C:253:ALA:HA	2.46	0.52
3:D:56:TYR:HA	3:D:80:VAL:HG13	1.92	0.51
4:E:84:ARG:O	4:E:87:LYS:HB3	2.10	0.51
5:F:321:ILE:HD13	5:F:332:PHE:CD2	2.45	0.51
3:D:560:GLN:O	5:F:132:ARG:NH1	2.42	0.51
2:C:44:ILE:HG13	2:C:340:MET:HE1	1.92	0.51
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.91	0.51
3:D:593:ASN:N	3:D:600:LEU:HD21	2.25	0.51
5:F:227:PHE:CD2	5:F:238:TYR:HD2	2.28	0.51
1:B:220:GLU:O	1:B:223:THR:OG1	2.20	0.51
2:C:1052:MET:HB3	3:D:623:VAL:HG11	1.92	0.51
3:D:706:PRO:HB2	3:D:708:LEU:HD21	1.92	0.51
3:D:792:ILE:HD13	3:D:941:PHE:CE2	2.46	0.51
1:A:156:HIS:O	1:A:157:GLY:C	2.53	0.51
1:A:178:ALA:HB2	2:C:864:GLY:HA3	1.92	0.51
2:C:1005:MET:HE3	3:D:645:PRO:HB2	1.92	0.51
3:D:534:ARG:HH21	5:F:313:GLU:H	1.57	0.51
3:D:1418:LYS:HG2	3:D:1419:PRO:HD2	1.93	0.51
1:A:123:MET:HA	1:A:123:MET:HE3	1.92	0.51
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.91	0.51
2:C:35:PRO:HG2	2:C:38:LYS:HB2	1.93	0.51
2:C:468:ARG:HG3	2:C:486:MET:C	2.36	0.51
5:F:238:TYR:HB2	7:H:2:DA:N3	2.25	0.51
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.25	0.51
2:C:520:GLU:HG3	2:C:521:PRO:HD2	1.93	0.51
3:D:1381:VAL:HG23	3:D:1393:GLN:O	2.11	0.51
6:G:17:DC:H2'	6:G:18:DA:O4'	2.10	0.51
1:A:74:ASP:OD2	1:A:76:VAL:HB	2.11	0.51
2:C:471:TYR:CD1	2:C:533:ASP:HA	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:169:TYR:CE2	3:D:198:ARG:HG2	2.46	0.51
3:D:813:LEU:HD22	3:D:836:VAL:HG13	1.93	0.51
5:F:252:ALA:CB	5:F:262:VAL:HG13	2.41	0.51
1:B:201:THR:HG21	1:B:205:VAL:O	2.12	0.51
3:D:996:TRP:CE2	3:D:1056:PRO:HG3	2.46	0.51
2:C:42:VAL:O	2:C:45:GLN:HB3	2.11	0.50
2:C:243:ARG:HH12	2:C:246:ASP:CB	2.25	0.50
2:C:437:ARG:HD3	2:C:467:ILE:HB	1.92	0.50
2:C:786:LYS:HG3	2:C:788:THR:HG23	1.92	0.50
3:D:421:LEU:HB2	3:D:427:VAL:HG12	1.93	0.50
5:F:273:ARG:O	5:F:277:GLN:HG3	2.11	0.50
1:A:117:VAL:HB	1:A:120:VAL:HG21	1.93	0.50
1:B:150:TYR:HB2	3:D:851:LEU:CD2	2.41	0.50
2:C:217:LEU:HB3	2:C:311:PHE:CE2	2.46	0.50
2:C:219:GLN:HA	2:C:222:MET:HG3	1.92	0.50
2:C:729:LEU:HD23	2:C:734:LEU:HD21	1.94	0.50
2:C:892:LEU:HD23	2:C:918:LEU:HD22	1.91	0.50
3:D:206:ARG:HB2	3:D:392:SER:O	2.11	0.50
1:A:86:VAL:HG21	1:A:202:ASP:HB2	1.94	0.50
1:B:9:PRO:HB3	1:B:27:PRO:O	2.11	0.50
1:B:88:ARG:HG2	1:B:90:LEU:HD13	1.93	0.50
1:B:90:LEU:HD22	1:B:90:LEU:H	1.76	0.50
2:C:45:GLN:O	2:C:49:ARG:HG2	2.12	0.50
2:C:198:ARG:NE	2:C:229:MET:O	2.44	0.50
2:C:292:ARG:HG2	2:C:299:LYS:O	2.11	0.50
2:C:473:ARG:NH1	2:C:482:GLU:OE2	2.45	0.50
2:C:927:GLY:HA2	2:C:930:LYS:HE2	1.93	0.50
3:D:65:ARG:HD2	5:F:378:GLY:C	2.36	0.50
2:C:471:TYR:HD1	2:C:533:ASP:HA	1.77	0.50
2:C:767:PRO:HG2	2:C:772:ARG:HH21	1.76	0.50
2:C:858:MET:HG2	2:C:867:VAL:O	2.11	0.50
3:D:401:TYR:OH	3:D:430:ASP:HB3	2.11	0.50
3:D:1147:ARG:HG2	3:D:1147:ARG:NH1	2.26	0.50
5:F:230:LYS:HB2	5:F:231:ARG:NH2	2.27	0.50
1:A:84:GLU:O	1:A:124:ASN:ND2	2.45	0.50
2:C:554:ASP:OD1	2:C:555:ALA:N	2.44	0.50
2:C:817:PRO:HA	5:F:305:GLU:HG3	1.92	0.50
3:D:683:ILE:HG21	3:D:688:TRP:CE2	2.45	0.50
3:D:1275:SER:OG	3:D:1277:ILE:O	2.27	0.50
2:C:77:PRO:HB2	2:C:78:PHE:HD1	1.77	0.50
2:C:971:LYS:HB3	2:C:986:PRO:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:485:SER:HB3	3:D:488:ARG:HG3	1.92	0.50
3:D:646:LYS:HA	3:D:720:LEU:HD13	1.94	0.50
1:A:20:TYR:CD1	1:A:21:GLY:N	2.80	0.50
2:C:86:LYS:HD3	2:C:813:VAL:HG23	1.93	0.50
2:C:165:LEU:HD23	2:C:166:PRO:O	2.12	0.50
3:D:1219:GLU:HG3	4:E:17:TYR:OH	2.11	0.50
6:G:11:DT:H2'	6:G:12:DG:C8	2.47	0.50
1:B:174:VAL:HG11	1:B:177:VAL:HG23	1.93	0.50
2:C:66:LEU:HD21	2:C:98:LEU:HD13	1.93	0.50
2:C:69:LEU:HB2	2:C:97:ARG:CB	2.42	0.50
2:C:987:ILE:HD11	3:D:946:GLY:HA2	1.94	0.50
5:F:392:VAL:CG1	5:F:396:ARG:HB3	2.42	0.50
1:A:52:ALA:HB3	1:A:171:PHE:HD1	1.77	0.50
1:B:132:LEU:HD21	1:B:138:LEU:HB2	1.94	0.50
2:C:911:GLU:HB2	2:C:912:PRO:HD3	1.94	0.50
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.94	0.50
3:D:1209:LEU:H	3:D:1209:LEU:HD22	1.77	0.50
5:F:162:LYS:HD3	5:F:162:LYS:O	2.12	0.50
5:F:268:ILE:HA	5:F:271:LEU:CD1	2.42	0.50
1:A:54:THR:OG1	1:A:143:ARG:HD2	2.11	0.49
2:C:212:GLY:HA2	2:C:218:VAL:HG11	1.94	0.49
2:C:217:LEU:HD12	2:C:217:LEU:H	1.77	0.49
2:C:351:LEU:O	2:C:355:VAL:HG23	2.11	0.49
2:C:471:TYR:CE1	2:C:496:ILE:HG21	2.46	0.49
3:D:60:CYS:H	3:D:76:CYS:HB3	1.76	0.49
3:D:176:ASP:CG	3:D:177:ALA:H	2.20	0.49
3:D:436:GLU:HG3	3:D:445:ARG:HB2	1.93	0.49
3:D:828:LYS:HD3	3:D:833:GLU:HB3	1.93	0.49
2:C:7:GLY:HA2	2:C:907:ASP:OD1	2.11	0.49
2:C:232:GLU:OE2	2:C:236:ILE:HG13	2.12	0.49
2:C:881:ASN:O	2:C:884:GLN:HG2	2.12	0.49
2:C:1048:THR:O	2:C:1052:MET:HG2	2.12	0.49
3:D:199:LEU:HD21	3:D:395:VAL:HB	1.95	0.49
3:D:400:VAL:C	3:D:401:TYR:CD1	2.90	0.49
2:C:268:ASP:OD1	2:C:288:ARG:NH1	2.45	0.49
2:C:395:LYS:HE2	2:C:397:GLU:HB3	1.94	0.49
2:C:793:PRO:HB2	2:C:796:GLU:HG3	1.93	0.49
3:D:690:ALA:O	3:D:693:GLU:HG3	2.12	0.49
3:D:1140:ILE:HG23	3:D:1144:LEU:HD12	1.93	0.49
3:D:1404:ASN:HD21	3:D:1415:VAL:HB	1.76	0.49
1:A:25:LEU:HD23	1:A:28:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:104:ARG:HG2	5:F:108:GLU:OE2	2.12	0.49
1:B:177:VAL:HG13	1:B:197:LEU:HD11	1.93	0.49
2:C:114:PHE:HB3	5:F:280:GLN:HA	1.93	0.49
2:C:1038:TRP:CH2	3:D:1096:ARG:HG3	2.47	0.49
3:D:435:VAL:HA	3:D:445:ARG:O	2.11	0.49
5:F:241:TRP:NE1	7:H:1:DT:H5"	2.27	0.49
2:C:162:ILE:HG21	2:C:290:LEU:HD11	1.95	0.49
3:D:664:LYS:NZ	3:D:693:GLU:OE1	2.45	0.49
1:A:54:THR:C	1:A:167:VAL:HG22	2.37	0.49
1:A:56:VAL:HG22	1:A:142:VAL:HG22	1.94	0.49
5:F:360:LYS:CB	5:F:411:HIS:CD2	2.94	0.49
3:D:67:ARG:HH21	5:F:379:ARG:CD	2.23	0.49
3:D:434:ARG:O	3:D:446:VAL:HA	2.12	0.49
3:D:527:MET:CG	3:D:537:THR:HB	2.39	0.49
3:D:1274:ILE:HG22	3:D:1324:PRO:HA	1.94	0.49
5:F:81:VAL:O	5:F:85:LEU:HG	2.13	0.49
1:A:157:GLY:HA2	1:A:166:PRO:HB3	1.95	0.49
1:B:84:GLU:OE2	3:D:867:ARG:NH2	2.46	0.49
2:C:721:ARG:HE	2:C:759:THR:CG2	2.26	0.49
2:C:874:LEU:HB3	3:D:1029:ARG:HG3	1.94	0.49
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.95	0.49
3:D:759:ALA:HA	3:D:763:MET:HB2	1.94	0.49
3:D:1094:LEU:HA	3:D:1097:LYS:HD2	1.94	0.49
1:A:184:THR:O	1:A:192:LEU:HB2	2.13	0.49
2:C:162:ILE:HB	2:C:172:ILE:HB	1.94	0.49
2:C:260:LEU:HD21	7:H:11:DG:O6	2.12	0.49
2:C:773:LEU:O	2:C:777:ILE:HG13	2.13	0.49
3:D:67:ARG:NH2	5:F:379:ARG:HD3	2.24	0.48
1:B:176:ARG:NH1	3:D:888:GLU:OE2	2.29	0.48
2:C:86:LYS:HB3	2:C:813:VAL:HG21	1.95	0.48
2:C:183:SER:HB2	2:C:190:LYS:HG2	1.95	0.48
2:C:419:THR:HG23	2:C:421:GLU:H	1.78	0.48
2:C:460:ARG:O	2:C:468:ARG:N	2.47	0.48
2:C:1008:ARG:HH21	2:C:1013:TYR:HE1	1.60	0.48
1:B:191:ASP:OD1	1:B:191:ASP:N	2.39	0.48
2:C:862:PRO:HD3	2:C:973:VAL:O	2.14	0.48
3:D:405:ASP:HB2	3:D:423:ASP:HA	1.95	0.48
2:C:846:LYS:NZ	9:C:1201:A1IF9:O18	2.46	0.48
3:D:403:PHE:CE2	3:D:444:VAL:HG23	2.48	0.48
3:D:458:ALA:HB1	3:D:513:ILE:CG2	2.43	0.48
5:F:114:LYS:HD3	5:F:114:LYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASN:N	1:A:39:PRO:HD2	2.28	0.48
2:C:290:LEU:HD22	2:C:302:VAL:HG21	1.96	0.48
2:C:712:ALA:HB3	2:C:821:GLU:CG	2.43	0.48
5:F:162:LYS:HD3	5:F:162:LYS:C	2.38	0.48
1:B:184:THR:HG23	1:B:192:LEU:HB2	1.96	0.48
2:C:18:LEU:CD1	2:C:404:LEU:HD11	2.43	0.48
2:C:539:VAL:O	2:C:539:VAL:HG12	2.14	0.48
3:D:101:HIS:HB3	3:D:104:PHE:HD1	1.79	0.48
3:D:411:THR:HG23	3:D:436:GLU:HA	1.96	0.48
3:D:702:LEU:HB3	3:D:745:MET:HE1	1.95	0.48
3:D:1147:ARG:NH1	3:D:1189:ARG:O	2.47	0.48
2:C:542:VAL:HG23	2:C:543:ASN:N	2.29	0.48
2:C:1066:ALA:O	2:C:1070:ILE:HG13	2.14	0.48
3:D:1211:MET:HE3	3:D:1213:ARG:HD2	1.96	0.48
2:C:18:LEU:HD12	2:C:590:ASP:HB2	1.96	0.48
2:C:144:PRO:O	2:C:273:GLY:HA2	2.13	0.48
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.48	0.48
3:D:401:TYR:OH	3:D:430:ASP:N	2.43	0.48
4:E:38:THR:HG22	4:E:40:LEU:H	1.79	0.48
4:E:40:LEU:HG	4:E:67:GLU:HG2	1.95	0.48
4:E:81:PRO:HB2	4:E:84:ARG:CB	2.43	0.48
1:B:132:LEU:HD21	1:B:138:LEU:CB	2.43	0.48
2:C:831:ARG:NE	2:C:1002:GLU:OE1	2.47	0.48
5:F:188:ILE:HG23	5:F:220:LEU:HD22	1.94	0.48
1:A:185:ARG:HG2	1:A:187:GLY:H	1.79	0.48
2:C:300:ASP:OD2	2:C:304:LEU:N	2.46	0.48
3:D:894:LYS:O	3:D:898:GLU:HG3	2.14	0.48
3:D:1459:LEU:HD23	3:D:1464:GLU:HB3	1.95	0.48
3:D:1487:VAL:HG22	3:D:1491:THR:OG1	2.14	0.48
5:F:316:SER:HB3	5:F:319:THR:HG23	1.95	0.48
1:A:40:LEU:O	1:A:44:LEU:HG	2.14	0.47
2:C:169:GLY:HA3	2:C:267:TYR:CD1	2.49	0.47
2:C:309:TYR:OH	2:C:320:HIS:HA	2.14	0.47
3:D:209:ARG:HA	3:D:347:VAL:HB	1.95	0.47
4:E:26:ARG:NH2	4:E:73:LEU:HD21	2.28	0.47
1:B:123:MET:HE3	1:B:123:MET:HB3	1.80	0.47
2:C:760:SER:HB3	2:C:786:LYS:HE2	1.96	0.47
3:D:423:ASP:HB3	3:D:426:LYS:HE2	1.96	0.47
3:D:690:ALA:C	3:D:693:GLU:HG3	2.39	0.47
3:D:969:ARG:HG2	3:D:969:ARG:NH1	2.30	0.47
3:D:1384:PRO:HB3	3:D:1389:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:194:LEU:HD21	7:H:5:DA:H2''	1.96	0.47
1:B:42:ARG:O	1:B:46:SER:OG	2.26	0.47
1:B:108:GLU:H	1:B:108:GLU:HG2	1.54	0.47
1:B:201:THR:HG22	1:B:202:ASP:H	1.78	0.47
3:D:102:ILE:HG12	3:D:586[A]:ARG:HD2	1.96	0.47
3:D:206:ARG:NH1	5:F:101:GLU:OE1	2.47	0.47
3:D:801:GLY:O	3:D:804:LEU:HD13	2.14	0.47
4:E:41:GLU:O	4:E:45:ARG:N	2.47	0.47
5:F:320:PRO:HB3	5:F:325:LYS:HD2	1.95	0.47
2:C:124:ASP:OD2	2:C:407:LYS:NZ	2.47	0.47
3:D:67:ARG:HB2	5:F:377:ASP:OD1	2.14	0.47
3:D:543:LEU:O	3:D:547:LEU:HD12	2.15	0.47
3:D:656:PHE:CB	3:D:694:VAL:HG21	2.42	0.47
3:D:714:GLN:HB2	3:D:736:PHE:HZ	1.79	0.47
3:D:729:HIS:O	3:D:732:VAL:HG22	2.14	0.47
3:D:869:MET:HE3	3:D:869:MET:HB3	1.75	0.47
5:F:227:PHE:HD2	5:F:238:TYR:HD2	1.62	0.47
2:C:65:VAL:O	2:C:100:LEU:HA	2.15	0.47
2:C:831:ARG:CZ	2:C:1002:GLU:OE1	2.63	0.47
2:C:910:LYS:HB2	2:C:913[B]:GLU:OE1	2.14	0.47
3:D:479:GLU:HA	3:D:482:LYS:HD3	1.96	0.47
3:D:1350:GLU:O	3:D:1354:LYS:HG3	2.14	0.47
2:C:926:PHE:HE2	2:C:960:GLU:HB2	1.78	0.47
2:C:1048:THR:HG22	2:C:1052:MET:HE3	1.96	0.47
3:D:416:ALA:HB1	3:D:417:PRO:HD2	1.96	0.47
4:E:41:GLU:O	4:E:44:GLU:N	2.47	0.47
4:E:86:GLN:O	4:E:89:MET:HB3	2.14	0.47
2:C:141:HIS:HE1	2:C:144:PRO:HD3	1.79	0.47
2:C:174:LEU:CD1	2:C:184:MET:HG3	2.44	0.47
2:C:329:GLY:HA3	2:C:489:THR:HG23	1.97	0.47
2:C:337:GLY:O	2:C:341:THR:HG23	2.13	0.47
2:C:419:THR:HG22	2:C:422:ARG:CG	2.41	0.47
2:C:436:GLY:HA2	2:C:538:GLN:O	2.15	0.47
2:C:475:VAL:O	2:C:478:VAL:HG22	2.14	0.47
2:C:582:GLY:O	2:C:583:LEU:HD12	2.15	0.47
2:C:711:GLU:HB2	2:C:713:ARG:NH2	2.29	0.47
2:C:958:THR:OG1	2:C:961:GLU:HG2	2.14	0.47
3:D:65:ARG:NH2	5:F:380:GLU:OE2	2.48	0.47
3:D:140:ALA:HA	3:D:450:TYR:CE2	2.49	0.47
3:D:140:ALA:HB3	3:D:147:VAL:HB	1.95	0.47
3:D:962:GLN:NE2	3:D:966:GLU:OE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:370:LYS:HB3	5:F:376:ILE:HB	1.97	0.47
1:A:153:ALA:C	1:A:155:LYS:H	2.22	0.47
1:B:186:LEU:O	1:B:189:ARG:HG3	2.15	0.47
2:C:141:HIS:CD2	2:C:334:ARG:HD2	2.50	0.47
2:C:151:ASP:HB3	2:C:157:ARG:HB2	1.95	0.47
2:C:344:PHE:CD1	2:C:378:LEU:HD11	2.50	0.47
1:B:108:GLU:HA	1:B:131:THR:HA	1.97	0.47
2:C:567:GLN:HB2	2:C:997:LEU:HD12	1.97	0.47
3:D:187:LYS:N	3:D:200:ASP:OD1	2.32	0.47
3:D:1281:VAL:HG11	3:D:1313:VAL:HG22	1.96	0.47
3:D:1479:ASP:CG	3:D:1482:ARG:HH21	2.23	0.47
5:F:379:ARG:CZ	5:F:381:HIS:CD2	2.98	0.47
1:B:104:GLU:HG2	1:B:137:ARG:CG	2.43	0.47
2:C:399:ASN:OD1	2:C:399:ASN:C	2.58	0.47
2:C:598:GLU:O	2:C:651:LYS:HG3	2.15	0.47
2:C:744:ARG:HD2	2:C:747:ALA:HB2	1.96	0.47
3:D:25:GLU:HA	3:D:92:HIS:O	2.15	0.47
3:D:79:GLU:HG2	3:D:80:VAL:N	2.29	0.47
3:D:962:GLN:O	3:D:966:GLU:HG3	2.15	0.47
2:C:396:ASP:CG	2:C:402:SER:HB3	2.40	0.46
2:C:631:SER:OG	2:C:635:THR:N	2.48	0.46
3:D:60:CYS:SG	3:D:76:CYS:HB3	2.54	0.46
3:D:553:ARG:O	3:D:557:LEU:HG	2.15	0.46
3:D:1397:LYS:O	3:D:1400:VAL:HG12	2.15	0.46
3:D:1462:LEU:HD22	3:D:1472:ILE:HB	1.97	0.46
5:F:332:PHE:HZ	6:G:19:DG:O6	1.98	0.46
2:C:662:GLU:OE2	2:C:900:ARG:NH1	2.47	0.46
2:C:1090:LYS:HD2	3:D:90:MET:HE2	1.98	0.46
3:D:155:ASP:O	3:D:159[B]:ARG:HG3	2.15	0.46
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.96	0.46
4:E:18:ARG:NH2	4:E:77:GLU:OE2	2.49	0.46
5:F:318:GLU:N	5:F:318:GLU:OE1	2.48	0.46
2:C:99:GLN:HB2	2:C:108:ILE:HG22	1.96	0.46
2:C:707:ARG:HH21	2:C:824:ARG:HD2	1.79	0.46
2:C:773:LEU:CD1	5:F:369:LEU:HD23	2.46	0.46
3:D:547:LEU:HD21	3:D:578:VAL:HA	1.96	0.46
3:D:565:ILE:HG21	5:F:88:ILE:HG22	1.96	0.46
5:F:209:PHE:O	5:F:213:ILE:HG13	2.15	0.46
1:A:206:THR:HG22	1:A:209:GLU:CD	2.40	0.46
2:C:168:ARG:HG3	2:C:268:ASP:N	2.30	0.46
2:C:436:GLY:HA2	2:C:539:VAL:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:533:ASP:HB3	2:C:538:GLN:NE2	2.31	0.46
2:C:605:LYS:HA	2:C:645:VAL:HG22	1.98	0.46
2:C:1093:GLN:OE1	3:D:90:MET:HE1	2.16	0.46
3:D:123:LEU:O	3:D:127:LEU:HD12	2.16	0.46
3:D:792:ILE:HG13	3:D:793:THR:N	2.31	0.46
3:D:914:LEU:CD2	3:D:930:LEU:HD21	2.45	0.46
3:D:1407:LEU:HG	3:D:1412:LYS:HD2	1.98	0.46
5:F:361:LEU:HD13	5:F:404:ALA:HB1	1.97	0.46
1:A:90[B]:LEU:HB3	1:A:119:ASP:OD1	2.16	0.46
2:C:328:LEU:HB2	2:C:433:THR:HB	1.97	0.46
2:C:846:LYS:HE3	3:D:741:ASP:HB2	1.97	0.46
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.15	0.46
2:C:99:GLN:HB2	2:C:108:ILE:CG2	2.45	0.46
2:C:886:LEU:HD21	3:D:951:ILE:HG12	1.98	0.46
5:F:127:ILE:HG13	5:F:128:ARG:N	2.31	0.46
5:F:187:LEU:HD23	5:F:224:VAL:HG13	1.97	0.46
5:F:382:THR:OG1	5:F:384:GLU:HG2	2.16	0.46
5:F:393:THR:HG23	5:F:396:ARG:H	1.81	0.46
1:A:64:GLU:O	1:A:75:VAL:HB	2.16	0.46
3:D:995:LEU:HA	3:D:998:GLU:OE1	2.16	0.46
3:D:1191:PRO:O	3:D:1373:ARG:HD2	2.15	0.46
1:A:29:GLU:HB2	1:A:32:PHE:CD2	2.51	0.46
2:C:244:PRO:HD2	5:F:82:ARG:HH22	1.81	0.46
2:C:309:TYR:CZ	2:C:320:HIS:HA	2.51	0.46
3:D:617:ASN:O	3:D:621:LYS:HE3	2.15	0.46
2:C:630:ARG:NE	2:C:705:ILE:O	2.49	0.46
3:D:602:SER:O	3:D:606:ILE:HG13	2.16	0.46
5:F:181:GLU:OE1	5:F:184:ARG:NH2	2.48	0.46
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.51	0.46
2:C:43:GLY:HA2	2:C:341:THR:HG21	1.98	0.46
2:C:44:ILE:HG12	2:C:344:PHE:CE2	2.50	0.46
2:C:109:LYS:HG3	2:C:369:PRO:HD2	1.98	0.46
3:D:33:ASN:O	3:D:37:LEU:HD23	2.16	0.46
3:D:60:CYS:CB	3:D:76:CYS:HB3	2.46	0.46
2:C:290:LEU:HB3	2:C:303:PHE:CE1	2.51	0.45
2:C:631:SER:HB3	2:C:637:LEU:HG	1.97	0.45
2:C:712:ALA:HB3	2:C:821:GLU:HG3	1.96	0.45
3:D:838:ARG:O	3:D:865:THR:OG1	2.31	0.45
3:D:1208:ASP:OD1	3:D:1208:ASP:C	2.59	0.45
3:D:1282:ARG:NE	3:D:1293:PHE:HB2	2.28	0.45
3:D:1375:MET:HB3	3:D:1422:MET:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:256:ARG:HB3	5:F:258:ILE:O	2.16	0.45
1:A:90[A]:LEU:HB2	1:A:119:ASP:OD1	2.15	0.45
1:B:38:ASN:HB2	1:B:39:PRO:HD3	1.97	0.45
2:C:462:ASP:OD1	2:C:462:ASP:C	2.59	0.45
3:D:33:ASN:N	3:D:38:LYS:O	2.49	0.45
3:D:65:ARG:HG3	5:F:379:ARG:HB2	1.98	0.45
3:D:1047:LYS:HG3	3:D:1051:GLU:O	2.17	0.45
2:C:13:ILE:HD13	2:C:483:VAL:HG11	1.97	0.45
2:C:69:LEU:HD12	2:C:97:ARG:HE	1.81	0.45
2:C:76:PRO:HA	2:C:77:PRO:HD2	1.87	0.45
2:C:99:GLN:O	2:C:100:LEU:CB	2.63	0.45
2:C:168:ARG:CD	2:C:268:ASP:HB3	2.47	0.45
2:C:196:LEU:O	2:C:200:LEU:HG	2.16	0.45
2:C:514:VAL:HA	2:C:523:ILE:HD13	1.97	0.45
3:D:573:MET:HE1	5:F:210:LEU:HB3	1.96	0.45
3:D:1135:ARG:HG2	3:D:1139:ASP:HB2	1.98	0.45
1:A:150:TYR:CD2	2:C:696:LYS:HG2	2.52	0.45
1:A:209:GLU:O	1:A:213:GLN:HG3	2.16	0.45
2:C:141:HIS:ND1	2:C:142:ARG:O	2.44	0.45
2:C:1005:MET:CE	3:D:648:MET:HG3	2.40	0.45
3:D:27:GLU:HB2	3:D:42:ASP:HB3	1.99	0.45
3:D:32:ILE:HD12	3:D:37:LEU:HB3	1.99	0.45
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.99	0.45
3:D:1277:ILE:HD11	3:D:1301:LYS:HG2	1.98	0.45
3:D:1282:ARG:HD2	3:D:1284:GLU:HG3	1.99	0.45
5:F:132:ARG:O	5:F:135:ILE:N	2.49	0.45
5:F:152:ASP:CG	5:F:153:PRO:HD2	2.42	0.45
2:C:23:VAL:HA	2:C:121:MET:CE	2.41	0.45
2:C:50:GLU:O	2:C:265:ARG:CZ	2.64	0.45
2:C:363:SER:O	2:C:367:LEU:HG	2.16	0.45
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.17	0.45
3:D:22:SER:HB2	3:D:92:HIS:HB3	1.98	0.45
3:D:952:ASP:HA	3:D:1062:ARG:NH1	2.30	0.45
1:B:30:ARG:NH1	2:C:854:PRO:HB3	2.31	0.45
3:D:492:ALA:O	3:D:496:LEU:HB2	2.17	0.45
3:D:640:HIS:CE1	4:E:2:ALA:N	2.85	0.45
3:D:924:MET:HG3	4:E:7:ASP:OD1	2.17	0.45
5:F:104:ARG:O	5:F:108:GLU:HG3	2.16	0.45
5:F:166:LEU:HD22	5:F:170:HIS:ND1	2.32	0.45
2:C:283:ILE:HD11	2:C:285:LEU:HD21	1.99	0.45
2:C:578:VAL:HG23	2:C:671:ASN:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:606:VAL:HG11	2:C:643:VAL:O	2.17	0.45
2:C:713:ARG:HG2	2:C:819:VAL:HG13	1.97	0.45
3:D:163:TYR:O	3:D:434:ARG:HD2	2.17	0.45
3:D:410:SER:OG	5:F:178:ARG:HG3	2.17	0.45
3:D:1471:LEU:HD21	3:D:1477:GLY:HA2	1.99	0.45
1:B:91:ASN:N	1:B:119:ASP:HB3	2.32	0.45
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.99	0.45
2:C:1012:PRO:C	2:C:1013:TYR:HD1	2.25	0.45
3:D:28:LYS:HB2	3:D:42:ASP:HB2	1.99	0.45
3:D:647:ARG:O	3:D:650:LEU:HB3	2.17	0.45
5:F:340:SER:O	5:F:343:ASP:N	2.50	0.45
1:A:221:HIS:HA	1:A:224:TYR:CE2	2.52	0.45
2:C:249:LYS:CD	2:C:252:LYS:HE2	2.46	0.45
2:C:312:ALA:HB1	2:C:317:VAL:CG2	2.44	0.45
2:C:1008:ARG:NH2	2:C:1013:TYR:CD1	2.85	0.45
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.51	0.45
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	1.99	0.45
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.31	0.45
3:D:1484:THR:CG2	4:E:18:ARG:HE	2.30	0.45
7:H:17:DA:H1'	7:H:18:DC:H5'	1.99	0.45
2:C:175:GLU:HG3	2:C:177:GLU:OE2	2.17	0.45
2:C:258:TYR:CD1	2:C:258:TYR:C	2.95	0.45
2:C:684:PHE:HB3	3:D:633:VAL:HG21	1.99	0.45
3:D:106:LYS:HB2	3:D:586[A]:ARG:HD3	1.99	0.45
3:D:1031:ASN:O	3:D:1035:ILE:HG12	2.16	0.45
5:F:134:LYS:HA	5:F:134:LYS:HD3	1.63	0.45
5:F:287:THR:OG1	5:F:288:TYR:N	2.49	0.45
5:F:369:LEU:HD11	5:F:404:ALA:HB3	1.98	0.45
1:A:94:LEU:O	1:A:146:ARG:HD3	2.17	0.44
1:A:124:ASN:OD1	1:A:124:ASN:N	2.51	0.44
2:C:69:LEU:HB2	2:C:97:ARG:HB3	1.99	0.44
3:D:978:TYR:HA	3:D:983:LEU:HG	1.98	0.44
3:D:1312:LEU:HD11	3:D:1324:PRO:O	2.17	0.44
2:C:211:LEU:HD22	2:C:221:LEU:HD22	1.98	0.44
2:C:557:ARG:HA	2:C:557:ARG:HD3	1.80	0.44
2:C:831:ARG:HH11	2:C:1000:MET:CE	2.30	0.44
5:F:169:GLU:O	5:F:172:ARG:HB3	2.17	0.44
5:F:373:LYS:HB2	5:F:375:LEU:CD1	2.48	0.44
2:C:205:GLU:O	2:C:209:ARG:HG3	2.17	0.44
2:C:695:LEU:HD21	2:C:833:LEU:HB3	2.00	0.44
3:D:171:LEU:CD1	3:D:393:ILE:HG12	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:574:LEU:O	3:D:578:VAL:HG23	2.17	0.44
2:C:20:GLU:HG3	2:C:21:ILE:N	2.32	0.44
2:C:880:MET:HE3	2:C:880:MET:HB2	1.80	0.44
3:D:363:ALA:HB2	3:D:381:ALA:HA	2.00	0.44
3:D:699:VAL:HG13	3:D:760:ARG:HD2	1.98	0.44
3:D:832:ARG:H	3:D:832:ARG:HG2	1.64	0.44
3:D:1285:GLU:HB3	3:D:1290:LEU:HD13	1.99	0.44
5:F:193:ARG:CB	7:H:6:DT:H1'	2.39	0.44
5:F:223:ALA:HB2	5:F:242:TRP:CG	2.52	0.44
1:A:11:PHE:HB3	1:B:227:ASN:O	2.17	0.44
2:C:400:PRO:HB3	2:C:591:SER:OG	2.18	0.44
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.99	0.44
3:D:1389:LEU:HD12	3:D:1415:VAL:HG11	1.99	0.44
3:D:1464:GLU:CD	3:D:1464:GLU:H	2.23	0.44
2:C:207:LEU:HD13	2:C:221:LEU:CD2	2.47	0.44
2:C:469:THR:HG23	2:C:471:TYR:CE2	2.53	0.44
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.17	0.44
4:E:61:VAL:O	4:E:65:MET:HG3	2.18	0.44
4:E:89:MET:SD	4:E:90:GLU:N	2.89	0.44
5:F:356:LYS:O	5:F:360:LYS:HG3	2.18	0.44
3:D:190:GLU:HB3	3:D:196:VAL:HG12	2.00	0.44
3:D:206:ARG:HA	3:D:206:ARG:HD3	1.82	0.44
3:D:421:LEU:HD13	3:D:444:VAL:HG11	2.00	0.44
1:A:6:LEU:HD22	1:A:6:LEU:HA	1.76	0.44
1:B:6:LEU:HD13	1:B:189:ARG:NH1	2.31	0.44
2:C:204:GLN:HB3	2:C:227:PHE:CE2	2.52	0.44
2:C:239:PHE:CD1	2:C:239:PHE:C	2.96	0.44
2:C:396:ASP:O	2:C:403:SER:N	2.51	0.44
2:C:626:ARG:HG3	2:C:626:ARG:NH1	2.32	0.44
3:D:401:TYR:CE2	3:D:428:LYS:O	2.71	0.44
3:D:433:GLY:HA2	3:D:449:SER:N	2.32	0.44
1:B:6:LEU:CD2	1:B:29:GLU:HG2	2.46	0.44
1:B:65:PHE:N	1:B:65:PHE:CD1	2.86	0.44
2:C:137:VAL:CG2	2:C:391:LEU:HD22	2.47	0.44
2:C:360:LEU:HD12	2:C:361:MET:CG	2.47	0.44
2:C:557:ARG:HG3	2:C:879:ARG:HB3	2.00	0.44
2:C:995:MET:HB2	2:C:995:MET:HE2	1.72	0.44
3:D:206:ARG:NH1	5:F:101:GLU:OE2	2.41	0.44
2:C:67:ASP:OD1	2:C:68:PHE:N	2.51	0.43
2:C:154:ARG:HB2	2:C:157:ARG:CG	2.48	0.43
2:C:580:MET:HE2	2:C:902:ILE:CD1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:700:TYR:OH	2:C:994:ILE:HB	2.18	0.43
3:D:86:ARG:CG	3:D:522:PRO:HG2	2.43	0.43
3:D:814:ALA:O	3:D:818:ARG:HG3	2.17	0.43
3:D:911:LEU:O	3:D:915:VAL:HG23	2.18	0.43
3:D:1208:ASP:OD1	3:D:1210:SER:N	2.50	0.43
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	2.00	0.43
4:E:41:GLU:O	4:E:45:ARG:HG3	2.17	0.43
2:C:192:PRO:HB2	2:C:194:VAL:HG22	1.99	0.43
2:C:272:ALA:N	2:C:464:LEU:HD22	2.33	0.43
2:C:998:TYR:CD1	2:C:998:TYR:C	2.96	0.43
3:D:767:HIS:HA	3:D:924:MET:CE	2.47	0.43
5:F:86:HIS:O	5:F:90:GLN:HG2	2.17	0.43
2:C:146:VAL:HG11	2:C:306:THR:HG23	2.00	0.43
2:C:156:GLY:C	2:C:157:ARG:NE	2.70	0.43
2:C:197:LEU:HA	2:C:200:LEU:HD12	1.99	0.43
2:C:393:GLN:OE1	9:C:1201:A1IF9:N44	2.51	0.43
3:D:420:VAL:HA	3:D:428:LYS:HA	1.99	0.43
3:D:491:LYS:HG3	3:D:492:ALA:N	2.33	0.43
3:D:544:TYR:O	3:D:548:ILE:HG13	2.18	0.43
3:D:1350:GLU:HG3	3:D:1354:LYS:HE3	1.98	0.43
3:D:1491:THR:O	3:D:1492:LEU:C	2.60	0.43
5:F:166:LEU:HD13	5:F:170:HIS:HB3	2.00	0.43
6:G:6:DA:H2'	6:G:7:DT:C6	2.53	0.43
7:H:10:DA:H2''	7:H:11:DG:O5'	2.18	0.43
1:A:201:THR:HG21	1:A:205:VAL:O	2.18	0.43
1:B:77:GLU:O	1:B:81:ASN:ND2	2.39	0.43
2:C:154:ARG:HB2	2:C:157:ARG:HG2	2.00	0.43
2:C:267:TYR:CE2	2:C:290:LEU:HG	2.54	0.43
2:C:750:LYS:HA	2:C:750:LYS:HD2	1.85	0.43
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.53	0.43
3:D:22:SER:HA	3:D:90:MET:O	2.18	0.43
3:D:25:GLU:HB3	3:D:92:HIS:NE2	2.33	0.43
3:D:646:LYS:HA	3:D:720:LEU:CD1	2.48	0.43
3:D:1057:VAL:CG1	3:D:1065:LEU:HD21	2.49	0.43
3:D:1208:ASP:OD1	3:D:1210:SER:HB3	2.18	0.43
3:D:1364:HIS:ND1	3:D:1366:LYS:HG3	2.33	0.43
3:D:1465:ASN:ND2	3:D:1473:PRO:HD3	2.33	0.43
5:F:340:SER:O	5:F:341:PRO:C	2.61	0.43
1:B:109:VAL:HG12	1:B:129:ILE:HB	1.99	0.43
2:C:50:GLU:CD	2:C:168:ARG:HH12	2.27	0.43
2:C:168:ARG:HD2	2:C:268:ASP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:729:LEU:HD23	2:C:734:LEU:HD11	2.00	0.43
3:D:1153:VAL:HG12	3:D:1160:LEU:HB2	1.99	0.43
3:D:1336:LEU:HD11	3:D:1419:PRO:HB2	2.00	0.43
4:E:87:LYS:HZ1	4:E:88:GLU:HG3	1.84	0.43
1:A:44:LEU:HB3	1:A:177:VAL:HG21	2.00	0.43
1:B:72:LYS:HG2	1:B:133:GLU:OE2	2.19	0.43
2:C:390:GLN:HE21	2:C:414:GLY:HA2	1.83	0.43
2:C:490:GLU:HA	2:C:493:ARG:HD2	2.00	0.43
3:D:187:LYS:NZ	3:D:198:ARG:HB2	2.32	0.43
3:D:637:LEU:O	3:D:935:LYS:NZ	2.51	0.43
5:F:360:LYS:O	5:F:361:LEU:HD23	2.18	0.43
1:A:55:SER:HB2	1:A:158:ILE:HB	2.01	0.43
2:C:26:TYR:OH	2:C:119:PRO:O	2.30	0.43
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.99	0.43
4:E:46:PRO:HB2	4:E:57:ASP:HB3	1.99	0.43
4:E:83:ASP:HA	4:E:86:GLN:CD	2.44	0.43
5:F:289:GLU:HG3	5:F:301:ALA:HB2	2.00	0.43
1:A:70:GLY:H	2:C:607:ASP:CG	2.27	0.43
2:C:168:ARG:HD2	2:C:268:ASP:CB	2.48	0.43
2:C:586:ARG:NH1	2:C:590:ASP:OD1	2.52	0.43
2:C:899:GLN:HG3	2:C:901:TYR:CZ	2.54	0.43
3:D:185:VAL:HG22	3:D:186:VAL:N	2.33	0.43
3:D:558:LEU:HD21	3:D:567:ILE:HG21	2.01	0.43
3:D:631:ILE:HG22	3:D:726:ILE:HB	2.01	0.43
3:D:674:ARG:O	3:D:678:GLU:HG2	2.18	0.43
3:D:1003:VAL:HG12	3:D:1003:VAL:H	1.52	0.43
5:F:86:HIS:HA	7:H:7:DG:H21	1.80	0.43
2:C:168:ARG:HG3	2:C:168:ARG:O	2.19	0.43
2:C:263:ASP:OD1	2:C:265:ARG:HG2	2.18	0.43
2:C:1067:TYR:CD1	2:C:1067:TYR:C	2.97	0.43
3:D:32:ILE:C	3:D:40:GLU:HG2	2.43	0.43
3:D:1281:VAL:CG1	3:D:1317:ASP:H	2.25	0.43
3:D:1433:SER:OG	3:D:1457:ASP:OD2	2.32	0.43
5:F:159:ILE:O	5:F:163:LEU:HG	2.19	0.43
5:F:323:ASP:OD1	5:F:323:ASP:C	2.62	0.43
1:A:79:ILE:CD1	1:A:167:VAL:HG11	2.49	0.43
1:A:215:VAL:CG1	1:B:222:LEU:HD12	2.36	0.43
1:B:32:PHE:HA	1:B:35:THR:HB	2.01	0.43
2:C:11:GLU:OE2	2:C:537:LYS:NZ	2.50	0.43
2:C:471:TYR:OH	2:C:516:ARG:NH2	2.52	0.43
3:D:519:VAL:HA	3:D:544:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:955:VAL:O	3:D:957:PRO:HD3	2.19	0.43
3:D:1311:LEU:HD12	3:D:1326:THR:HG22	2.00	0.43
1:B:211:LEU:O	1:B:215:VAL:HG23	2.18	0.42
2:C:170:PRO:HA	7:H:13:DT:H3	1.84	0.42
2:C:286:SER:OG	2:C:301:GLU:OE2	2.37	0.42
2:C:325:ILE:H	2:C:325:ILE:HG12	1.67	0.42
2:C:567:GLN:HB2	2:C:997:LEU:CD1	2.49	0.42
2:C:703:ILE:HG23	2:C:830:LYS:HG3	2.01	0.42
3:D:60:CYS:HB3	3:D:76:CYS:HB3	2.01	0.42
3:D:556:LYS:HE3	5:F:218:GLN:CG	2.48	0.42
3:D:991:GLN:HA	3:D:994:GLN:OE1	2.19	0.42
3:D:1046:GLN:CG	3:D:1052:THR:HG22	2.46	0.42
5:F:236:SER:HB2	7:H:5:DA:C8	2.54	0.42
1:A:169:ALA:HB1	1:A:171:PHE:CE1	2.54	0.42
2:C:64:LEU:HD22	2:C:102:HIS:CG	2.54	0.42
2:C:167:LYS:HB3	2:C:345:ARG:NH2	2.33	0.42
2:C:419:THR:H	2:C:422:ARG:HG2	1.85	0.42
2:C:901:TYR:CE2	2:C:917:LEU:HD13	2.54	0.42
2:C:1067:TYR:C	2:C:1067:TYR:HD1	2.27	0.42
3:D:172:PRO:O	3:D:175:VAL:HG12	2.18	0.42
3:D:584:ASN:OD1	3:D:585:GLY:N	2.52	0.42
3:D:681:ARG:H	3:D:681:ARG:HG2	1.61	0.42
3:D:867:ARG:HA	3:D:871:LYS:O	2.19	0.42
3:D:951:ILE:HG13	3:D:1062:ARG:HG3	2.01	0.42
3:D:1038:LEU:HD23	3:D:1061:PHE:HB2	2.01	0.42
4:E:89:MET:O	4:E:90:GLU:HB3	2.19	0.42
1:A:65:PHE:HB3	2:C:628:PHE:CD2	2.54	0.42
2:C:484:VAL:HG12	2:C:486:MET:HG2	2.00	0.42
2:C:517:ARG:NH2	2:C:524:VAL:HG11	2.34	0.42
2:C:596:TYR:CD1	2:C:654:LEU:HA	2.53	0.42
2:C:724:ARG:HD2	2:C:739:GLU:HA	2.00	0.42
3:D:963:TYR:CD1	3:D:1002:LYS:HD3	2.54	0.42
3:D:1304:LYS:O	3:D:1305:LEU:HD13	2.19	0.42
1:A:169:ALA:HB1	1:A:171:PHE:CZ	2.54	0.42
2:C:41:ASN:CG	2:C:41:ASN:O	2.62	0.42
2:C:98:LEU:HD12	2:C:113:VAL:HG21	2.00	0.42
2:C:222:MET:HE3	2:C:222:MET:HB3	1.84	0.42
2:C:417:GLY:C	2:C:418:LEU:HD23	2.44	0.42
2:C:726:ILE:HB	2:C:729:LEU:HD22	2.01	0.42
3:D:18:ILE:HG23	3:D:518:PRO:HG3	2.02	0.42
3:D:122:GLU:HA	3:D:125:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:505:SER:HB2	3:D:507:ASN:HD22	1.85	0.42
3:D:659:LYS:HD2	3:D:659:LYS:O	2.19	0.42
3:D:673:ALA:O	3:D:677:LEU:HG	2.19	0.42
3:D:1150:ALA:C	3:D:1151:ARG:HD3	2.44	0.42
5:F:188:ILE:O	5:F:192:LEU:HG	2.19	0.42
5:F:226:LYS:NZ	5:F:226:LYS:HB3	2.34	0.42
2:C:408:ARG:NH2	2:C:455:LEU:HD23	2.35	0.42
2:C:535:SER:HB2	2:C:536:PRO:HD2	2.01	0.42
2:C:600:ASP:OD1	2:C:651:LYS:N	2.52	0.42
2:C:1018:GLN:HG3	2:C:1063:ARG:HH22	1.84	0.42
3:D:86:ARG:HG2	3:D:523:ASP:CG	2.45	0.42
3:D:90:MET:HG3	3:D:521:PRO:HD3	2.01	0.42
3:D:92:HIS:CD2	3:D:92:HIS:C	2.97	0.42
3:D:696:HIS:CE1	4:E:57:ASP:OD1	2.73	0.42
5:F:130:VAL:HG21	5:F:159:ILE:HG21	2.00	0.42
2:C:164:PRO:HB3	2:C:267:TYR:CE1	2.54	0.42
2:C:202:TYR:OH	2:C:300:ASP:HB3	2.19	0.42
2:C:385:PHE:HD2	2:C:386:PHE:CE1	2.38	0.42
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.84	0.42
2:C:538:GLN:HG3	2:C:539:VAL:HG23	2.01	0.42
2:C:735:ARG:HH21	3:D:681:ARG:HH12	1.67	0.42
2:C:806:LEU:HA	2:C:806:LEU:HD12	1.77	0.42
3:D:105:VAL:HG22	3:D:112:ILE:HD12	2.00	0.42
3:D:569:ASN:O	3:D:573:MET:HG3	2.20	0.42
3:D:775:GLY:CA	3:D:1209:LEU:HB3	2.49	0.42
3:D:1126:ASP:O	3:D:1130:ARG:N	2.44	0.42
1:B:72:LYS:HG3	1:B:131:THR:HB	2.02	0.42
2:C:251:ASP:HB2	2:C:252:LYS:NZ	2.34	0.42
2:C:542:VAL:HG23	2:C:543:ASN:H	1.85	0.42
2:C:805:ARG:HG3	2:C:823:VAL:HG22	2.01	0.42
3:D:350:HIS:ND1	3:D:350:HIS:N	2.67	0.42
3:D:410:SER:HB3	5:F:178:ARG:NH1	2.35	0.42
3:D:907:GLU:OE2	3:D:910:SER:HB3	2.20	0.42
3:D:1036:ARG:O	3:D:1040:GLY:N	2.49	0.42
1:A:221:HIS:CE1	1:B:32:PHE:CE2	3.08	0.42
2:C:541:SER:OG	2:C:542:VAL:N	2.52	0.42
2:C:874:LEU:HG	3:D:1023:MET:SD	2.60	0.42
3:D:162:ARG:O	3:D:414:ARG:NH1	2.53	0.42
3:D:416:ALA:O	3:D:429:SER:HB3	2.20	0.42
3:D:434:ARG:HG2	3:D:447:VAL:HB	2.01	0.42
3:D:845:ASN:OD1	3:D:848:GLU:N	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:HIS:HD2	1:A:129:ILE:N	2.16	0.42
2:C:100:LEU:HG	2:C:102:HIS:NE2	2.34	0.42
2:C:710:ILE:CG1	2:C:790:LEU:HD22	2.50	0.42
2:C:722:ILE:HA	2:C:758:ARG:HA	2.01	0.42
2:C:874:LEU:HD11	3:D:787:LEU:HD22	2.02	0.42
3:D:95:LEU:HD11	3:D:517:VAL:HG13	2.02	0.42
3:D:849:ALA:O	3:D:853:VAL:HG23	2.20	0.42
3:D:1304:LYS:C	3:D:1304:LYS:HD2	2.44	0.42
3:D:1491:THR:O	3:D:1494:ALA:N	2.53	0.42
5:F:194:LEU:HD23	5:F:194:LEU:HA	1.81	0.42
1:A:58:ILE:O	1:A:61:VAL:HG22	2.20	0.42
1:B:41:ARG:HA	1:B:177:VAL:HG11	2.02	0.42
2:C:627:ARG:NH1	2:C:640:ARG:HG2	2.35	0.42
3:D:1190:SER:OG	3:D:1369:GLU:OE1	2.23	0.42
4:E:68:LEU:CD1	4:E:73:LEU:HB2	2.49	0.42
4:E:84:ARG:HA	4:E:87:LYS:HE3	2.02	0.42
5:F:276:ARG:O	5:F:280:GLN:HG2	2.20	0.42
5:F:300:ASP:OD1	5:F:303:ARG:HB2	2.20	0.42
1:B:209:GLU:O	1:B:213:GLN:HG3	2.19	0.41
2:C:355:VAL:O	2:C:359:MET:HE3	2.19	0.41
2:C:468:ARG:HD3	2:C:485:TYR:O	2.20	0.41
2:C:486:MET:HB3	2:C:490:GLU:HG2	2.02	0.41
3:D:350:HIS:HA	5:F:100:VAL:HG11	2.02	0.41
4:E:89:MET:SD	4:E:93:TYR:CD2	3.11	0.41
4:E:91:ARG:NH2	4:E:92:LEU:HD11	2.35	0.41
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.55	0.41
3:D:3:LYS:HD3	3:D:3:LYS:HA	1.97	0.41
3:D:206:ARG:NH1	5:F:101:GLU:CD	2.78	0.41
3:D:567:ILE:CG2	3:D:571:LYS:HE2	2.49	0.41
3:D:701:LEU:HD13	3:D:763:MET:HE1	2.03	0.41
1:B:42:ARG:NH2	10:D:1605:TRS:N	2.68	0.41
2:C:159:ILE:HD11	2:C:173:ASP:HB3	2.02	0.41
2:C:247:PRO:HG2	2:C:249:LYS:HE3	2.02	0.41
2:C:875:GLY:O	2:C:879:ARG:HD3	2.19	0.41
3:D:205:TYR:CD1	3:D:390:PRO:HG3	2.56	0.41
3:D:435:VAL:CG2	3:D:444:VAL:HG13	2.48	0.41
3:D:895:VAL:O	3:D:899:LEU:HG	2.20	0.41
3:D:984:THR:HG23	3:D:987:GLU:OE1	2.20	0.41
5:F:207:LEU:HD23	5:F:207:LEU:HA	1.83	0.41
1:A:143:ARG:HH11	1:A:143:ARG:HG3	1.86	0.41
1:A:186:LEU:O	1:A:188:GLN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:376:ARG:N	2:C:377:PRO:HD2	2.35	0.41
2:C:854:PRO:HB2	2:C:856:GLU:CD	2.46	0.41
2:C:893:ALA:HB2	2:C:918:LEU:HD23	2.02	0.41
3:D:81:THR:OG1	3:D:82:LYS:N	2.53	0.41
3:D:169:TYR:OH	3:D:198:ARG:CG	2.69	0.41
3:D:447:VAL:O	3:D:448:GLU:C	2.63	0.41
3:D:543:LEU:CD2	3:D:600:LEU:HD12	2.51	0.41
3:D:1484:THR:O	4:E:25:LYS:NZ	2.51	0.41
4:E:88:GLU:HB3	4:E:91:ARG:HH21	1.85	0.41
2:C:417:GLY:O	2:C:418:LEU:HD23	2.20	0.41
2:C:513:VAL:HG23	2:C:526:PRO:HD3	2.02	0.41
2:C:715:THR:HG22	2:C:717:LEU:H	1.85	0.41
3:D:176:ASP:OD1	3:D:388:HIS:HB3	2.20	0.41
3:D:1133:ARG:HE	3:D:1133:ARG:HB3	1.45	0.41
3:D:1277:ILE:O	3:D:1277:ILE:HD12	2.20	0.41
3:D:1278:ASP:HB3	3:D:1321:ALA:H	1.85	0.41
5:F:101:GLU:O	5:F:105:LYS:HG3	2.21	0.41
5:F:277:GLN:HA	5:F:280:GLN:HE21	1.84	0.41
5:F:302:LYS:O	5:F:306:GLU:HG3	2.20	0.41
5:F:380:GLU:CD	5:F:380:GLU:H	2.27	0.41
1:A:48:ILE:HG22	1:A:173:PRO:HD2	2.03	0.41
1:A:53:VAL:CG2	1:A:82:LEU:CD2	2.92	0.41
1:B:206:THR:HG22	1:B:207:PRO:HD2	2.03	0.41
2:C:129:ILE:HB	2:C:134:ARG:HD2	2.02	0.41
2:C:595:LEU:HG	2:C:655:LEU:HD12	2.02	0.41
2:C:1013:TYR:HD2	2:C:1063:ARG:NH2	2.18	0.41
2:C:1099:VAL:HA	3:D:9:ARG:O	2.20	0.41
5:F:95:THR:O	5:F:96:LEU:C	2.64	0.41
2:C:16:PRO:HG3	2:C:460:ARG:HH21	1.86	0.41
2:C:276:LYS:HD2	2:C:276:LYS:HA	1.73	0.41
2:C:878:SER:HA	3:D:1034:GLN:OE1	2.21	0.41
2:C:1008:ARG:NE	3:D:624:ASP:OD1	2.53	0.41
3:D:41:ARG:HG3	3:D:48:ARG:NH2	2.34	0.41
3:D:505:SER:HB2	3:D:507:ASN:ND2	2.36	0.41
3:D:676:MET:HE3	3:D:682:ASP:O	2.21	0.41
4:E:36:LYS:HB2	4:E:93:TYR:CD1	2.55	0.41
5:F:267:THR:O	5:F:271:LEU:HD12	2.20	0.41
1:A:51:THR:HG22	1:A:146:ARG:CB	2.48	0.41
2:C:19:THR:O	2:C:23:VAL:HG22	2.20	0.41
2:C:580:MET:HB2	2:C:902:ILE:HG13	2.01	0.41
2:C:620:LEU:HD23	2:C:620:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:710:ILE:HG12	2:C:790:LEU:HD22	2.02	0.41
2:C:876:VAL:HG22	2:C:884:GLN:NE2	2.36	0.41
3:D:39:PRO:HG2	3:D:47:GLU:HG3	2.01	0.41
3:D:104:PHE:O	3:D:112:ILE:HG13	2.19	0.41
4:E:38:THR:HG23	4:E:67:GLU:OE2	2.20	0.41
1:A:53:VAL:CB	1:A:82:LEU:HD21	2.48	0.41
1:A:190:THR:HG23	1:A:191:ASP:H	1.86	0.41
1:B:63:HIS:CD2	1:B:63:HIS:H	2.38	0.41
1:B:73:GLU:OE2	1:B:128:HIS:CE1	2.73	0.41
2:C:8:ARG:N	2:C:907:ASP:OD1	2.52	0.41
2:C:121:MET:HB2	2:C:127:PHE:CE1	2.56	0.41
2:C:477:GLY:O	2:C:507:ARG:HG3	2.20	0.41
2:C:498:GLN:HB2	2:C:514:VAL:HG23	2.03	0.41
2:C:690:ILE:HG13	2:C:852:ILE:HG23	2.02	0.41
3:D:132:TYR:HA	3:D:456:MET:HG3	2.02	0.41
3:D:169:TYR:HE2	3:D:198:ARG:HG2	1.86	0.41
3:D:477:LEU:HD21	3:D:495:ARG:NH1	2.36	0.41
3:D:792:ILE:HG13	3:D:793:THR:HG23	2.02	0.41
3:D:1144:LEU:O	3:D:1147:ARG:HB2	2.21	0.41
3:D:1149:LEU:HD13	3:D:1166:LEU:HD21	2.02	0.41
3:D:1290:LEU:HB3	3:D:1307:LYS:HA	2.03	0.41
3:D:1471:LEU:HD21	3:D:1477:GLY:CA	2.50	0.41
5:F:353:GLU:HG3	5:F:421:PHE:CZ	2.55	0.41
1:A:226:SER:O	1:A:228:PRO:HD3	2.20	0.41
2:C:95:TYR:HB3	2:C:112:GLU:HG2	2.02	0.41
2:C:146:VAL:CG2	2:C:162:ILE:HG12	2.40	0.41
2:C:437:ARG:HB3	2:C:467:ILE:HG21	2.02	0.41
2:C:458:TYR:HB3	2:C:470:PRO:HG3	2.02	0.41
2:C:491:GLU:O	2:C:496:ILE:HD11	2.21	0.41
2:C:749:VAL:O	2:C:750:LYS:HD2	2.21	0.41
2:C:772:ARG:HG3	5:F:373:LYS:HD2	2.02	0.41
3:D:401:TYR:HE2	3:D:429:SER:CA	2.31	0.41
3:D:421:LEU:HD13	3:D:444:VAL:CG1	2.51	0.41
5:F:327:SER:HG	6:G:19:DG:H1	1.69	0.41
1:A:156:HIS:CE1	1:A:167:VAL:O	2.72	0.40
1:A:201:THR:HG22	1:A:202:ASP:N	2.36	0.40
1:B:106:PRO:HB3	1:B:133:GLU:HA	2.03	0.40
2:C:56:GLU:HB2	2:C:359:MET:SD	2.61	0.40
2:C:169:GLY:HA3	2:C:267:TYR:HD1	1.85	0.40
2:C:439:CYS:HB2	2:C:541:SER:HB2	2.03	0.40
2:C:588:VAL:HG23	2:C:588:VAL:H	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:901:TYR:HE2	2:C:917:LEU:HD13	1.85	0.40
3:D:416:ALA:HA	3:D:432:TYR:HA	2.02	0.40
3:D:508:ARG:HD3	3:D:508:ARG:HA	1.85	0.40
3:D:875:THR:HG21	3:D:902:LEU:HD23	2.02	0.40
3:D:1166:LEU:HD23	3:D:1166:LEU:HA	1.82	0.40
3:D:1463:LYS:HE2	3:D:1463:LYS:HB3	1.85	0.40
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.89	0.40
1:A:107:LYS:HE3	1:A:107:LYS:HB3	1.94	0.40
1:A:206:THR:OG1	1:A:207:PRO:HD2	2.21	0.40
1:B:38:ASN:O	1:B:39:PRO:C	2.63	0.40
2:C:13:ILE:CD1	2:C:483:VAL:HG11	2.51	0.40
2:C:230:ARG:HB3	2:C:233:GLU:OE1	2.21	0.40
2:C:344:PHE:HD1	2:C:382:ILE:HD11	1.86	0.40
3:D:984:THR:OG1	3:D:987:GLU:HG3	2.20	0.40
2:C:247:PRO:HG3	7:H:7:DG:C5	2.57	0.40
3:D:207:PHE:HB2	3:D:391:ALA:HB3	2.04	0.40
3:D:1139:ASP:OD1	3:D:1357:ARG:HD3	2.21	0.40
5:F:113:ILE:HD13	5:F:128:ARG:HA	2.02	0.40
5:F:131:VAL:O	5:F:135:ILE:HG12	2.21	0.40
2:C:833:LEU:HD12	2:C:833:LEU:HA	1.92	0.40
2:C:1067:TYR:HE1	2:C:1071:ILE:HG21	1.87	0.40
3:D:824:ASN:ND2	3:D:862:ASP:OD1	2.38	0.40
5:F:131:VAL:CG1	5:F:181:GLU:HG3	2.49	0.40
1:A:20:TYR:HD1	1:A:21:GLY:H	1.69	0.40
1:A:97:VAL:HG22	1:A:98:THR:H	1.87	0.40
1:A:156:HIS:ND1	1:A:157:GLY:N	2.70	0.40
2:C:468:ARG:CD	2:C:485:TYR:HB3	2.52	0.40
2:C:535:SER:O	2:C:538:GLN:HG2	2.21	0.40
3:D:112:ILE:HG12	3:D:512:MET:CE	2.37	0.40
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.54	0.40
3:D:171:LEU:HD13	3:D:392:SER:HA	2.04	0.40
3:D:500:ARG:HH11	3:D:500:ARG:HG3	1.87	0.40
3:D:591:VAL:O	3:D:600:LEU:HG	2.21	0.40
3:D:633:VAL:HB	3:D:740:PHE:CE2	2.56	0.40
3:D:797:LYS:HZ2	3:D:826:PRO:HG3	1.87	0.40
3:D:1031:ASN:OD1	3:D:1034:GLN:CD	2.65	0.40
4:E:48:MET:O	4:E:48:MET:HG3	2.22	0.40
5:F:236:SER:OG	7:H:5:DA:OP2	2.34	0.40
5:F:354:LEU:HD13	5:F:418:LEU:HD21	2.03	0.40
5:F:360:LYS:HD3	5:F:411:HIS:HB3	2.04	0.40
5:F:386:VAL:CG1	5:F:397:ILE:HD12	2.39	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	226/315 (72%)	202 (89%)	24 (11%)	0	100	100
1	B	224/315 (71%)	216 (96%)	8 (4%)	0	100	100
2	C	1110/1119 (99%)	1037 (93%)	73 (7%)	0	100	100
3	D	1353/1524 (89%)	1287 (95%)	66 (5%)	0	100	100
4	E	92/99 (93%)	86 (94%)	6 (6%)	0	100	100
5	F	335/444 (76%)	318 (95%)	17 (5%)	0	100	100
All	All	3340/3816 (88%)	3146 (94%)	194 (6%)	0	100	100

There are no Ramachandran outliers to report.

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%)	193 (97%)	6 (3%)	36	69
1	B	198/273 (72%)	196 (99%)	2 (1%)	73	88
2	C	935/941 (99%)	928 (99%)	7 (1%)	81	91
3	D	1128/1279 (88%)	1111 (98%)	17 (2%)	60	83
4	E	81/88 (92%)	81 (100%)	0	100	100
5	F	293/389 (75%)	283 (97%)	10 (3%)	32	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2834/3243 (87%)	2792 (98%)	42 (2%)	60 83

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	62	LEU
1	A	107	LYS
1	A	129	ILE
1	A	132	LEU
1	A	158	ILE
1	B	25	LEU
1	B	112	ARG
2	C	3	ILE
2	C	111	ASP
2	C	310	LEU
2	C	375	SER
2	C	581	THR
2	C	806	LEU
2	C	1084	SER
3	D	154	THR
3	D	396	VAL
3	D	459	GLU
3	D	496	LEU
3	D	525	ARG
3	D	547	LEU
3	D	693	GLU
3	D	720	LEU
3	D	808	THR
3	D	1003	VAL
3	D	1149	LEU
3	D	1209	LEU
3	D	1261	GLU
3	D	1282	ARG
3	D	1304	LYS
3	D	1346	ARG
3	D	1394	VAL
5	F	115	LYS
5	F	151	LEU
5	F	228	GLU
5	F	333	ILE
5	F	335	ASP

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Mol	Chain	Res	Type
5	F	338	LEU
5	F	375	LEU
5	F	380	GLU
5	F	394	ARG
5	F	414	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	A	212	ASN
1	B	63	HIS
1	B	124	ASN
1	B	188	GLN
2	C	22	GLN
2	C	117	HIS
2	C	179	ASN
2	C	538	GLN
2	C	563	ASN
2	C	565	GLN
2	C	884	GLN
2	C	962	GLN
2	C	1100	GLN
3	D	125	GLN
3	D	569	ASN
3	D	617	ASN
3	D	640	HIS
3	D	696	HIS
3	D	703	ASN
3	D	724	GLN
3	D	762	GLN
3	D	1254	GLN
3	D	1359	GLN
3	D	1404	ASN
3	D	1485	GLN
4	E	28	GLN
5	F	86	HIS
5	F	214	GLN
5	F	280	GLN
5	F	337	HIS
5	F	411	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\# Z > 2$
10	TRS	C	1202	-	7,7,7	0.14	0	9,9,9	0.20	0
10	TRS	D	1605	-	7,7,7	0.13	0	9,9,9	0.25	0
9	A1IF9	C	1201	8	46,59,59	0.93	3 (6%)	50,93,93	0.85	1 (2%)

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
10	TRS	C	1202	-	-	0/9/9/9	-
10	TRS	D	1605	-	-	0/9/9/9	-
9	A1IF9	C	1201	8	-	10/30/70/70	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1201	A1IF9	C10-N9	-2.72	1.30	1.35
9	C	1201	A1IF9	C8-C2	-2.23	1.42	1.47
9	C	1201	A1IF9	O46-C31	2.18	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1201	A1IF9	O1-C2-C8	2.19	128.64	124.37

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1201	A1IF9	C15-O16-P17-O19
9	C	1201	A1IF9	C29-O28-P26-O27
9	C	1201	A1IF9	C29-O28-P26-O47
9	C	1201	A1IF9	C30-C29-O28-P26
9	C	1201	A1IF9	P20-O22-P23-O24
9	C	1201	A1IF9	C15-O16-P17-O18
9	C	1201	A1IF9	C15-O16-P17-O50
9	C	1201	A1IF9	C29-O28-P26-O25
9	C	1201	A1IF9	P23-O25-P26-O27
9	C	1201	A1IF9	O28-C29-C30-O34

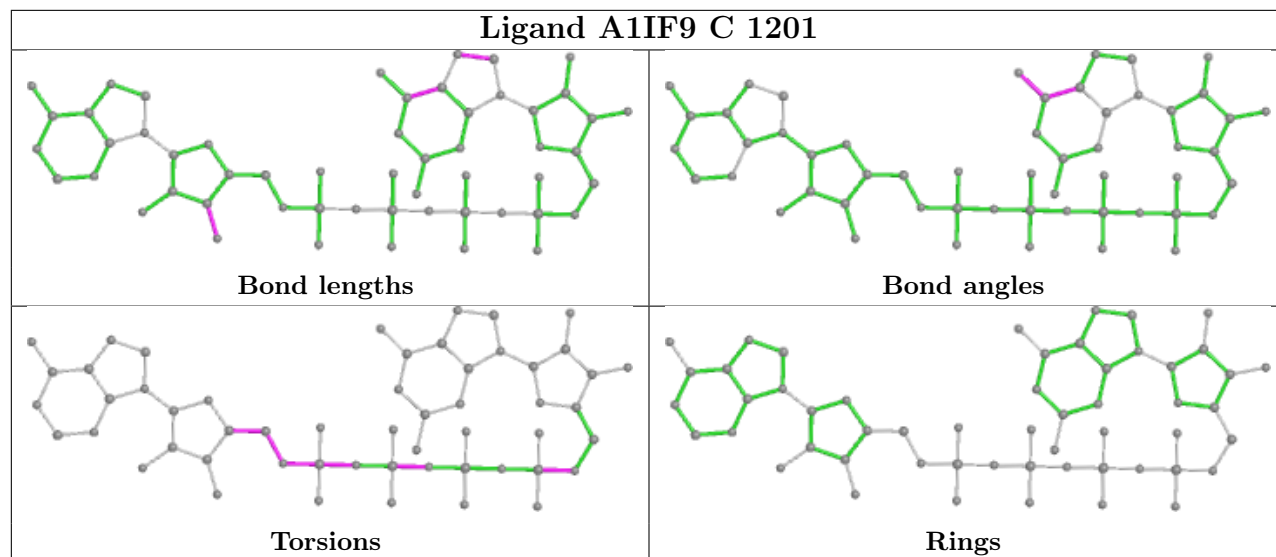
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	1605	TRS	1	0
9	C	1201	A1IF9	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	227/315 (72%)	0.69	19 (8%) 18 10	37, 71, 91, 105	1 (0%)
1	B	226/315 (71%)	0.12	0 100 100	33, 54, 79, 93	0
2	C	1113/1119 (99%)	0.71	84 (7%) 22 12	20, 75, 119, 146	1 (0%)
3	D	1357/1524 (89%)	0.55	148 (10%) 12 7	19, 56, 174, 222	3 (0%)
4	E	94/99 (94%)	0.79	7 (7%) 22 12	39, 75, 104, 109	0
5	F	338/444 (76%)	1.34	71 (21%) 3 2	43, 89, 114, 143	1 (0%)
6	G	15/22 (68%)	0.82	2 (13%) 8 5	43, 69, 127, 130	0
7	H	22/27 (81%)	1.78	7 (31%) 1 1	88, 109, 144, 157	0
All	All	3392/3865 (87%)	0.68	338 (9%) 14 8	19, 70, 136, 222	6 (0%)

All (338) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	216	VAL	6.4
3	D	409	VAL	5.3
3	D	365	ASP	5.1
2	C	63	GLY	4.9
3	D	207	PHE	4.7
3	D	354	VAL	4.7
3	D	355	VAL	4.6
3	D	408	GLU	4.6
3	D	367	ILE	4.6
2	C	372	LEU	4.5
5	F	418	LEU	4.3
3	D	566	ILE	4.3
3	D	349	PRO	4.3
3	D	202	VAL	4.3
7	H	5	DA	4.2
3	D	390	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
3	D	211	VAL	4.2
5	F	196	VAL	4.2
5	F	156	VAL	4.2
3	D	374	GLU	4.2
3	D	377	VAL	4.1
3	D	362	GLU	4.0
2	C	92	ALA	4.0
3	D	393	ILE	3.9
3	D	353	VAL	3.9
3	D	204	LEU	3.9
3	D	443	VAL	3.9
3	D	205	TYR	3.9
3	D	558	LEU	3.9
3	D	445	ARG	3.9
3	D	212	ARG	3.8
3	D	440	VAL	3.8
3	D	380	GLU	3.8
3	D	49	ILE	3.8
3	D	350	HIS	3.8
3	D	356	PRO	3.7
3	D	436	GLU	3.7
3	D	381	ALA	3.7
3	D	395	VAL	3.7
5	F	216	GLY	3.6
3	D	394	LEU	3.6
5	F	131	VAL	3.6
5	F	310	ILE	3.6
3	D	368	VAL	3.6
5	F	375	LEU	3.6
3	D	371	ILE	3.6
5	F	243	ILE	3.6
3	D	366	LYS	3.6
3	D	370	ALA	3.6
3	D	352	ASN	3.6
3	D	159[A]	ARG	3.5
3	D	361	VAL	3.5
2	C	25	SER	3.5
3	D	343	LYS	3.5
3	D	215	TYR	3.5
3	D	43	GLY	3.5
7	H	1	DT	3.5
3	D	386	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
3	D	470	LEU	3.4
5	F	221	ILE	3.4
2	C	771	GLU	3.4
3	D	407	VAL	3.4
5	F	217	ASN	3.4
3	D	171	LEU	3.4
3	D	666	ILE	3.4
5	F	229	TYR	3.4
3	D	203	ALA	3.4
5	F	195	VAL	3.4
3	D	360	ARG	3.3
5	F	224	VAL	3.3
2	C	776	SER	3.3
3	D	437	VAL	3.3
3	D	452	ILE	3.3
3	D	410	SER	3.3
3	D	347	VAL	3.3
3	D	446	VAL	3.3
2	C	778	PHE	3.3
1	A	99	LEU	3.3
2	C	18	LEU	3.3
2	C	618	GLY	3.2
3	D	44	LEU	3.2
2	C	485	TYR	3.2
3	D	384	VAL	3.2
3	D	379	ALA	3.2
3	D	378	ILE	3.2
3	D	422	ALA	3.2
3	D	183	GLU	3.2
1	A	68	ILE	3.2
6	G	19	DG	3.2
5	F	151	LEU	3.2
5	F	210	LEU	3.2
5	F	124	PRO	3.1
2	C	605	LYS	3.1
2	C	608	GLY	3.1
3	D	430	ASP	3.1
5	F	174	LEU	3.1
3	D	687	VAL	3.1
3	D	1486	VAL	3.1
6	G	20	DC	3.1
3	D	80	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
3	D	214	GLU	3.0
3	D	444	VAL	3.0
5	F	377	ASP	3.0
4	E	39	VAL	3.0
2	C	269	LEU	3.0
3	D	387	LEU	3.0
3	D	449	SER	3.0
2	C	469	THR	3.0
3	D	415	VAL	3.0
3	D	434	ARG	3.0
3	D	369	ALA	3.0
3	D	385	VAL	2.9
3	D	421	LEU	2.9
2	C	789	SER	2.9
3	D	680	GLN	2.9
3	D	382	GLU	2.9
5	F	190	ALA	2.9
3	D	178	LEU	2.9
4	E	30	LEU	2.9
5	F	364	ARG	2.9
3	D	425	GLY	2.9
5	F	127	ILE	2.9
5	F	95	THR	2.9
3	D	424	GLY	2.9
5	F	81	VAL	2.9
3	D	208	PRO	2.9
3	D	345	TYR	2.9
1	A	73	GLU	2.8
2	C	764	GLU	2.8
2	C	376	ARG	2.8
2	C	207	LEU	2.8
3	D	166	GLN	2.8
3	D	213	VAL	2.8
3	D	442	ASN	2.8
2	C	711	GLU	2.8
1	A	67	THR	2.8
5	F	91	VAL	2.8
5	F	183	ALA	2.8
5	F	422	LEU	2.8
2	C	606	VAL	2.8
2	C	607	ASP	2.8
3	D	426	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
5	F	325	LYS	2.8
1	A	135	GLY	2.8
2	C	763	GLY	2.8
3	D	560	GLN	2.8
5	F	381	HIS	2.8
4	E	85	LEU	2.8
3	D	1319	VAL	2.8
5	F	244[A]	ARG	2.7
3	D	179	VAL	2.7
3	D	439	LEU	2.7
5	F	202	TYR	2.7
2	C	638	ASP	2.7
5	F	260	ILE	2.7
5	F	163	LEU	2.7
2	C	458	TYR	2.7
3	D	979	GLU	2.7
7	H	4	DA	2.7
3	D	412	GLY	2.6
2	C	102	HIS	2.6
2	C	825	VAL	2.6
5	F	247	ILE	2.6
5	F	236	SER	2.6
3	D	547	LEU	2.6
5	F	180	GLY	2.6
3	D	657	LEU	2.6
3	D	84	ILE	2.6
5	F	373	LYS	2.6
2	C	741	GLY	2.6
5	F	130	VAL	2.6
5	F	165	SER	2.6
2	C	632	ASN	2.6
3	D	1495	ILE	2.5
5	F	404	ALA	2.5
3	D	413	ASP	2.5
3	D	71	LYS	2.5
3	D	36	THR	2.5
2	C	57	GLU	2.5
2	C	65	VAL	2.5
3	D	181	ASP	2.5
5	F	253	ASP	2.5
2	C	823	VAL	2.5
4	E	42	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	397	GLU	2.5
2	C	748	GLU	2.5
3	D	74	GLU	2.5
2	C	754	ILE	2.5
1	A	101	LEU	2.5
2	C	320	HIS	2.5
7	H	20	DG	2.5
3	D	432	TYR	2.5
5	F	291	ILE	2.4
3	D	359	ALA	2.4
3	D	1318	TYR	2.4
2	C	382	ILE	2.4
5	F	215	GLU	2.4
2	C	781	LYS	2.4
2	C	223	ASP	2.4
3	D	406	ASP	2.4
3	D	76	CYS	2.4
2	C	101	ILE	2.4
2	C	460	ARG	2.4
2	C	755	LEU	2.4
4	E	92	LEU	2.4
1	A	133	GLU	2.4
2	C	262	ALA	2.4
3	D	373	PRO	2.4
3	D	176	ASP	2.4
3	D	685	ASP	2.4
3	D	1279	GLY	2.4
3	D	63	TYR	2.4
2	C	115	LEU	2.4
3	D	161	LEU	2.4
2	C	111	ASP	2.4
2	C	191	PHE	2.4
5	F	111	GLU	2.4
3	D	454	ALA	2.4
2	C	149	THR	2.4
3	D	411	THR	2.4
3	D	1128	VAL	2.4
1	A	85	LEU	2.3
1	A	129	ILE	2.3
7	H	6	DT	2.3
2	C	1061	GLU	2.3
1	A	70	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	272	ALA	2.3
3	D	670	VAL	2.3
5	F	242	TRP	2.3
5	F	341	PRO	2.3
2	C	749	VAL	2.3
3	D	447	VAL	2.3
3	D	180	LYS	2.3
3	D	981	GLY	2.3
5	F	171	LYS	2.3
2	C	806	LEU	2.3
1	A	58	ILE	2.3
2	C	54	ILE	2.3
2	C	37	GLU	2.3
2	C	804	VAL	2.3
3	D	564	GLU	2.3
5	F	189	GLU	2.3
2	C	736	ASP	2.3
4	E	58	PRO	2.3
5	F	280	GLN	2.3
7	H	2	DA	2.3
5	F	164	LYS	2.3
1	A	130	ALA	2.3
2	C	260	LEU	2.3
5	F	116	LEU	2.3
3	D	405	ASP	2.2
2	C	51	THR	2.2
3	D	535	PHE	2.2
1	A	57	TYR	2.2
3	D	34	TYR	2.2
1	A	72	LYS	2.2
2	C	125	GLY	2.2
2	C	242	LEU	2.2
2	C	620	LEU	2.2
3	D	182	GLY	2.2
5	F	126	LEU	2.2
5	F	248	ASN	2.2
5	F	178	ARG	2.2
3	D	39	PRO	2.2
3	D	81	THR	2.2
2	C	219	GLN	2.2
5	F	214	GLN	2.2
3	D	26	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
4	E	95	VAL	2.2
5	F	258	ILE	2.2
5	F	235	PHE	2.2
3	D	668	PRO	2.2
2	C	461	VAL	2.2
2	C	645	VAL	2.2
2	C	655	LEU	2.2
3	D	189	GLN	2.2
1	A	164	ALA	2.2
2	C	459	ALA	2.2
5	F	175	HIS	2.2
5	F	241	TRP	2.2
2	C	1009	SER	2.2
3	D	429	SER	2.2
2	C	352	ALA	2.1
3	D	348	GLN	2.2
5	F	83	GLN	2.2
7	H	13	DT	2.2
3	D	565	ILE	2.1
2	C	298	PHE	2.1
2	C	513	VAL	2.1
2	C	534	VAL	2.1
2	C	774	LEU	2.1
2	C	790	LEU	2.1
3	D	431	VAL	2.1
3	D	1294	VAL	2.1
2	C	289	THR	2.1
3	D	669	ASN	2.1
2	C	457	ALA	2.1
3	D	66	GLN	2.1
3	D	139	GLY	2.1
3	D	364	GLY	2.1
5	F	219	GLY	2.1
2	C	466	PHE	2.1
3	D	1295	GLU	2.1
5	F	383	LEU	2.1
3	D	1286	THR	2.1
5	F	176	ILE	2.1
3	D	165	LYS	2.1
2	C	344	PHE	2.1
2	C	233	GLU	2.1
3	D	52	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	357	GLU	2.1
3	D	191	LEU	2.1
1	A	71	VAL	2.1
2	C	355	VAL	2.1
5	F	160	ASP	2.1
1	A	94	LEU	2.1
2	C	244	PRO	2.1
3	D	396	VAL	2.1
5	F	234	LYS	2.1
2	C	615	TYR	2.1
2	C	810	ASP	2.1
2	C	77	PRO	2.1
2	C	613	VAL	2.1
5	F	135	ILE	2.0
5	F	162	LYS	2.0
2	C	812	GLY	2.0
1	A	131	THR	2.0
3	D	392	SER	2.0
1	A	163	ASN	2.0
5	F	255	ALA	2.0
3	D	520	LEU	2.0
3	D	1492	LEU	2.0
5	F	304	VAL	2.0
2	C	36	PRO	2.0
5	F	396	ARG	2.0
3	D	40	GLU	2.0
5	F	336	GLU	2.0
5	F	380	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

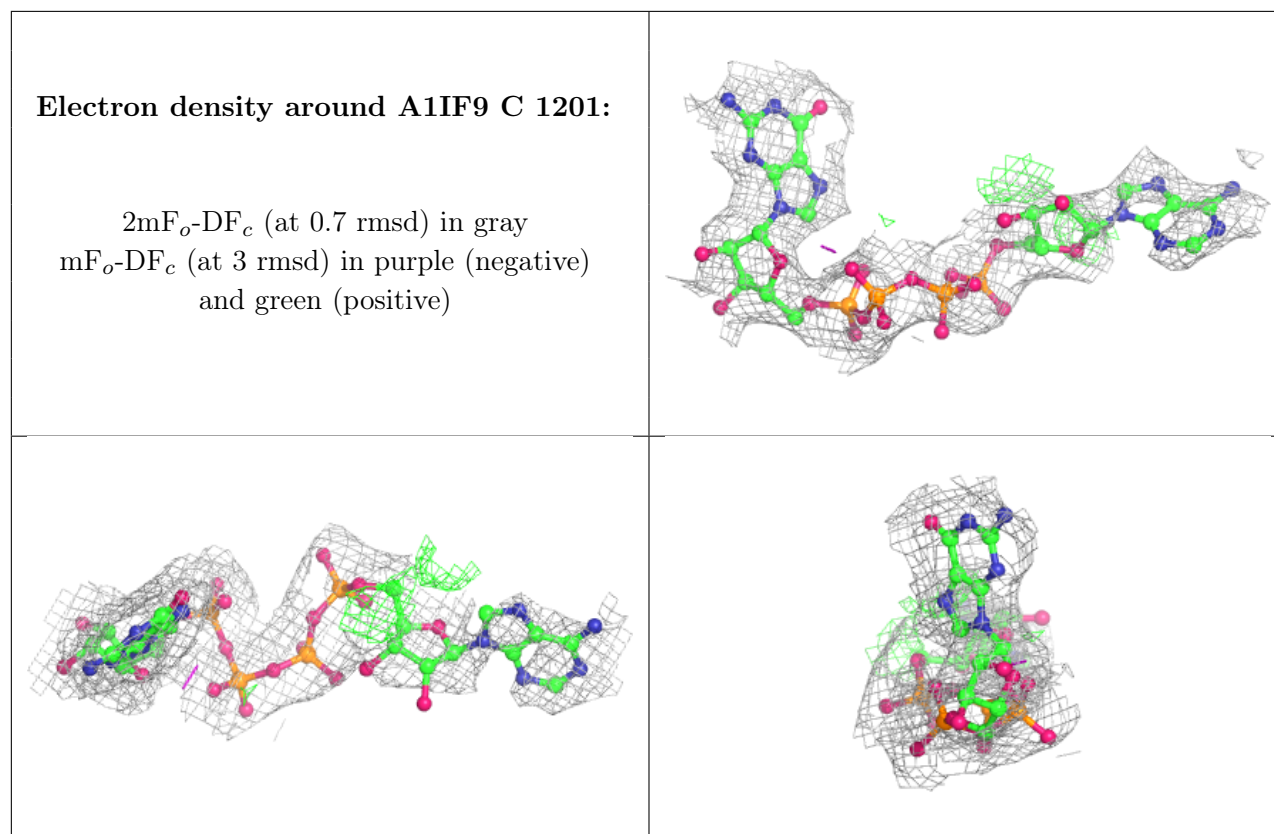
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
10	TRS	D	1605	8/8	0.61	0.21	31,37,45,47	0
10	TRS	C	1202	8/8	0.64	0.21	41,51,56,56	0
11	ZN	D	1602	1/1	0.80	0.12	174,174,174,174	0
8	MG	A	401	1/1	0.83	0.24	60,60,60,60	0
9	A1IF9	C	1201	54/54	0.89	0.11	37,47,66,68	21
8	MG	B	401	1/1	0.90	0.20	32,32,32,32	0
8	MG	D	1604	1/1	0.93	0.08	36,36,36,36	0
11	ZN	D	1601	1/1	0.97	0.04	36,36,36,36	0
8	MG	D	1603	1/1	0.98	0.03	25,25,25,25	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 ⓘ

There are no such residues in this entry.