



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2023 – 11:52 AM EDT

PDB ID : 4OIR
Title : Crystal structure of Thermus thermophilus RNA polymerase transcription initiation complex soaked with GE23077 and rifamycin SV
Authors : Zhang, Y.; Ebright, R.H.; Arnold, E.
Deposited on : 2014-01-20
Resolution : 3.10 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

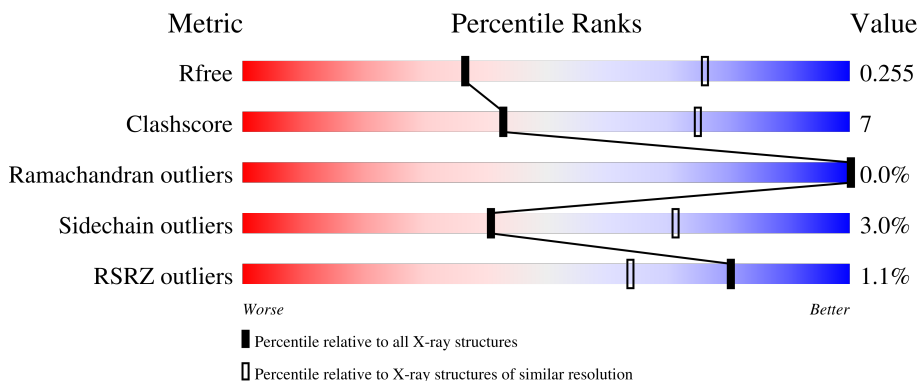
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



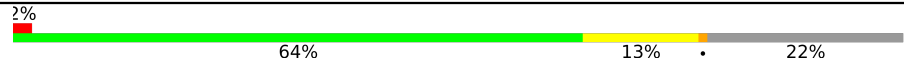
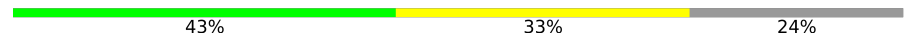
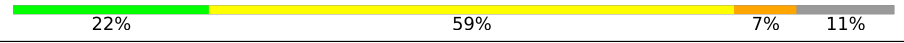

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	305	
1	B	305	
2	C	1119	
3	D	1524	
4	E	99	

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Mol	Chain	Length	Quality of chain
5	F	443	 <p>2% 64% 13% 22%</p>
6	G	21	 <p>43% 33% 24%</p>
7	H	27	 <p>22% 59% 7% 11%</p>
8	I	7	 <p>43% 29% 29%</p>

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 28730 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
			Total	C	N	O	S			
1	A	231	Total	C	N	O	S	0	0	0
			1809	1155	315	337	2			
1	B	227	Total	C	N	O	S	0	0	0
			1789	1143	310	334	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1112	Total	C	N	O	S	0	0	0
			8774	5550	1565	1635	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1485	Total	C	N	O	S	0	1	0
			11739	7441	2069	2193	36			

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

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

- Molecule 5 is a protein called DNA directed RNA polymerase sigma factor A.

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

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	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	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	16	Total	C	N	O	P	0	0	0
			328	156	63	94	15			

- Molecule 7 is a DNA chain called 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*C P*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

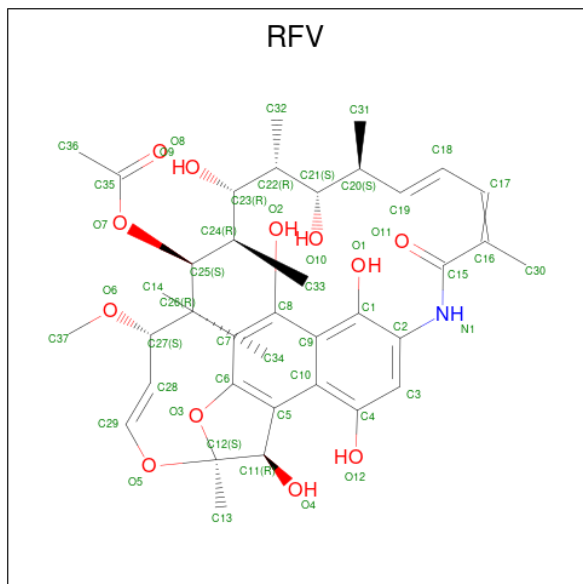
- Molecule 8 is a protein called GE23077.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	7	Total	C	N	O	0	0	0
			50	26	9	15			

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Mg 1 1	0	0
9	D	2	Total Mg 2 2	0	0
9	F	1	Total Mg 1 1	0	0

- Molecule 10 is rifamycin SV (three-letter code: RFV) (formula: C₃₇H₄₉NO₁₂).

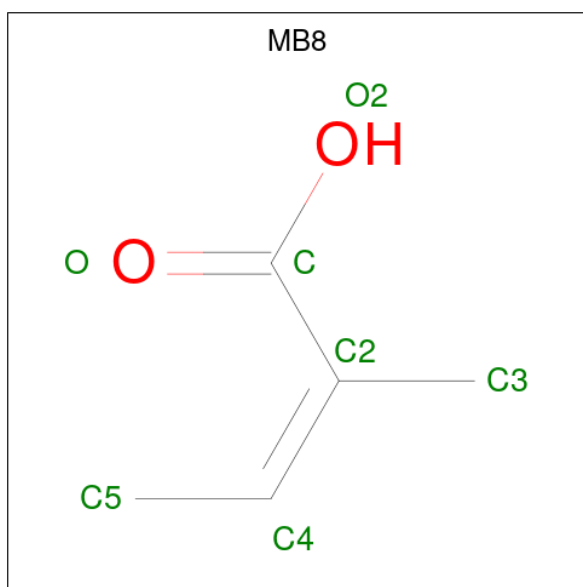


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total C N O 50 37 1 12	0	0

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

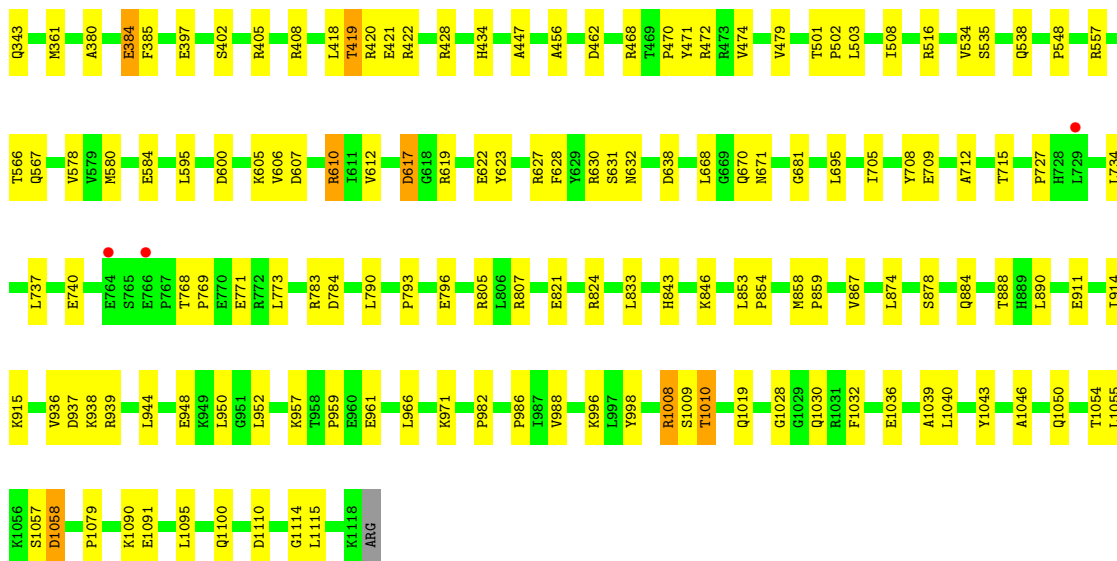
- Molecule 12 is (2Z)-2-methylbut-2-enoic acid (three-letter code: MB8) (formula: C₅H₈O₂).



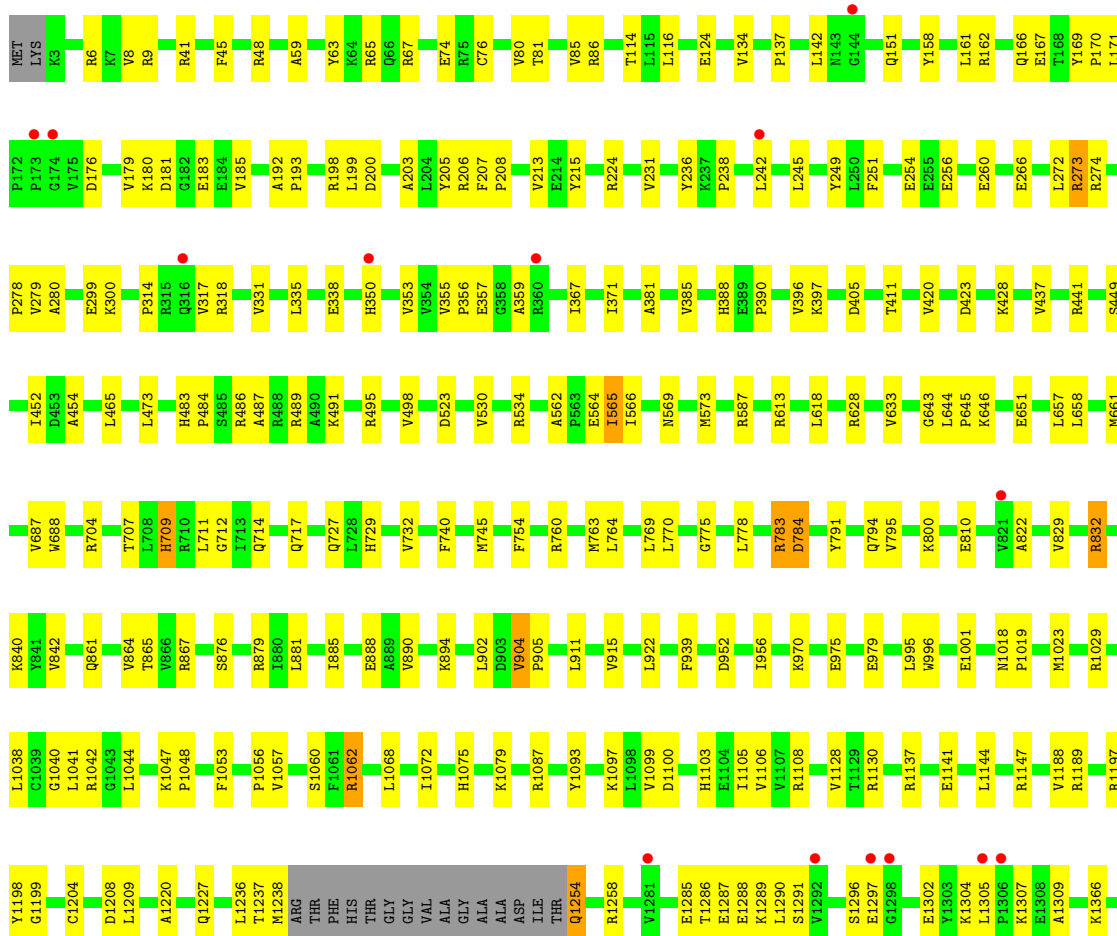
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	I	1	Total	C O	0	0
			2	1 1		

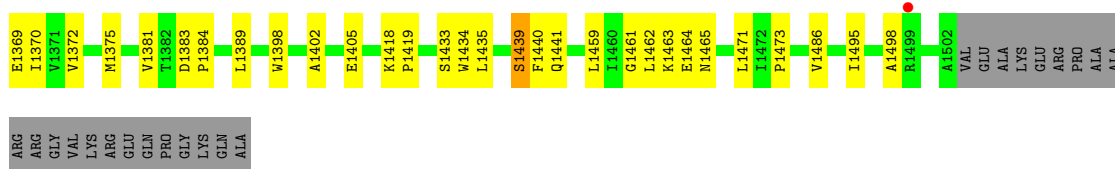
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	8	Total	O	0	0
			8	8		
13	B	6	Total	O	0	0
			6	6		
13	C	46	Total	O	0	0
			46	46		
13	D	46	Total	O	0	0
			46	46		
13	E	3	Total	O	0	0
			3	3		
13	F	9	Total	O	0	0
			9	9		
13	G	4	Total	O	0	0
			4	4		
13	H	1	Total	O	0	0
			1	1		



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





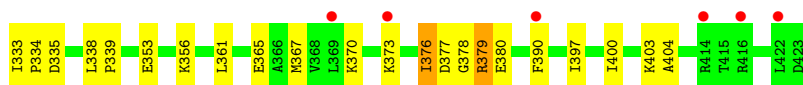
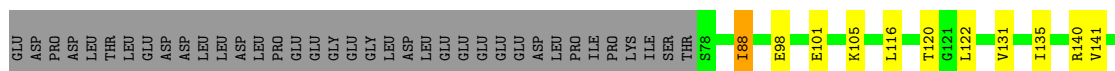
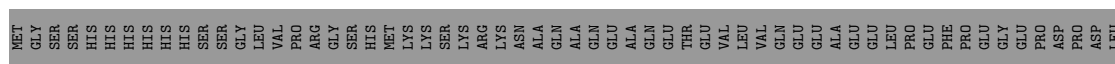
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 82% 12% 5%



- Molecule 5: DNA directed RNA polymerase sigma factor A

Chain F: 2% 64% 13% 22%



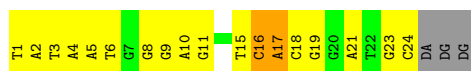
- Molecule 6: 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'

Chain G: 43% 33% 24%



- Molecule 7: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'

Chain H: 22% 59% 7% 11%



- Molecule 8: GE23077

Chain I: 43% 29% 29%



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.70Å 105.01Å 295.36Å 90.00° 98.79° 90.00°	Depositor
Resolution (Å)	47.50 – 3.10 47.50 – 3.11	Depositor EDS
% Data completeness (in resolution range)	82.6 (47.50-3.10) 82.7 (47.50-3.11)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 3.12Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.206 , 0.253 0.208 , 0.255	Depositor DCC
R_{free} test set	4160 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.5	Xtrriage
Anisotropy	0.074	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 25.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.018 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-1$ 0.015 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-1$	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	28730	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: R2T, FGL, 2RA, 0QZ, MG, DVA, ZN, RFV, 2TL, DSN, MB8

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	0.24	0/1841	0.46	0/2504
1	B	0.23	0/1821	0.46	0/2476
2	C	0.24	0/8941	0.45	0/12092
3	D	0.24	0/11948	0.45	0/16152
4	E	0.24	0/772	0.41	0/1040
5	F	0.23	0/2852	0.40	0/3837
6	G	0.48	0/368	1.06	2/567 (0.4%)
7	H	0.50	0/556	1.14	3/858 (0.3%)
All	All	0.25	0/29099	0.49	5/39526 (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
8	I	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	5	DC	O4'-C4'-C3'	-9.49	100.30	106.00
7	H	17	DA	O4'-C1'-N9	7.70	113.39	108.00
7	H	23	DG	C4'-C3'-C2'	-5.43	98.22	103.10
7	H	16	DC	O4'-C1'-N1	5.04	111.53	108.00
6	G	5	DC	C4'-C3'-C2'	-5.01	98.59	103.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	I	5	2TL	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1809	0	1863	32	0
1	B	1789	0	1841	33	0
2	C	8774	0	8877	129	0
3	D	11739	0	11975	173	0
4	E	758	0	770	10	0
5	F	2807	0	2882	46	0
6	G	328	0	181	5	0
7	H	495	0	272	12	0
8	I	50	0	37	3	0
9	B	1	0	0	0	0
9	D	2	0	0	0	0
9	F	1	0	0	0	0
10	C	50	0	48	2	0
11	D	2	0	0	0	0
12	I	2	0	0	0	0
13	A	8	0	0	0	0
13	B	6	0	0	0	0
13	C	46	0	0	1	0
13	D	46	0	0	4	0
13	E	3	0	0	0	0
13	F	9	0	0	2	0
13	G	4	0	0	0	0
13	H	1	0	0	0	0
All	All	28730	0	28746	392	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 7.

All (392) 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)
5:F:321:ILE:HD11	5:F:329:TYR:HA	1.69	0.74
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.69	0.74
3:D:256:GLU:HG3	3:D:300:LYS:HG3	1.69	0.74
2:C:428:ARG:NH2	2:C:447:ALA:O	2.22	0.72
10:C:1201:RFV:H51	10:C:1201:RFV:H48	1.33	0.72
3:D:956:ILE:HD11	3:D:1062:ARG:HD2	1.71	0.72
6:G:16:DC:H2'	6:G:17:DG:H8	1.54	0.71
3:D:208:PRO:HA	3:D:390:PRO:HA	1.72	0.70
2:C:1091:GLU:OE2	3:D:613:ARG:NH2	2.23	0.69
3:D:65:ARG:NH1	5:F:378:GLY:O	2.26	0.69
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.75	0.69
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.76	0.68
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.27	0.68
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.76	0.67
2:C:1019:GLN:HG2	2:C:1058:ASP:HB3	1.77	0.67
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.76	0.66
3:D:1285:GLU:HG3	3:D:1290:LEU:HD13	1.76	0.66
2:C:793:PRO:HB2	2:C:796:GLU:HG3	1.77	0.66
1:A:36:LEU:HD11	1:B:221:HIS:HB3	1.78	0.66
3:D:791:TYR:O	13:D:2135:HOH:O	2.12	0.66
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.79	0.65
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.26	0.65
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.27	0.65
5:F:370:LYS:HB3	5:F:376:ILE:HD13	1.79	0.64
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.31	0.64
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.30	0.64
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.32	0.63
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.80	0.63
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.31	0.63
3:D:1237:THR:OG1	3:D:1238:MET:N	2.31	0.63
2:C:397:GLU:HB3	2:C:631:SER:HB2	1.79	0.63
2:C:24:GLU:OE2	2:C:27:ARG:NH2	2.32	0.63
3:D:134:VAL:HG22	3:D:151:GLN:H	1.63	0.63
3:D:970:LYS:HD3	3:D:995:LEU:HD13	1.80	0.62
3:D:41:ARG:HE	3:D:48:ARG:HH22	1.47	0.62
1:B:80:LEU:HB3	3:D:867:ARG:HH21	1.63	0.62
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.80	0.62
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.82	0.61
2:C:197:LEU:HD12	2:C:221:LEU:HD11	1.83	0.61
2:C:595:LEU:HD11	2:C:623:TYR:HB3	1.82	0.60
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.84	0.60
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1498:ALA:HB1	4:E:84:ARG:HH21	1.66	0.60
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.84	0.60
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.83	0.59
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.83	0.59
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.85	0.59
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.36	0.59
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.84	0.59
2:C:278:GLU:OE2	2:C:284:ARG:NH2	2.36	0.58
2:C:612:VAL:HG22	2:C:622:GLU:HG3	1.85	0.58
1:A:112:ARG:HG3	1:A:125:PRO:HB2	1.85	0.58
3:D:371:ILE:HG23	5:F:230:LYS:HD2	1.85	0.58
7:H:10:DA:H2 ^{''}	7:H:11:DG:H5 ^{''}	1.86	0.58
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.86	0.58
2:C:628:PHE:H	2:C:638:ASP:HB3	1.67	0.58
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.34	0.58
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.85	0.58
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.85	0.58
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.85	0.57
6:G:11:DT:H3	7:H:17:DA:H61	1.51	0.57
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.19	0.57
6:G:4:DG:H1	7:H:24:DC:H42	1.53	0.57
1:A:185:ARG:NH2	1:A:187:GLY:O	2.39	0.56
2:C:807:ARG:HG2	2:C:821:GLU:HB3	1.87	0.56
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.88	0.56
2:C:1050:GLN:O	2:C:1054:THR:OG1	2.18	0.56
2:C:503:LEU:HD23	2:C:508:ILE:HA	1.88	0.56
3:D:411:THR:O	5:F:178:ARG:NH1	2.34	0.55
3:D:171:LEU:HD12	3:D:390:PRO:HG2	1.88	0.55
5:F:323:ASP:OD2	5:F:323:ASP:N	2.37	0.55
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.87	0.55
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.39	0.55
3:D:1105:ILE:HG23	3:D:1199:GLY:HA2	1.88	0.55
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.88	0.55
2:C:420:ARG:O	2:C:421:GLU:HB3	2.07	0.54
5:F:367:MET:HB3	5:F:390:PHE:HZ	1.72	0.54
2:C:628:PHE:H	2:C:638:ASP:CB	2.21	0.54
3:D:231:VAL:O	3:D:236:TYR:OH	2.25	0.54
1:A:133:GLU:OE2	2:C:606:VAL:N	2.40	0.54
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.43	0.54
3:D:534:ARG:NH1	5:F:312:GLN:OE1	2.37	0.54
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1038:LEU:O	3:D:1060:SER:HB2	2.08	0.54
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.89	0.54
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.90	0.54
2:C:200:LEU:HG	2:C:300:ASP:HB2	1.89	0.54
3:D:1100:ASP:OD1	3:D:1463:LYS:NZ	2.35	0.54
2:C:1030:GLN:OE1	3:D:628:ARG:NH1	2.36	0.53
3:D:63:TYR:OH	3:D:74:GLU:OE2	2.23	0.53
5:F:144:ILE:HB	5:F:147:LEU:HD13	1.91	0.53
5:F:88:ILE:HG23	5:F:193:ARG:HG2	1.90	0.53
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.90	0.53
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.90	0.52
3:D:569:ASN:ND2	5:F:214:GLN:OE1	2.37	0.52
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.91	0.52
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.90	0.52
3:D:707:THR:HG23	3:D:712:GLY:HA3	1.91	0.52
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.92	0.52
2:C:937:ASP:OD2	2:C:939:ARG:NH1	2.43	0.52
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.92	0.52
3:D:1048:PRO:O	3:D:1079:LYS:NZ	2.35	0.52
2:C:884:GLN:O	2:C:888:THR:OG1	2.21	0.51
2:C:168:ARG:O	2:C:267:TYR:HA	2.10	0.51
2:C:607:ASP:HB3	2:C:610:ARG:HG3	1.93	0.51
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.43	0.51
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.92	0.51
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.92	0.51
2:C:402:SER:HA	2:C:566:THR:HG23	1.92	0.51
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.45	0.51
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.39	0.51
3:D:1093:TYR:CZ	3:D:1097:LYS:HE3	2.46	0.51
6:G:7:DT:H3	7:H:21:DA:H61	1.59	0.51
3:D:142:LEU:HB2	3:D:161:LEU:HD11	1.93	0.51
3:D:162:ARG:NH2	13:D:2130:HOH:O	2.41	0.51
3:D:794:GLN:HB3	13:D:2135:HOH:O	2.11	0.51
5:F:370:LYS:HD3	5:F:376:ILE:HD11	1.92	0.51
2:C:343:GLN:NE2	2:C:384:GLU:OE2	2.42	0.50
3:D:1486:VAL:HG21	4:E:22:VAL:HG13	1.93	0.50
4:E:44:GLU:OE2	4:E:72:ARG:NH1	2.43	0.50
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.93	0.50
1:A:70:GLY:N	2:C:607:ASP:OD1	2.44	0.50
5:F:316:SER:HB3	5:F:319:THR:HG23	1.93	0.50
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.93	0.50
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.93	0.50
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.47	0.50
3:D:256:GLU:O	3:D:274:ARG:NH1	2.45	0.50
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.94	0.50
2:C:186:VAL:HG11	2:C:260:LEU:HD21	1.93	0.50
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.11	0.50
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.93	0.50
1:B:108:GLU:HG2	1:B:131:THR:HB	1.95	0.49
5:F:101:GLU:HG2	5:F:105:LYS:HE2	1.93	0.49
2:C:769:PRO:HG3	3:D:65:ARG:HH12	1.77	0.49
1:A:99:LEU:HB2	1:A:142:VAL:HG22	1.93	0.49
2:C:617:ASP:OD1	2:C:617:ASP:N	2.45	0.49
2:C:911:GLU:OE2	3:D:1062:ARG:NE	2.43	0.49
3:D:116:LEU:HD21	3:D:465:LEU:HD23	1.93	0.49
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.94	0.49
3:D:1435:LEU:O	3:D:1439:SER:OG	2.31	0.49
3:D:1462:LEU:HD23	3:D:1473:PRO:HD2	1.95	0.49
3:D:134:VAL:CG2	3:D:151:GLN:H	2.26	0.49
1:B:185:ARG:NH1	1:B:187:GLY:O	2.46	0.49
5:F:236:SER:OG	7:H:5:DA:OP2	2.26	0.49
1:B:30:ARG:HH21	2:C:854:PRO:HB3	1.77	0.49
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.48	0.49
2:C:727:PRO:HB3	2:C:783:ARG:HD3	1.94	0.48
3:D:350:HIS:HE1	5:F:232:ARG:HB3	1.79	0.48
4:E:49:GLN:HG2	4:E:54:LEU:HG	1.94	0.48
3:D:633:VAL:HB	3:D:740:PHE:CE2	2.48	0.48
3:D:1459:LEU:HD22	3:D:1464:GLU:HB3	1.94	0.48
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.94	0.48
2:C:630:ARG:HG3	2:C:705:ILE:HB	1.95	0.48
1:A:193:ASP:OD2	2:C:938:LYS:NZ	2.31	0.48
1:B:104:GLU:OE2	1:B:137:ARG:NH1	2.47	0.48
3:D:256:GLU:HG2	3:D:299:GLU:HA	1.96	0.48
3:D:894:LYS:H	3:D:894:LYS:HD2	1.79	0.48
3:D:864:VAL:HG22	3:D:865:THR:H	1.78	0.48
2:C:405:ARG:NH1	2:C:566:THR:OG1	2.45	0.48
3:D:114:THR:HG21	3:D:498:VAL:HG21	1.95	0.48
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.96	0.48
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.96	0.48
5:F:400:ILE:HG22	5:F:403:LYS:HE2	1.96	0.48
2:C:129:ILE:HB	2:C:134:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.49	0.47
3:D:1381:VAL:HG21	3:D:1389:LEU:HD23	1.96	0.47
2:C:1100:GLN:HG3	3:D:9:ARG:HH21	1.78	0.47
3:D:657:LEU:HG	3:D:661:MET:HE1	1.95	0.47
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.96	0.47
1:A:26:GLU:HB3	1:A:194:LYS:HG3	1.96	0.47
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.96	0.47
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.95	0.47
4:E:14:ASP:OD2	4:E:14:ASP:N	2.47	0.47
1:B:185:ARG:HB3	1:B:190:THR:HA	1.96	0.47
2:C:223:ASP:OD1	2:C:225:SER:OG	2.28	0.47
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.96	0.47
2:C:890:LEU:HD13	2:C:914:ILE:HG12	1.97	0.47
2:C:1055:LEU:HG	2:C:1079:PRO:HB3	1.96	0.47
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.97	0.47
3:D:775:GLY:HA2	3:D:1209:LEU:HB3	1.96	0.47
3:D:1286:THR:HG22	3:D:1288:GLU:H	1.79	0.47
2:C:567:GLN:NE2	8:I:7:FGL:OG1	2.47	0.47
3:D:711:LEU:HB3	3:D:714:GLN:HE21	1.80	0.46
2:C:408:ARG:NH1	2:C:456:ALA:O	2.48	0.46
3:D:658:LEU:HA	3:D:661:MET:HE2	1.97	0.46
5:F:172:ARG:O	5:F:176:ILE:HG12	2.15	0.46
2:C:179:ASN:HD21	2:C:181:VAL:HG12	1.79	0.46
2:C:1009:SER:OG	2:C:1010:THR:N	2.48	0.46
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.97	0.46
1:B:91:ASN:OD1	1:B:92:PRO:HD2	2.15	0.46
1:B:154:GLU:HG3	3:D:840:LYS:HE3	1.98	0.46
2:C:773:LEU:HD13	5:F:373:LYS:HG3	1.97	0.46
3:D:842:VAL:HG22	3:D:865:THR:HB	1.98	0.46
3:D:795:VAL:HG12	3:D:876:SER:HB3	1.97	0.46
1:B:92:PRO:O	1:B:146:ARG:NH2	2.49	0.46
3:D:41:ARG:HE	3:D:48:ARG:NH2	2.13	0.46
3:D:274:ARG:NH2	3:D:279:VAL:HG21	2.31	0.46
5:F:193:ARG:HB2	7:H:6:DT:H1'	1.96	0.46
3:D:1305:LEU:HD13	3:D:1309:ALA:HB3	1.98	0.46
3:D:562:ALA:O	5:F:140:ARG:NH1	2.27	0.46
2:C:734:LEU:HD22	2:C:737:LEU:HD12	1.97	0.46
3:D:487:ALA:O	3:D:491:LYS:HG2	2.16	0.46
1:B:100:LEU:HG	1:B:141:GLU:HG2	1.98	0.45
2:C:535:SER:O	2:C:538:GLN:HG2	2.16	0.45
3:D:1302:GLU:OE1	3:D:1304:LYS:HE3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:333:ILE:HA	5:F:334:PRO:HD3	1.80	0.45
2:C:937:ASP:OD1	2:C:938:LYS:N	2.49	0.45
3:D:486:ARG:HA	3:D:489:ARG:HE	1.81	0.45
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.96	0.45
2:C:209:ARG:NH1	2:C:210:GLU:OE1	2.50	0.45
3:D:8:VAL:HG12	3:D:1434:TRP:HZ2	1.80	0.45
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.99	0.45
3:D:179:VAL:O	3:D:205:TYR:OH	2.23	0.45
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.52	0.45
3:D:1286:THR:HB	3:D:1289:LYS:H	1.81	0.45
4:E:50:THR:HG22	4:E:51:LEU:H	1.82	0.45
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.97	0.45
3:D:760:ARG:O	3:D:764:LEU:HB2	2.16	0.45
7:H:3:DT:H2'	7:H:4:DA:C8	2.51	0.45
1:B:73:GLU:HB3	1:B:77:GLU:HB3	1.98	0.45
2:C:27:ARG:HB3	2:C:27:ARG:HH21	1.82	0.45
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.98	0.45
2:C:768:THR:HB	2:C:771:GLU:OE1	2.17	0.45
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.44	0.45
3:D:911:LEU:O	3:D:915:VAL:HG23	2.17	0.45
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.52	0.45
1:B:12:THR:HB	1:B:24:VAL:HB	1.98	0.45
3:D:171:LEU:HD23	3:D:171:LEU:HA	1.81	0.45
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.99	0.45
7:H:8:DG:H2''	7:H:9:DG:O4'	2.17	0.45
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.99	0.45
3:D:881:LEU:O	3:D:885:ILE:HG13	2.17	0.45
3:D:1018:ASN:HA	3:D:1019:PRO:HD3	1.83	0.45
1:B:155:LYS:HA	1:B:155:LYS:HD3	1.85	0.44
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.65	0.44
2:C:419:THR:O	2:C:422:ARG:HB3	2.17	0.44
2:C:858:MET:HG2	2:C:867:VAL:O	2.17	0.44
3:D:318:ARG:NH1	3:D:338:GLU:OE1	2.44	0.44
3:D:405:ASP:HB3	3:D:423:ASP:HA	2.00	0.44
3:D:613:ARG:HG3	3:D:618:LEU:HD23	2.00	0.44
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.98	0.44
3:D:709:HIS:HA	3:D:1227:GLN:HB3	1.97	0.44
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.99	0.44
5:F:353:GLU:HA	5:F:356:LYS:HD2	1.98	0.44
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.17	0.44
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:548:PRO:O	2:C:843:HIS:HE1	2.01	0.44
3:D:646:LYS:HB3	3:D:688:TRP:CZ3	2.52	0.44
3:D:729:HIS:O	3:D:732:VAL:HG22	2.18	0.44
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.67	0.44
2:C:708:TYR:HB3	2:C:790:LEU:HD21	2.00	0.44
2:C:971:LYS:HG2	2:C:988:VAL:HG22	1.99	0.44
5:F:338:LEU:HA	5:F:339:PRO:HD3	1.84	0.44
2:C:471:TYR:OH	2:C:516:ARG:NH2	2.51	0.44
2:C:627:ARG:HA	2:C:638:ASP:HB2	1.99	0.44
7:H:16:DC:H2''	7:H:17:DA:H8	1.83	0.44
1:B:90:LEU:HD21	1:B:121:GLU:HB2	1.99	0.44
2:C:695:LEU:HD21	2:C:833:LEU:HB3	1.99	0.44
1:A:209:GLU:O	1:A:213:GLN:HG2	2.18	0.44
3:D:573:MET:SD	5:F:210:LEU:HB3	2.57	0.44
3:D:956:ILE:H	3:D:956:ILE:HG13	1.66	0.44
5:F:373:LYS:HA	5:F:373:LYS:HD3	1.88	0.44
4:E:14:ASP:OD1	4:E:18:ARG:NH1	2.50	0.44
1:A:87:VAL:HG21	1:A:144:VAL:HG21	1.99	0.43
2:C:317:VAL:HA	2:C:318:PRO:HD3	1.91	0.43
3:D:314:PRO:HB2	3:D:317:VAL:HG12	2.00	0.43
3:D:1290:LEU:HD12	3:D:1291:SER:N	2.34	0.43
2:C:419:THR:HG22	2:C:422:ARG:HB3	2.00	0.43
7:H:1:DT:H71	7:H:2:DA:H62	1.83	0.43
2:C:578:VAL:HG23	2:C:671:ASN:CG	2.39	0.43
3:D:473:LEU:HD21	3:D:495:ARG:HH21	1.82	0.43
3:D:861:GLN:OE1	3:D:861:GLN:N	2.51	0.43
2:C:64:LEU:HD22	2:C:100:LEU:HD21	1.99	0.43
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.81	0.43
3:D:176:ASP:OD2	3:D:388:HIS:ND1	2.52	0.43
3:D:245:LEU:HD23	3:D:249:TYR:HB3	2.01	0.43
2:C:1032:PHE:CZ	2:C:1036:GLU:HB3	2.54	0.43
3:D:166:GLN:HB2	3:D:396:VAL:HG22	2.00	0.43
2:C:194:VAL:HG12	2:C:226:VAL:HG11	1.99	0.43
3:D:1418:LYS:HG2	3:D:1419:PRO:HD2	2.01	0.43
2:C:878:SER:HB2	3:D:1029:ARG:HD2	2.00	0.43
3:D:207:PHE:HE2	5:F:98:GLU:HG2	1.83	0.43
3:D:1296:SER:OG	3:D:1297:GLU:N	2.52	0.43
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.91	0.43
1:B:23:PHE:HB2	1:B:197:LEU:HB3	2.01	0.43
1:B:113:ASP:N	1:B:113:ASP:OD2	2.51	0.43
1:B:128:HIS:CE1	1:B:131:THR:HG22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:397:GLU:OE2	2:C:632:ASN:N	2.49	0.43
3:D:45:PHE:O	3:D:86:ARG:NH2	2.52	0.43
3:D:769:LEU:O	3:D:770:LEU:HD23	2.18	0.43
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.59	0.43
2:C:160:ALA:HB3	2:C:174:LEU:HB2	2.02	0.42
3:D:67:ARG:HD2	5:F:379:ARG:HB3	2.02	0.42
10:C:1201:RFV:H22	5:F:323:ASP:HB3	2.00	0.42
3:D:1144:LEU:HD23	3:D:1144:LEU:HA	1.84	0.42
7:H:18:DC:H2'	7:H:19:DG:C8	2.54	0.42
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.51	0.42
2:C:957:LYS:HD3	2:C:961:GLU:HB3	2.01	0.42
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.77	0.42
3:D:272:LEU:O	3:D:279:VAL:N	2.53	0.42
1:A:54:THR:N	1:A:143:ARG:O	2.50	0.42
1:A:112:ARG:NH1	1:A:126:ASP:OD2	2.47	0.42
1:B:32:PHE:HA	1:B:35:THR:HB	2.01	0.42
2:C:229:MET:HB2	2:C:233:GLU:HB2	2.02	0.42
2:C:271:GLU:OE1	2:C:288:ARG:NH1	2.52	0.42
2:C:853:LEU:HB2	2:C:858:MET:CE	2.49	0.42
1:A:31:GLY:N	1:A:193:ASP:OD1	2.52	0.42
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.87	0.42
1:A:172:SER:HA	1:A:173:PRO:HD2	1.90	0.42
1:A:228:PRO:HB3	1:B:13:VAL:HG21	2.01	0.42
2:C:380:ALA:O	2:C:384:GLU:HB3	2.20	0.42
3:D:644:LEU:HD12	3:D:645:PRO:HD2	2.00	0.42
1:A:110:LYS:HD3	1:A:128:HIS:HA	2.02	0.42
1:B:143:ARG:NH1	1:B:158:ILE:HD12	2.34	0.42
2:C:1040:LEU:HD23	2:C:1040:LEU:HA	1.83	0.42
3:D:975:GLU:O	3:D:979:GLU:HG2	2.20	0.42
1:A:183:ASP:HA	2:C:938:LYS:HE3	2.01	0.42
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.20	0.42
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.54	0.42
2:C:92:ALA:HB2	2:C:120:LEU:HD11	2.02	0.42
2:C:474:VAL:HG22	2:C:479:VAL:HG22	2.01	0.42
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	2.00	0.42
4:E:44:GLU:OE1	4:E:72:ARG:NH2	2.50	0.42
3:D:213:VAL:HG21	3:D:367:ILE:HD13	2.02	0.42
3:D:236:TYR:CE1	3:D:242:LEU:HD12	2.55	0.42
3:D:1440:PHE:CD1	3:D:1441:GLN:HB2	2.55	0.42
2:C:217:LEU:HD22	2:C:217:LEU:H	1.85	0.41
2:C:966:LEU:HD13	2:C:986:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:200:ASP:O	3:D:397:LYS:HG2	2.20	0.41
2:C:580:MET:HB3	2:C:584:GLU:OE2	2.19	0.41
3:D:224:ARG:H	3:D:251:PHE:HE1	1.67	0.41
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.21	0.41
5:F:164:LYS:HA	5:F:171:LYS:HE3	2.02	0.41
2:C:944:LEU:O	2:C:948:GLU:HB2	2.21	0.41
2:C:1008:ARG:HD3	2:C:1028:GLY:C	2.41	0.41
3:D:162:ARG:O	3:D:449:SER:HB2	2.21	0.41
3:D:784:ASP:HB2	3:D:939:PHE:CE2	2.54	0.41
2:C:93:PRO:HB2	2:C:95:TYR:CE1	2.55	0.41
3:D:1087:ARG:HD2	3:D:1236:LEU:O	2.20	0.41
1:A:25:LEU:HD23	1:A:28:LEU:HD11	2.01	0.41
2:C:422:ARG:HG2	7:H:15:DT:O4'	2.21	0.41
2:C:853:LEU:HB2	2:C:858:MET:HE2	2.03	0.41
3:D:1291:SER:OG	3:D:1304:LYS:HG2	2.21	0.41
5:F:376:ILE:HG22	5:F:377:ASP:N	2.35	0.41
2:C:668:LEU:HD23	2:C:668:LEU:HA	1.89	0.41
2:C:950:LEU:HB3	2:C:952:LEU:HD13	2.03	0.41
1:A:99:LEU:HB3	1:A:114:PHE:CD2	2.56	0.41
2:C:859:PRO:O	2:C:867:VAL:HG22	2.21	0.41
2:C:224:GLU:H	2:C:224:GLU:CD	2.24	0.41
2:C:501:THR:HA	2:C:502:PRO:HD3	1.86	0.41
2:C:890:LEU:HD12	2:C:890:LEU:HA	1.93	0.41
3:D:185:VAL:HG21	3:D:203:ALA:HB2	2.03	0.41
3:D:428:LYS:HB3	13:D:2145:HOH:O	2.20	0.41
3:D:832:ARG:H	3:D:832:ARG:HG2	1.71	0.41
5:F:217:ASN:OD1	13:F:2102:HOH:O	2.22	0.41
8:I:4:R2T:NE2	8:I:4:R2T:OB1	2.54	0.41
3:D:180:LYS:NZ	3:D:357:GLU:OE1	2.48	0.41
3:D:879:ARG:HD3	3:D:902:LEU:O	2.21	0.41
3:D:1106:VAL:HG13	3:D:1220:ALA:HA	2.01	0.41
3:D:1383:ASP:HA	3:D:1384:PRO:HD3	1.82	0.41
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.86	0.40
2:C:996:LYS:HG2	13:C:1329:HOH:O	2.21	0.40
3:D:215:TYR:HE1	3:D:381:ALA:H	1.68	0.40
3:D:530:VAL:HG22	3:D:534:ARG:O	2.21	0.40
3:D:564:GLU:HG3	3:D:565:ILE:H	1.86	0.40
5:F:193:ARG:NH1	13:F:2109:HOH:O	2.55	0.40
1:B:150:TYR:CE1	1:B:170:VAL:HG22	2.57	0.40
2:C:605:LYS:HB3	2:C:610:ARG:NH1	2.35	0.40
2:C:846:LYS:HZ1	8:I:4:R2T:HG2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1046:ALA:HB1	3:D:1471:LEU:HG	2.02	0.40
3:D:783:ARG:HB3	3:D:784:ASP:H	1.56	0.40
3:D:1048:PRO:HG3	3:D:1075:HIS:ND1	2.35	0.40
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.21	0.40
1:A:41:ARG:HA	1:A:177:VAL:HG11	2.03	0.40
1:A:206:THR:OG1	1:A:209:GLU:HG3	2.21	0.40
1:B:227:ASN:HA	1:B:228:PRO:HD3	1.86	0.40
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.92	0.40
2:C:470:PRO:HB2	2:C:534:VAL:HG21	2.02	0.40
2:C:1009:SER:HB3	3:D:651:GLU:O	2.20	0.40
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.88	0.40
6:G:17:DG:H2'	6:G:18:DA:C8	2.56	0.40
1:A:133:GLU:HG2	1:A:134:GLU:H	1.86	0.40
2:C:681:GLY:HA3	3:D:939:PHE:CD1	2.56	0.40
2:C:712:ALA:HB3	2:C:821:GLU:HG3	2.02	0.40
2:C:740:GLU:HB3	2:C:805:ARG:NH1	2.37	0.40
2:C:784:ASP:OD1	2:C:784:ASP:N	2.41	0.40
2:C:1039:ALA:HB2	3:D:707:THR:HG21	2.02	0.40
2:C:76:PRO:HG3	2:C:120:LEU:HD12	2.03	0.40
3:D:59:ALA:HB3	3:D:76:CYS:HB2	2.04	0.40
3:D:353:VAL:HG12	3:D:355:VAL:H	1.86	0.40
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	229/305 (75%)	226 (99%)	3 (1%)	0	100	100
1	B	225/305 (74%)	223 (99%)	2 (1%)	0	100	100
2	C	1108/1119 (99%)	1080 (98%)	28 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1482/1524 (97%)	1450 (98%)	31 (2%)	1 (0%)	51	83
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
5	F	344/443 (78%)	339 (98%)	5 (2%)	0	100	100
All	All	3480/3795 (92%)	3408 (98%)	71 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	565	ILE

5.3.2 Protein sidechains [i](#)

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	200/264 (76%)	196 (98%)	4 (2%)	55	80
1	B	200/264 (76%)	190 (95%)	10 (5%)	24	57
2	C	936/941 (100%)	906 (97%)	30 (3%)	39	69
3	D	1253/1279 (98%)	1219 (97%)	34 (3%)	44	74
4	E	82/88 (93%)	81 (99%)	1 (1%)	71	88
5	F	301/388 (78%)	290 (96%)	11 (4%)	34	66
All	All	2972/3224 (92%)	2882 (97%)	90 (3%)	41	71

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	134	GLU
1	A	142	VAL
1	A	176	ARG
1	B	6	LEU
1	B	95	GLN
1	B	131	THR

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Mol	Chain	Res	Type
1	B	133	GLU
1	B	139	ASN
1	B	154	GLU
1	B	160	ASP
1	B	188	GLN
1	B	189	ARG
1	B	192	LEU
2	C	1	MET
2	C	5	ARG
2	C	27	ARG
2	C	81	ASP
2	C	138	SER
2	C	141	HIS
2	C	177	GLU
2	C	210	GLU
2	C	217	LEU
2	C	224	GLU
2	C	257	VAL
2	C	301	GLU
2	C	342	ASP
2	C	361	MET
2	C	384	GLU
2	C	418	LEU
2	C	419	THR
2	C	434	HIS
2	C	557	ARG
2	C	600	ASP
2	C	610	ARG
2	C	617	ASP
2	C	670	GLN
2	C	715	THR
2	C	998	TYR
2	C	1008	ARG
2	C	1010	THR
2	C	1057	SER
2	C	1058	ASP
2	C	1095	LEU
3	D	6	ARG
3	D	80	VAL
3	D	81	THR
3	D	183	GLU
3	D	199	LEU

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Mol	Chain	Res	Type
3	D	206	ARG
3	D	273	ARG
3	D	331	VAL
3	D	335	LEU
3	D	420	VAL
3	D	523	ASP
3	D	687	VAL
3	D	709	HIS
3	D	717	GLN
3	D	754	PHE
3	D	778	LEU
3	D	783	ARG
3	D	784	ASP
3	D	810	GLU
3	D	829	VAL
3	D	832	ARG
3	D	904	VAL
3	D	1001	GLU
3	D	1041	LEU
3	D	1062	ARG
3	D	1128	VAL
3	D	1130	ARG
3	D	1188	VAL
3	D	1208	ASP
3	D	1254	GLN
3	D	1287	GLU
3	D	1307	LYS
3	D	1433	SER
3	D	1439	SER
4	E	50	THR
5	F	88	ILE
5	F	116	LEU
5	F	141	VAL
5	F	205	ARG
5	F	295	MET
5	F	321	ILE
5	F	323	ASP
5	F	335	ASP
5	F	376	ILE
5	F	379	ARG
5	F	380	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
2	C	1047	HIS
3	D	66	GLN
3	D	350	HIS
3	D	696	HIS
3	D	714	GLN
3	D	724	GLN
3	D	976	GLN
3	D	1195	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FGL	I	7	8	5,6,7	1.04	0	1,7,9	2.03	1 (100%)
8	2TL	I	5	8	5,6,7	1.08	0	6,7,9	0.91	0
8	0QZ	I	6	8	4,5,6	1.60	1 (25%)	2,5,7	0.90	0
8	R2T	I	4	8	8,10,11	1.92	2 (25%)	6,13,15	0.90	0
8	2RA	I	1	12,8	3,5,6	0.58	0	1,5,7	0.45	0

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
8	FGL	I	7	8	-	2/4/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2TL	I	5	8	-	1/5/6/8	-
8	0QZ	I	6	8	-	1/3/4/6	-
8	R2T	I	4	8	-	6/13/14/16	-
8	2RA	I	1	12,8	-	2/2/4/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	4	R2T	CD-NE2	4.29	1.43	1.32
8	I	6	0QZ	OB-CA	-3.04	1.38	1.43
8	I	4	R2T	OB1-CB	-2.26	1.37	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	7	FGL	OG1-CB-OG2	-2.03	119.48	124.09

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	2RA	C-CA-CB-NG
8	I	1	2RA	N-CA-CB-NG
8	I	7	FGL	C-CA-CB-OG1
8	I	7	FGL	C-CA-CB-OG2
8	I	4	R2T	OE1-CD-CG-OG1
8	I	4	R2T	NE2-CD-CG-OG1
8	I	5	2TL	O-C-CA-CB
8	I	6	0QZ	N-C1-CA-C
8	I	4	R2T	OE1-CD-CG-CB
8	I	4	R2T	NE2-CD-CG-CB
8	I	4	R2T	OB1-CB-CG-CD
8	I	4	R2T	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	7	FGL	1	0
8	I	4	R2T	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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
12	MB8	I	101	8	0,1,6	-	-	-		
10	RFV	C	1201	-	52,53,53	3.52	12 (23%)	72,80,80	2.44	16 (22%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	RFV	C	1201	-	-	10/55/70/70	0/3/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1201	RFV	C12-C11	-20.64	1.40	1.55
10	C	1201	RFV	C17-C16	6.85	1.54	1.34
10	C	1201	RFV	C15-N1	5.38	1.47	1.35
10	C	1201	RFV	O7-C25	-5.03	1.37	1.44
10	C	1201	RFV	C5-C11	-3.78	1.47	1.50
10	C	1201	RFV	C18-C17	3.36	1.53	1.43
10	C	1201	RFV	C6-C7	3.13	1.45	1.39
10	C	1201	RFV	C2-N1	3.11	1.47	1.41
10	C	1201	RFV	O3-C12	2.71	1.49	1.45
10	C	1201	RFV	O9-C23	-2.20	1.37	1.43
10	C	1201	RFV	C3-C4	2.10	1.42	1.37
10	C	1201	RFV	C29-C28	2.08	1.41	1.30

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1201	RFV	C12-C11-C5	12.67	111.13	101.52
10	C	1201	RFV	C30-C16-C17	-6.44	107.83	123.42
10	C	1201	RFV	O3-C6-C7	5.47	130.54	121.14
10	C	1201	RFV	O4-C11-C12	5.35	122.85	113.41
10	C	1201	RFV	O7-C35-C36	4.23	118.88	111.09
10	C	1201	RFV	O4-C11-C5	3.91	122.69	112.56
10	C	1201	RFV	O3-C6-C5	-3.55	109.81	113.15
10	C	1201	RFV	C13-C12-C11	-3.35	110.02	117.78
10	C	1201	RFV	C37-O6-C27	3.05	120.32	113.01
10	C	1201	RFV	C33-C24-C25	-3.04	105.95	111.40
10	C	1201	RFV	C23-C24-C25	2.76	116.02	110.61
10	C	1201	RFV	C20-C19-C18	-2.54	120.81	126.16
10	C	1201	RFV	C12-O5-C29	2.53	123.98	117.84
10	C	1201	RFV	C18-C17-C16	-2.33	119.75	126.61
10	C	1201	RFV	C34-C26-C27	-2.10	106.64	110.93
10	C	1201	RFV	C25-O7-C35	2.02	120.84	117.72

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	1201	RFV	C16-C17-C18-C19
10	C	1201	RFV	C26-C27-C28-C29
10	C	1201	RFV	C26-C27-O6-C37
10	C	1201	RFV	C28-C27-O6-C37
10	C	1201	RFV	C18-C19-C20-C31
10	C	1201	RFV	C1-C2-N1-C15
10	C	1201	RFV	C15-C16-C17-C18
10	C	1201	RFV	C28-C29-O5-C12
10	C	1201	RFV	N1-C15-C16-C17
10	C	1201	RFV	O11-C15-C16-C17

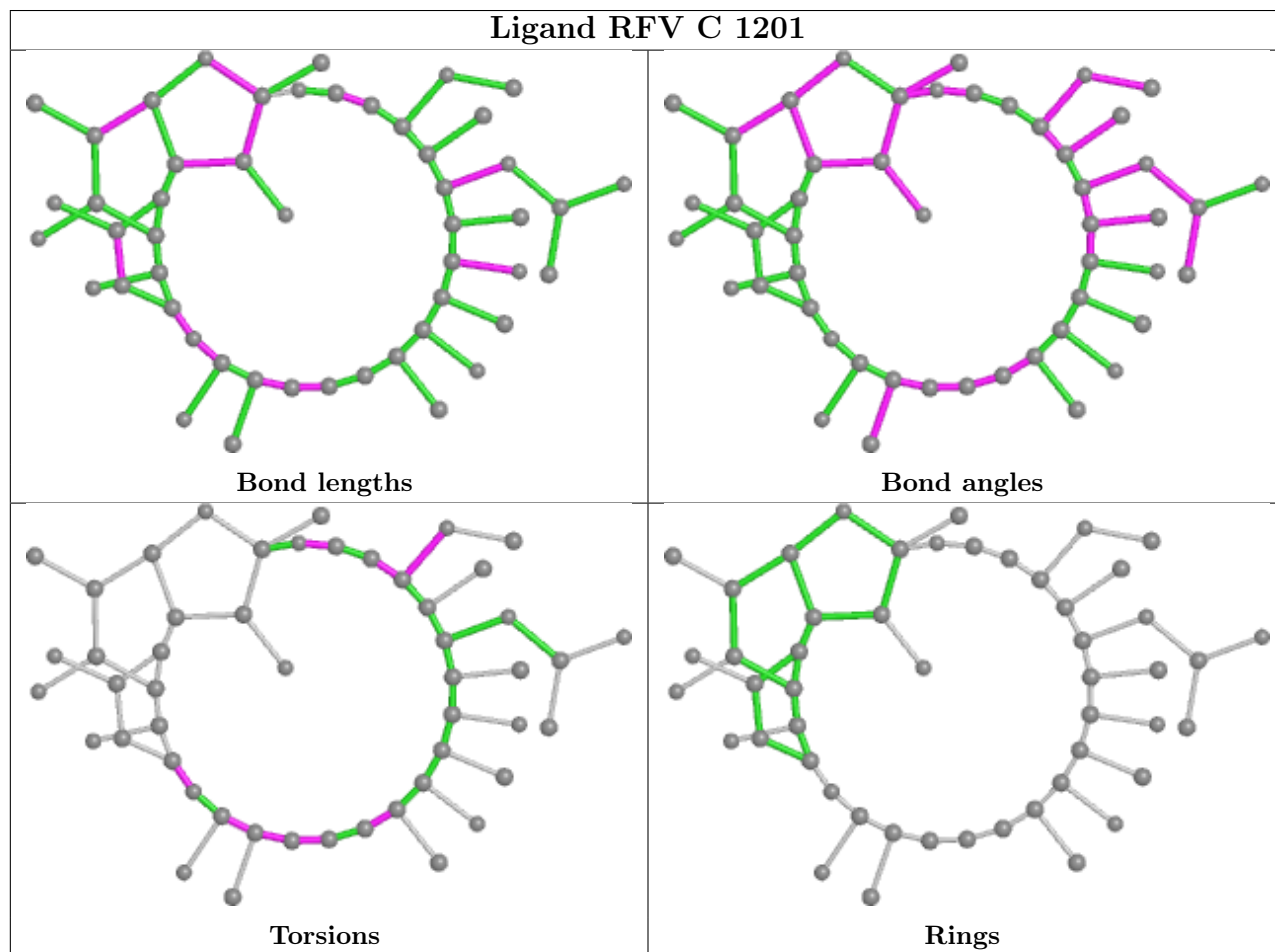
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1201	RFV	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	231/305 (75%)	-0.43	4 (1%) 70 49	31, 50, 79, 128	0
1	B	227/305 (74%)	-0.36	2 (0%) 84 69	35, 65, 92, 125	0
2	C	1112/1119 (99%)	-0.35	10 (0%) 84 69	15, 44, 109, 139	0
3	D	1485/1524 (97%)	-0.28	15 (1%) 82 67	15, 50, 111, 156	0
4	E	94/99 (94%)	-0.40	0 100 100	27, 55, 99, 107	0
5	F	346/443 (78%)	-0.17	7 (2%) 65 44	24, 66, 122, 138	0
6	G	16/21 (76%)	-0.32	0 100 100	66, 101, 179, 183	0
7	H	24/27 (88%)	-0.24	0 100 100	58, 110, 171, 185	0
8	I	0/7	-	-	-	-
All	All	3535/3850 (91%)	-0.31	38 (1%) 80 64	15, 52, 112, 185	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	ALA	4.0
2	C	766	GLU	3.2
3	D	1281	VAL	2.9
1	A	233	VAL	2.9
5	F	149	GLU	2.9
3	D	821	VAL	2.7
5	F	390	PHE	2.7
2	C	176	VAL	2.7
3	D	1305	LEU	2.7
3	D	360	ARG	2.7
3	D	242	LEU	2.6
3	D	174	GLY	2.6
1	B	2	LEU	2.6
3	D	1297	GLU	2.6
2	C	226	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	173	PRO	2.5
1	A	234	ALA	2.5
3	D	1298	GLY	2.5
2	C	729	LEU	2.5
3	D	1499	ARG	2.4
5	F	369	LEU	2.4
3	D	350	HIS	2.4
2	C	189	ARG	2.3
5	F	414	ARG	2.3
2	C	107	LEU	2.3
3	D	1292	VAL	2.3
3	D	144	GLY	2.3
1	A	231	ALA	2.2
2	C	159	ILE	2.2
2	C	174	LEU	2.2
2	C	764	GLU	2.2
5	F	422	LEU	2.1
3	D	316	GLN	2.1
3	D	1306	PRO	2.1
5	F	416	ARG	2.1
5	F	373	LYS	2.1
1	B	93	SER	2.1
2	C	221	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
8	FGL	I	7	7/8	0.93	0.15	19,25,27,29	0
8	DSN	I	2	6/7	0.95	0.17	20,21,29,31	0
8	R2T	I	4	11/12	0.95	0.16	21,25,32,33	0
8	2RA	I	1	6/7	0.96	0.11	24,25,29,34	0
8	DVA	I	3	7/8	0.97	0.17	13,17,21,22	0
8	0QZ	I	6	6/7	0.97	0.15	23,25,25,28	0
8	2TL	I	5	7/8	0.98	0.18	21,21,24,29	0

6.3 Carbohydrates [i](#)

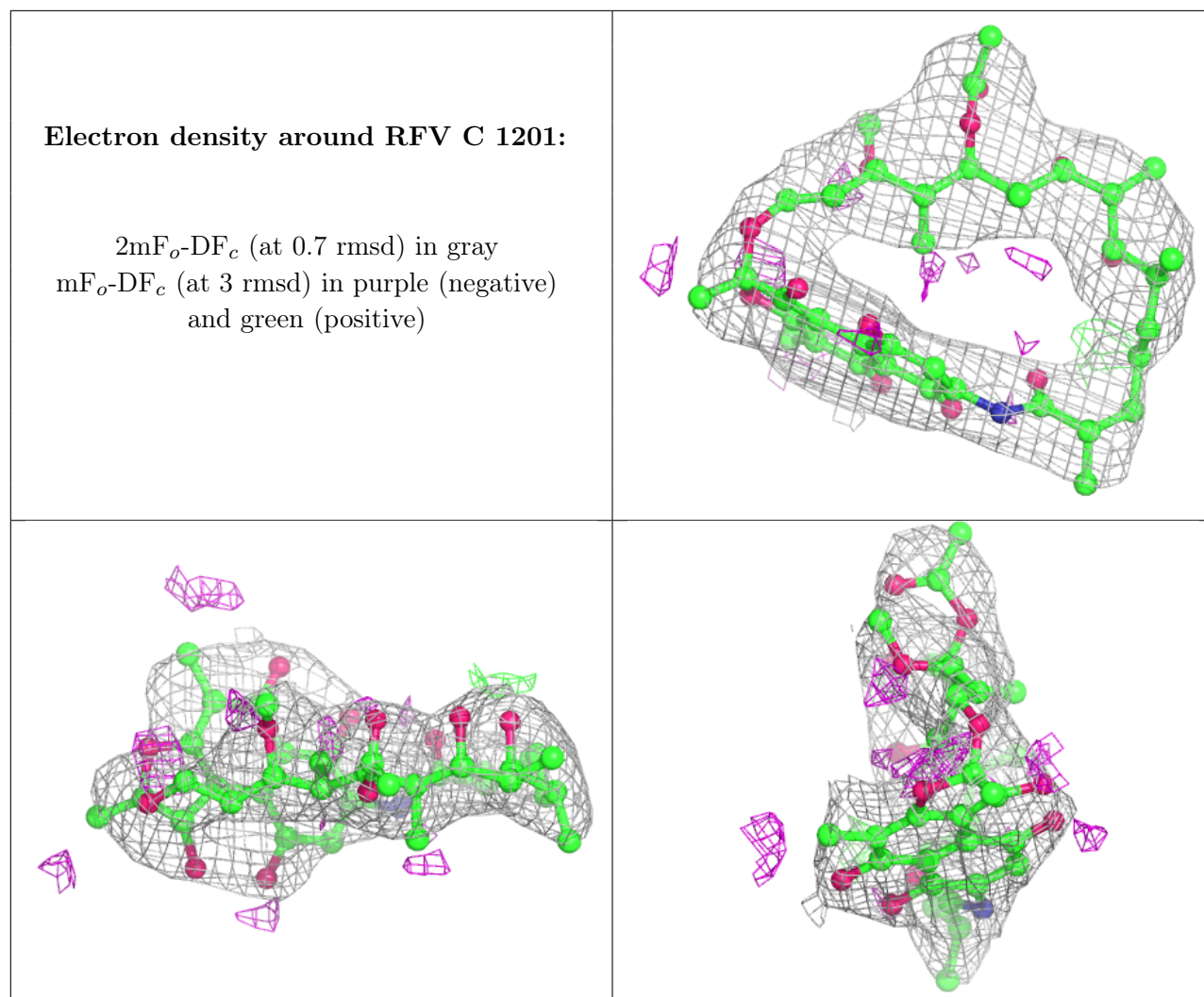
There are no monosaccharides in this entry.

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(\AA^2)	Q<0.9
9	MG	D	2004	1/1	0.77	0.18	50,50,50,50	0
10	RFV	C	1201	50/50	0.95	0.24	19,30,47,53	0
9	MG	F	2001	1/1	0.96	0.17	55,55,55,55	0
9	MG	B	401	1/1	0.96	0.25	25,25,25,25	0
12	MB8	I	101	2/7	0.96	0.13	26,26,26,31	0
11	ZN	D	2001	1/1	0.97	0.17	43,43,43,43	0
11	ZN	D	2002	1/1	0.97	0.08	79,79,79,79	0
9	MG	D	2003	1/1	0.97	0.17	14,14,14,14	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.