



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:21 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

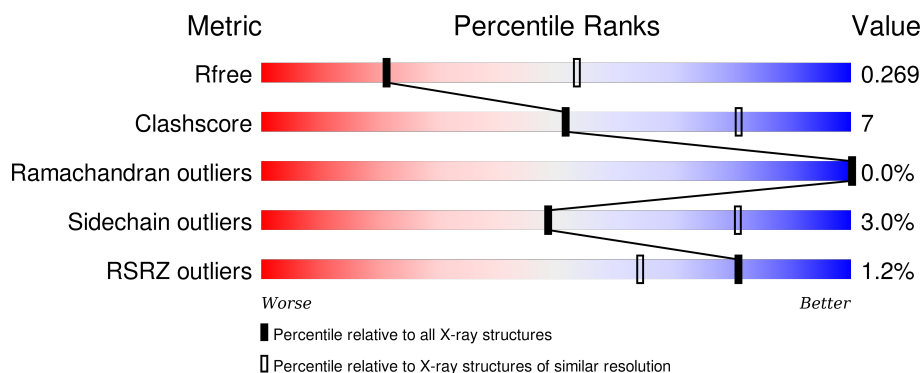
1 Overall quality at a glance

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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div></div> <div>59% 16% • 24%</div> </div>
1	B	305	<div> <div></div> <div>56% 18% • 26%</div> </div>
2	C	1119	<div> <div></div> <div>81% 17% ••</div> </div>
3	D	1524	<div> <div></div> <div>79% 18% ••</div> </div>
4	E	99	<div> <div></div> <div>82% 12% • 5%</div> </div>

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Mol	Chain	Length	Quality of chain
5	F	443	<div><div><div></div><div></div><div></div></div><div>2%64%13%22%</div></div>
6	G	21	<div><div><div></div><div></div><div></div></div><div>43%33%24%</div></div>
7	H	27	<div><div><div></div><div></div><div></div></div><div>22%59%7%11%</div></div>
8	I	7	<div><div><div></div><div></div><div></div></div><div>57%43%</div></div>

2 Entry composition

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
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
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
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
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
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			

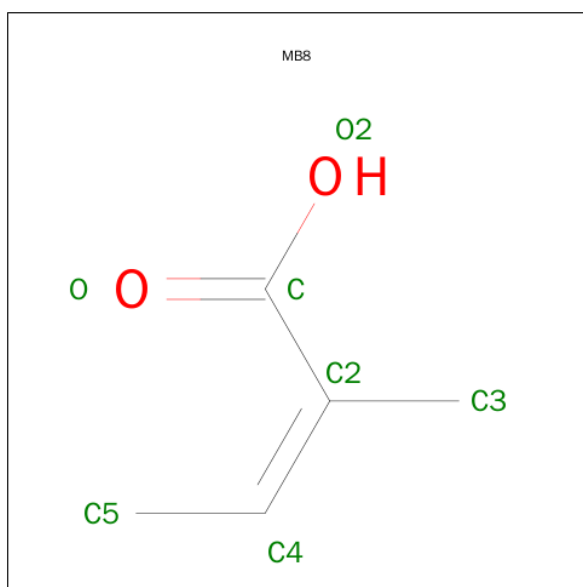
- Molecule 7 is a DNA chain called 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*C
P*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'.

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 (2Z)-2-METHYLBUT-2-ENOIC ACID (three-letter code: MB8) (formula: C₅H₈O₂).

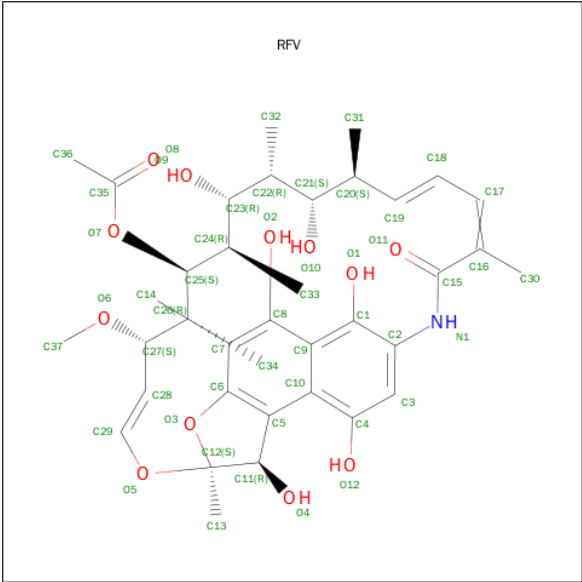


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	I	1	Total	C	O	0	0
			2	1	1		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 11 is RIFAMYCIN SV (three-letter code: RFV) (formula: C₃₇H₄₉NO₁₂).



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

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

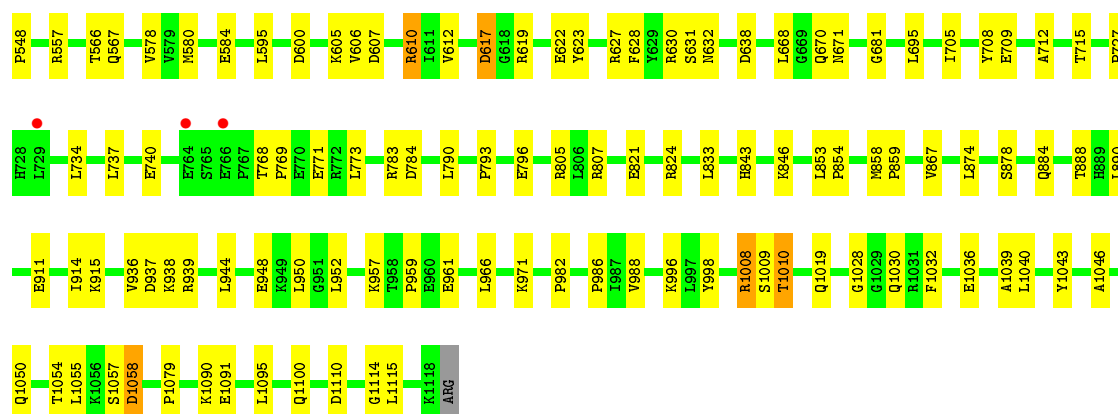
- Molecule 13 is water.

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		

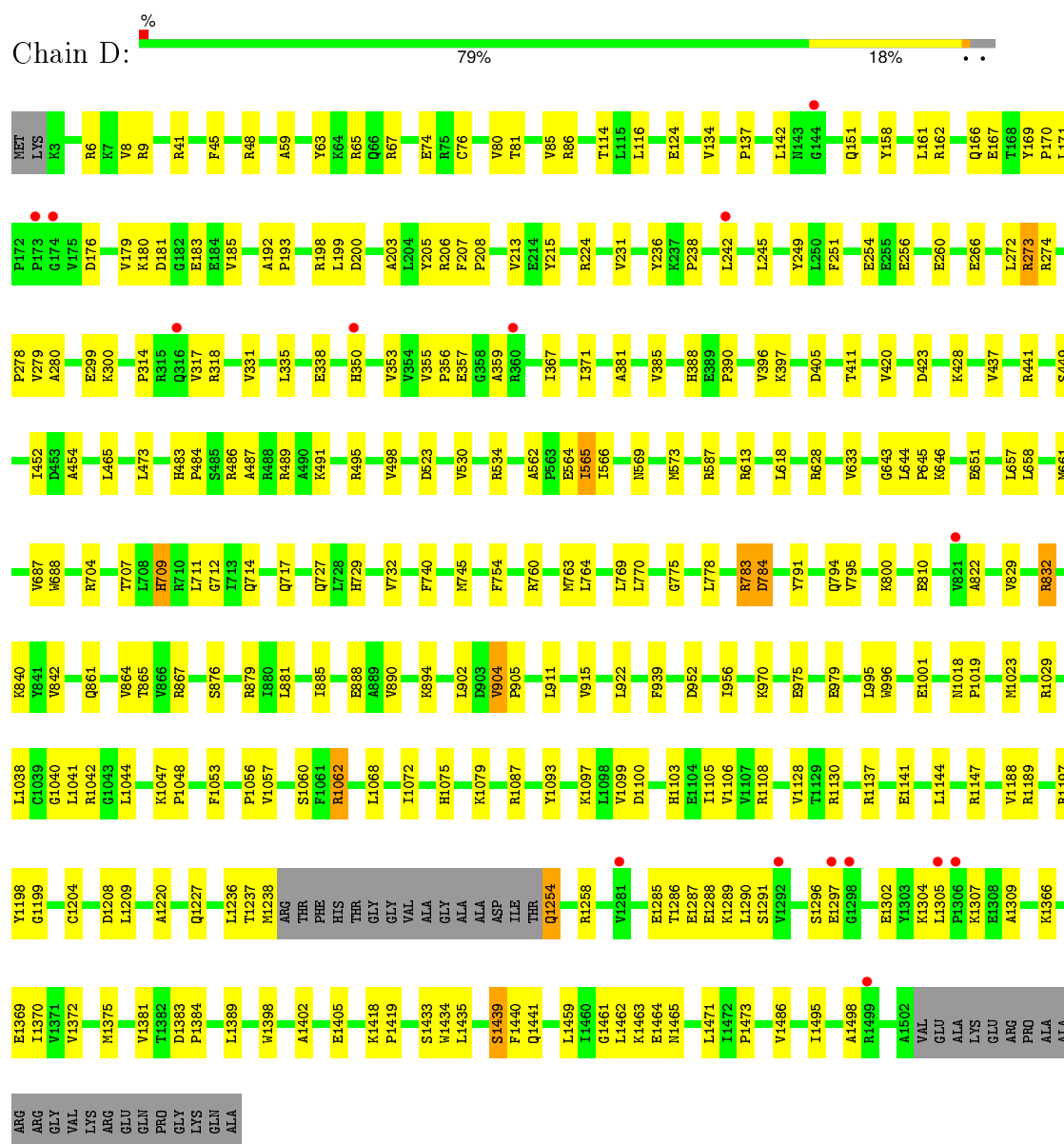
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	H	1	Total	O	0	0
			1	1		



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



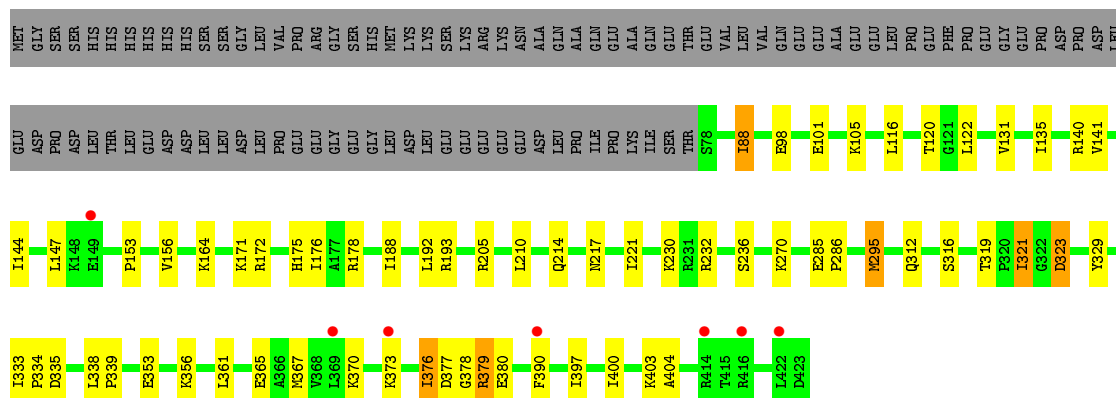
- Molecule 4: DNA-directed RNA polymerase subunit omega

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%



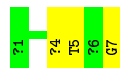
- Molecule 7: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'

Chain H:  22% 59% 7% 11%



- Molecule 8: GE23077

Chain I:  57% 43%



4 Data and refinement statistics

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)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.206 , 0.253 0.228 , 0.269	Depositor DCC
R_{free} test set	4160 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	63.5	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 25.3	EDS
Estimated twinning fraction	0.018 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.015 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 83148 reflections	Xtriage
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

Xtriage'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, 0.375 respectively for untwinned datasets, and 0.333, 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: FGL, ZN, RFV, 2TL, DVA, MG, 2RA, DSN, MB8, 0QZ, R2T

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 ⓘ

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	I	2	0	0	0	0
10	B	1	0	0	0	0
10	D	2	0	0	0	0
10	F	1	0	0	0	0
11	C	50	0	48	2	0
12	D	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
11:C:1201:RFV:H51	11:C:1201:RFV:H48	1.33	0.72
2:C:428:ARG:NH2	2:C:447:ALA:O	2.22	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
3:D:1237:THR:OG1	3:D:1238:MET:N	2.31	0.63
2:C:1110:ASP:OD2	2:C:1114:GLY: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:1498:ALA:HB1	4:E:84:ARG:HH21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.83	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
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.84	0.59
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.36	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
7:H:10:DA:H2"	7:H:11:DG:H5"	1.86	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
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.34	0.58
2:C:628:PHE:H	2:C:638:ASP:HB3	1.67	0.58
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.86	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
2:C:807:ARG:HG2	2:C:821:GLU:HB3	1.87	0.56
1:A:185:ARG:NH2	1:A:187:GLY:O	2.39	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
5:F:323:ASP:N	5:F:323:ASP:OD2	2.37	0.55
3:D:171:LEU:HD12	3:D:390:PRO:HG2	1.88	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
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.88	0.55
3:D:1105:ILE:HG23	3:D:1199:GLY:HA2	1.88	0.55
5:F:367:MET:HB3	5:F:390:PHE:HZ	1.72	0.54
2:C:420:ARG:O	2:C:421:GLU:HB3	2.07	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:1038:LEU:O	3:D:1060:SER:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.89	0.54
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.90	0.54
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.89	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
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.90	0.52
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.91	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
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.45	0.51
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.92	0.51
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.92	0.51
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.39	0.51
2:C:402:SER:HA	2:C:566:THR:HG23	1.92	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: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
3:D:162:ARG:NH2	13:D:2130:HOH:O	2.41	0.51
4:E:44:GLU:OE2	4:E:72:ARG:NH1	2.43	0.50
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
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
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.47	0.50
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.93	0.50
3:D:256:GLU:O	3:D:274:ARG:NH1	2.45	0.50
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.11	0.50
2:C:186:VAL:HG11	2:C:260:LEU:HD21	1.93	0.50
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.94	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
2:C:911:GLU:OE2	3:D:1062:ARG:NE	2.43	0.49
2:C:617:ASP:N	2:C:617:ASP:OD1	2.45	0.49
1:A:99:LEU:HB2	1:A:142:VAL:HG22	1.93	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
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.48	0.49
1:B:30:ARG:HH21	2:C:854:PRO:HB3	1.77	0.49
2:C:727:PRO:HB3	2:C:783:ARG:HD3	1.94	0.48
4:E:49:GLN:HG2	4:E:54:LEU:HG	1.94	0.48
3:D:350:HIS:HE1	5:F:232:ARG:HB3	1.79	0.48
3:D:1459:LEU:HD22	3:D:1464:GLU:HB3	1.94	0.48
3:D:633:VAL:HB	3:D:740:PHE:CE2	2.48	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
3:D:256:GLU:HG2	3:D:299:GLU:HA	1.96	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:894:LYS:HD2	3:D:894:LYS:H	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:1381:VAL:HG21	3:D:1389:LEU:HD23	1.96	0.47
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.49	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
2:C:1100:GLN:HG3	3:D:9:ARG:HH21	1.78	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
1:A:26:GLU:HB3	1:A:194:LYS:HG3	1.96	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
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.97	0.47
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.96	0.47
2:C:223:ASP:OD1	2:C:225:SER:OG	2.28	0.47
3:D:775:GLY:HA2	3:D:1209:LEU:HB3	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: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
3:D:658:LEU:HA	3:D:661:MET:HE2	1.97	0.46
2:C:408:ARG:NH1	2:C:456:ALA:O	2.48	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
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.97	0.46
2:C:1009:SER:OG	2:C:1010:THR:N	2.48	0.46
3:D:842:VAL:HG22	3:D:865:THR:HB	1.98	0.46
1:B:91:ASN:OD1	1:B:92:PRO:HD2	2.15	0.46
2:C:773:LEU:HD13	5:F:373:LYS:HG3	1.97	0.46
1:B:154:GLU:HG3	3:D:840:LYS:HE3	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:274:ARG:NH2	3:D:279:VAL:HG21	2.31	0.46
3:D:41:ARG:HE	3:D:48:ARG:NH2	2.13	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
3:D:487:ALA:O	3:D:491:LYS:HG2	2.16	0.46
2:C:734:LEU:HD22	2:C:737:LEU:HD12	1.97	0.46
3:D:1302:GLU:OE1	3:D:1304:LYS:HE3	2.16	0.45
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

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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:179:VAL:O	3:D:205:TYR:OH	2.23	0.45
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.99	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
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.52	0.45
3:D:8:VAL:HG12	3:D:1434:TRP:HZ2	1.80	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:A:55:SER:HB3	1:A:143:ARG:HB3	1.97	0.45
1:B:73:GLU:HB3	1:B:77:GLU:HB3	1.98	0.45
2:C:27:ARG:HH21	2:C:27:ARG:HB3	1.82	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
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.98	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
3:D:171:LEU:HA	3:D:171:LEU:HD23	1.81	0.45
1:B:12:THR:HB	1:B:24:VAL:HB	1.98	0.45
7:H:8:DG:H2''	7:H:9:DG:O4'	2.17	0.45
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.99	0.45
3:D:1018:ASN:HA	3:D:1019:PRO:HD3	1.83	0.45
3:D:881:LEU:O	3:D:885:ILE:HG13	2.17	0.45
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.99	0.45
3:D:613:ARG:HG3	3:D:618:LEU:HD23	2.00	0.44
3:D:318:ARG:NH1	3:D:338:GLU:OE1	2.44	0.44
2:C:419:THR:O	2:C:422:ARG:HB3	2.17	0.44
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.99	0.44
3:D:709:HIS:HA	3:D:1227:GLN:HB3	1.97	0.44
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.65	0.44
3:D:405:ASP:HB3	3:D:423:ASP:HA	2.00	0.44
1:B:155:LYS:HD3	1:B:155:LYS:HA	1.85	0.44
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.98	0.44
2:C:858:MET:HG2	2:C:867:VAL:O	2.17	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:729:HIS:O	3:D:732:VAL:HG22	2.18	0.44
3:D:646:LYS:HB3	3:D:688:TRP:CZ3	2.52	0.44
2:C:971:LYS:HG2	2:C:988:VAL:HG22	1.99	0.44
2:C:708:TYR:HB3	2:C:790:LEU:HD21	2.00	0.44
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.67	0.44
5:F:338:LEU:HA	5:F:339:PRO:HD3	1.84	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
2:C:471:TYR:OH	2:C:516:ARG:NH2	2.51	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
3:D:956:ILE:H	3:D:956:ILE:HG13	1.66	0.44
5:F:373:LYS:HD3	5:F:373:LYS:HA	1.88	0.44
3:D:573:MET:SD	5:F:210:LEU:HB3	2.57	0.44
1:A:209:GLU:O	1:A:213:GLN:HG2	2.18	0.44
4:E:14:ASP:OD1	4:E:18:ARG:NH1	2.50	0.44
2:C:317:VAL:HA	2:C:318:PRO:HD3	1.91	0.43
1:A:87:VAL:HG21	1:A:144:VAL:HG21	1.99	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
3:D:473:LEU:HD21	3:D:495:ARG:HH21	1.82	0.43
3:D:861:GLN:N	3:D:861:GLN:OE1	2.51	0.43
2:C:578:VAL:HG23	2:C:671:ASN:CG	2.39	0.43
3:D:245:LEU:HD23	3:D:249:TYR:HB3	2.01	0.43
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.81	0.43
2:C:64:LEU:HD22	2:C:100:LEU:HD21	1.99	0.43
3:D:176:ASP:OD2	3:D:388:HIS:ND1	2.52	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
3:D:207:PHE:HE2	5:F:98:GLU:HG2	1.83	0.43
2:C:878:SER:HB2	3:D:1029:ARG:HD2	2.00	0.43
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.91	0.43
3:D:1296:SER:OG	3:D:1297:GLU:N	2.52	0.43
2:C:397:GLU:OE2	2:C:632:ASN:N	2.49	0.43
1:B:128:HIS:CE1	1:B:131:THR:HG22	2.54	0.43
3:D:769:LEU:O	3:D:770:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:45:PHE:O	3:D:86:ARG:NH2	2.52	0.43
1:B:23:PHE:HB2	1:B:197:LEU:HB3	2.01	0.43
1:B:113:ASP:OD2	1:B:113:ASP:N	2.51	0.43
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.59	0.43
3:D:67:ARG:HD2	5:F:379:ARG:HB3	2.02	0.42
2:C:160:ALA:HB3	2:C:174:LEU:HB2	2.02	0.42
11:C:1201:RFV:H22	5:F:323:ASP:HB3	2.00	0.42
7:H:18:DC:H2'	7:H:19:DG:C8	2.54	0.42
3:D:1144:LEU:HA	3:D:1144:LEU:HD23	1.84	0.42
3:D:272:LEU:O	3:D:279:VAL:N	2.53	0.42
2:C:957:LYS:HD3	2:C:961:GLU:HB3	2.01	0.42
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.51	0.42
2:C:1090:LYS:HD3	2:C:1090:LYS:HA	1.77	0.42
1:A:112:ARG:NH1	1:A:126:ASP:OD2	2.47	0.42
1:A:54:THR:N	1:A:143:ARG:O	2.50	0.42
2:C:853:LEU:HB2	2:C:858:MET:CE	2.49	0.42
2:C:229:MET:HB2	2:C:233:GLU:HB2	2.02	0.42
1:B:32:PHE:HA	1:B:35:THR:HB	2.01	0.42
2:C:271:GLU:OE1	2:C:288:ARG:NH1	2.52	0.42
1:A:31:GLY:N	1:A:193:ASP:OD1	2.52	0.42
2:C:380:ALA:O	2:C:384:GLU:HB3	2.20	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
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.87	0.42
3:D:644:LEU:HD12	3:D:645:PRO:HD2	2.00	0.42
1:B:143:ARG:NH1	1:B:158:ILE:HD12	2.34	0.42
1:A:110:LYS:HD3	1:A:128:HIS:HA	2.02	0.42
3:D:975:GLU:O	3:D:979:GLU:HG2	2.20	0.42
2:C:1040:LEU:HA	2:C:1040:LEU:HD23	1.83	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
4:E:44:GLU:OE1	4:E:72:ARG:NH2	2.50	0.42
2:C:92:ALA:HB2	2:C:120:LEU:HD11	2.02	0.42
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	2.00	0.42
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.54	0.42
2:C:474:VAL:HG22	2:C:479:VAL:HG22	2.01	0.42
3:D:236:TYR:CE1	3:D:242:LEU:HD12	2.55	0.42
3:D:213:VAL:HG21	3:D:367:ILE:HD13	2.02	0.42
3:D:1440:PHE:CD1	3:D:1441:GLN:HB2	2.55	0.42
3:D:200:ASP:O	3:D:397:LYS:HG2	2.20	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)
2:C:217:LEU:H	2:C:217:LEU:HD22	1.85	0.41
3:D:224:ARG:H	3:D:251:PHE:HE1	1.67	0.41
2:C:580:MET:HB3	2:C:584:GLU:OE2	2.19	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
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:1008:ARG:HD3	2:C:1028:GLY:C	2.41	0.41
2:C:944:LEU:O	2:C:948:GLU:HB2	2.21	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
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: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
1:A:25:LEU:HD23	1:A:28:LEU:HD11	2.01	0.41
2:C:950:LEU:HB3	2:C:952:LEU:HD13	2.03	0.41
2:C:668:LEU:HA	2:C:668:LEU:HD23	1.89	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:890:LEU:HA	2:C:890:LEU:HD12	1.93	0.41
3:D:185:VAL:HG21	3:D:203:ALA:HB2	2.03	0.41
2:C:501:THR:HA	2:C:502:PRO:HD3	1.86	0.41
3:D:428:LYS:HB3	13:D:2145:HOH:O	2.20	0.41
5:F:217:ASN:OD1	13:F:2102:HOH:O	2.22	0.41
2:C:224:GLU:CD	2:C:224:GLU:H	2.24	0.41
3:D:832:ARG:HG2	3:D:832:ARG:H	1.71	0.41
8:I:4:R2T:NE2	8:I:4:R2T:OB1	2.54	0.41
3:D:1106:VAL:HG13	3:D:1220:ALA:HA	2.01	0.41
3:D:879:ARG:HD3	3:D:902:LEU:O	2.21	0.41
3:D:180:LYS:NZ	3:D:357:GLU:OE1	2.48	0.41
3:D:1383:ASP:HA	3:D:1384:PRO:HD3	1.82	0.41
3:D:530:VAL:HG22	3:D:534:ARG:O	2.21	0.40
5:F:193:ARG:NH1	13:F:2109:HOH:O	2.55	0.40
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:564:GLU:HG3	3:D:565:ILE:H	1.86	0.40
3:D:215:TYR:HE1	3:D:381:ALA:H	1.68	0.40
2:C:605:LYS:HB3	2:C:610:ARG:NH1	2.35	0.40
3:D:1048:PRO:HG3	3:D:1075:HIS:ND1	2.35	0.40
3:D:783:ARG:HB3	3:D:784:ASP:H	1.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:846:LYS:HZ1	8:I:4:R2T:HG2	1.86	0.40
1:B:150:TYR:CE1	1:B:170:VAL:HG22	2.57	0.40
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.21	0.40
2:C:1046:ALA:HB1	3:D:1471:LEU:HG	2.02	0.40
6:G:17:DG:H2'	6:G:18:DA:C8	2.56	0.40
2:C:1009:SER:HB3	3:D:651:GLU:O	2.20	0.40
1:A:206:THR:OG1	1:A:209:GLU:HG3	2.21	0.40
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.88	0.40
1:A:41:ARG:HA	1:A:177:VAL:HG11	2.03	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
1:B:227:ASN:HA	1:B:228:PRO:HD3	1.86	0.40
2:C:712:ALA:HB3	2:C:821:GLU:HG3	2.02	0.40
1:A:133:GLU:HG2	1:A:134:GLU:H	1.86	0.40
2:C:1039:ALA:HB2	3:D:707:THR:HG21	2.02	0.40
2:C:740:GLU:HB3	2:C:805:ARG:NH1	2.37	0.40
2:C:681:GLY:HA3	3:D:939:PHE:CD1	2.56	0.40
2:C:784:ASP:OD1	2:C:784:ASP:N	2.41	0.40
3:D:353:VAL:HG12	3:D:355:VAL:H	1.86	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: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%)	56	88
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 ⓘ

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%)	63	86
1	B	200/264 (76%)	190 (95%)	10 (5%)	30	67
2	C	936/941 (100%)	906 (97%)	30 (3%)	46	79
3	D	1253/1279 (98%)	1219 (97%)	34 (3%)	52	82
4	E	82/88 (93%)	81 (99%)	1 (1%)	78	92
5	F	301/388 (78%)	290 (96%)	11 (4%)	41	76
All	All	2972/3224 (92%)	2882 (97%)	90 (3%)	48	81

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

Some 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 ⓘ

There are no RNA molecules in this entry.

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

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	2RA	I	1	9,8	3,5,6	0.54	0	1,5,7	2.11	1 (100%)
8	DSN	I	2	8	4,5,6	0.51	0	2,5,7	1.34	0
8	DVA	I	3	8	5,6,7	0.49	0	5,7,9	1.36	1 (20%)
8	R2T	I	4	8	9,10,11	2.15	2 (22%)	10,13,15	1.21	1 (10%)
8	2TL	I	5	8	5,6,7	1.23	1 (20%)	5,7,9	1.12	0
8	0QZ	I	6	8	5,5,6	1.37	1 (20%)	4,5,7	1.36	1 (25%)
8	FGL	I	7	8	2,6,7	0.60	0	1,7,9	0.50	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	2RA	I	1	9,8	-	0/1/4/6	0/0/0/0
8	DSN	I	2	8	-	0/2/4/6	0/0/0/0
8	DVA	I	3	8	-	0/4/6/8	0/0/0/0
8	R2T	I	4	8	-	0/12/14/16	0/0/0/0
8	2TL	I	5	8	-	0/4/6/8	0/0/0/0
8	0QZ	I	6	8	-	0/2/4/6	0/0/0/0
8	FGL	I	7	8	-	0/0/6/8	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	6	0QZ	OB-CA	-2.87	1.38	1.43
8	I	5	2TL	OG1-CB	-2.38	1.37	1.43
8	I	4	R2T	OB1-CB	-2.21	1.37	1.43
8	I	4	R2T	CD-NE2	5.49	1.43	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	3	DVA	O-C-CA	-2.74	118.20	125.44
8	I	6	0QZ	O-C-CA	-2.46	119.14	125.35
8	I	1	2RA	O-C-CA	-2.11	119.98	125.49
8	I	4	R2T	C-CA-N	2.30	114.63	109.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z > 2$
11	RFV	C	1201	-	50,53,53	1.86	8 (16%)	64,80,80	1.85	16 (25%)
9	MB8	I	101	8	0,1,6	0.00	-	0,0,7	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	RFV	C	1201	-	-	0/55/70/70	0/1/4/4
9	MB8	I	101	8	-	0/0/0/6	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1201	RFV	O7-C25	-4.90	1.37	1.44
11	C	1201	RFV	O9-C23	-2.16	1.37	1.43
11	C	1201	RFV	C5-C10	2.05	1.46	1.42
11	C	1201	RFV	C6-C7	2.93	1.45	1.39
11	C	1201	RFV	C2-N1	3.09	1.47	1.41
11	C	1201	RFV	C18-C17	3.26	1.53	1.43
11	C	1201	RFV	C15-N1	5.00	1.47	1.35
11	C	1201	RFV	C17-C16	5.98	1.54	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1201	RFV	C30-C16-C17	-6.49	107.83	123.22
11	C	1201	RFV	C13-C12-C11	-3.26	110.02	117.83
11	C	1201	RFV	C5-C6-C7	-2.98	119.63	124.47
11	C	1201	RFV	C33-C24-C25	-2.91	105.95	111.38
11	C	1201	RFV	C18-C17-C16	-2.41	119.75	126.82
11	C	1201	RFV	C20-C19-C18	-2.34	120.81	126.07
11	C	1201	RFV	C17-C16-C15	-2.14	115.89	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1201	RFV	C34-C26-C27	-2.05	106.64	110.97
11	C	1201	RFV	C25-O7-C35	2.03	120.84	117.70
11	C	1201	RFV	C6-C5-C10	2.08	121.40	119.95
11	C	1201	RFV	C23-C24-C25	2.67	116.02	110.82
11	C	1201	RFV	C12-O5-C29	2.93	123.98	116.72
11	C	1201	RFV	C37-O6-C27	3.43	120.32	113.20
11	C	1201	RFV	O4-C11-C5	3.52	122.69	113.15
11	C	1201	RFV	O7-C35-C36	4.12	118.88	111.10
11	C	1201	RFV	O3-C6-C7	4.48	130.54	121.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	1201	RFV	2	0

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%)	-0.41	4 (1%) 73 52	31, 50, 79, 128	0
1	B	227/305 (74%)	-0.34	2 (0%) 85 72	35, 65, 92, 125	0
2	C	1112/1119 (99%)	-0.33	14 (1%) 79 62	15, 44, 109, 139	0
3	D	1485/1524 (97%)	-0.26	15 (1%) 84 69	15, 50, 111, 156	0
4	E	94/99 (94%)	-0.39	0 100 100	27, 55, 99, 107	0
5	F	346/443 (78%)	-0.15	7 (2%) 68 46	24, 66, 122, 138	0
6	G	16/21 (76%)	-0.29	0 100 100	66, 101, 179, 183	0
7	H	24/27 (88%)	-0.21	0 100 100	58, 110, 171, 185	0
8	I	0/7	-	-	-	-
All	All	3535/3850 (91%)	-0.29	42 (1%) 81 64	15, 52, 112, 185	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	ALA	4.1
2	C	766	GLU	3.3
3	D	1281	VAL	3.0
1	A	233	VAL	3.0
5	F	149	GLU	3.0
5	F	390	PHE	2.8
3	D	821	VAL	2.8
2	C	176	VAL	2.8
3	D	360	ARG	2.8
3	D	1305	LEU	2.7
3	D	242	LEU	2.7
1	B	2	LEU	2.7
3	D	174	GLY	2.7
3	D	1297	GLU	2.7
2	C	226	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	173	PRO	2.6
2	C	729	LEU	2.6
3	D	1298	GLY	2.6
1	A	234	ALA	2.6
3	D	1499	ARG	2.5
5	F	369	LEU	2.5
3	D	350	HIS	2.4
2	C	189	ARG	2.4
5	F	414	ARG	2.4
2	C	107	LEU	2.4
3	D	144	GLY	2.3
3	D	1292	VAL	2.3
1	A	231	ALA	2.3
2	C	174	LEU	2.3
2	C	159	ILE	2.3
2	C	764	GLU	2.2
5	F	422	LEU	2.2
5	F	416	ARG	2.2
3	D	1306	PRO	2.2
3	D	316	GLN	2.2
5	F	373	LYS	2.1
1	B	93	SER	2.1
2	C	221	LEU	2.1
2	C	157	ARG	2.1
2	C	217	LEU	2.1
2	C	207	LEU	2.0
2	C	64	LEU	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
8	FGL	I	7	7/8	0.93	0.15	-	19,25,27,29	0
8	2TL	I	5	7/8	0.98	0.18	-	21,21,24,29	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	DSN	I	2	6/7	0.95	0.17	-	20,21,29,31	0
8	0QZ	I	6	6/7	0.97	0.15	-	23,25,25,28	0
8	R2T	I	4	11/12	0.95	0.16	-	21,25,32,33	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
11	RFV	C	1201	50/50	0.95	0.24	0.86	19,30,47,53	0
10	MG	B	401	1/1	0.96	0.25	0.32	25,25,25,25	0
10	MG	F	2001	1/1	0.96	0.17	-0.06	55,55,55,55	0
12	ZN	D	2002	1/1	0.97	0.08	-0.81	79,79,79,79	0
12	ZN	D	2001	1/1	0.97	0.17	-0.88	43,43,43,43	0
10	MG	D	2004	1/1	0.77	0.18	-	50,50,50,50	0
10	MG	D	2003	1/1	0.97	0.17	-	14,14,14,14	0
9	MB8	I	101	2/7	0.96	0.13	-	26,26,26,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.