



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:49 AM UTC

PDB ID : 4OIR / pdb_00004oir
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

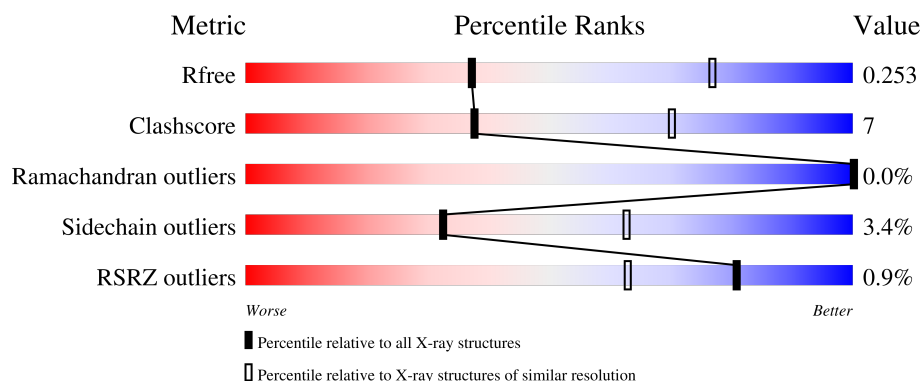
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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	% 59% 15% • 24%
1	B	305	55% 19% • 26%
2	C	1119	80% 19% ••
3	D	1524	% 78% 19% ••
4	E	99	% 76% 18% • 5%

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Mol	Chain	Length	Quality of chain
5	F	443	2% 63% 13% 22%
6	G	21	10% 48% 29% 24%
7	H	27	4% 33% 56% 11%
8	I	7	43% 29% 29%

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			

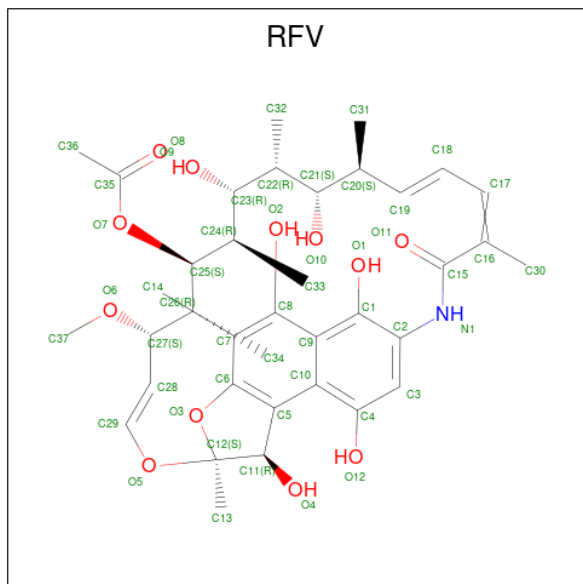
- Molecule 8 is a protein called GE23077.

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

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

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

- Molecule 10 is rifamycin SV (CCD ID: RFV) (formula: $C_{37}H_{49}NO_{12}$).

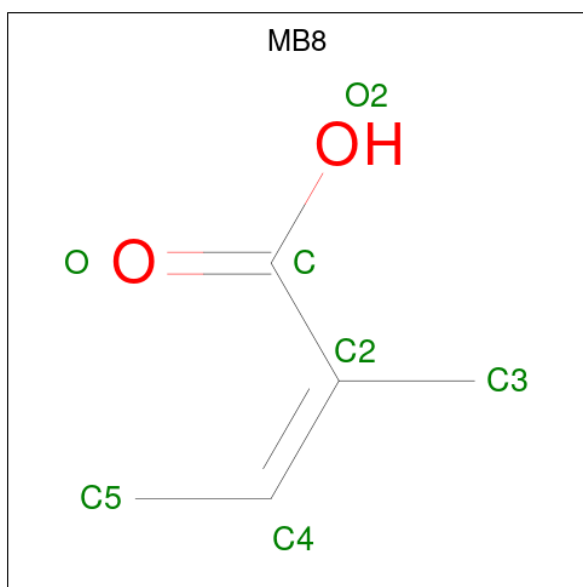


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	N	O	0	0
			50	37	1	12		

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

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

- Molecule 12 is (2Z)-2-methylbut-2-enoic acid (CCD ID: MB8) (formula: $C_5H_8O_2$).



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

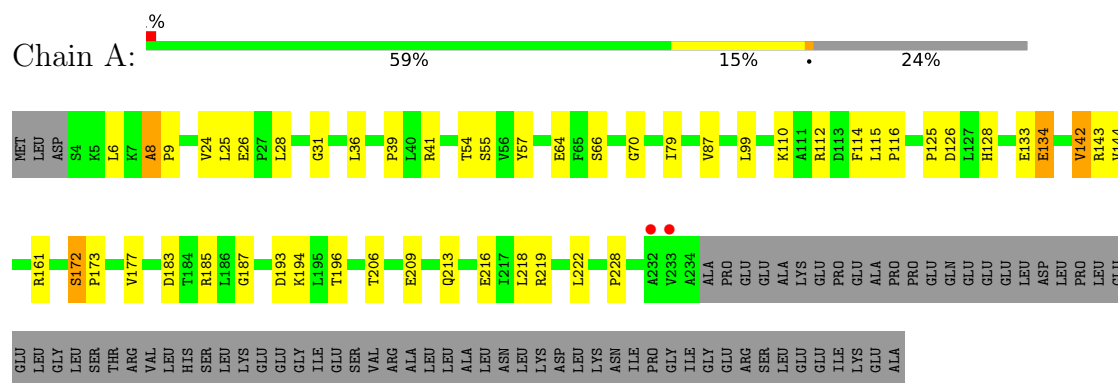
- Molecule 13 is water.

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		

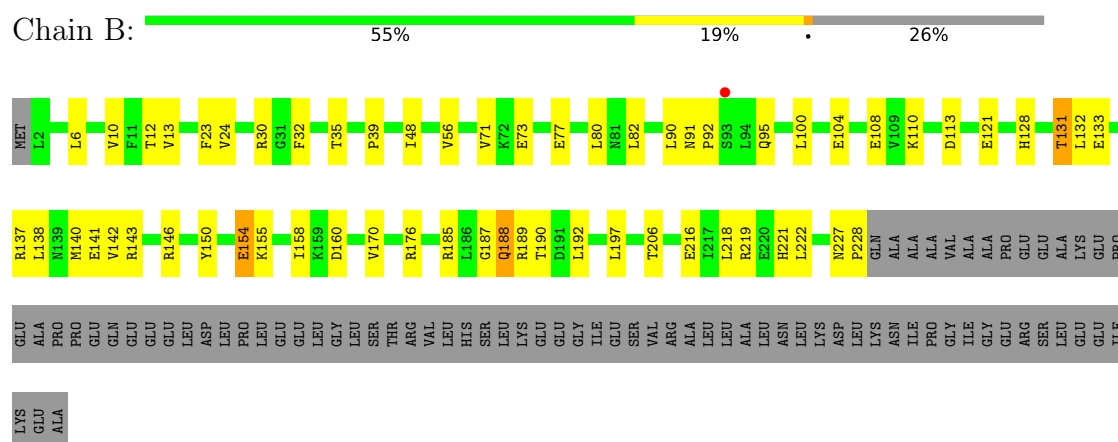
3 Residue-property plots [i](#)

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.

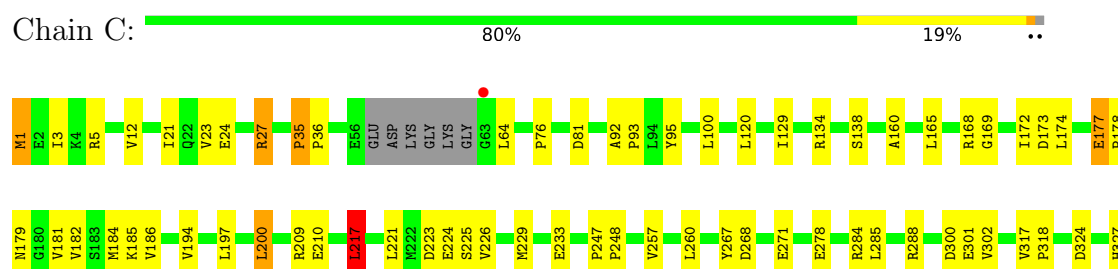
- Molecule 1: DNA-directed RNA polymerase subunit alpha

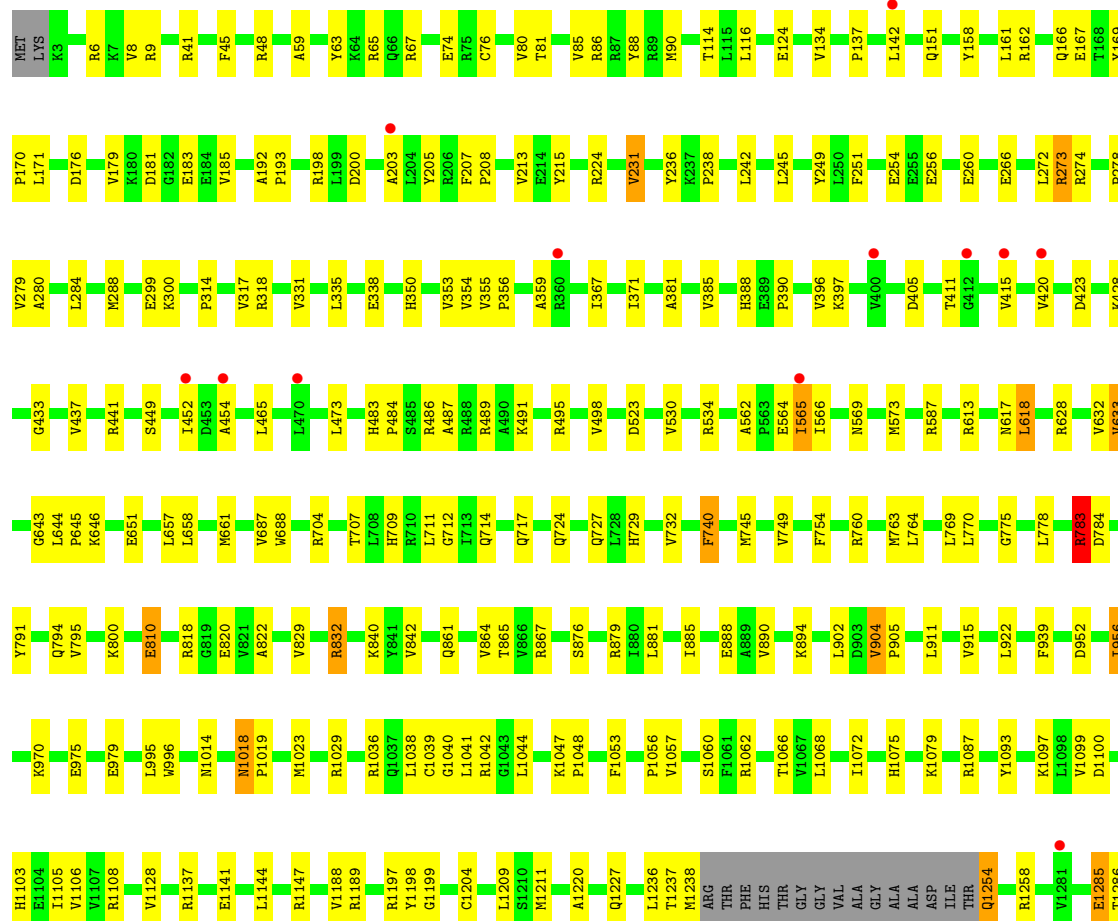


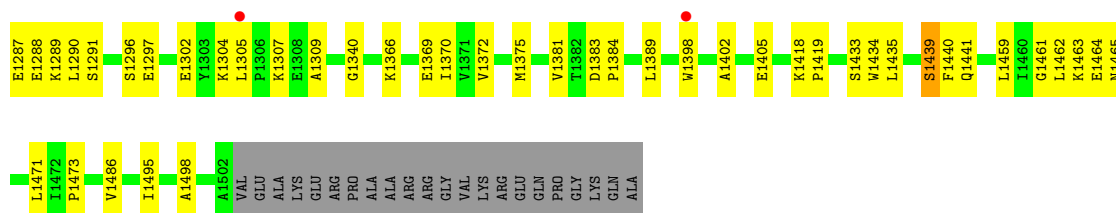
- Molecule 1: DNA-directed RNA polymerase subunit alpha



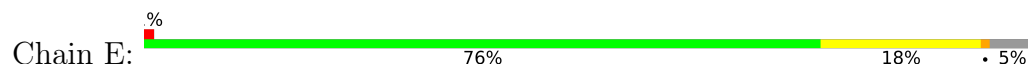
- Molecule 2: DNA-directed RNA polymerase subunit beta



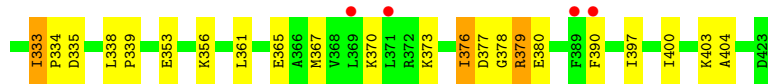
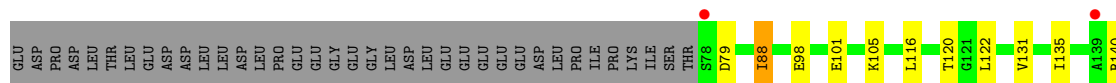
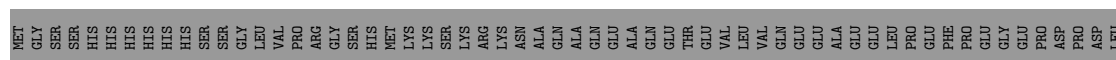




- Molecule 4: DNA-directed RNA polymerase subunit omega



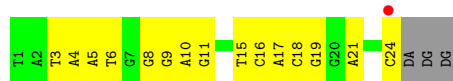
- Molecule 5: DNA directed RNA polymerase sigma factor A



- 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'



- 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'



- Molecule 8: GE23077



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 – 3.10	Depositor EDS
% Data completeness (in resolution range)	82.6 (47.50-3.10) 82.6 (47.50-3.10)	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 0.208 , 0.253	Depositor DCC
R_{free} test set	4160 reflections (3.97%)	wwPDB-VP
Wilson B-factor (Å ²)	63.5	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 23.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
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
F_o, F_c correlation	0.91	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, 0.333 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: FGL, RFV, DVA, ZN, 2RA, 0QZ, DSN, MB8, MG, 2TL, 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	0.30	0/1841	0.83	4/2504 (0.2%)
1	B	0.31	0/1821	0.82	3/2476 (0.1%)
2	C	0.32	0/8941	0.79	9/12092 (0.1%)
3	D	0.31	0/11948	0.79	10/16152 (0.1%)
4	E	0.31	0/772	0.76	0/1040
5	F	0.30	0/2852	0.75	5/3837 (0.1%)
6	G	0.11	0/368	0.51	0/567
7	H	0.13	0/556	0.60	0/858
All	All	0.31	0/29099	0.78	31/39526 (0.1%)

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 (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	433	GLY	N-CA-C	6.73	119.96	110.74
3	D	1340	GLY	CA-C-N	6.24	126.43	119.32
3	D	1340	GLY	C-N-CA	6.24	126.43	119.32
1	B	48	ILE	CA-C-N	6.15	126.51	119.93
1	B	48	ILE	C-N-CA	6.15	126.51	119.93
1	A	8	ALA	CA-C-N	6.10	126.29	120.31
1	A	8	ALA	C-N-CA	6.10	126.29	120.31
1	A	172	SER	CA-C-N	6.01	125.63	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	SER	C-N-CA	6.01	125.63	119.56
3	D	1014	ASN	N-CA-C	5.80	118.82	111.69
2	C	980	GLY	N-CA-C	-5.75	107.13	114.37
5	F	333	ILE	N-CA-C	5.64	113.13	107.55
2	C	169	GLY	CA-C-N	5.63	125.83	120.31
2	C	169	GLY	C-N-CA	5.63	125.83	120.31
3	D	1018	ASN	CA-C-N	5.47	124.93	119.24
3	D	1018	ASN	C-N-CA	5.47	124.93	119.24
3	D	783	ARG	CB-CA-C	-5.44	110.31	116.63
2	C	35	PRO	CA-C-N	5.43	125.51	119.32
2	C	35	PRO	C-N-CA	5.43	125.51	119.32
3	D	617	ASN	N-CA-C	5.38	119.95	113.17
1	B	188	GLN	N-CA-C	5.32	117.15	111.36
2	C	439	CYS	CA-C-N	5.27	124.89	119.56
2	C	439	CYS	C-N-CA	5.27	124.89	119.56
5	F	333	ILE	CA-C-N	5.27	125.03	119.76
5	F	333	ILE	C-N-CA	5.27	125.03	119.76
3	D	88	TYR	N-CA-C	5.20	119.63	113.28
2	C	217	LEU	N-CA-C	-5.17	105.82	111.82
3	D	740	PHE	N-CA-C	5.14	119.19	113.02
5	F	79	ASP	CA-C-N	5.08	124.69	119.05
5	F	79	ASP	C-N-CA	5.08	124.69	119.05
2	C	302	VAL	N-CA-C	5.07	116.25	111.48

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	34	0
2	C	8774	0	8877	136	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	11739	0	11975	179	0
4	E	758	0	770	13	0
5	F	2807	0	2882	45	0
6	G	328	0	181	5	0
7	H	495	0	272	11	0
8	I	50	0	37	2	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	404	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 (404) 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
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
3:D:657:LEU:HG	3:D:661:MET:HE2	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.76	0.67
2:C:1019:GLN:HG2	2:C:1058:ASP:HB3	1.77	0.67
2:C:1:MET:HE3	2:C:3:ILE:HD11	1.76	0.66
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
4:E:37:ASN:HD22	4:E:89:MET:HE1	1.63	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:193:ASP:OD2	2:C:938:LYS:NZ	2.31	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:C:1201:RFV:O4	10:C:1201:RFV:O12	2.25	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
2:C:223:ASP:OD1	2:C:225:SER:OG	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:138:LEU:HD11	1:B:140:MET:HE3	1.95	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
2:C:1056:LYS:NZ	3:D:749:VAL:O	2.45	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
2:C:578:VAL:HG23	2:C:671:ASN:CG	2.39	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
2:C:704:HIS:CE1	2:C:1000:MET:HE1	2.49	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
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:284:LEU:HD22	3:D:288:MET:HE3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:853:LEU:HB2	2:C:858:MET:HE1	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: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:172:ILE:HD13	2:C:184:MET:HE3	1.96	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:HE3	1.98	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
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
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.44	0.46
3:D:842:VAL:HG22	3:D:865:THR:HB	1.98	0.46
2:C:1008:ARG:HD3	2:C:1028:GLY:C	2.41	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:1372:VAL:HA	3:D:1375:MET:HE3	1.97	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:224:GLU:CD	2:C:224:GLU:H	2.24	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
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: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
2:C:548:PRO:O	2:C:843:HIS:HE1	2.01	0.44
2:C:1005:MET:HE2	3:D:724:GLN:HE21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:905:ILE:C	2:C:907:ASP:H	2.26	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:420:ARG:C	2:C:422:ARG:H	2.25	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
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
2:C:397:GLU:OE2	2:C:632:ASN:N	2.49	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
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
3:D:818:ARG:HE	3:D:820:GLU:CD	2.27	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:810:GLU:CD	3:D:810:GLU:H	2.28	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
2:C:580:MET:HB3	2:C:584:GLU:CD	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1211:MET:HE1	4:E:16:LYS:HD2	2.00	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
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
3:D:90:MET:HE3	3:D:90:MET:HB3	1.92	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: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
4:E:12:MET:HE1	4:E:69:LEU:HA	2.02	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: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

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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%)	48	78
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%)	48	72
1	B	200/264 (76%)	189 (94%)	11 (6%)	19	50
2	C	936/941 (100%)	902 (96%)	34 (4%)	31	62
3	D	1253/1279 (98%)	1216 (97%)	37 (3%)	36	65
4	E	82/88 (93%)	80 (98%)	2 (2%)	43	69
5	F	301/388 (78%)	288 (96%)	13 (4%)	26	57
All	All	2972/3224 (92%)	2871 (97%)	101 (3%)	32	63

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	66	SER
1	A	134	GLU
1	A	142	VAL
1	B	6	LEU
1	B	10	VAL
1	B	95	GLN

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Mol	Chain	Res	Type
1	B	131	THR
1	B	133	GLU
1	B	154	GLU
1	B	160	ASP
1	B	188	GLN
1	B	189	ARG
1	B	192	LEU
1	B	206	THR
2	C	1	MET
2	C	5	ARG
2	C	21	ILE
2	C	23	VAL
2	C	27	ARG
2	C	81	ASP
2	C	138	SER
2	C	177	GLU
2	C	182	VAL
2	C	200	LEU
2	C	217	LEU
2	C	257	VAL
2	C	285	LEU
2	C	301	GLU
2	C	342	ASP
2	C	348	LEU
2	C	361	MET
2	C	384	GLU
2	C	398	THR
2	C	418	LEU
2	C	419	THR
2	C	557	ARG
2	C	600	ASP
2	C	617	ASP
2	C	620	LEU
2	C	674	VAL
2	C	715	THR
2	C	722	ILE
2	C	968	LEU
2	C	998	TYR
2	C	1008	ARG
2	C	1010	THR
2	C	1058	ASP
2	C	1095	LEU

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Mol	Chain	Res	Type
3	D	6	ARG
3	D	80	VAL
3	D	81	THR
3	D	183	GLU
3	D	231	VAL
3	D	273	ARG
3	D	331	VAL
3	D	335	LEU
3	D	354	VAL
3	D	415	VAL
3	D	420	VAL
3	D	523	ASP
3	D	618	LEU
3	D	632	VAL
3	D	633	VAL
3	D	687	VAL
3	D	717	GLN
3	D	754	PHE
3	D	778	LEU
3	D	783	ARG
3	D	810	GLU
3	D	829	VAL
3	D	832	ARG
3	D	904	VAL
3	D	956	ILE
3	D	1036	ARG
3	D	1039	CYS
3	D	1041	LEU
3	D	1066	THR
3	D	1128	VAL
3	D	1188	VAL
3	D	1254	GLN
3	D	1285	GLU
3	D	1287	GLU
3	D	1307	LYS
3	D	1433	SER
3	D	1439	SER
4	E	50	THR
4	E	80	VAL
5	F	88	ILE
5	F	116	LEU
5	F	141	VAL

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Mol	Chain	Res	Type
5	F	156	VAL
5	F	205	ARG
5	F	279	GLN
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 (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	99	GLN
2	C	187	ASN
2	C	538	GLN
2	C	563	ASN
2	C	575	GLN
2	C	647	GLN
2	C	670	GLN
2	C	991	GLN
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	1018	ASN
3	D	1172	HIS
3	D	1195	GLN
5	F	402	ASN

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	8,12	4,5,6	0.55	0	1,5,7	0.45	0
8	R2T	I	4	8	8,10,11	2.00	2 (25%)	6,13,15	0.92	0
8	2TL	I	5	8	5,6,7	1.11	0	5,7,9	1.00	0
8	0QZ	I	6	8	4,5,6	1.67	1 (25%)	2,5,7	0.80	0
8	FGL	I	7	8	5,6,7	1.08	0	1,7,9	2.03	1 (100%)

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	8,12	-	2/2/4/6	-
8	R2T	I	4	8	-	6/13/14/16	-
8	2TL	I	5	8	-	1/5/6/8	-
8	0QZ	I	6	8	-	1/3/4/6	-
8	FGL	I	7	8	-	2/4/6/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	4	R2T	CD-NE2	4.59	1.43	1.32
8	I	6	0QZ	OB-CA	-3.23	1.38	1.43
8	I	4	R2T	OB1-CB	-2.14	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	124.08

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 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	-	51,53,53	3.55	14 (27%)	73,80,80	2.47	16 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

All (14) 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	7.30	1.54	1.34
10	C	1201	RFV	C15-N1	5.61	1.47	1.35
10	C	1201	RFV	O7-C25	-5.12	1.37	1.44
10	C	1201	RFV	C18-C17	3.44	1.53	1.43
10	C	1201	RFV	C6-C7	3.07	1.45	1.39
10	C	1201	RFV	C2-N1	3.02	1.47	1.41
10	C	1201	RFV	O3-C12	2.74	1.49	1.45
10	C	1201	RFV	C29-C28	2.10	1.41	1.30
10	C	1201	RFV	O9-C23	-2.08	1.37	1.43
10	C	1201	RFV	C4-C10	2.07	1.46	1.43
10	C	1201	RFV	O6-C27	-2.04	1.38	1.43
10	C	1201	RFV	O3-C6	2.02	1.41	1.37
10	C	1201	RFV	C3-C4	2.01	1.42	1.37

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	-6.52	107.83	123.67
10	C	1201	RFV	O3-C6-C7	5.53	130.54	121.16
10	C	1201	RFV	O4-C11-C12	5.35	122.85	113.41
10	C	1201	RFV	C5-C6-C7	-4.69	119.63	124.50
10	C	1201	RFV	O7-C35-C36	4.37	118.88	111.09
10	C	1201	RFV	O3-C6-C5	-3.90	109.81	113.06
10	C	1201	RFV	C13-C12-C11	-3.35	110.02	117.78
10	C	1201	RFV	C37-O6-C27	3.20	120.32	112.99
10	C	1201	RFV	C33-C24-C25	-3.10	105.95	111.40
10	C	1201	RFV	C23-C24-C25	2.85	116.02	110.58
10	C	1201	RFV	C20-C19-C18	-2.57	120.81	126.11
10	C	1201	RFV	C12-O5-C29	2.56	123.98	117.82
10	C	1201	RFV	C18-C17-C16	-2.44	119.75	126.64
10	C	1201	RFV	C34-C26-C27	-2.13	106.64	110.95
10	C	1201	RFV	C25-O7-C35	2.01	120.84	117.72

There are no chirality outliers.

All (10) torsion outliers are listed below:

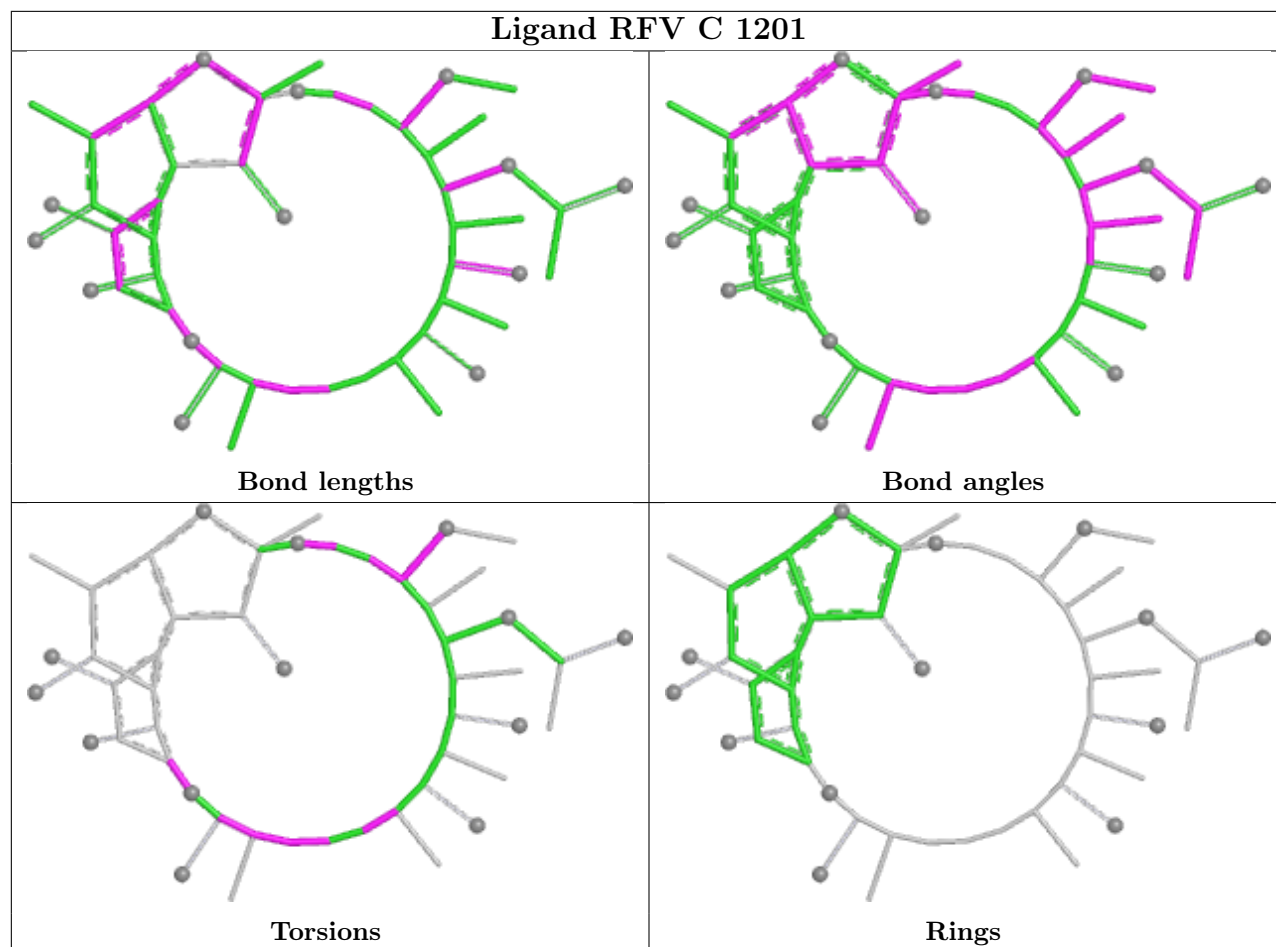
Mol	Chain	Res	Type	Atoms
10	C	1201	RFV	C16-C17-C18-C19
10	C	1201	RFV	C26-C27-C28-C29
10	C	1201	RFV	C26-C27-O6-C37
10	C	1201	RFV	C28-C27-O6-C37
10	C	1201	RFV	C18-C19-C20-C31
10	C	1201	RFV	C1-C2-N1-C15
10	C	1201	RFV	C15-C16-C17-C18
10	C	1201	RFV	C28-C29-O5-C12
10	C	1201	RFV	N1-C15-C16-C17
10	C	1201	RFV	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%)	-0.21	2 (0%) 81 63	31, 50, 79, 128	0
1	B	227/305 (74%)	0.06	1 (0%) 88 76	35, 65, 92, 125	0
2	C	1112/1119 (99%)	-0.20	2 (0%) 91 83	15, 44, 109, 139	0
3	D	1485/1524 (97%)	-0.06	14 (0%) 81 63	15, 50, 111, 156	1 (0%)
4	E	94/99 (94%)	-0.06	1 (1%) 78 59	27, 55, 99, 107	0
5	F	346/443 (78%)	0.17	8 (2%) 61 39	24, 66, 122, 138	0
6	G	16/21 (76%)	0.60	2 (12%) 8 5	66, 101, 179, 183	0
7	H	24/27 (88%)	0.37	1 (4%) 40 22	58, 110, 171, 185	0
8	I	0/7	-	-	-	-
All	All	3535/3850 (91%)	-0.08	31 (0%) 81 63	15, 52, 112, 185	1 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	93	SER	3.4
3	D	412	GLY	3.0
2	C	63	GLY	2.9
5	F	78	SER	2.9
3	D	203	ALA	2.8
6	G	19	DG	2.7
4	E	95	VAL	2.6
3	D	454	ALA	2.6
5	F	390	PHE	2.6
5	F	369	LEU	2.6
3	D	420	VAL	2.6
5	F	323	ASP	2.5
3	D	400	VAL	2.5
5	F	145	PRO	2.5
7	H	24	DC	2.4

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Mol	Chain	Res	Type	RSRZ
5	F	371	LEU	2.3
3	D	565	ILE	2.3
5	F	389	PHE	2.3
3	D	1281	VAL	2.3
3	D	142	LEU	2.3
6	G	4	DG	2.3
3	D	360	ARG	2.2
3	D	452	ILE	2.2
3	D	1305	LEU	2.2
5	F	139	ALA	2.2
2	C	766	GLU	2.2
3	D	1398	TRP	2.2
1	A	232	ALA	2.1
3	D	470	LEU	2.1
3	D	415	VAL	2.0
1	A	233	VAL	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	2RA	I	1	6/7	0.89	0.10	24,25,29,34	0
8	FGL	I	7	7/8	0.90	0.09	19,25,27,29	0
8	R2T	I	4	11/12	0.94	0.07	21,25,32,33	0
8	DVA	I	3	7/8	0.96	0.09	13,17,21,22	0
8	DSN	I	2	6/7	0.96	0.08	20,21,29,31	0
8	2TL	I	5	7/8	0.96	0.08	21,21,24,29	0
8	0QZ	I	6	6/7	0.97	0.06	23,25,25,28	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

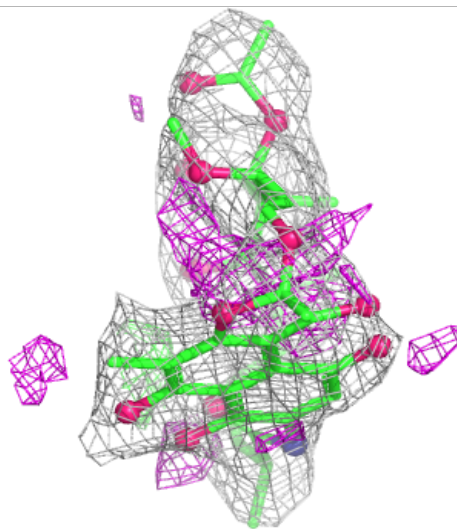
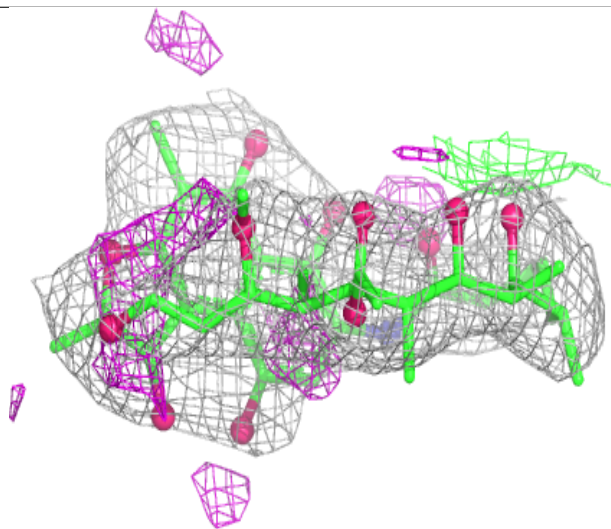
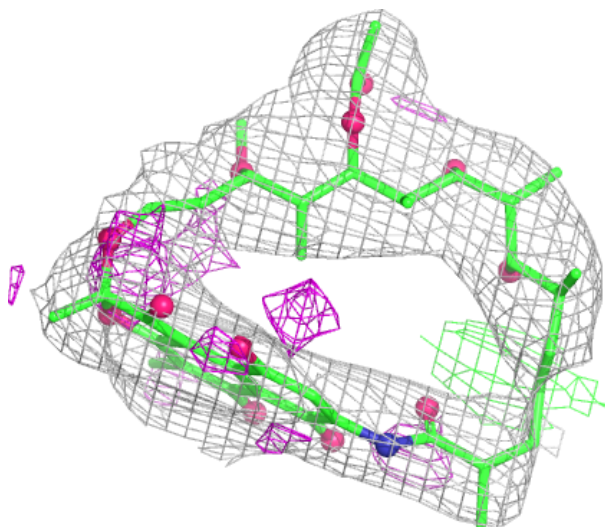
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	MG	D	2004	1/1	0.71	0.15	50,50,50,50	0
12	MB8	I	101	2/7	0.89	0.11	26,26,26,31	0
9	MG	F	2001	1/1	0.91	0.04	55,55,55,55	0
10	RFV	C	1201	50/50	0.92	0.12	19,30,47,53	0
9	MG	B	401	1/1	0.95	0.17	25,25,25,25	0
11	ZN	D	2002	1/1	0.99	0.02	79,79,79,79	0
11	ZN	D	2001	1/1	0.99	0.03	43,43,43,43	0
9	MG	D	2003	1/1	1.00	0.02	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.

Electron density around RFV C 1201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.