



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:18 PM EDT

PDB ID : 4OIN / pdb_00004oin
Title : Crystal structure of Thermus thermophilus transcription initiation complex soaked with GE23077
Authors : Zhang, Y.; Ebright, R.H.; Arnold, E.
Deposited on : 2014-01-20
Resolution : 2.80 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
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

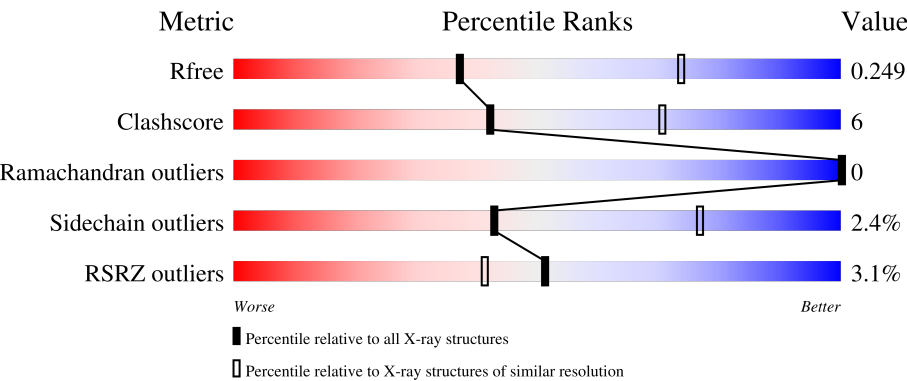
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	315	% 58%15%27%
1	B	315	2% 58%14%28%
2	C	1119	2% 82%17%..
3	D	1524	4% 78%18%..
4	E	99	% 82%13%5%

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Mol	Chain	Length	Quality of chain
5	F	443	
6	G	19	
7	H	27	
8	I	7	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 29180 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	7442	2069	2193	35			

- 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*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			

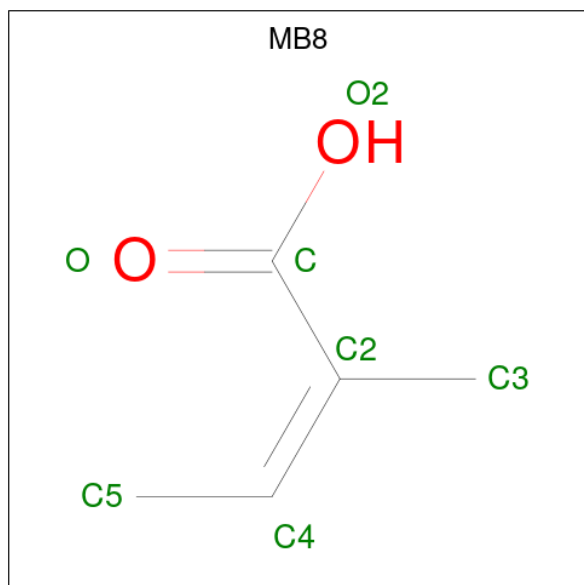
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		
9	D	3	Total	Mg	0	0
			3	3		
9	F	1	Total	Mg	0	0
			1	1		

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 11 is (2Z)-2-methylbut-2-enoic acid (CCD ID: MB8) (formula: C₅H₈O₂).



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

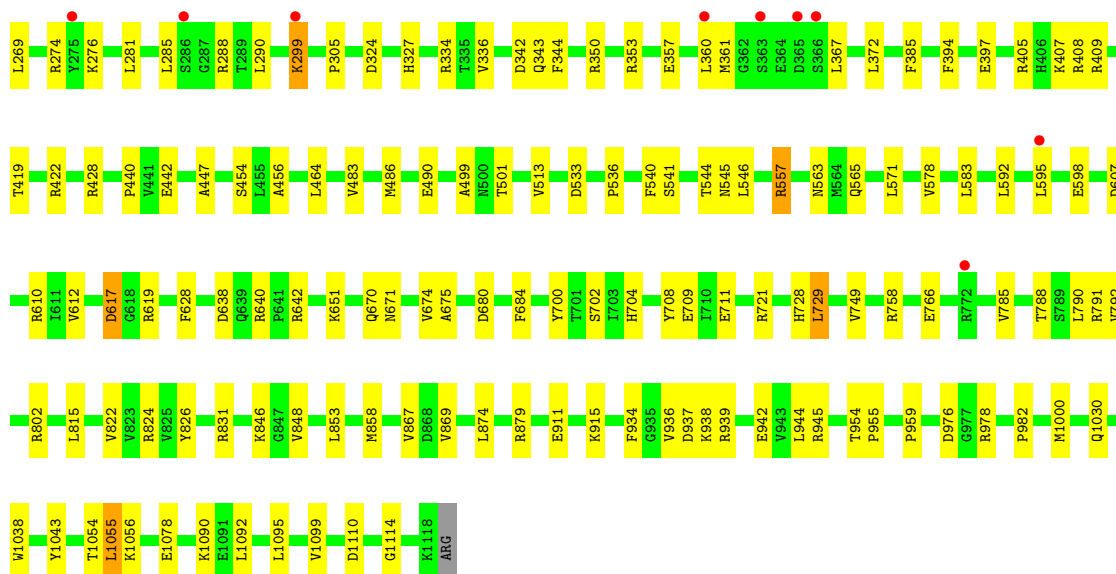
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	27	Total	O	0	0
			27	27		
12	B	25	Total	O	0	0
			25	25		

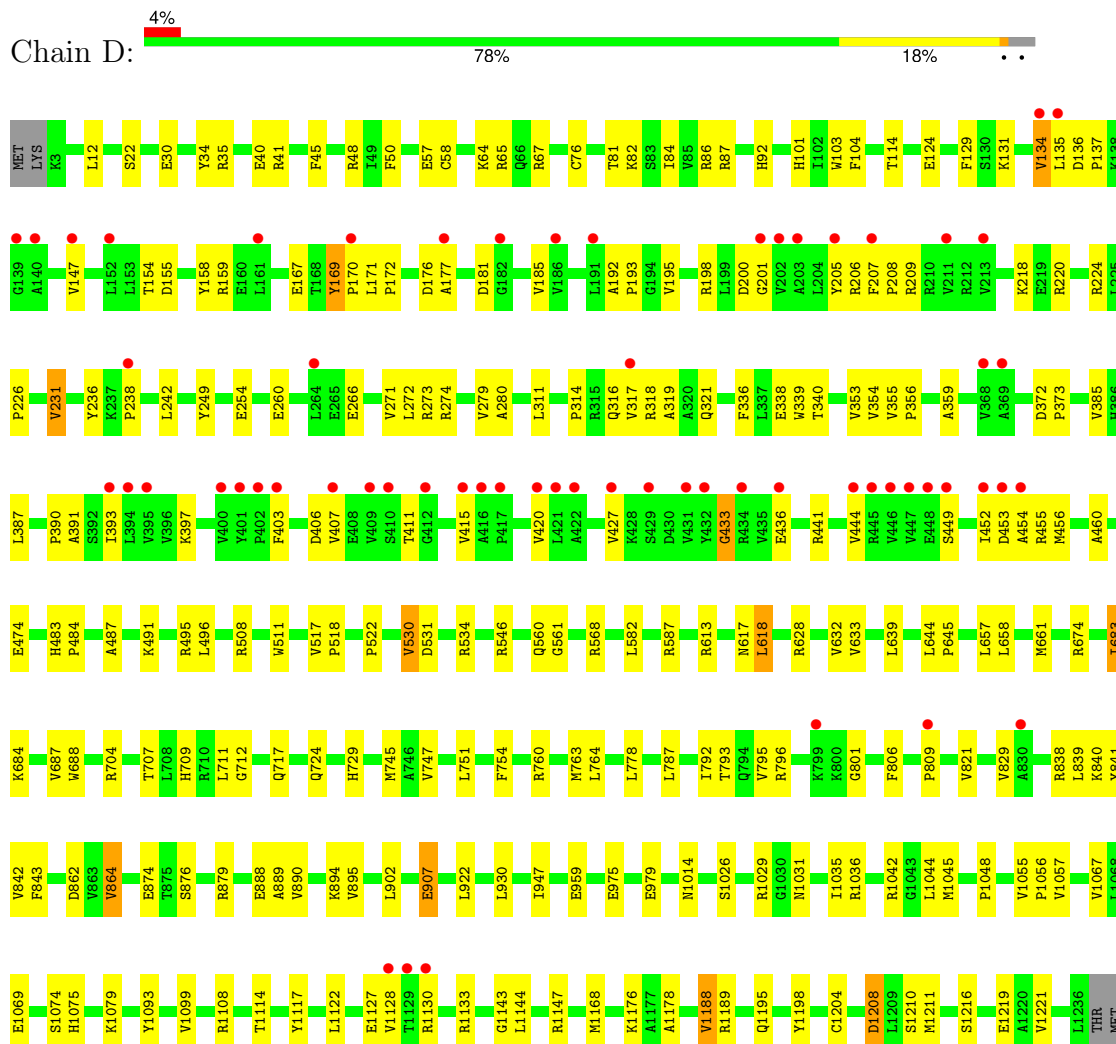
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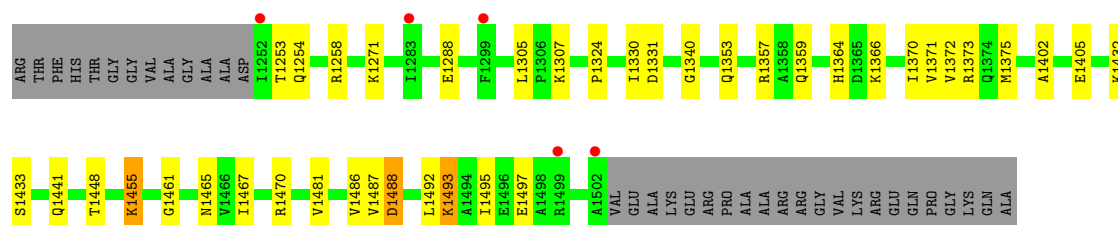
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	221	Total 221	O 221	0	0
12	D	269	Total 269	O 269	0	0
12	E	22	Total 22	O 22	0	0
12	F	36	Total 36	O 36	0	0
12	G	10	Total 10	O 10	0	0
12	H	4	Total 4	O 4	0	0
12	I	8	Total 8	O 8	0	0

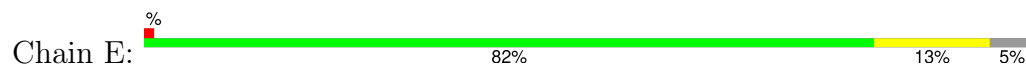


• Molecule 3: DNA-directed RNA polymerase subunit beta'

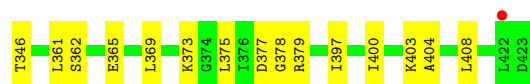
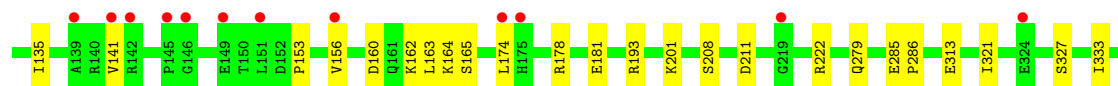
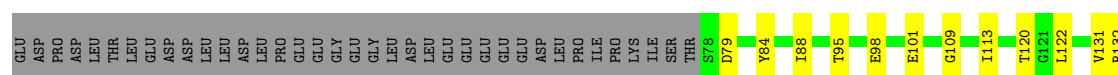
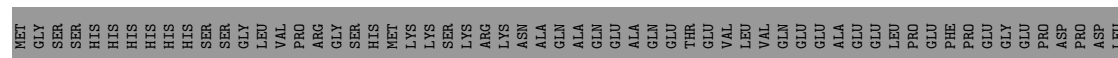




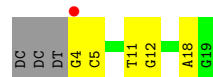
- Molecule 4: DNA-directed RNA polymerase subunit omega



- 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*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	183.77Å 103.20Å 294.77Å 90.00° 99.18° 90.00°	Depositor
Resolution (Å)	48.50 – 2.80 48.50 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.50-2.80) 98.0 (48.50-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.206 , 0.252 0.206 , 0.249	Depositor DCC
R_{free} test set	6582 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.017 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	0.92	EDS
Total number of atoms	29180	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: 0QZ, MB8, FGL, DSN, MG, ZN, R2T, 2RA, 2TL, DVA

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	0.31	0/1841	0.81	4/2504 (0.2%)
1	B	0.29	0/1821	0.79	0/2476
2	C	0.31	0/8941	0.76	4/12092 (0.0%)
3	D	0.32	0/11948	0.79	12/16153 (0.1%)
4	E	0.29	0/772	0.70	0/1040
5	F	0.29	0/2852	0.74	3/3837 (0.1%)
6	G	0.10	0/368	0.48	0/567
7	H	0.12	0/556	0.54	0/858
All	All	0.31	0/29099	0.76	23/39527 (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 (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1208	ASP	N-CA-C	-6.26	99.67	109.25
3	D	433	GLY	N-CA-C	6.14	119.46	110.80
1	A	8	ALA	CA-C-N	6.11	126.62	120.14
1	A	8	ALA	C-N-CA	6.11	126.62	120.14
2	C	169	GLY	CA-C-N	6.04	125.94	119.85
2	C	169	GLY	C-N-CA	6.04	125.94	119.85
1	A	172	SER	CA-C-N	5.77	125.39	119.56
1	A	172	SER	C-N-CA	5.77	125.39	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1144	LEU	N-CA-C	5.59	120.26	113.38
3	D	1340	GLY	CA-C-N	5.56	124.76	118.97
3	D	1340	GLY	C-N-CA	5.56	124.76	118.97
2	C	35	PRO	CA-C-N	5.53	125.62	119.32
2	C	35	PRO	C-N-CA	5.53	125.62	119.32
5	F	333	ILE	N-CA-C	5.42	112.92	107.55
3	D	169	TYR	CA-C-N	5.33	125.74	119.99
3	D	169	TYR	C-N-CA	5.33	125.74	119.99
3	D	1481	VAL	N-CA-C	5.25	119.68	113.22
3	D	617	ASN	N-CA-C	5.19	119.71	113.17
3	D	1014	ASN	N-CA-C	5.10	117.96	111.69
3	D	136	ASP	CA-C-N	5.03	124.69	119.56
3	D	136	ASP	C-N-CA	5.03	124.69	119.56
5	F	79	ASP	CA-C-N	5.02	125.04	119.32
5	F	79	ASP	C-N-CA	5.02	125.04	119.32

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	29	0
1	B	1789	0	1841	27	0
2	C	8774	0	8877	115	0
3	D	11739	0	11977	172	0
4	E	758	0	770	9	0
5	F	2807	0	2882	36	0
6	G	328	0	181	5	0
7	H	495	0	272	9	0
8	I	50	0	37	3	0
9	B	1	0	0	0	0
9	D	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	1	0	0	0	0
10	D	2	0	0	0	0
11	I	2	0	0	0	0
12	A	27	0	0	0	0
12	B	25	0	0	0	0
12	C	221	0	0	5	0
12	D	269	0	0	7	0
12	E	22	0	0	0	0
12	F	36	0	0	0	0
12	G	10	0	0	1	0
12	H	4	0	0	2	0
12	I	8	0	0	0	0
All	All	29180	0	28700	360	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 6.

All (360) 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)
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.62	0.81
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.66	0.75
2:C:428:ARG:NH2	2:C:447:ALA:O	2.20	0.75
2:C:409:ARG:HH11	2:C:454:SER:HB2	1.53	0.74
2:C:758:ARG:HH21	2:C:788:THR:HB	1.53	0.74
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.68	0.73
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.73	0.70
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.73	0.70
2:C:628:PHE:H	2:C:638:ASP:HB3	1.58	0.69
6:G:4:DG:H1	7:H:24:DC:H42	1.40	0.69
3:D:657:LEU:HG	3:D:661:MET:HE2	1.75	0.69
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.75	0.68
7:H:2:DA:N7	12:H:102:HOH:O	2.25	0.68
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.75	0.68
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.27	0.68
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.76	0.67
3:D:65:ARG:NH1	5:F:378:GLY:O	2.27	0.67
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.75	0.67
3:D:208:PRO:HA	3:D:390:PRO:HA	1.77	0.67
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.75	0.66
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:230:ARG:HD3	2:C:231:PRO:HD2	1.78	0.66
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.77	0.65
2:C:670:GLN:HE21	2:C:700:TYR:H	1.42	0.65
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.79	0.65
3:D:717:GLN:NE2	12:D:2345:HOH:O	2.29	0.65
3:D:433:GLY:HA2	3:D:449:SER:H	1.62	0.65
3:D:534:ARG:NH2	5:F:313:GLU:O	2.31	0.64
3:D:318:ARG:NH1	3:D:338:GLU:OE1	2.30	0.64
2:C:1030:GLN:OE1	3:D:628:ARG:NH1	2.31	0.63
3:D:316:GLN:NE2	3:D:340:THR:O	2.31	0.63
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.80	0.63
3:D:711:LEU:HD13	3:D:778:LEU:HD23	1.80	0.63
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.81	0.63
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.31	0.62
3:D:895:VAL:HG11	3:D:922:LEU:HD21	1.81	0.62
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.82	0.61
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.82	0.61
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.32	0.61
2:C:350:ARG:NH1	12:C:1466:HOH:O	2.32	0.61
3:D:959:GLU:OE1	3:D:959:GLU:N	2.30	0.61
1:A:231:ALA:HB2	1:B:12:THR:HG22	1.82	0.60
2:C:274:ARG:HD2	2:C:288:ARG:HG2	1.83	0.60
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.83	0.60
3:D:1048:PRO:O	3:D:1079:LYS:NZ	2.34	0.60
3:D:1432:LYS:O	3:D:1455:LYS:NZ	2.34	0.60
2:C:598:GLU:O	2:C:651:LYS:NZ	2.35	0.60
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.66	0.60
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.32	0.60
3:D:1093:TYR:OH	3:D:1441:GLN:NE2	2.35	0.60
5:F:193:ARG:HB2	7:H:6:DT:H1'	1.84	0.60
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.82	0.59
3:D:206:ARG:NH2	5:F:101:GLU:OE2	2.35	0.59
1:B:100:LEU:HG	1:B:141:GLU:HG2	1.86	0.58
3:D:1371:VAL:HG12	3:D:1375:MET:HE2	1.85	0.58
3:D:1133:ARG:NH1	12:D:2120:HOH:O	2.36	0.57
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.86	0.57
1:B:94:LEU:O	1:B:146:ARG:NH2	2.36	0.57
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.37	0.57
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.87	0.57
3:D:45:PHE:O	3:D:86:ARG:NH2	2.37	0.57
3:D:207:PHE:HE2	5:F:98:GLU:HG2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:223:ASP:OD1	2:C:225:SER:OG	2.24	0.56
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.40	0.56
3:D:1168:MET:HE3	3:D:1168:MET:HA	1.88	0.56
1:A:106:PRO:HD3	1:A:134:GLU:HG2	1.88	0.56
2:C:628:PHE:H	2:C:638:ASP:CB	2.19	0.56
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.88	0.56
2:C:164:PRO:HA	2:C:269:LEU:HD23	1.87	0.56
2:C:721:ARG:HH22	2:C:785:VAL:HG11	1.71	0.56
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.87	0.55
2:C:419:THR:HG22	2:C:422:ARG:HE	1.71	0.55
2:C:198:ARG:HE	2:C:227:PHE:HA	1.71	0.55
3:D:546:ARG:NH2	12:D:2252:HOH:O	2.38	0.55
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.89	0.55
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.88	0.55
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.87	0.55
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.41	0.55
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.87	0.55
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.88	0.55
1:B:93:SER:O	1:B:95:GLN:NE2	2.39	0.55
3:D:411:THR:HG23	3:D:436:GLU:HA	1.89	0.55
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.88	0.55
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.88	0.54
3:D:658:LEU:HA	3:D:661:MET:HE3	1.89	0.54
3:D:1143:GLY:O	3:D:1147:ARG:HD2	2.06	0.54
2:C:939:ARG:NH2	12:C:1491:HOH:O	2.40	0.54
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.87	0.54
2:C:353:ARG:NH1	2:C:357:GLU:OE2	2.40	0.54
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.08	0.54
3:D:618:LEU:HG	3:D:1467:ILE:HG23	1.90	0.53
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.89	0.53
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.90	0.53
2:C:64:LEU:HB3	2:C:100:LEU:HD11	1.90	0.53
3:D:894:LYS:H	3:D:894:LYS:HD2	1.74	0.53
2:C:557:ARG:HD3	2:C:879:ARG:HB3	1.90	0.53
1:A:199:ILE:HB	1:A:207:PRO:HB3	1.91	0.52
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.90	0.52
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.92	0.52
2:C:260:LEU:HB3	2:C:261:ILE:HD12	1.91	0.52
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.91	0.52
6:G:4:DG:N2	6:G:5:DC:O2	2.41	0.52
3:D:684:LYS:O	3:D:687:VAL:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:217:LEU:HD12	2:C:217:LEU:H	1.73	0.52
3:D:67:ARG:HD2	5:F:379:ARG:HB3	1.92	0.52
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.90	0.52
3:D:200:ASP:O	3:D:397:LYS:HG2	2.10	0.52
3:D:67:ARG:HB3	5:F:377:ASP:O	2.09	0.52
3:D:321:GLN:HB2	3:D:336:PHE:HB2	1.92	0.52
3:D:1042:ARG:HG3	3:D:1045:MET:HE3	1.91	0.52
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.92	0.51
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.91	0.51
2:C:729:LEU:HD11	2:C:791:ARG:HH22	1.75	0.51
3:D:231:VAL:O	3:D:236:TYR:OH	2.28	0.51
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.93	0.51
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.31	0.51
1:A:70:GLY:N	2:C:607:ASP:OD1	2.42	0.51
3:D:1048:PRO:HG3	3:D:1075:HIS:ND1	2.25	0.51
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.75	0.51
1:B:138:LEU:HD11	1:B:140:MET:HE3	1.93	0.51
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.93	0.51
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.91	0.51
3:D:1045:MET:HG3	12:D:2221:HOH:O	2.11	0.51
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.93	0.51
1:B:54:THR:OG1	1:B:145:ASP:OD1	2.27	0.51
3:D:411:THR:O	5:F:178:ARG:NH1	2.36	0.51
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.93	0.50
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.93	0.50
2:C:704:HIS:CE1	2:C:1000:MET:HE1	2.46	0.50
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.92	0.50
3:D:975:GLU:O	3:D:979:GLU:HG2	2.12	0.50
2:C:15:LEU:HD11	2:C:583:LEU:HD11	1.93	0.50
3:D:209:ARG:HE	3:D:391:ALA:HB2	1.74	0.50
3:D:1271:LYS:HE2	3:D:1331:ASP:HB2	1.93	0.50
5:F:160:ASP:O	5:F:164:LYS:HG2	2.12	0.49
2:C:610:ARG:HD3	2:C:612:VAL:HG23	1.92	0.49
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.47	0.49
3:D:67:ARG:CZ	5:F:379:ARG:HD3	2.42	0.49
3:D:809:PRO:HB3	3:D:839:LEU:HD13	1.94	0.49
3:D:560:GLN:HE22	5:F:222:ARG:HH12	1.60	0.49
2:C:168:ARG:O	2:C:267:TYR:HA	2.13	0.49
2:C:167:LYS:HD3	7:H:12:DC:H5	1.78	0.49
2:C:405:ARG:NE	2:C:442:GLU:OE2	2.36	0.49
1:A:209:GLU:O	1:A:213:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:846:LYS:NZ	8:I:4:R2T:HG2	2.27	0.49
7:H:16:DC:H2''	7:H:17:DA:C8	2.47	0.49
3:D:274:ARG:NH2	3:D:279:VAL:HG21	2.27	0.49
3:D:508:ARG:HB2	3:D:511:TRP:CE2	2.48	0.49
3:D:155:ASP:OD1	3:D:159:ARG:NH1	2.46	0.49
1:B:54:THR:HG22	1:B:169:ALA:HB2	1.95	0.48
2:C:65:VAL:HG21	2:C:103:LYS:HE3	1.95	0.48
2:C:874:LEU:O	3:D:1029:ARG:HG3	2.12	0.48
3:D:530:VAL:HG12	3:D:531:ASP:H	1.77	0.48
3:D:1114:THR:OG1	3:D:1195:GLN:NE2	2.45	0.48
2:C:218:VAL:HG22	2:C:222:MET:HE2	1.95	0.48
3:D:207:PHE:CE2	5:F:98:GLU:HG2	2.47	0.48
7:H:18:DC:H2'	7:H:19:DG:C8	2.49	0.48
2:C:124:ASP:OD2	2:C:407:LYS:NZ	2.44	0.48
2:C:361:MET:HE1	5:F:201:LYS:HD2	1.96	0.48
3:D:22:SER:HB2	3:D:92:HIS:HB3	1.94	0.48
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.95	0.48
1:B:58:ILE:HG12	1:B:140:MET:HE2	1.95	0.48
2:C:501:THR:HG22	12:C:1472:HOH:O	2.13	0.48
6:G:12:DG:N2	7:H:16:DC:O2	2.35	0.48
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.36	0.48
3:D:1128:VAL:HG23	3:D:1130:ARG:H	1.79	0.48
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.95	0.48
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.95	0.48
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.47	0.47
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.95	0.47
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.96	0.47
2:C:540:PHE:HB3	2:C:544:THR:HB	1.95	0.47
3:D:137:PRO:HB3	3:D:147:VAL:HG12	1.96	0.47
1:B:90:LEU:HD21	1:B:121:GLU:HB2	1.97	0.47
2:C:541:SER:O	2:C:545:ASN:ND2	2.43	0.47
2:C:976:ASP:OD1	2:C:978:ARG:HG3	2.15	0.47
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.97	0.47
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.97	0.47
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.96	0.47
3:D:683:ILE:HD11	3:D:688:TRP:CZ2	2.50	0.47
3:D:658:LEU:HD11	3:D:674[A]:ARG:HH11	1.80	0.47
3:D:806:PHE:HB2	3:D:829:VAL:HG22	1.97	0.47
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.96	0.47
3:D:272:LEU:O	3:D:279:VAL:N	2.47	0.46
5:F:84:TYR:O	5:F:88:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.96	0.46
2:C:299:LYS:HE2	2:C:299:LYS:HA	1.96	0.46
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.97	0.46
2:C:680:ASP:OD2	2:C:978:ARG:NH2	2.48	0.46
6:G:18:DA:N6	12:G:101:HOH:O	2.49	0.46
2:C:440:PRO:HB2	3:D:1074:SER:OG	2.15	0.46
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.65	0.46
2:C:167:LYS:HD3	7:H:12:DC:C5	2.51	0.46
3:D:879:ARG:HD3	3:D:902:LEU:O	2.16	0.46
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.51	0.46
1:A:90:LEU:HB2	1:A:119:ASP:HB3	1.98	0.46
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.98	0.45
3:D:1122:LEU:HD13	3:D:1178:ALA:HB2	1.99	0.45
6:G:11:DT:H2"	6:G:12:DG:C8	2.52	0.45
3:D:30:GLU:OE1	3:D:40:GLU:HG2	2.17	0.45
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.51	0.45
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.39	0.45
1:A:100:LEU:HD22	1:A:141:GLU:HG2	1.98	0.45
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.98	0.45
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.99	0.45
1:B:78:ILE:HG21	1:B:140:MET:HE1	1.98	0.45
2:C:334:ARG:NH2	2:C:342:ASP:OD2	2.45	0.45
3:D:41:ARG:HE	3:D:48:ARG:CZ	2.30	0.45
3:D:353:VAL:HG11	3:D:387:LEU:HD11	1.98	0.45
3:D:560:GLN:NE2	5:F:222:ARG:HH12	2.14	0.45
3:D:456:MET:HE1	3:D:568:ARG:NE	2.32	0.45
1:B:32:PHE:HA	1:B:35:THR:HB	1.98	0.45
2:C:76:PRO:HG3	2:C:120:LEU:HD12	1.99	0.45
2:C:132:ALA:HB1	2:C:394:PHE:HE1	1.82	0.45
2:C:172:ILE:HD13	2:C:184:MET:HE3	1.97	0.45
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.50	0.45
3:D:238:PRO:HG3	3:D:318:ARG:HB2	1.99	0.45
3:D:487:ALA:O	3:D:491:LYS:HG2	2.16	0.45
2:C:911:GLU:O	2:C:915:LYS:HG2	2.16	0.45
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.52	0.44
3:D:1211:MET:HE1	4:E:16:LYS:HD2	1.99	0.44
2:C:41:ASN:O	2:C:46:ALA:HB2	2.17	0.44
3:D:260:GLU:HB3	3:D:271:VAL:HB	2.00	0.44
1:A:54:THR:HG21	1:A:145:ASP:HB2	2.00	0.44
2:C:118:ILE:HD11	2:C:344:PHE:HE2	1.82	0.44
2:C:367:LEU:HD13	2:C:372:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:220:ARG:NH1	12:D:2339:HOH:O	2.51	0.44
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.16	0.44
5:F:109:GLY:O	5:F:113:ILE:HG13	2.17	0.44
3:D:1353:GLN:O	3:D:1357:ARG:HG3	2.17	0.44
5:F:362:SER:OG	5:F:365:GLU:HG2	2.18	0.44
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.99	0.44
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.87	0.44
3:D:1253:THR:HG21	3:D:1359:GLN:HE22	1.83	0.44
3:D:1176:LYS:HB3	3:D:1176:LYS:HE2	1.79	0.44
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.68	0.44
2:C:324:ASP:HB3	2:C:327:HIS:HB2	2.00	0.44
3:D:135:LEU:O	3:D:453:ASP:HB3	2.18	0.44
3:D:171:LEU:HA	3:D:172:PRO:HD2	1.89	0.44
1:A:6:LEU:HD11	1:A:27:PRO:HG2	1.99	0.43
1:A:159:LYS:HE3	1:A:164:ALA:O	2.17	0.43
1:A:183:ASP:HA	2:C:938:LYS:HE3	1.99	0.43
3:D:792:ILE:HG13	3:D:793:THR:HG23	2.00	0.43
3:D:1487:VAL:HG11	3:D:1492:LEU:HD13	2.00	0.43
3:D:1492:LEU:HD22	4:E:74:VAL:HG21	2.01	0.43
2:C:194:VAL:HA	2:C:197:LEU:HD12	2.00	0.43
3:D:84:ILE:O	3:D:87:ARG:HG2	2.18	0.43
2:C:617:ASP:HB2	2:C:619:ARG:HG2	2.00	0.43
2:C:708:TYR:HB3	2:C:790:LEU:HD21	2.00	0.43
2:C:97:ARG:HG2	2:C:112:GLU:HB2	2.00	0.43
3:D:176:ASP:OD1	3:D:177:ALA:N	2.44	0.43
1:A:57:TYR:CE1	1:A:161:ARG:HD2	2.53	0.43
4:E:14:ASP:OD2	4:E:18:ARG:NH1	2.50	0.43
2:C:563:ASN:HB3	8:I:7:FGL:OG1	2.19	0.43
1:A:20:TYR:C	1:A:207:PRO:HG2	2.44	0.43
2:C:499:ALA:HB2	2:C:533:ASP:HB2	2.00	0.43
3:D:317:VAL:HG23	3:D:339:TRP:HB3	2.00	0.43
2:C:1056:LYS:HE2	3:D:751:LEU:HG	2.00	0.43
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.50	0.43
2:C:101:ILE:HG12	2:C:108:ILE:HG12	2.01	0.43
3:D:1208:ASP:OD1	3:D:1210:SER:OG	2.34	0.43
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.54	0.43
1:B:94:LEU:HD11	1:B:97:VAL:HG22	2.01	0.42
2:C:954:THR:HA	2:C:955:PRO:HD3	1.91	0.42
3:D:81:THR:OG1	3:D:82:LYS:N	2.52	0.42
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.50	0.42
3:D:1373:ARG:HD3	12:D:2140:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.19	0.42
2:C:154:ARG:H	2:C:154:ARG:HG2	1.68	0.42
2:C:684:PHE:HB3	3:D:633:VAL:HG21	2.01	0.42
3:D:103:TRP:HB3	3:D:1448:THR:HG21	2.02	0.42
3:D:129:PHE:HD1	3:D:456:MET:HE3	1.83	0.42
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.73	0.42
3:D:372:ASP:HA	3:D:373:PRO:HD3	1.88	0.42
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.54	0.42
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.87	0.42
2:C:546:LEU:HB2	2:C:565:GLN:HE22	1.84	0.42
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.53	0.42
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.77	0.42
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	2.00	0.42
3:D:1031:ASN:O	3:D:1035:ILE:HG12	2.19	0.42
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	2.01	0.42
3:D:795:VAL:HG12	3:D:876:SER:HB3	2.00	0.42
3:D:796:ARG:NH1	3:D:862:ASP:OD2	2.47	0.42
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.55	0.42
2:C:218:VAL:O	2:C:222:MET:HG2	2.20	0.42
2:C:642:ARG:HD3	2:C:642:ARG:HA	1.87	0.42
3:D:131:LYS:NZ	3:D:154:THR:HG22	2.34	0.42
3:D:838:ARG:HD3	3:D:874:GLU:OE1	2.20	0.42
2:C:858:MET:HE2	2:C:858:MET:HB2	1.86	0.42
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.55	0.42
3:D:801:GLY:HA3	3:D:821:VAL:HG13	2.01	0.42
3:D:1036:ARG:NH2	3:D:1042:ARG:O	2.52	0.42
3:D:1216:SER:N	12:D:2247:HOH:O	2.52	0.42
3:D:67:ARG:CD	5:F:379:ARG:HB3	2.49	0.42
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.84	0.42
1:A:133:GLU:HG2	1:A:134:GLU:N	2.35	0.41
2:C:239:PHE:CD2	2:C:253:ALA:HA	2.54	0.41
3:D:1057:VAL:HG13	3:D:1069:GLU:CD	2.44	0.41
3:D:1117:TYR:HB2	3:D:1188:VAL:O	2.20	0.41
1:B:83:LYS:HE2	1:B:168:ASP:HB2	2.02	0.41
3:D:455:ARG:HB2	3:D:460:ALA:HB2	2.02	0.41
3:D:1219:GLU:OE1	4:E:17:TYR:OH	2.35	0.41
2:C:545:ASN:HB3	2:C:583:LEU:HD22	2.02	0.41
2:C:766:GLU:HG3	3:D:64:LYS:HD3	2.02	0.41
3:D:517:VAL:HA	3:D:518:PRO:HD3	1.95	0.41
7:H:13:DT:O4	12:H:104:HOH:O	2.21	0.41
2:C:13:ILE:HD13	2:C:483:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:408:ARG:NH1	2:C:456:ALA:O	2.53	0.41
3:D:644:LEU:HD12	3:D:645:PRO:HD2	2.02	0.41
3:D:704:ARG:HB2	3:D:745:MET:HG2	2.03	0.41
5:F:321:ILE:O	5:F:327:SER:HB3	2.20	0.41
1:B:56:VAL:HG21	1:B:82:LEU:HD13	2.02	0.41
1:B:124:ASN:OD1	1:B:124:ASN:N	2.53	0.41
2:C:486:MET:HB3	2:C:490:GLU:HB3	2.01	0.41
2:C:536:PRO:HB3	3:D:1067:VAL:HG21	2.03	0.41
2:C:942:GLU:HG3	2:C:945:ARG:HH21	1.85	0.41
3:D:707:THR:HG23	3:D:712:GLY:HA3	2.01	0.41
3:D:889:ALA:HB1	3:D:930:LEU:HA	2.02	0.41
5:F:162:LYS:O	5:F:165:SER:OG	2.33	0.41
1:A:196:THR:HG21	2:C:934:PHE:HE2	1.86	0.41
2:C:124:ASP:HB3	2:C:592:LEU:HD12	2.02	0.41
3:D:185:VAL:N	3:D:201:GLY:O	2.45	0.41
3:D:192:ALA:HB1	3:D:193:PRO:HD2	2.02	0.41
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.20	0.41
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.95	0.41
2:C:409:ARG:HD2	12:C:1339:HOH:O	2.20	0.41
5:F:88:ILE:CG2	5:F:193:ARG:HG2	2.50	0.41
1:A:102:LYS:HE3	1:A:102:LYS:HB2	1.75	0.41
2:C:571:LEU:HD23	2:C:702:SER:HB3	2.03	0.41
2:C:578:VAL:HG23	2:C:671:ASN:CG	2.46	0.41
2:C:749:VAL:HB	2:C:792:VAL:HG21	2.03	0.41
2:C:944:LEU:HD23	2:C:944:LEU:HA	1.97	0.41
3:D:50:PHE:CD2	3:D:522:PRO:HD3	2.55	0.41
3:D:171:LEU:HD11	3:D:393:ILE:HD11	2.03	0.41
3:D:760:ARG:O	3:D:764:LEU:HB2	2.21	0.41
2:C:1054:THR:OG1	2:C:1055:LEU:N	2.53	0.41
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.56	0.41
5:F:373:LYS:HA	5:F:373:LYS:HD3	1.93	0.41
1:B:51:THR:OG1	1:B:87:VAL:O	2.32	0.40
1:B:143:ARG:NH1	1:B:158:ILE:HD12	2.36	0.40
3:D:403:PHE:CD2	3:D:444:VAL:HG23	2.56	0.40
3:D:613:ARG:HG3	3:D:618:LEU:HD22	2.04	0.40
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.56	0.40
5:F:408:LEU:HD23	5:F:408:LEU:HA	1.89	0.40
2:C:265:ARG:NH1	12:C:1417:HOH:O	2.55	0.40
3:D:226:PRO:HD3	3:D:249:TYR:CE2	2.56	0.40
3:D:843:PHE:HE1	3:D:864:VAL:HG21	1.86	0.40
3:D:907:GLU:HB2	3:D:1026:SER:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.21	0.40
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.21	0.40
2:C:17:PRO:HB2	2:C:20:GLU:HB3	2.02	0.40
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.79	0.40
3:D:134:VAL:C	3:D:135:LEU:HD12	2.46	0.40
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.96	0.40
1:A:31:GLY:N	1:A:193:ASP:OD1	2.53	0.40
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.57	0.40
2:C:846:LYS:HZ3	8:I:4:R2T:HG2	1.85	0.40
3:D:58:CYS:HB2	3:D:76:CYS:SG	2.62	0.40
5:F:135:ILE:HG13	5:F:181:GLU:HB2	2.03	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	229/315 (73%)	226 (99%)	3 (1%)	0	100	100
1	B	225/315 (71%)	222 (99%)	3 (1%)	0	100	100
2	C	1108/1119 (99%)	1088 (98%)	20 (2%)	0	100	100
3	D	1482/1524 (97%)	1451 (98%)	31 (2%)	0	100	100
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
5	F	344/443 (78%)	340 (99%)	4 (1%)	0	100	100
All	All	3480/3815 (91%)	3416 (98%)	64 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	200/273 (73%)	194 (97%)	6 (3%)	36	72
1	B	200/273 (73%)	196 (98%)	4 (2%)	48	80
2	C	936/941 (100%)	912 (97%)	24 (3%)	40	75
3	D	1253/1279 (98%)	1223 (98%)	30 (2%)	43	77
4	E	82/88 (93%)	81 (99%)	1 (1%)	63	87
5	F	301/388 (78%)	295 (98%)	6 (2%)	48	80
All	All	2972/3242 (92%)	2901 (98%)	71 (2%)	43	77

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	66	SER
1	A	96	THR
1	A	104	GLU
1	A	205	VAL
1	A	233	VAL
1	B	7	LYS
1	B	10	VAL
1	B	91	ASN
1	B	154	GLU
2	C	11	GLU
2	C	81	ASP
2	C	194	VAL
2	C	210	GLU
2	C	219	GLN
2	C	257	VAL
2	C	276	LYS
2	C	285	LEU
2	C	299	LYS
2	C	336	VAL
2	C	360	LEU
2	C	397	GLU

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Mol	Chain	Res	Type
2	C	464	LEU
2	C	513	VAL
2	C	557	ARG
2	C	595	LEU
2	C	617	ASP
2	C	640	ARG
2	C	728	HIS
2	C	729	LEU
2	C	815	LEU
2	C	848	VAL
2	C	1055	LEU
2	C	1078	GLU
3	D	134	VAL
3	D	231	VAL
3	D	354	VAL
3	D	406	ASP
3	D	407	VAL
3	D	415	VAL
3	D	420	VAL
3	D	427	VAL
3	D	530	VAL
3	D	618	LEU
3	D	632	VAL
3	D	683	ILE
3	D	709	HIS
3	D	724	GLN
3	D	747	VAL
3	D	754	PHE
3	D	864	VAL
3	D	907	GLU
3	D	1055	VAL
3	D	1127	GLU
3	D	1188	VAL
3	D	1221	VAL
3	D	1288	GLU
3	D	1305	LEU
3	D	1307	LYS
3	D	1433	SER
3	D	1455	LYS
3	D	1486	VAL
3	D	1488	ASP
3	D	1493	LYS

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Mol	Chain	Res	Type
4	E	37	ASN
5	F	95	THR
5	F	141	VAL
5	F	279	GLN
5	F	346	THR
5	F	369	LEU
5	F	375	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	63	HIS
1	B	95	GLN
1	B	188	GLN
2	C	565	GLN
2	C	670	GLN
2	C	860	HIS
2	C	1047	HIS
3	D	66	GLN
3	D	560	GLN
3	D	696	HIS
3	D	714	GLN
3	D	717	GLN
3	D	724	GLN
3	D	768	ASN
3	D	994	GLN
3	D	1046	GLN
3	D	1124	GLN
3	D	1195	GLN
3	D	1202	GLN
3	D	1359	GLN
3	D	1441	GLN
4	E	33	HIS
5	F	83	GLN
5	F	312	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	2TL	I	5	8	5,6,7	1.08	0	5,7,9	1.00	1 (20%)
8	R2T	I	4	8	8,10,11	1.96	2 (25%)	6,13,15	0.91	0
8	2RA	I	1	11,8	4,5,6	0.55	0	1,5,7	0.39	0
8	FGL	I	7	8	5,6,7	1.05	0	1,7,9	1.98	0
8	0QZ	I	6	8	4,5,6	1.72	1 (25%)	2,5,7	0.66	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	2TL	I	5	8	-	1/5/6/8	-
8	R2T	I	4	8	-	7/13/14/16	-
8	2RA	I	1	11,8	-	0/2/4/6	-
8	FGL	I	7	8	-	0/4/6/8	-
8	0QZ	I	6	8	-	1/3/4/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	4	R2T	CD-NE2	4.50	1.43	1.32
8	I	6	0QZ	OB-CA	-3.34	1.37	1.43
8	I	4	R2T	OB1-CB	-2.21	1.37	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	5	2TL	O-C-CA	-2.07	119.45	124.77

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	4	R2T	2	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, 7 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	MB8	I	101	8	0,1,6	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	231/315 (73%)	-0.14	2 (0%) 81 74	16, 33, 61, 102	0
1	B	227/315 (72%)	0.17	5 (2%) 62 52	21, 43, 78, 108	0
2	C	1112/1119 (99%)	-0.18	18 (1%) 70 61	4, 25, 84, 113	0
3	D	1485/1524 (97%)	0.10	67 (4%) 38 30	2, 33, 94, 121	1 (0%)
4	E	94/99 (94%)	-0.32	1 (1%) 78 70	7, 28, 63, 73	0
5	F	346/443 (78%)	0.34	13 (3%) 44 35	14, 47, 87, 113	0
6	G	16/19 (84%)	0.71	1 (6%) 26 19	44, 77, 145, 154	0
7	H	24/27 (88%)	0.65	2 (8%) 17 12	43, 83, 136, 156	0
8	I	0/7	-	-	-	-
All	All	3535/3868 (91%)	0.02	109 (3%) 51 41	2, 34, 89, 156	1 (0%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	449	SER	4.2
3	D	447	VAL	4.2
5	F	141	VAL	4.2
3	D	420	VAL	4.1
1	B	6	LEU	3.6
3	D	203	ALA	3.5
3	D	402	PRO	3.4
3	D	434	ARG	3.3
3	D	1283	ILE	3.3
6	G	4	DG	3.3
3	D	161	LEU	3.3
3	D	409	VAL	3.2
3	D	135	LEU	3.2
2	C	207	LEU	3.1
1	B	190	THR	3.1

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Mol	Chain	Res	Type	RSRZ
7	H	24	DC	3.0
2	C	208	ALA	3.0
3	D	432	TYR	3.0
3	D	452	ILE	3.0
1	A	233	VAL	3.0
3	D	415	VAL	2.9
2	C	299	LYS	2.9
3	D	1252	ILE	2.9
1	A	234	ALA	2.9
3	D	393	ILE	2.9
3	D	1502	ALA	2.8
3	D	205	TYR	2.8
3	D	211	VAL	2.8
3	D	444	VAL	2.8
1	B	93	SER	2.8
3	D	799	LYS	2.8
5	F	149	GLU	2.8
3	D	412	GLY	2.8
3	D	170	PRO	2.8
3	D	368	VAL	2.7
3	D	422	ALA	2.7
5	F	139	ALA	2.7
3	D	394	LEU	2.7
3	D	445	ARG	2.7
3	D	317	VAL	2.7
3	D	177	ALA	2.7
3	D	429	SER	2.7
3	D	401	TYR	2.6
3	D	1128	VAL	2.6
3	D	416	ALA	2.6
3	D	1299	PHE	2.6
3	D	431	VAL	2.6
3	D	417	PRO	2.5
2	C	221	LEU	2.5
5	F	151	LEU	2.5
3	D	147	VAL	2.5
2	C	231	PRO	2.5
5	F	156	VAL	2.5
3	D	213	VAL	2.4
3	D	410	SER	2.4
3	D	1130	ARG	2.4
3	D	182	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	395	VAL	2.4
3	D	446	VAL	2.4
3	D	140	ALA	2.4
3	D	202	VAL	2.4
5	F	146	GLY	2.4
3	D	454	ALA	2.4
3	D	191	LEU	2.4
3	D	134	VAL	2.3
3	D	400	VAL	2.3
1	B	2	LEU	2.3
3	D	427	VAL	2.3
5	F	219	GLY	2.3
3	D	264	LEU	2.3
3	D	421	LEU	2.3
5	F	422	LEU	2.3
3	D	1499	ARG	2.3
2	C	203	ASP	2.2
3	D	186	VAL	2.2
2	C	275	TYR	2.2
2	C	366	SER	2.2
3	D	448	GLU	2.2
5	F	324	GLU	2.2
4	E	95	VAL	2.2
3	D	407	VAL	2.2
2	C	360	LEU	2.2
3	D	152	LEU	2.2
5	F	174	LEU	2.2
2	C	63	GLY	2.2
2	C	365	ASP	2.1
3	D	201	GLY	2.1
3	D	1129	THR	2.1
1	B	100	LEU	2.1
3	D	830	ALA	2.1
3	D	403	PHE	2.1
5	F	142	ARG	2.1
2	C	236	ILE	2.1
2	C	286	SER	2.1
2	C	363	SER	2.1
2	C	103	LYS	2.1
5	F	145	PRO	2.1
2	C	245	GLY	2.1
3	D	369	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
5	F	175	HIS	2.1
7	H	12	DC	2.1
2	C	595	LEU	2.1
3	D	207	PHE	2.1
3	D	238	PRO	2.0
2	C	772	ARG	2.0
3	D	453	ASP	2.0
3	D	809	PRO	2.0
3	D	139	GLY	2.0
3	D	436	GLU	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	0.91	0.10	8,10,16,18	0
8	DVA	I	3	7/8	0.95	0.09	8,9,13,13	0
8	FGL	I	7	7/8	0.96	0.05	8,9,10,11	0
8	R2T	I	4	11/12	0.96	0.07	7,8,9,11	0
8	2TL	I	5	7/8	0.96	0.07	6,7,8,9	0
8	DSN	I	2	6/7	0.97	0.07	7,9,15,15	0
8	0QZ	I	6	6/7	0.98	0.07	7,7,10,11	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	MG	B	2001	1/1	0.80	0.11	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	MB8	I	101	2/7	0.92	0.08	6,6,6,11	0
9	MG	D	2005	1/1	0.93	0.11	31,31,31,31	0
9	MG	F	2001	1/1	0.97	0.04	22,22,22,22	0
10	ZN	D	2002	1/1	0.99	0.03	56,56,56,56	0
9	MG	D	2004	1/1	0.99	0.02	31,31,31,31	0
9	MG	D	2003	1/1	1.00	0.02	5,5,5,5	0
10	ZN	D	2001	1/1	1.00	0.01	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.