



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:20 PM GMT

PDB ID : 4OIN
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
<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

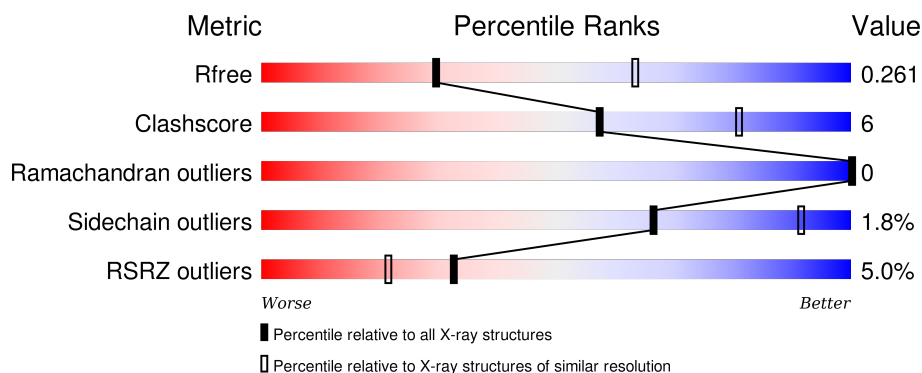
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 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	315	<div> <div>2%</div> <div>59%14%27%</div> </div>
1	B	315	<div> <div>2%</div> <div>60%12%28%</div> </div>
2	C	1119	<div> <div>3%</div> <div>83%16%..</div> </div>
3	D	1524	<div> <div>7%</div> <div>80%17%..</div> </div>
4	E	99	<div> <div></div> <div>85%10%5%</div> </div>

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MG	B	2001	-	-	-	X

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			

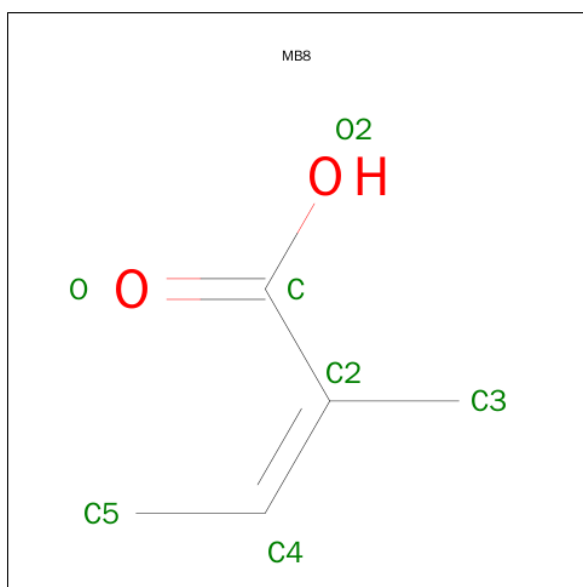
- Molecule 7 is a DNA chain called 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*C P*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'.

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 (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 1 1	0	0
10	D	3	Total Mg 3 3	0	0
10	F	1	Total Mg 1 1	0	0

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

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

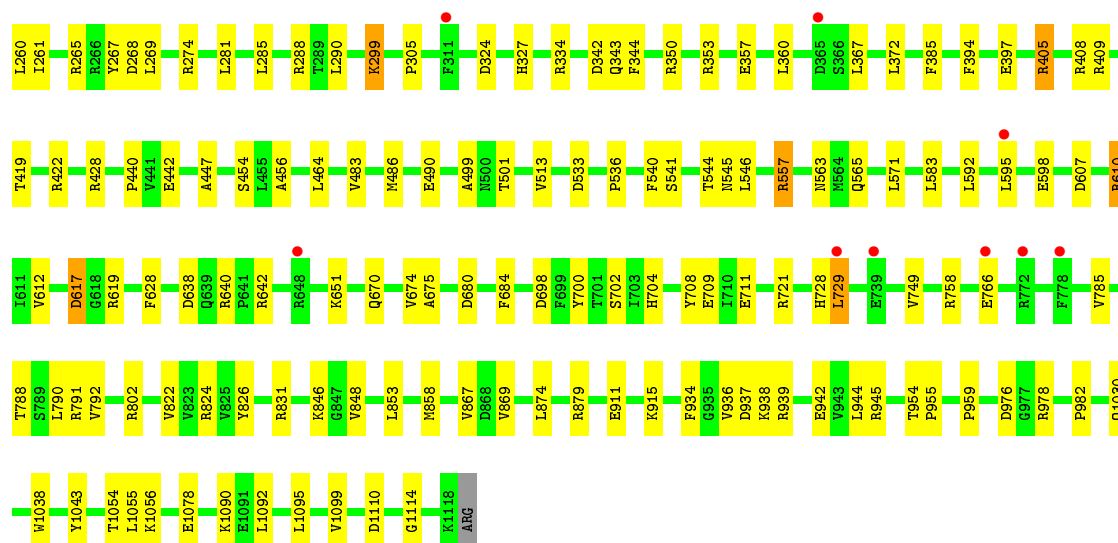
- Molecule 12 is water.

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

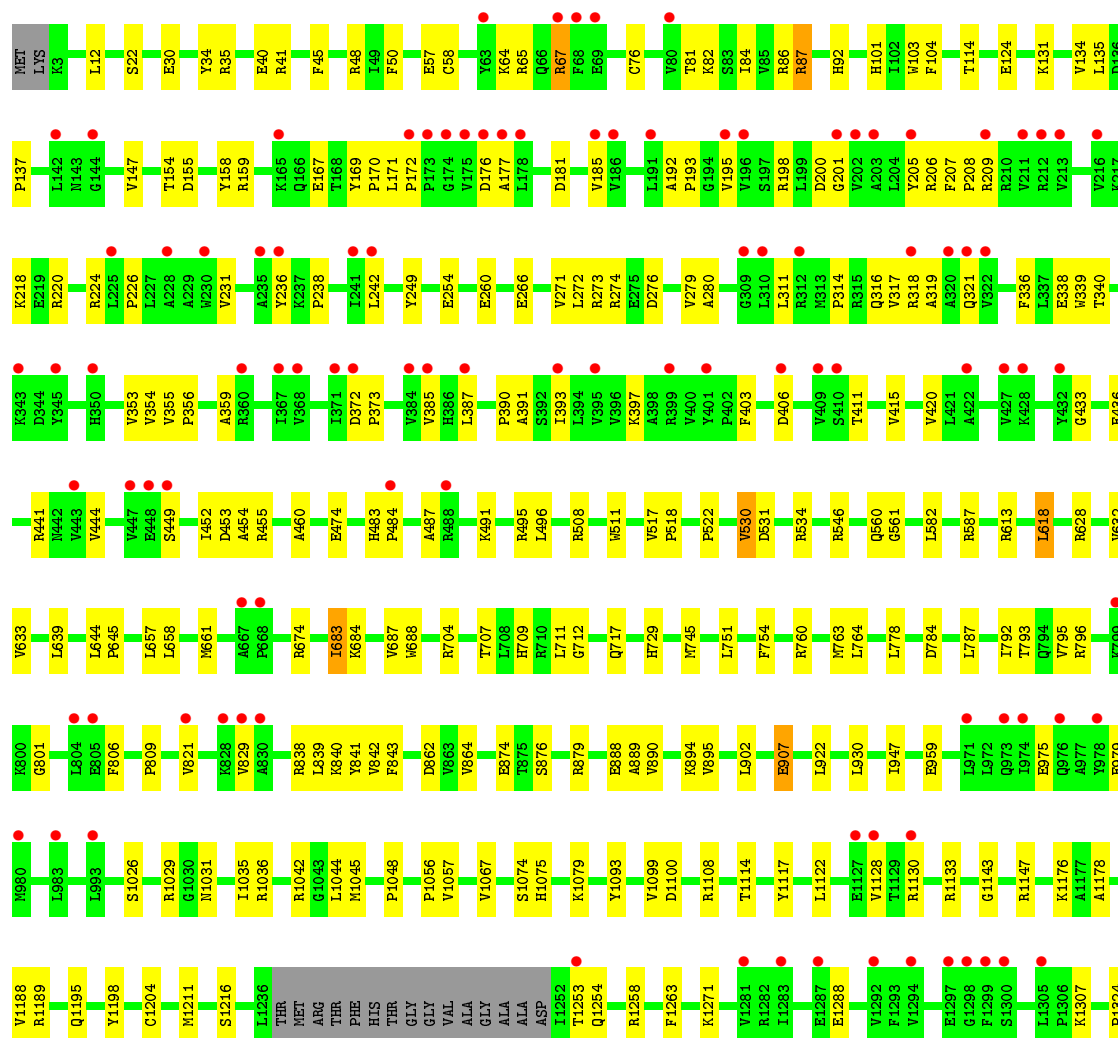
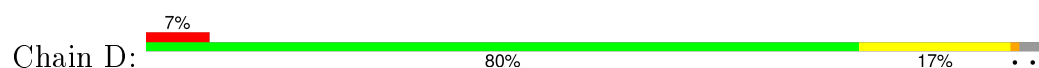
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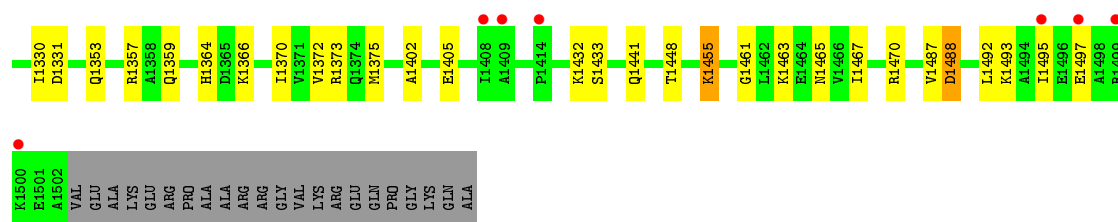
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	221	Total 221	O 221	0	0
12	D	269	Total 269	O 269	0	0
12	E	22	Total 22	O 22	0	0
12	F	36	Total 36	O 36	0	0
12	G	10	Total 10	O 10	0	0
12	H	4	Total 4	O 4	0	0
12	I	8	Total 8	O 8	0	0



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





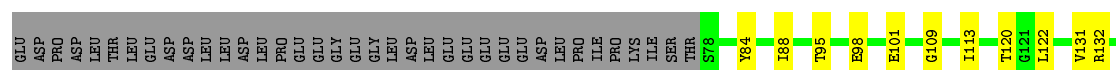
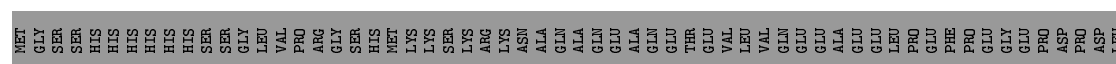
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 85% 10% 5%



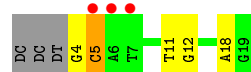
- Molecule 5: DNA directed RNA polymerase sigma factor A

Chain F: 3% 68% 10% 22%



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

Chain G: 16% 58% 21% 5% 16%



- 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: 11% 56% 33% 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	183.77Å 103.20Å 294.77Å 90.00° 99.18° 90.00°	Depositor
Resolution (Å)	48.50 – 2.80 48.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.50-2.80) 98.1 (48.84-2.80)	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 0.218 , 0.261	Depositor DCC
R_{free} test set	6582 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.8	EDS
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
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 131690 reflections	Xtriage
F_o, F_c correlation	0.91	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, 0.375 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, 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	0.22	0/1821	0.44	0/2476
2	C	0.24	0/8941	0.45	0/12092
3	D	0.24	0/11948	0.46	0/16153
4	E	0.24	0/772	0.41	0/1040
5	F	0.23	0/2852	0.39	0/3837
6	G	0.47	0/368	1.00	1/567 (0.2%)
7	H	0.45	0/556	1.04	0/858
All	All	0.25	0/29099	0.48	1/39527 (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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	5	DC	O4'-C4'-C3'	-7.59	101.44	106.00

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	28	0
1	B	1789	0	1841	23	0
2	C	8774	0	8877	109	0
3	D	11739	0	11977	165	0
4	E	758	0	770	7	0
5	F	2807	0	2882	35	0
6	G	328	0	181	5	0
7	H	495	0	272	9	0
8	I	50	0	37	3	0
9	I	2	0	0	0	0
10	B	1	0	0	0	0
10	D	3	0	0	0	0
10	F	1	0	0	0	0
11	D	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	342	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 (342) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:D:208:PRO:HA	3:D:390:PRO:HA	1.77	0.67
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.29	0.66
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
3:D:717:GLN:NE2	12:D:2345:HOH:O	2.29	0.65
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.79	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:1432:LYS:O	3:D:1455:LYS:NZ	2.34	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
5:F:193:ARG:HB2	7:H:6:DT:H1'	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1093:TYR:OH	3:D:1441:GLN:NE2	2.35	0.60
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.82	0.59
3:D:1048:PRO:O	3:D:1079:LYS:NZ	2.34	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: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
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.37	0.57
1:B:94:LEU:O	1:B:146:ARG:NH2	2.36	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
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.40	0.56
2:C:628:PHE:H	2:C:638:ASP:CB	2.19	0.56
1:A:106:PRO:HD3	1:A:134:GLU:HG2	1.88	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:419:THR:HG22	2:C:422:ARG:HE	1.71	0.55
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.87	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:B:128:HIS:CE1	1:B:131:THR:HG23	2.41	0.55
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.87	0.55
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.88	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: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
3:D:657:LEU:HG	3:D:661:MET:HE2	1.90	0.53
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.90	0.53
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:64:LEU:HB3	2:C:100:LEU:HD11	1.90	0.53
3:D:894:LYS:HD2	3:D:894:LYS:H	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
2:C:598:GLU:O	2:C:651:LYS:NZ	2.35	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
6:G:4:DG:N2	6:G:5:DC:O2	2.41	0.52
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.91	0.52
2:C:260:LEU:HB3	2:C:261:ILE:HD12	1.91	0.52
2:C:846:LYS:HZ1	8:I:4:R2T:HG2	1.73	0.52
3:D:684:LYS:O	3:D:687:VAL:HG12	2.09	0.52
2:C:217:LEU:H	2:C:217:LEU:HD12	1.73	0.52
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.90	0.52
2:C:223:ASP:OD1	2:C:225:SER:OG	2.24	0.52
3:D:67:ARG:HD2	5:F:379:ARG:HB3	1.92	0.52
3:D:200:ASP:O	3:D:397:LYS:HG2	2.10	0.52
3:D:658:LEU:HA	3:D:661:MET:HE3	1.92	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
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
3:D:231:VAL:O	3:D:236:TYR:OH	2.28	0.51
2:C:729:LEU:HD11	2:C:791:ARG:HH22	1.75	0.51
3:D:1488:ASP:N	3:D:1488:ASP:OD1	2.31	0.51
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.93	0.51
3:D:1048:PRO:HG3	3:D:1075:HIS:ND1	2.25	0.51
1:A:70:GLY:N	2:C:607:ASP:OD1	2.42	0.51
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.75	0.51
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.93	0.51
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.93	0.51
3:D:1045:MET:HG3	12:D:2221:HOH:O	2.11	0.51
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.91	0.51
3:D:411:THR:O	5:F:178:ARG:NH1	2.36	0.51
1:B:54:THR:OG1	1:B:145:ASP:OD1	2.27	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.47	0.49
2:C:610:ARG:HD3	2:C:612:VAL:HG23	1.92	0.49
3:D:1263:PHE:HD2	3:D:1375:MET:HE2	1.77	0.49
3:D:1100:ASP:OD1	3:D:1463:LYS:NZ	2.37	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
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
1:A:209:GLU:O	1:A:213:GLN:HG2	2.12	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
3:D:1114:THR:OG1	3:D:1195:GLN:NE2	2.45	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
2:C:853:LEU:HB2	2:C:858:MET:HE1	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
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
6:G:12:DG:N2	7:H:16:DC:O2	2.35	0.48
2:C:501:THR:HG22	12:C:1472:HOH:O	2.13	0.48
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.95	0.48
3:D:1128:VAL:HG23	3:D:1130:ARG:H	1.79	0.48
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.36	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
3:D:137:PRO:HB3	3:D:147:VAL:HG12	1.96	0.47
2:C:540:PHE:HB3	2:C:544:THR:HB	1.95	0.47
2:C:541:SER:O	2:C:545:ASN:ND2	2.43	0.47
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:976:ASP:OD1	2:C:978:ARG:HG3	2.15	0.47
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.97	0.47
1:B:90:LEU:HD21	1:B:121:GLU:HB2	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
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.96	0.46
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.96	0.46
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.97	0.46
2:C:299:LYS:HE2	2:C:299:LYS:HA	1.96	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
2:C:167:LYS:HD3	7:H:12:DC:C5	2.51	0.46
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.65	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
6:G:11:DT:H2"	6:G:12:DG:C8	2.52	0.45
3:D:1122:LEU:HD13	3:D:1178:ALA:HB2	1.99	0.45
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.51	0.45
3:D:30:GLU:OE1	3:D:40:GLU:HG2	2.17	0.45
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.39	0.45
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.98	0.45
1:A:100:LEU:HD22	1:A:141:GLU:HG2	1.98	0.45
3:D:560:GLN:NE2	5:F:222:ARG:HH12	2.14	0.45
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.99	0.45
2:C:334:ARG:NH2	2:C:342:ASP:OD2	2.45	0.45
3:D:353:VAL:HG11	3:D:387:LEU:HD11	1.98	0.45
3:D:41:ARG:HE	3:D:48:ARG:CZ	2.30	0.45
1:B:32:PHE:HA	1:B:35:THR:HB	1.98	0.45
2:C:132:ALA:HB1	2:C:394:PHE:HE1	1.82	0.45
2:C:76:PRO:HG3	2:C:120:LEU:HD12	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:260:GLU:HB3	3:D:271:VAL:HB	2.00	0.44
2:C:41:ASN:O	2:C:46:ALA:HB2	2.17	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
1:A:54:THR:HG21	1:A:145:ASP:HB2	2.00	0.44
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.16	0.44
3:D:220:ARG:NH1	12:D:2339:HOH:O	2.51	0.44
5:F:109:GLY:O	5:F:113:ILE:HG13	2.17	0.44
5:F:362:SER:OG	5:F:365:GLU:HG2	2.18	0.44
3:D:1353:GLN:O	3:D:1357:ARG:HG3	2.17	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:HE2	3:D:1176:LYS:HB3	1.79	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
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.68	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:183:ASP:HA	2:C:938:LYS:HE3	1.99	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
3:D:792:ILE:HG13	3:D:793:THR:HG23	2.00	0.43
1:A:159:LYS:HE3	1:A:164:ALA:O	2.17	0.43
3:D:84:ILE:O	3:D:87:ARG:HG2	2.18	0.43
2:C:194:VAL:HA	2:C:197:LEU:HD12	2.00	0.43
2:C:708:TYR:HB3	2:C:790:LEU:HD21	2.00	0.43
2:C:617:ASP:HB2	2:C:619:ARG:HG2	2.00	0.43
3:D:176:ASP:OD1	3:D:177:ALA:N	2.44	0.43
2:C:97:ARG:HG2	2:C:112:GLU:HB2	2.00	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
3:D:317:VAL:HG23	3:D:339:TRP:HB3	2.00	0.43
2:C:499:ALA:HB2	2:C:533:ASP:HB2	2.00	0.43
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.50	0.43
2:C:1056:LYS:HE2	3:D:751:LEU:HG	2.00	0.43
2:C:101:ILE:HG12	2:C:108:ILE:HG12	2.01	0.43
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1211:MET:HE3	3:D:1211:MET:HB2	1.90	0.43
1:B:94:LEU:HD11	1:B:97:VAL:HG22	2.01	0.42
3:D:81:THR:OG1	3:D:82:LYS:N	2.52	0.42
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.19	0.42
3:D:1373:ARG:HD3	12:D:2140:HOH:O	2.19	0.42
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.50	0.42
2:C:954:THR:HA	2:C:955:PRO:HD3	1.91	0.42
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.73	0.42
2:C:154:ARG:H	2:C:154:ARG:HG2	1.68	0.42
3:D:103:TRP:HB3	3:D:1448:THR:HG21	2.02	0.42
2:C:684:PHE:HB3	3:D:633:VAL:HG21	2.01	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
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.77	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
3:D:1031:ASN:O	3:D:1035:ILE:HG12	2.19	0.42
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	2.00	0.42
3:D:796:ARG:NH1	3:D:862:ASP:OD2	2.47	0.42
3:D:795:VAL:HG12	3:D:876:SER:HB3	2.00	0.42
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	2.01	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
3:D:838:ARG:HD3	3:D:874:GLU:OE1	2.20	0.42
3:D:131:LYS:NZ	3:D:154:THR:HG22	2.34	0.42
2:C:642:ARG:HA	2:C:642:ARG:HD3	1.87	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
3:D:1117:TYR:HB2	3:D:1188:VAL:O	2.20	0.41
2:C:239:PHE:CD2	2:C:253:ALA:HA	2.54	0.41
3:D:455:ARG:HB2	3:D:460:ALA:HB2	2.02	0.41
1:B:83:LYS:HE2	1:B:168:ASP:HB2	2.02	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
7:H:13:DT:O4	12:H:104:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:517:VAL:HA	3:D:518:PRO:HD3	1.95	0.41
2:C:408:ARG:NH1	2:C:456:ALA:O	2.53	0.41
5:F:321:ILE:O	5:F:327:SER:HB3	2.20	0.41
2:C:13:ILE:HD13	2:C:483:VAL:HG11	2.03	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
1:B:56:VAL:HG21	1:B:82:LEU:HD13	2.02	0.41
3:D:889:ALA:HB1	3:D:930:LEU:HA	2.02	0.41
2:C:536:PRO:HB3	3:D:1067:VAL:HG21	2.03	0.41
3:D:707:THR:HG23	3:D:712:GLY:HA3	2.01	0.41
1:B:124:ASN:N	1:B:124:ASN:OD1	2.53	0.41
2:C:486:MET:HB3	2:C:490:GLU:HB3	2.01	0.41
2:C:942:GLU:HG3	2:C:945:ARG:HH21	1.85	0.41
1:A:196:THR:HG21	2:C:934:PHE:HE2	1.86	0.41
3:D:192:ALA:HB1	3:D:193:PRO:HD2	2.02	0.41
3:D:185:VAL:N	3:D:201:GLY:O	2.45	0.41
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.20	0.41
2:C:124:ASP:HB3	2:C:592:LEU:HD12	2.02	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:80:LEU:HD23	1:A:80:LEU:HA	1.95	0.41
5:F:162:LYS:O	5:F:165:SER:OG	2.33	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:944:LEU:HD23	2:C:944:LEU:HA	1.97	0.41
1:A:102:LYS:HB2	1:A:102:LYS:HE3	1.75	0.41
2:C:571:LEU:HD23	2:C:702:SER:HB3	2.03	0.41
3:D:50:PHE:CD2	3:D:522:PRO:HD3	2.55	0.41
2:C:749:VAL:HB	2:C:792:VAL:HG21	2.03	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
3:D:613:ARG:HG3	3:D:618:LEU:HD22	2.04	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
5:F:408:LEU:HD23	5:F:408:LEU:HA	1.89	0.40
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.56	0.40
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.21	0.40
2:C:853:LEU:HB2	2:C:858:MET:CE	2.50	0.40
3:D:907:GLU:HB2	3:D:1026:SER:HA	2.03	0.40
3:D:843:PHE:HE1	3:D:864:VAL:HG21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:226:PRO:HD3	3:D:249:TYR:CE2	2.56	0.40
2:C:265:ARG:NH1	12:C:1417:HOH:O	2.55	0.40
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.96	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
5:F:135:ILE:HG13	5:F:181:GLU:HB2	2.03	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
3:D:58:CYS:HB2	3:D:76:CYS:SG	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	196 (98%)	4 (2%)	63	90
1	B	200/273 (73%)	196 (98%)	4 (2%)	63	90
2	C	936/941 (100%)	915 (98%)	21 (2%)	60	89
3	D	1253/1279 (98%)	1232 (98%)	21 (2%)	68	92
4	E	82/88 (93%)	82 (100%)	0	100	100
5	F	301/388 (78%)	297 (99%)	4 (1%)	76	94
All	All	2972/3242 (92%)	2918 (98%)	54 (2%)	66	91

All (54) 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	219	ARG
1	B	7	LYS
1	B	14	ARG
1	B	91	ASN
1	B	154	GLU
2	C	81	ASP
2	C	141	HIS
2	C	194	VAL
2	C	219	GLN
2	C	285	LEU
2	C	299	LYS
2	C	360	LEU
2	C	397	GLU
2	C	405	ARG
2	C	464	LEU
2	C	513	VAL
2	C	557	ARG
2	C	595	LEU
2	C	610	ARG

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Mol	Chain	Res	Type
2	C	617	ASP
2	C	640	ARG
2	C	698	ASP
2	C	728	HIS
2	C	729	LEU
2	C	848	VAL
2	C	1078	GLU
3	D	67	ARG
3	D	87	ARG
3	D	134	VAL
3	D	276	ASP
3	D	354	VAL
3	D	406	ASP
3	D	415	VAL
3	D	420	VAL
3	D	530	VAL
3	D	618	LEU
3	D	632	VAL
3	D	683	ILE
3	D	709	HIS
3	D	754	PHE
3	D	784	ASP
3	D	907	GLU
3	D	1288	GLU
3	D	1307	LYS
3	D	1433	SER
3	D	1455	LYS
3	D	1488	ASP
5	F	95	THR
5	F	141	VAL
5	F	279	GLN
5	F	369	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
2	C	390	GLN
2	C	506	ASN
2	C	670	GLN
2	C	860	HIS
2	C	1047	HIS

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Mol	Chain	Res	Type
3	D	66	GLN
3	D	316	GLN
3	D	560	GLN
3	D	696	HIS
3	D	709	HIS
3	D	855	HIS
3	D	976	GLN
3	D	1124	GLN
3	D	1195	GLN
3	D	1359	GLN
3	D	1441	GLN
5	F	83	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	0.48	0	1,5,7	2.22	1 (100%)
8	DSN	I	2	8	4,5,6	0.56	0	2,5,7	1.57	1 (50%)
8	DVA	I	3	8	5,6,7	0.54	0	5,7,9	1.28	1 (20%)
8	R2T	I	4	8	9,10,11	2.11	2 (22%)	10,13,15	1.42	2 (20%)
8	2TL	I	5	8	5,6,7	1.20	1 (20%)	5,7,9	1.28	1 (20%)
8	0QZ	I	6	8	5,5,6	1.45	1 (20%)	4,5,7	1.19	1 (25%)
8	FGL	I	7	8	2,6,7	0.55	0	1,7,9	0.06	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	-2.97	1.37	1.43
8	I	5	2TL	OG1-CB	-2.36	1.37	1.43
8	I	4	R2T	OB1-CB	-2.29	1.37	1.43
8	I	4	R2T	CD-NE2	5.38	1.43	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	3	DVA	O-C-CA	-2.84	117.95	125.44
8	I	5	2TL	O-C-CA	-2.27	119.45	125.44
8	I	6	0QZ	O-C-CA	-2.24	119.69	125.35
8	I	1	2RA	O-C-CA	-2.22	119.72	125.49
8	I	2	DSN	O-C-CA	-2.18	119.81	125.49
8	I	4	R2T	CG-CD-NE2	2.28	120.36	116.90
8	I	4	R2T	C-CA-N	2.88	115.85	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
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
9	MB8	I	101	8	-	0/0/0/6	0/0/0/0

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%)	-0.12	6 (2%) 59 47	16, 33, 61, 102	0
1	B	227/315 (72%)	0.06	6 (2%) 59 47	21, 43, 78, 108	0
2	C	1112/1119 (99%)	-0.06	36 (3%) 51 39	4, 25, 84, 113	0
3	D	1485/1524 (97%)	0.18	109 (7%) 18 10	2, 33, 94, 121	0
4	E	94/99 (94%)	-0.29	0 100 100	7, 28, 63, 73	0
5	F	346/443 (78%)	0.13	13 (3%) 44 32	14, 47, 87, 113	0
6	G	16/19 (84%)	0.70	3 (18%) 2 1	44, 77, 145, 154	0
7	H	24/27 (88%)	0.41	3 (12%) 5 2	43, 83, 136, 156	0
8	I	0/7	-	-	-	-
All	All	3535/3868 (91%)	0.06	176 (4%) 32 21	2, 34, 89, 156	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	191	LEU	5.5
3	D	1499	ARG	5.3
2	C	207	LEU	5.1
2	C	365	ASP	5.1
3	D	422	ALA	4.9
3	D	241	ILE	4.7
2	C	203	ASP	4.4
1	B	6	LEU	4.4
3	D	185	VAL	4.4
3	D	1287	GLU	4.3
3	D	173	PRO	4.3
2	C	219	GLN	4.3
3	D	393	ILE	4.1
2	C	221	LEU	4.1
3	D	409	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
2	C	222	MET	4.0
3	D	242	LEU	3.9
3	D	178	LEU	3.9
3	D	144	GLY	3.8
3	D	174	GLY	3.8
3	D	345	TYR	3.8
3	D	201	GLY	3.8
2	C	217	LEU	3.7
2	C	227	PHE	3.7
3	D	68	PHE	3.7
3	D	196	VAL	3.7
2	C	208	ALA	3.6
3	D	974	ILE	3.6
3	D	1130	ARG	3.5
3	D	186	VAL	3.5
3	D	447	VAL	3.5
3	D	1408	ILE	3.4
3	D	432	TYR	3.4
2	C	218	VAL	3.4
2	C	228	ALA	3.4
5	F	422	LEU	3.4
3	D	406	ASP	3.3
1	A	234	ALA	3.3
1	B	2	LEU	3.3
7	H	23	DG	3.3
2	C	64	LEU	3.2
2	C	778	PHE	3.2
2	C	107	LEU	3.2
3	D	449	SER	3.2
3	D	322	VAL	3.1
3	D	312	ARG	3.1
3	D	310	LEU	3.1
3	D	203	ALA	3.0
3	D	1299	PHE	3.0
3	D	211	VAL	3.0
2	C	729	LEU	3.0
3	D	385	VAL	3.0
6	G	5	DC	2.9
3	D	488	ARG	2.9
2	C	205	GLU	2.9
3	D	395	VAL	2.9
3	D	175	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
3	D	387	LEU	2.9
1	A	137	ARG	2.9
3	D	205	TYR	2.9
3	D	212	ARG	2.9
3	D	368	VAL	2.9
3	D	202	VAL	2.9
3	D	401	TYR	2.9
3	D	971	LEU	2.8
3	D	195	VAL	2.8
3	D	213	VAL	2.8
5	F	415	THR	2.8
3	D	978	TYR	2.8
3	D	360	ARG	2.8
3	D	343	LYS	2.8
3	D	1297	GLU	2.7
3	D	1298	GLY	2.7
3	D	427	VAL	2.7
3	D	176	ASP	2.7
2	C	766	GLU	2.7
3	D	448	GLU	2.7
5	F	149	GLU	2.7
3	D	384	VAL	2.7
1	B	138	LEU	2.7
3	D	799	LYS	2.6
3	D	236	TYR	2.6
3	D	67	ARG	2.6
3	D	1305	LEU	2.6
5	F	169	GLU	2.6
2	C	254	VAL	2.6
2	C	105	THR	2.6
3	D	320	ALA	2.6
3	D	805	GLU	2.6
5	F	174	LEU	2.6
5	F	416	ARG	2.5
3	D	142	LEU	2.5
2	C	648	ARG	2.5
3	D	367	ILE	2.5
2	C	216	GLU	2.5
7	H	24	DC	2.5
1	A	231	ALA	2.5
5	F	420	ASP	2.5
2	C	311	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	63	TYR	2.5
3	D	209	ARG	2.5
3	D	1127	GLU	2.5
3	D	372	ASP	2.5
3	D	1253	THR	2.5
3	D	976	GLN	2.4
3	D	1409	ALA	2.4
3	D	371	ILE	2.4
5	F	414	ARG	2.4
5	F	147	LEU	2.4
3	D	1294	VAL	2.4
2	C	242	LEU	2.4
2	C	188	LYS	2.4
3	D	1281	VAL	2.4
6	G	6	DA	2.4
3	D	1495	ILE	2.4
5	F	411	HIS	2.4
3	D	983	LEU	2.4
3	D	309	GLY	2.4
1	B	186	LEU	2.3
3	D	1414	PRO	2.3
3	D	230	TRP	2.3
3	D	804	LEU	2.3
2	C	226	VAL	2.3
3	D	443	VAL	2.3
3	D	1292	VAL	2.3
1	A	138	LEU	2.3
2	C	245	GLY	2.3
3	D	69	GLU	2.3
3	D	973	GLN	2.3
3	D	830	ALA	2.3
3	D	1500	LYS	2.3
3	D	1300	SER	2.3
3	D	428	LYS	2.3
3	D	235	ALA	2.3
3	D	177	ALA	2.3
6	G	7	DT	2.3
2	C	772	ARG	2.3
2	C	204	GLN	2.3
2	C	104	ASP	2.2
5	F	156	VAL	2.2
3	D	321	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	234	ALA	2.2
7	H	22	DT	2.2
3	D	1497	GLU	2.2
2	C	220	GLY	2.2
3	D	821	VAL	2.2
5	F	379	ARG	2.2
1	A	233	VAL	2.2
1	B	93	SER	2.2
3	D	410	SER	2.2
1	A	230	ALA	2.2
5	F	233	PHE	2.2
1	B	7	LYS	2.2
2	C	176	VAL	2.2
3	D	993	LEU	2.2
3	D	228	ALA	2.2
3	D	667	ALA	2.2
3	D	172	PRO	2.1
3	D	1283	ILE	2.1
3	D	80	VAL	2.1
3	D	1128	VAL	2.1
3	D	980	MET	2.1
3	D	350	HIS	2.1
3	D	668	PRO	2.1
2	C	595	LEU	2.1
2	C	739	GLU	2.1
3	D	225	LEU	2.0
3	D	318	ARG	2.0
3	D	829	VAL	2.0
2	C	224	GLU	2.0
3	D	484	PRO	2.0
3	D	828	LYS	2.0
2	C	197	LEU	2.0
3	D	399	ARG	2.0
3	D	165	LYS	2.0
3	D	216	VAL	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	2RA	I	1	6/7	0.92	0.17	-	8,10,16,18	0
8	DSN	I	2	6/7	0.97	0.15	-	7,9,15,15	0
8	DVA	I	3	7/8	0.98	0.17	-	8,9,13,13	0
8	FGL	I	7	7/8	0.97	0.13	-	8,9,10,11	0
8	0QZ	I	6	6/7	0.98	0.18	-	7,7,10,11	0
8	2TL	I	5	7/8	0.97	0.17	-	6,7,8,9	0
8	R2T	I	4	11/12	0.98	0.15	-	7,8,9,11	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(Å ²)	Q<0.9
10	MG	B	2001	1/1	0.82	0.25	2.10	50,50,50,50	0
11	ZN	D	2002	1/1	0.98	0.05	-1.47	56,56,56,56	0
11	ZN	D	2001	1/1	1.00	0.13	-1.50	10,10,10,10	0
10	MG	D	2004	1/1	0.97	0.08	-1.62	31,31,31,31	0
10	MG	F	2001	1/1	0.95	0.10	-6.23	22,22,22,22	0
10	MG	D	2003	1/1	0.97	0.17	-	5,5,5,5	0
9	MB8	I	101	2/7	0.95	0.14	-	6,6,6,11	0
10	MG	D	2005	1/1	0.83	0.10	-	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.