



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:00 PM UTC

PDB ID : 6KQG / pdb_00006kqg
Title : Thermus thermophilus initial transcription complex comprising sigma A and 5'-OH RNA of 6 nt
Authors : Zhang, Y.; Li, L.; Ebright, R.H.
Deposited on : 2019-08-17
Resolution : 2.78 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
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

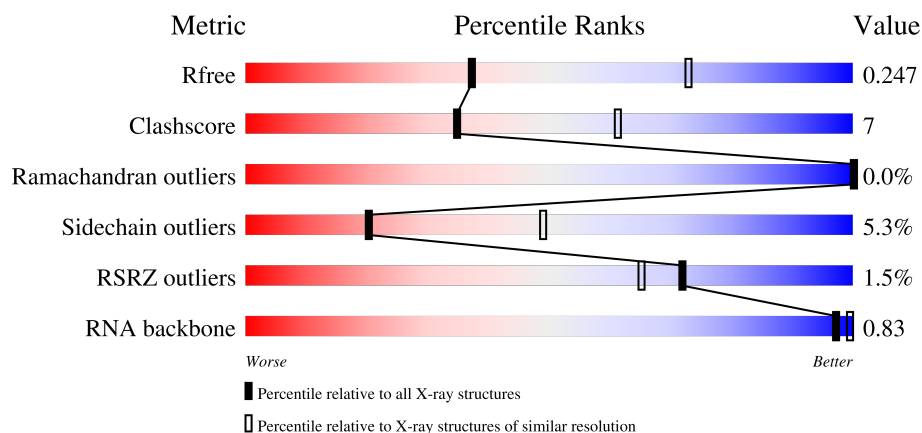
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)
RNA backbone	3983	1133 (3.00-2.56)

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	2% 54% 17% 27%
1	B	315	2% 52% 17% 29%
2	C	1119	0% 79% 19% ..
3	D	1524	2% 78% 19% ..

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Mol	Chain	Length	Quality of chain
4	E	99	% 84% 11% 5%
5	F	443	2% 64% 12% 24%
6	G	21	10% 24% 62% 14%
7	H	27	4% 41% 48% 11%
8	I	6	83% 17%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28816 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	1	0
			1814	1158	316	338	2			
1	B	223	Total	C	N	O	S	0	0	0
			1758	1124	305	327	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	3	0
			8788	5560	1570	1634	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1486	Total	C	N	O	S	0	3	0
			11732	7442	2063	2191	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
			761	486	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	338	Total	C	N	O	S	0	0	0
			2748	1735	500	509	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	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 DNA (5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*T
P*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	18	Total	C	N	O	P	0	0	0
			372	176	73	106	17			

- Molecule 7 is a DNA chain called DNA (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').

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 RNA chain called RNA (5'-R(*CP*CP*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	6	Total	C	N	O	P	0	0	0
			122	56	21	40	5			

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

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

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

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

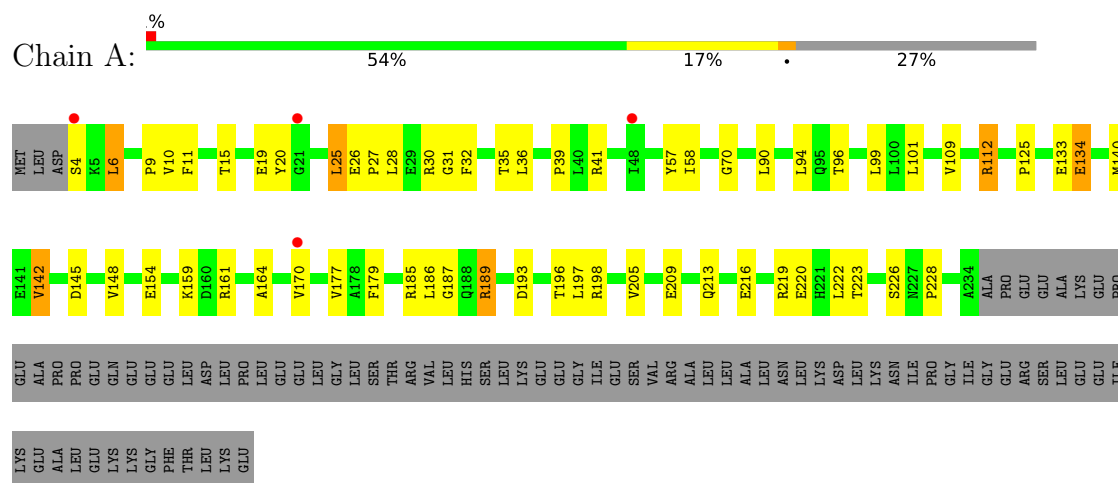
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	9	Total O 9 9	0	0
11	B	9	Total O 9 9	0	0
11	C	60	Total O 60 60	0	0
11	D	94	Total O 94 94	0	0
11	E	8	Total O 8 8	0	0
11	F	23	Total O 23 23	0	0
11	G	10	Total O 10 10	0	0
11	H	6	Total O 6 6	0	0
11	I	1	Total O 1 1	0	0

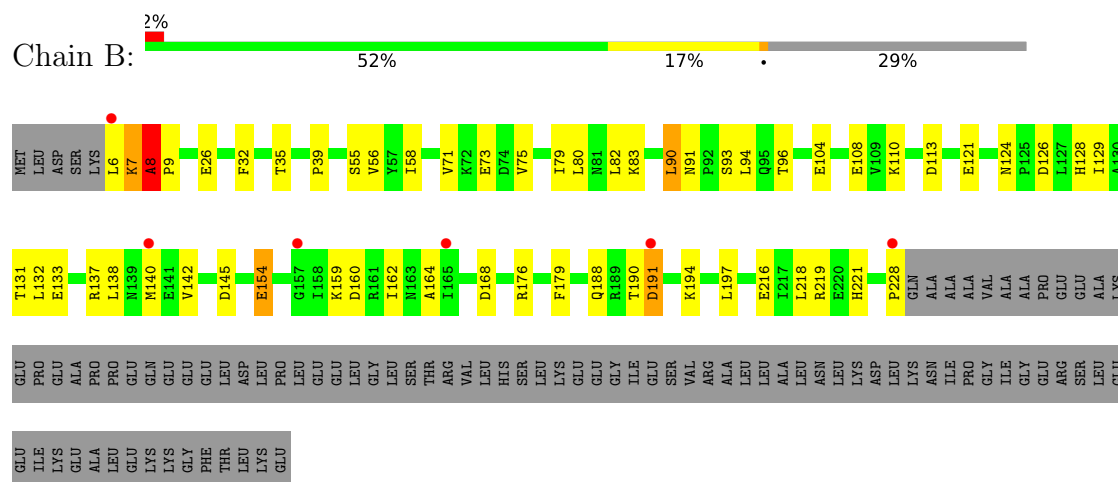
3 Residue-property plots [i](#)

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.

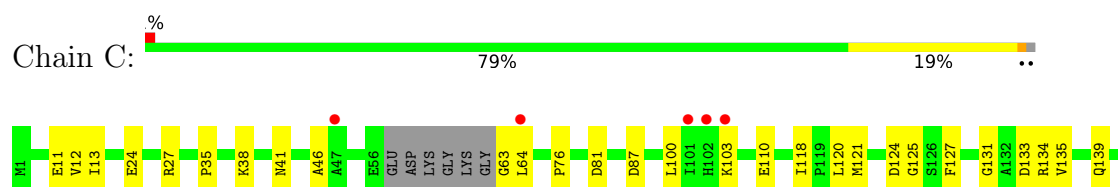
- Molecule 1: DNA-directed RNA polymerase subunit alpha

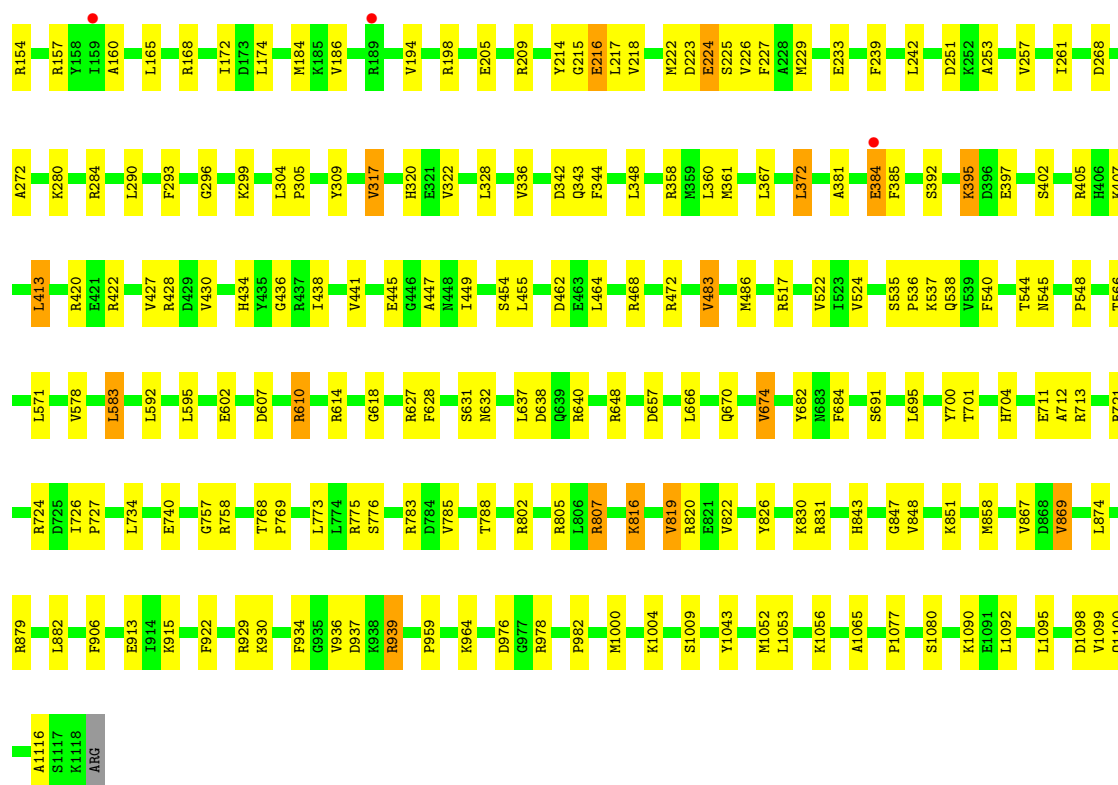


- Molecule 1: DNA-directed RNA polymerase subunit alpha

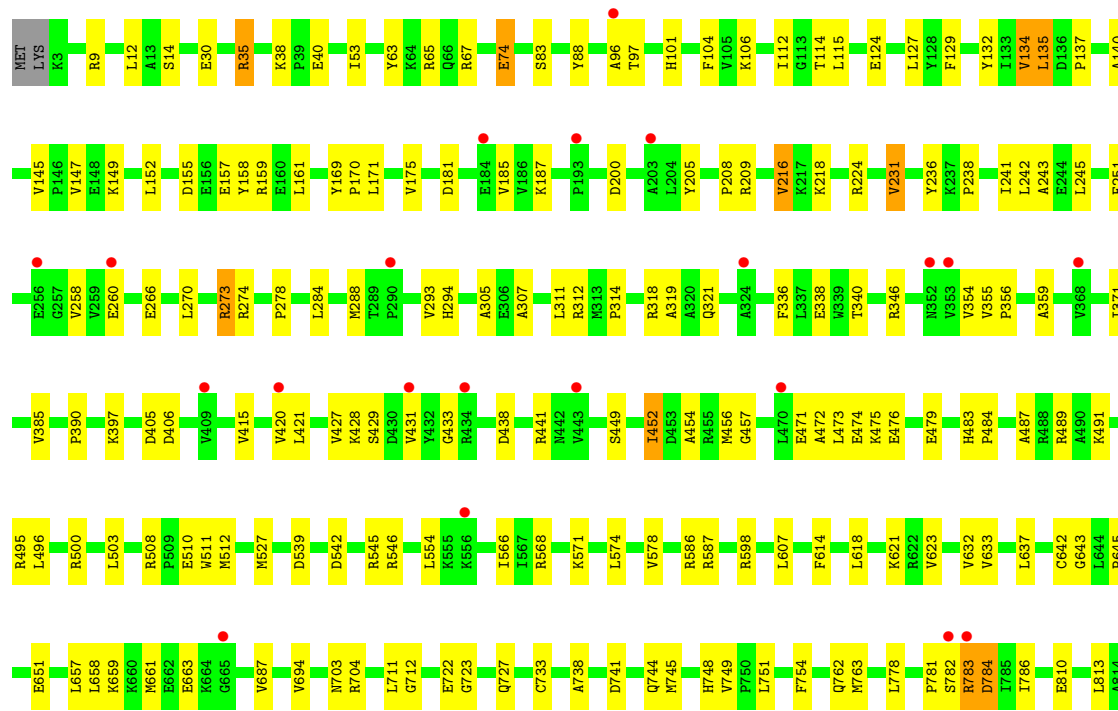
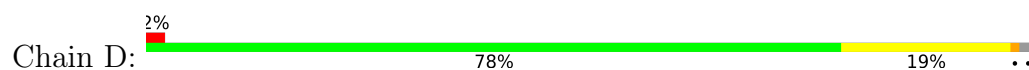


- Molecule 2: DNA-directed RNA polymerase subunit beta



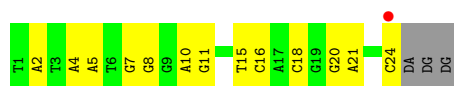


• Molecule 3: DNA-directed RNA polymerase subunit beta'

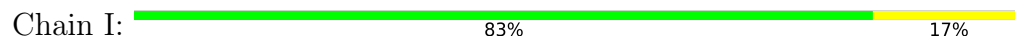




- Molecule 7: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G*)-3')



- Molecule 8: RNA (5'-R(*CP*CP*UP*CP*GP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.24Å 104.04Å 296.85Å 90.00° 98.65° 90.00°	Depositor
Resolution (Å)	49.03 – 2.78 49.03 – 2.78	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.03-2.78) 98.3 (49.03-2.78)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.205 , 0.248 0.205 , 0.247	Depositor DCC
R_{free} test set	6829 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	74.1	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28816	wwPDB-VP
Average B, all atoms (Å ²)	88.0	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: MG, ZN

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	0.21	0/1849	0.46	0/2515
1	B	0.26	0/1790	0.49	2/2435 (0.1%)
2	C	0.21	0/8965	0.45	0/12124
3	D	0.23	0/11948	0.45	1/16157 (0.0%)
4	E	0.34	0/775	0.54	2/1045 (0.2%)
5	F	0.22	0/2791	0.42	2/3753 (0.1%)
6	G	0.33	0/418	0.45	0/645
7	H	0.27	0/556	0.49	0/858
8	I	0.27	0/135	0.47	0/208
All	All	0.23	0/29227	0.46	7/39740 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	376	ILE	N-CA-C	6.75	117.51	110.62
4	E	93	TYR	CA-C-N	-5.97	114.45	120.31
4	E	93	TYR	C-N-CA	-5.97	114.45	120.31
1	B	8	ALA	CA-C-N	-5.75	113.83	119.76
1	B	8	ALA	C-N-CA	-5.75	113.83	119.76
5	F	375	LEU	N-CA-C	5.30	117.06	111.28
3	D	274	ARG	N-CA-C	-5.27	100.30	108.90

There are no chirality outliers.

There are no planarity outliers.

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	1814	0	1869	34	0
1	B	1758	0	1808	48	0
2	C	8788	0	8898	136	0
3	D	11732	0	11952	189	0
4	E	761	0	778	8	0
5	F	2748	0	2828	29	0
6	G	372	0	203	18	0
7	H	495	0	272	11	0
8	I	122	0	66	1	0
9	B	1	0	0	0	0
9	D	2	0	0	0	0
9	F	1	0	0	0	0
10	D	2	0	0	0	0
11	A	9	0	0	0	0
11	B	9	0	0	0	0
11	C	60	0	0	4	0
11	D	94	0	0	5	0
11	E	8	0	0	1	0
11	F	23	0	0	0	0
11	G	10	0	0	1	0
11	H	6	0	0	0	0
11	I	1	0	0	0	0
All	All	28816	0	28674	423	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 (423) 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)
6:G:20:DG:H2'	6:G:21:DG:C4'	1.81	1.11
3:D:783:ARG:HB3	3:D:1028:ALA:O	1.54	1.06
6:G:20:DG:H2'	6:G:21:DG:O4'	1.60	1.02
1:B:6:LEU:HD12	1:B:7:LYS:H	1.26	0.99
2:C:684:PHE:HE1	3:D:782:SER:OG	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LYS:NZ	1:B:8:ALA:HB2	1.83	0.94
1:B:7:LYS:HZ1	1:B:8:ALA:HB2	1.36	0.89
3:D:783:ARG:CB	3:D:1028:ALA:O	2.24	0.85
6:G:20:DG:H2'	6:G:21:DG:H4'	1.58	0.85
6:G:19:DG:H2''	6:G:20:DG:H5'	1.59	0.85
6:G:20:DG:C2'	6:G:21:DG:H4'	2.07	0.85
3:D:827:ILE:HG12	3:D:834:THR:O	1.77	0.84
1:B:6:LEU:O	1:B:9:PRO:HD3	1.79	0.81
2:C:684:PHE:CE1	3:D:782:SER:OG	2.27	0.80
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.64	0.79
1:B:7:LYS:HD2	1:B:8:ALA:N	2.00	0.77
2:C:628:PHE:H	2:C:638:ASP:HB3	1.49	0.76
1:B:7:LYS:HD2	1:B:8:ALA:H	1.50	0.74
3:D:782:SER:O	3:D:786:ILE:HG13	1.84	0.74
6:G:20:DG:C2'	6:G:21:DG:C4'	2.61	0.73
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.71	0.73
6:G:20:DG:H1	8:I:2:C:H42	1.36	0.73
1:B:6:LEU:CD1	1:B:7:LYS:H	1.98	0.73
3:D:273:ARG:HG3	3:D:278:PRO:HA	1.70	0.73
5:F:374:GLY:HA2	5:F:379:ARG:O	1.88	0.72
3:D:241:ILE:HA	3:D:312:ARG:HG2	1.71	0.72
6:G:19:DG:H2'	6:G:20:DG:C8	2.24	0.72
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.72	0.71
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.73	0.71
3:D:835:SER:OG	3:D:838:ARG:HG3	1.92	0.70
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.74	0.69
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.73	0.69
2:C:24:GLU:OE2	2:C:27:ARG:NH2	2.25	0.69
2:C:428:ARG:NH2	2:C:447:ALA:O	2.24	0.69
2:C:198:ARG:HE	2:C:227:PHE:HA	1.58	0.69
3:D:97:THR:HG21	3:D:571:LYS:HG2	1.74	0.69
3:D:65:ARG:NH1	5:F:378:GLY:O	2.25	0.69
6:G:15:DT:H2'	6:G:16:DC:C6	2.29	0.68
3:D:260:GLU:HG2	3:D:294:HIS:HE1	1.58	0.68
6:G:18:DA:H2'	6:G:19:DG:C8	2.30	0.67
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.28	0.67
2:C:63:GLY:HA3	2:C:100:LEU:HD21	1.77	0.67
1:B:104:GLU:OE2	1:B:137:ARG:NH1	2.28	0.66
1:B:6:LEU:HD12	1:B:7:LYS:N	2.08	0.66
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.26	0.66
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:HG3	1:A:125:PRO:HB2	1.78	0.65
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.29	0.65
3:D:1450:ALA:HA	3:D:1455:LYS:HE3	1.78	0.65
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.79	0.64
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.79	0.64
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.80	0.63
6:G:4:DG:H1	7:H:24:DC:H42	1.47	0.63
3:D:657:LEU:HG	3:D:661:MET:HE2	1.80	0.63
3:D:959:GLU:OE1	3:D:959:GLU:N	2.31	0.63
3:D:1045[B]:MET:HE1	3:D:1057:VAL:HG23	1.81	0.63
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.81	0.63
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.32	0.63
2:C:124:ASP:OD2	2:C:407:LYS:NZ	2.29	0.63
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.81	0.63
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.82	0.62
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.80	0.62
1:A:6:LEU:HD21	1:A:27:PRO:HG2	1.82	0.62
3:D:1053[B]:PHE:CZ	3:D:1055:VAL:HG13	2.36	0.61
1:A:31:GLY:N	1:A:193:ASP:OD2	2.34	0.60
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.84	0.60
1:A:209:GLU:O	1:A:213:GLN:HG2	2.02	0.60
1:A:185:ARG:NH2	1:A:187:GLY:O	2.34	0.60
7:H:10:DA:H2''	7:H:11:DG:H5''	1.84	0.60
2:C:773:LEU:HB2	5:F:373:LYS:HG3	1.83	0.60
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.84	0.59
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.84	0.59
2:C:721:ARG:HH22	2:C:785:VAL:HG11	1.67	0.59
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.85	0.59
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.01	0.59
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.84	0.58
5:F:395:GLU:OE2	5:F:398:ARG:NH2	2.30	0.58
3:D:835:SER:OG	3:D:838:ARG:CG	2.50	0.58
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.85	0.58
2:C:224:GLU:CD	2:C:224:GLU:H	2.10	0.58
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.86	0.58
2:C:713:ARG:HA	2:C:819:VAL:HA	1.85	0.58
3:D:208:PRO:HA	3:D:390:PRO:HA	1.86	0.58
3:D:288:MET:HE2	3:D:307:ALA:HB2	1.85	0.58
3:D:783:ARG:HA	3:D:1028:ALA:HA	1.86	0.57
3:D:155:ASP:OD2	3:D:159:ARG:NH1	2.37	0.57
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:63:TYR:OH	3:D:74:GLU:OE2	2.23	0.57
1:B:191:ASP:OD1	1:B:191:ASP:N	2.30	0.57
3:D:231:VAL:O	3:D:236:TYR:OH	2.22	0.57
3:D:954:ALA:O	3:D:1062:ARG:NH2	2.37	0.57
6:G:11:DT:H2"	6:G:12:DG:C8	2.39	0.57
3:D:273:ARG:HG3	3:D:278:PRO:CA	2.33	0.56
7:H:15:DT:H2"	7:H:16:DC:C6	2.40	0.56
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.87	0.56
3:D:783:ARG:HB3	3:D:1028:ALA:C	2.28	0.56
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.38	0.56
2:C:536:PRO:HB3	3:D:1067:VAL:HG11	1.87	0.56
2:C:874:LEU:HD12	3:D:784:ASP:OD1	2.04	0.56
1:B:7:LYS:O	1:B:8:ALA:HB3	2.05	0.56
2:C:727:PRO:HB3	2:C:783:ARG:HD3	1.88	0.56
3:D:1444:THR:O	3:D:1448:THR:HG23	2.05	0.56
2:C:684:PHE:HB3	3:D:633:VAL:HG21	1.88	0.56
1:A:36:LEU:HD11	1:B:221:HIS:HB3	1.88	0.56
2:C:614:ARG:NH2	2:C:618:GLY:O	2.39	0.56
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.87	0.56
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.88	0.56
2:C:816:LYS:HG3	2:C:819:VAL:HG11	1.89	0.55
3:D:1003:VAL:HG21	3:D:1041:LEU:HG	1.88	0.55
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.89	0.55
2:C:317:VAL:HG22	2:C:320:HIS:HD1	1.72	0.55
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.88	0.55
3:D:835:SER:O	3:D:836:VAL:C	2.48	0.55
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.35	0.55
5:F:172:ARG:O	5:F:176:ILE:HG12	2.06	0.55
3:D:815:ALA:HB3	11:D:2137:HOH:O	2.06	0.55
3:D:959:GLU:HB3	3:D:963:TYR:CE2	2.42	0.55
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.88	0.55
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.07	0.55
4:E:95:VAL:HG12	4:E:95:VAL:O	2.06	0.55
2:C:684:PHE:HE1	3:D:782:SER:HG	0.66	0.54
3:D:783:ARG:HD3	3:D:1028:ALA:O	2.07	0.54
3:D:975:GLU:O	3:D:979:GLU:HG2	2.07	0.54
2:C:906:PHE:CG	3:D:1067:VAL:HG12	2.43	0.54
2:C:139:GLN:NE2	2:C:413:LEU:O	2.41	0.54
2:C:776:SER:OG	5:F:373:LYS:NZ	2.41	0.54
2:C:11:GLU:HG2	2:C:535:SER:HB2	1.90	0.54
3:D:438:ASP:OD2	3:D:441:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1499:ARG:HH21	4:E:81:PRO:HD3	1.73	0.54
3:D:1084:THR:O	3:D:1088:THR:HG23	2.07	0.53
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.43	0.53
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.43	0.53
3:D:288:MET:HG2	3:D:305:ALA:HB1	1.91	0.53
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.90	0.53
2:C:13:ILE:HD13	2:C:483:VAL:HG21	1.91	0.53
2:C:405:ARG:HD3	2:C:566:THR:HG21	1.90	0.53
1:B:91:ASN:OD1	1:B:93:SER:N	2.36	0.53
2:C:41:ASN:O	2:C:46:ALA:HB2	2.09	0.53
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.44	0.53
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.31	0.52
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.08	0.52
3:D:827:ILE:O	3:D:834:THR:N	2.24	0.52
1:A:32:PHE:HA	1:A:35:THR:HB	1.92	0.52
3:D:1168:MET:HE3	3:D:1168:MET:HA	1.90	0.52
2:C:682:TYR:CE1	2:C:851:LYS:HD3	2.44	0.52
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.92	0.52
3:D:1296:SER:OG	3:D:1297:GLU:N	2.42	0.52
5:F:236:SER:OG	7:H:5:DA:OP2	2.21	0.52
1:B:6:LEU:CG	1:B:7:LYS:N	2.73	0.52
3:D:487:ALA:O	3:D:491:LYS:HG2	2.10	0.52
5:F:94:LEU:HD21	5:F:102:LEU:HD12	1.91	0.52
2:C:1052:MET:HE1	3:D:748:HIS:HB3	1.92	0.52
3:D:137:PRO:HA	3:D:452:ILE:HG23	1.92	0.52
2:C:134:ARG:NH1	2:C:392:SER:O	2.39	0.52
2:C:205:GLU:O	2:C:209:ARG:HG2	2.10	0.52
2:C:118:ILE:HD11	2:C:344:PHE:HE2	1.74	0.52
2:C:127:PHE:O	2:C:133:ASP:HA	2.10	0.52
2:C:704:HIS:CE1	2:C:1000:MET:HE1	2.45	0.52
2:C:1100:GLN:HG3	3:D:9:ARG:HH21	1.75	0.52
2:C:1056:LYS:HE2	3:D:751:LEU:HG	1.92	0.51
1:B:32:PHE:HA	1:B:35:THR:HB	1.93	0.51
2:C:805:ARG:O	2:C:807[A]:ARG:NH2	2.43	0.51
2:C:328:LEU:HD11	2:C:438:ILE:HD12	1.91	0.51
3:D:472:ALA:O	3:D:476:GLU:HG2	2.09	0.51
3:D:828:LYS:HA	3:D:833:GLU:HA	1.92	0.51
3:D:841:TYR:HB2	3:D:864:VAL:HG22	1.92	0.51
2:C:631:SER:HB3	2:C:637:LEU:HG	1.93	0.51
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.91	0.51
1:B:58:ILE:HG12	1:B:140:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:381:ALA:O	2:C:384:GLU:HG3	2.10	0.51
3:D:1093:TYR:O	3:D:1097:LYS:HG3	2.11	0.51
1:A:133:GLU:HG2	1:A:134:GLU:H	1.75	0.51
2:C:740:GLU:OE1	2:C:807[B]:ARG:NH2	2.44	0.51
3:D:956:ILE:HD11	3:D:1062:ARG:HG2	1.92	0.51
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.45	0.50
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.11	0.50
3:D:959:GLU:HB3	3:D:963:TYR:HE2	1.74	0.50
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.93	0.50
1:B:138:LEU:HD11	1:B:140:MET:HE3	1.94	0.50
2:C:64:LEU:HD12	2:C:103:LYS:HB2	1.92	0.50
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.77	0.50
6:G:10:DG:N2	7:H:18:DC:O2	2.45	0.50
1:B:154:GLU:CD	1:B:154:GLU:H	2.20	0.50
2:C:517:ARG:HD2	2:C:522:VAL:HG11	1.93	0.50
3:D:106:LYS:O	3:D:586:ARG:NH1	2.45	0.50
3:D:781:PRO:HG2	3:D:911:LEU:HB3	1.93	0.50
5:F:167:PRO:O	5:F:171:LYS:N	2.45	0.49
7:H:10:DA:H2''	7:H:11:DG:C8	2.47	0.49
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.94	0.49
1:B:6:LEU:HG	1:B:7:LYS:N	2.27	0.49
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.12	0.49
5:F:89:GLY:HA3	7:H:7:DG:C6	2.47	0.49
3:D:546:ARG:NH2	11:D:2104:HOH:O	2.45	0.49
2:C:218:VAL:HG22	2:C:222:MET:HE2	1.95	0.49
3:D:1057:VAL:HG22	3:D:1069:GLU:HG2	1.94	0.49
6:G:17:DG:N3	6:G:17:DG:H2'	2.28	0.49
1:B:73:GLU:OE1	1:B:73:GLU:N	2.44	0.49
2:C:627:ARG:HA	2:C:638:ASP:HB2	1.95	0.49
2:C:628:PHE:H	2:C:638:ASP:CB	2.22	0.49
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.48	0.49
3:D:187:LYS:N	3:D:200:ASP:OD1	2.37	0.48
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.94	0.48
2:C:724:ARG:NH2	2:C:734:LEU:O	2.45	0.48
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.48	0.48
3:D:968:ASP:OD1	3:D:1058:ARG:NH2	2.45	0.48
1:A:9:PRO:HB3	1:A:27:PRO:O	2.14	0.48
6:G:6:DA:C8	6:G:7:DT:H72	2.49	0.48
2:C:602:GLU:HB2	2:C:648:ARG:HH21	1.78	0.48
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.44	0.48
1:A:226:SER:O	1:A:228:PRO:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.94	0.48
3:D:134:VAL:HG22	3:D:149:LYS:HA	1.94	0.48
3:D:658:LEU:HA	3:D:661:MET:HE3	1.96	0.48
1:A:186:LEU:O	1:A:189:ARG:HG3	2.13	0.48
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.14	0.48
1:A:99:LEU:HB2	1:A:142:VAL:HG22	1.96	0.48
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.96	0.48
2:C:816:LYS:O	2:C:819:VAL:HG13	2.13	0.48
3:D:132:TYR:OH	3:D:568:ARG:NH1	2.47	0.48
5:F:276:ARG:O	5:F:279:GLN:HG3	2.14	0.48
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.47	0.48
2:C:436:GLY:HA2	2:C:538:GLN:O	2.13	0.47
3:D:224:ARG:H	3:D:251:PHE:HE1	1.61	0.47
5:F:127:ILE:O	5:F:131:VAL:HG23	2.14	0.47
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.96	0.47
2:C:1009:SER:HB3	3:D:651:GLU:O	2.14	0.47
5:F:237:THR:OG1	7:H:4:DA:H8	1.96	0.47
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.79	0.47
3:D:704:ARG:HB2	3:D:745:MET:HE2	1.96	0.47
1:A:4:SER:O	1:A:189:ARG:NH2	2.48	0.47
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.79	0.47
2:C:172:ILE:HD13	2:C:184:MET:HE3	1.96	0.47
2:C:758:ARG:HH21	2:C:788:THR:HB	1.79	0.47
1:A:25:LEU:HB3	1:A:28:LEU:HD11	1.96	0.47
3:D:260:GLU:HG2	3:D:294:HIS:CE1	2.44	0.47
3:D:1208:ASP:OD2	3:D:1211:MET:HE2	2.15	0.47
2:C:420:ARG:C	2:C:422:ARG:H	2.23	0.47
3:D:784:ASP:HB3	3:D:939:PHE:HE1	1.79	0.47
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.50	0.47
3:D:421:LEU:HD11	3:D:429:SER:HB2	1.96	0.47
1:B:6:LEU:CD1	1:B:7:LYS:N	2.73	0.47
3:D:489:ARG:NH1	3:D:1391:GLU:OE2	2.47	0.47
2:C:674:VAL:HG22	2:C:869:VAL:HG22	1.97	0.47
3:D:1341:PRO:O	3:D:1345:GLU:HG3	2.15	0.47
4:E:39:VAL:O	4:E:72:ARG:NH1	2.41	0.47
1:B:7:LYS:CD	1:B:8:ALA:N	2.73	0.47
2:C:214:TYR:HB3	2:C:217:LEU:HD12	1.97	0.47
3:D:200:ASP:O	3:D:397:LYS:HG2	2.15	0.47
3:D:542:ASP:OD1	3:D:545:ARG:NH2	2.41	0.46
2:C:317:VAL:HG22	2:C:320:HIS:ND1	2.30	0.46
2:C:361:MET:HE2	5:F:201:LYS:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:607:ASP:HB3	2:C:610:ARG:H	1.79	0.46
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.97	0.46
5:F:88:ILE:HD11	5:F:192:LEU:HD13	1.96	0.46
1:B:8:ALA:N	1:B:9:PRO:CD	2.78	0.46
3:D:1485:GLN:O	4:E:75:PHE:HA	2.16	0.46
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.96	0.46
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.97	0.46
1:B:179:PHE:HB3	1:B:197:LEU:HD13	1.97	0.46
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.98	0.46
2:C:1056:LYS:NZ	3:D:749:VAL:O	2.41	0.46
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.74	0.46
6:G:19:DG:N7	11:G:101:HOH:O	2.36	0.46
2:C:1098:ASP:OD2	2:C:1100:GLN:NE2	2.49	0.46
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.44	0.46
3:D:999:THR:O	3:D:1003:VAL:HG13	2.16	0.46
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.31	0.46
2:C:1116:ALA:HB2	3:D:88:TYR:HB3	1.98	0.46
3:D:733:CYS:HB3	3:D:738:ALA:O	2.16	0.46
3:D:921:ARG:NH1	11:D:2106:HOH:O	2.49	0.46
1:B:75:VAL:O	1:B:79:ILE:HG13	2.16	0.46
2:C:712:ALA:O	2:C:820:ARG:N	2.44	0.46
1:A:70:GLY:N	2:C:607:ASP:OD1	2.48	0.45
2:C:879:ARG:NE	11:C:1202:HOH:O	2.39	0.45
2:C:1065:ALA:HB1	2:C:1077:PRO:HG3	1.98	0.45
3:D:35:ARG:HH21	3:D:35:ARG:HB3	1.81	0.45
5:F:374:GLY:CA	5:F:379:ARG:O	2.62	0.45
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	1.97	0.45
5:F:370:LYS:HD3	5:F:376:ILE:HD11	1.98	0.45
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.51	0.45
3:D:659:LYS:HE3	3:D:663:GLU:OE2	2.17	0.45
5:F:82:ARG:HB2	7:H:8:DG:O6	2.16	0.45
2:C:328:LEU:HA	2:C:328:LEU:HD23	1.82	0.45
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.16	0.45
4:E:14:ASP:OD1	4:E:18:ARG:NH1	2.43	0.45
5:F:80:PRO:HB2	5:F:210:LEU:HD11	1.99	0.45
3:D:74:GLU:CD	3:D:74:GLU:H	2.24	0.45
2:C:280:LYS:HE3	2:C:309:TYR:CZ	2.51	0.45
2:C:293:PHE:CZ	2:C:296:GLY:HA2	2.51	0.45
2:C:769:PRO:HG3	3:D:65:ARG:HH12	1.81	0.45
3:D:371:ILE:HD12	5:F:230:LYS:HA	1.98	0.45
2:C:726:ILE:HD11	2:C:757:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.98	0.45
2:C:239:PHE:CD1	2:C:253:ALA:HA	2.52	0.45
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.98	0.45
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.52	0.44
2:C:121:MET:SD	2:C:125:GLY:HA2	2.58	0.44
2:C:226:VAL:HA	2:C:229:MET:HE2	1.99	0.44
1:A:154:GLU:CD	1:A:154:GLU:H	2.26	0.44
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.98	0.44
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	2.00	0.44
3:D:473:LEU:HD21	3:D:495:ARG:HH21	1.81	0.44
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.52	0.44
3:D:137:PRO:HB3	3:D:147:VAL:HG12	2.00	0.44
3:D:475:LYS:O	3:D:479:GLU:HG2	2.18	0.44
3:D:171:LEU:HD12	3:D:390:PRO:HG2	1.99	0.44
3:D:405:ASP:CG	3:D:406:ASP:H	2.26	0.44
1:B:7:LYS:CE	1:B:8:ALA:HB2	2.47	0.44
3:D:645:PRO:HB3	3:D:723:GLY:O	2.17	0.44
3:D:1271:LYS:HG3	3:D:1272:ALA:O	2.18	0.44
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.52	0.43
2:C:674:VAL:CG2	2:C:869:VAL:HG22	2.48	0.43
2:C:691:SER:HB2	2:C:858:MET:HG3	1.99	0.43
3:D:30:GLU:OE1	3:D:40:GLU:HG2	2.17	0.43
3:D:1045[B]:MET:HE3	3:D:1045[B]:MET:HB2	1.58	0.43
2:C:135:VAL:HG23	2:C:395:LYS:HG3	2.00	0.43
3:D:1144:LEU:O	3:D:1147:ARG:HG3	2.18	0.43
7:H:20:DG:H1'	7:H:21:DA:C8	2.53	0.43
2:C:215:GLY:O	2:C:216:GLU:HG3	2.18	0.43
3:D:1011:PHE:HB3	3:D:1021:TYR:CD1	2.54	0.43
3:D:1362:LYS:HE3	3:D:1362:LYS:HB2	1.84	0.43
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.77	0.43
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.99	0.43
3:D:420:VAL:HA	11:D:2182:HOH:O	2.19	0.43
3:D:112:ILE:HD11	3:D:512:MET:HB3	2.01	0.43
3:D:1458:GLU:HG3	11:D:2143:HOH:O	2.19	0.43
1:B:190:THR:HG21	3:D:722:GLU:CD	2.44	0.43
3:D:879:ARG:HD3	3:D:902:LEU:O	2.18	0.43
1:A:101:LEU:HD21	1:A:109:VAL:HG11	2.01	0.43
1:B:159:LYS:HE3	1:B:164:ALA:O	2.19	0.43
2:C:261:ILE:HG13	2:C:290:LEU:HD12	2.01	0.43
2:C:272:ALA:HB2	2:C:464:LEU:HB3	2.00	0.43
2:C:882:LEU:HD11	3:D:1038:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1004:LYS:HD3	3:D:744:GLN:OE1	2.18	0.43
1:A:11:PHE:O	1:B:228:PRO:HA	2.18	0.43
1:B:113:ASP:OD1	1:B:113:ASP:N	2.52	0.43
2:C:540:PHE:HB3	2:C:544:THR:HB	2.01	0.43
2:C:627:ARG:NH2	2:C:640:ARG:HG3	2.34	0.43
2:C:816:LYS:HG3	2:C:819:VAL:CG1	2.48	0.43
2:C:858:MET:HE3	2:C:867:VAL:HG23	2.00	0.43
3:D:129:PHE:CD1	3:D:456:MET:HB3	2.54	0.43
3:D:236:TYR:CE1	3:D:242:LEU:HD12	2.54	0.43
3:D:508:ARG:HD3	3:D:510:GLU:OE1	2.19	0.43
1:B:124:ASN:OD1	1:B:124:ASN:N	2.52	0.42
2:C:11:GLU:OE2	2:C:537:LYS:HE2	2.19	0.42
3:D:321:GLN:HB2	3:D:336:PHE:HD2	1.83	0.42
3:D:574:LEU:O	3:D:578:VAL:HG23	2.19	0.42
3:D:1045[B]:MET:CE	3:D:1057:VAL:HG23	2.48	0.42
3:D:1101:VAL:HG23	3:D:1102:THR:HG23	2.01	0.42
2:C:304:LEU:HB3	2:C:305:PRO:HD3	2.01	0.42
2:C:468:ARG:HA	2:C:486:MET:O	2.18	0.42
3:D:527:MET:HB2	3:D:527:MET:HE2	1.86	0.42
3:D:1281:VAL:HG21	3:D:1313:VAL:CG2	2.49	0.42
3:D:614:PHE:HA	3:D:618:LEU:HD12	2.01	0.42
5:F:362:SER:OG	5:F:365:GLU:HG2	2.19	0.42
3:D:158:TYR:HE1	3:D:454:ALA:HB3	1.83	0.42
1:B:56:VAL:HG21	1:B:82:LEU:HD13	2.01	0.42
2:C:571:LEU:HD22	2:C:700:TYR:HA	2.02	0.42
2:C:936:VAL:HG11	2:C:959:PRO:HB2	2.01	0.42
2:C:1053:LEU:HA	3:D:621:LYS:HD2	2.01	0.42
3:D:115:LEU:HD23	3:D:115:LEU:HA	1.89	0.42
3:D:539:ASP:CG	3:D:598:ARG:HH22	2.27	0.42
3:D:876:SER:OG	3:D:879:ARG:HG3	2.20	0.42
5:F:233:PHE:CD2	7:H:2:DA:H1'	2.53	0.42
5:F:373:LYS:HA	5:F:373:LYS:HD3	1.64	0.42
1:B:110:LYS:HD2	1:B:126:ASP:O	2.20	0.42
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.91	0.42
3:D:231:VAL:HG23	3:D:243:ALA:HA	2.02	0.42
2:C:110:GLU:HB2	11:C:1235:HOH:O	2.19	0.42
2:C:124:ASP:HB3	2:C:592:LEU:HD12	2.01	0.42
3:D:127:LEU:HA	3:D:457:GLY:HA2	2.02	0.42
2:C:63:GLY:N	2:C:367:LEU:HD12	2.35	0.42
2:C:372:LEU:HD12	2:C:372:LEU:HA	1.89	0.42
1:A:196:THR:HG21	2:C:934:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:930:LYS:HD2	2:C:930:LYS:HA	1.81	0.42
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.20	0.42
3:D:428:LYS:HE2	3:D:428:LYS:HB3	1.85	0.42
3:D:956:ILE:H	3:D:956:ILE:HG12	1.66	0.42
3:D:157:GLU:O	3:D:161:LEU:HG	2.19	0.41
2:C:194:VAL:HG23	11:C:1201:HOH:O	2.21	0.41
2:C:462:ASP:HB3	2:C:468:ARG:HD2	2.02	0.41
3:D:258:VAL:HG12	3:D:273:ARG:O	2.20	0.41
3:D:433:GLY:HA2	3:D:449:SER:H	1.85	0.41
6:G:16:DC:H2'	6:G:17:DG:H8	1.85	0.41
1:A:41:ARG:HA	1:A:177:VAL:HG11	2.03	0.41
2:C:548:PRO:O	2:C:843:HIS:HE1	2.03	0.41
3:D:961:LYS:HB2	3:D:961:LYS:HE3	1.80	0.41
3:D:1096:ARG:NH1	3:D:1440:PHE:O	2.53	0.41
1:A:10:VAL:HG12	1:A:26:GLU:O	2.20	0.41
3:D:135:LEU:N	3:D:135:LEU:HD23	2.36	0.41
3:D:703:ASN:HA	3:D:712:GLY:O	2.20	0.41
1:A:220:GLU:O	1:A:223:THR:HB	2.21	0.41
2:C:701:THR:HA	2:C:831:ARG:O	2.21	0.41
2:C:847:GLY:HA2	3:D:741:ASP:HA	2.01	0.41
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.56	0.41
1:B:96:THR:HB	1:B:145:ASP:OD1	2.21	0.41
3:D:762:GLN:HA	11:E:104:HOH:O	2.20	0.41
1:B:90:LEU:HD11	1:B:121:GLU:HB2	2.02	0.41
3:D:784:ASP:HB3	3:D:939:PHE:CE1	2.56	0.41
1:A:133:GLU:HG2	1:A:134:GLU:N	2.36	0.41
2:C:76:PRO:HG3	2:C:120:LEU:HD12	2.03	0.41
2:C:154:ARG:HH21	2:C:157:ARG:HG3	1.86	0.41
3:D:140:ALA:HB2	3:D:452:ILE:HG12	2.02	0.41
3:D:209:ARG:O	3:D:346:ARG:HD3	2.21	0.41
3:D:844:ALA:O	3:D:867:ARG:HB3	2.21	0.41
1:A:159:LYS:HE3	1:A:164:ALA:O	2.21	0.41
2:C:223:ASP:OD2	2:C:225:SER:OG	2.35	0.41
2:C:229:MET:HB2	2:C:233:GLU:HB2	2.02	0.41
5:F:260:ILE:HG22	5:F:265:VAL:HG23	2.03	0.41
1:A:196:THR:HG21	2:C:934:PHE:HE1	1.86	0.40
3:D:270:LEU:HD12	3:D:284:LEU:HD11	2.03	0.40
3:D:783:ARG:H	3:D:783:ARG:HG2	1.55	0.40
2:C:168:ARG:HD3	2:C:268:ASP:HB3	2.04	0.40
2:C:434:HIS:HE1	11:C:1203:HOH:O	2.03	0.40
6:G:17:DG:H3'	6:G:18:DA:H8	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:114:THR:HG23	3:D:495:ARG:HG2	2.02	0.40
2:C:87:ASP:HA	2:C:131:GLY:HA3	2.02	0.40
2:C:397:GLU:HG2	2:C:632:ASN:HB2	2.02	0.40
3:D:38:LYS:HA	3:D:38:LYS:HD3	1.83	0.40
3:D:216:VAL:HA	3:D:340:THR:HG22	2.02	0.40
3:D:355:VAL:HG11	3:D:385:VAL:HG21	2.02	0.40
1:A:133:GLU:OE1	2:C:610:ARG:NH1	2.55	0.40
3:D:904:VAL:CG2	3:D:905:PRO:HD2	2.50	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	230/315 (73%)	229 (100%)	1 (0%)	0	100	100
1	B	221/315 (70%)	218 (99%)	2 (1%)	1 (0%)	24	52
2	C	1111/1119 (99%)	1091 (98%)	20 (2%)	0	100	100
3	D	1485/1524 (97%)	1461 (98%)	24 (2%)	0	100	100
4	E	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
5	F	334/443 (75%)	333 (100%)	1 (0%)	0	100	100
All	All	3473/3815 (91%)	3423 (99%)	49 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	ALA

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	201/273 (74%)	185 (92%)	16 (8%)	11	31
1	B	196/273 (72%)	185 (94%)	11 (6%)	19	46
2	C	938/941 (100%)	885 (94%)	53 (6%)	18	46
3	D	1250/1279 (98%)	1192 (95%)	58 (5%)	24	55
4	E	83/88 (94%)	82 (99%)	1 (1%)	63	84
5	F	294/388 (76%)	275 (94%)	19 (6%)	15	40
All	All	2962/3242 (91%)	2804 (95%)	158 (5%)	20	49

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	15	THR
1	A	19	GLU
1	A	25	LEU
1	A	30	ARG
1	A	90	LEU
1	A	94	LEU
1	A	96	THR
1	A	112	ARG
1	A	134	GLU
1	A	142	VAL
1	A	145	ASP
1	A	148	VAL
1	A	170	VAL
1	A	189	ARG
1	A	205	VAL
1	B	7	LYS
1	B	55	SER
1	B	90	LEU
1	B	94	LEU
1	B	129	ILE
1	B	133	GLU

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Mol	Chain	Res	Type
1	B	154	GLU
1	B	160	ASP
1	B	162	ILE
1	B	188	GLN
1	B	191	ASP
2	C	81	ASP
2	C	186	VAL
2	C	216	GLU
2	C	224	GLU
2	C	242	LEU
2	C	251	ASP
2	C	257	VAL
2	C	284	ARG
2	C	299	LYS
2	C	317	VAL
2	C	322	VAL
2	C	336	VAL
2	C	342	ASP
2	C	348	LEU
2	C	358	ARG
2	C	360	LEU
2	C	372	LEU
2	C	384	GLU
2	C	395	LYS
2	C	402	SER
2	C	413	LEU
2	C	427	VAL
2	C	430	VAL
2	C	441	VAL
2	C	445	GLU
2	C	449	ILE
2	C	454	SER
2	C	455	LEU
2	C	483	VAL
2	C	524	VAL
2	C	578	VAL
2	C	583	LEU
2	C	595	LEU
2	C	610	ARG
2	C	657	ASP
2	C	666	LEU
2	C	670	GLN

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Mol	Chain	Res	Type
2	C	674	VAL
2	C	695	LEU
2	C	768	THR
2	C	775	ARG
2	C	807[A]	ARG
2	C	807[B]	ARG
2	C	816	LYS
2	C	819	VAL
2	C	830	LYS
2	C	848	VAL
2	C	869	VAL
2	C	913	GLU
2	C	929	ARG
2	C	939	ARG
2	C	1080	SER
2	C	1095	LEU
3	D	35	ARG
3	D	53	ILE
3	D	67	ARG
3	D	74	GLU
3	D	83	SER
3	D	134	VAL
3	D	135	LEU
3	D	145	VAL
3	D	152	LEU
3	D	175	VAL
3	D	185	VAL
3	D	216	VAL
3	D	231	VAL
3	D	245	LEU
3	D	273	ARG
3	D	293	VAL
3	D	354	VAL
3	D	415	VAL
3	D	427	VAL
3	D	431	VAL
3	D	452	ILE
3	D	471	GLU
3	D	503	LEU
3	D	607	LEU
3	D	623	VAL
3	D	632	VAL

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Mol	Chain	Res	Type
3	D	687	VAL
3	D	694	VAL
3	D	711	LEU
3	D	754	PHE
3	D	778	LEU
3	D	783	ARG
3	D	784	ASP
3	D	810	GLU
3	D	813	LEU
3	D	864	VAL
3	D	892	ASP
3	D	899	LEU
3	D	956	ILE
3	D	1055	VAL
3	D	1067	VAL
3	D	1083	ASP
3	D	1100	ASP
3	D	1101	VAL
3	D	1129	THR
3	D	1188	VAL
3	D	1193	THR
3	D	1200	VAL
3	D	1221	VAL
3	D	1252	ILE
3	D	1295	GLU
3	D	1312	LEU
3	D	1313	VAL
3	D	1424	VAL
3	D	1468	LEU
3	D	1486	VAL
3	D	1488	ASP
3	D	1493	LYS
4	E	50	THR
5	F	81	VAL
5	F	88	ILE
5	F	94	LEU
5	F	95	THR
5	F	96	LEU
5	F	141	VAL
5	F	179	GLU
5	F	257	THR
5	F	262	VAL

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Mol	Chain	Res	Type
5	F	295	MET
5	F	310	ILE
5	F	315	VAL
5	F	338	LEU
5	F	358	LEU
5	F	369	LEU
5	F	373	LYS
5	F	380	GLU
5	F	392	VAL
5	F	399	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	B	63	HIS
2	C	139	GLN
2	C	556	ASN
3	D	125	GLN
3	D	352	ASN
3	D	696	HIS
3	D	703	ASN
3	D	762	GLN
3	D	1033	GLN
3	D	1184	GLN
5	F	83	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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 [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	231/315 (73%)	-0.02	4 (1%) 69 62	55, 85, 111, 148	1 (0%)
1	B	223/315 (70%)	0.19	6 (2%) 56 48	68, 94, 122, 133	0
2	C	1112/1119 (99%)	-0.03	8 (0%) 84 79	40, 78, 132, 155	3 (0%)
3	D	1486/1524 (97%)	0.08	23 (1%) 72 65	46, 79, 135, 160	4 (0%)
4	E	94/99 (94%)	0.08	1 (1%) 78 72	61, 83, 115, 136	0
5	F	338/443 (76%)	0.21	7 (2%) 63 56	64, 93, 130, 147	0
6	G	18/21 (85%)	0.12	2 (11%) 10 8	67, 100, 176, 181	0
7	H	24/27 (88%)	-0.13	1 (4%) 40 34	84, 105, 167, 193	0
8	I	6/6 (100%)	-0.36	0 100 100	66, 70, 84, 103	0
All	All	3532/3869 (91%)	0.05	52 (1%) 72 65	40, 83, 133, 193	8 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	782	SER	5.5
1	B	6	LEU	4.9
2	C	64	LEU	3.7
3	D	1252	ILE	3.7
1	B	157	GLY	3.6
1	B	228	PRO	3.5
3	D	409	VAL	3.4
2	C	102[A]	HIS	3.3
2	C	384	GLU	3.2
3	D	184	GLU	3.0
5	F	78	SER	2.9
6	G	21	DG	2.9
5	F	319	THR	2.9
5	F	318	GLU	2.8
1	B	191	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	256	GLU	2.8
3	D	324	ALA	2.8
4	E	95	VAL	2.8
2	C	159	ILE	2.7
3	D	203	ALA	2.7
5	F	139	ALA	2.7
3	D	434	ARG	2.7
3	D	368	VAL	2.7
3	D	1053[A]	PHE	2.6
3	D	420	VAL	2.6
3	D	556	LYS	2.5
6	G	4	DG	2.5
3	D	353	VAL	2.5
3	D	431	VAL	2.5
2	C	189	ARG	2.4
3	D	470	LEU	2.4
5	F	375	LEU	2.3
2	C	47	ALA	2.2
1	B	165	ILE	2.2
3	D	96	ALA	2.2
1	A	170	VAL	2.2
1	A	48	ILE	2.2
3	D	260	GLU	2.2
3	D	352	ASN	2.2
2	C	103	LYS	2.1
2	C	101	ILE	2.1
3	D	290	PRO	2.1
3	D	193	PRO	2.1
1	B	140	MET	2.1
5	F	328	PHE	2.1
1	A	4	SER	2.1
1	A	21	GLY	2.1
3	D	783	ARG	2.0
3	D	665	GLY	2.0
3	D	443	VAL	2.0
5	F	141	VAL	2.0
7	H	24	DC	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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	0.76	0.25	83,83,83,83	0
9	MG	B	2001	1/1	0.83	0.10	97,97,97,97	0
9	MG	F	2001	1/1	0.87	0.08	83,83,83,83	0
10	ZN	D	2002	1/1	0.99	0.03	107,107,107,107	0
10	ZN	D	2001	1/1	1.00	0.04	66,66,66,66	0
9	MG	D	2003	1/1	1.00	0.04	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.