



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:20 AM UTC

PDB ID : 6LTS / pdb_00006lts
Title : Crystal structure of Thermus thermophilus transcription initiation complex comprising a truncated sigma finger
Authors : Zhang, Y.; Ebright, R.H.
Deposited on : 2020-01-23
Resolution : 3.45 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:

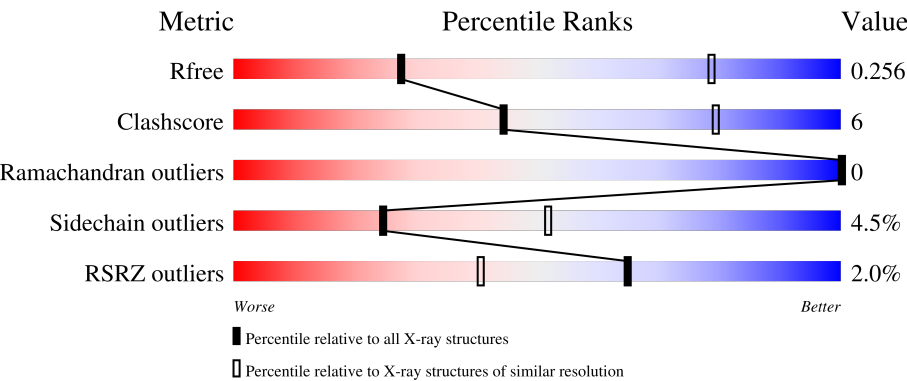
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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%13%28%
1	B	315	% 56%14%30%
2	C	1119	% 81%17%..
3	D	1524	3% 79%17%..
4	E	99	% 79%15%5%

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Mol	Chain	Length	Quality of chain
5	F	443	% 63% 12% 24%
6	H	27	41% 48% 11%
7	G	19	11% 26% 26% 47%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28227 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	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	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	0	0
			11738	7441	2067	2195	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 RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	336	Total	C	N	O	S	0	0	0
			2725	1717	498	506	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 nontemplate DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

- Molecule 7 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	10	Total	C	N	O	P	0	0	0
			202	97	38	58	9			

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

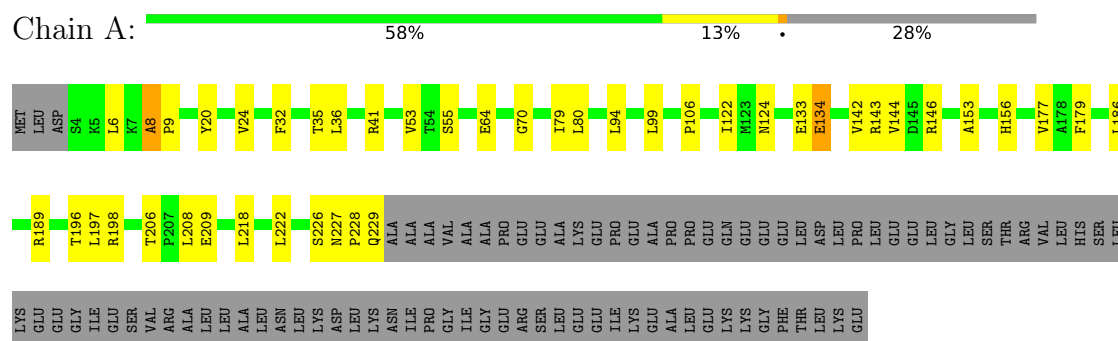
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

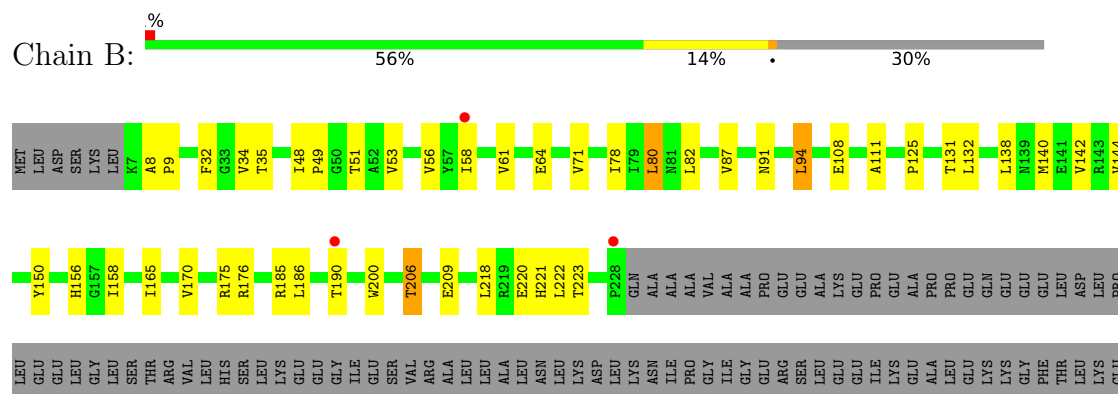
3 Residue-property plots [i](#)

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.

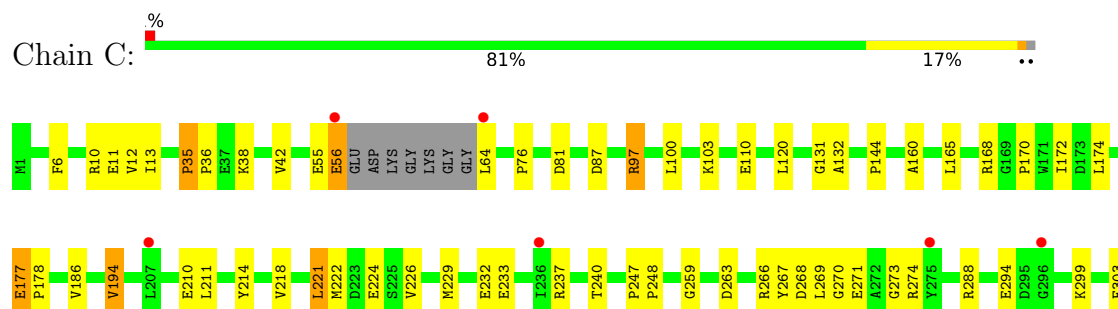
• Molecule 1: DNA-directed RNA polymerase subunit alpha

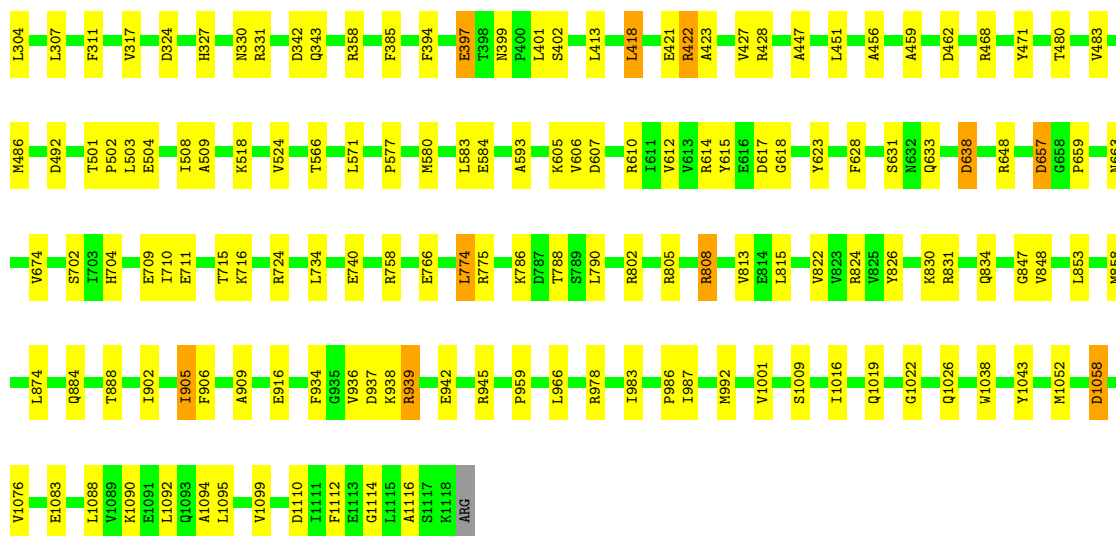


• Molecule 1: DNA-directed RNA polymerase subunit alpha

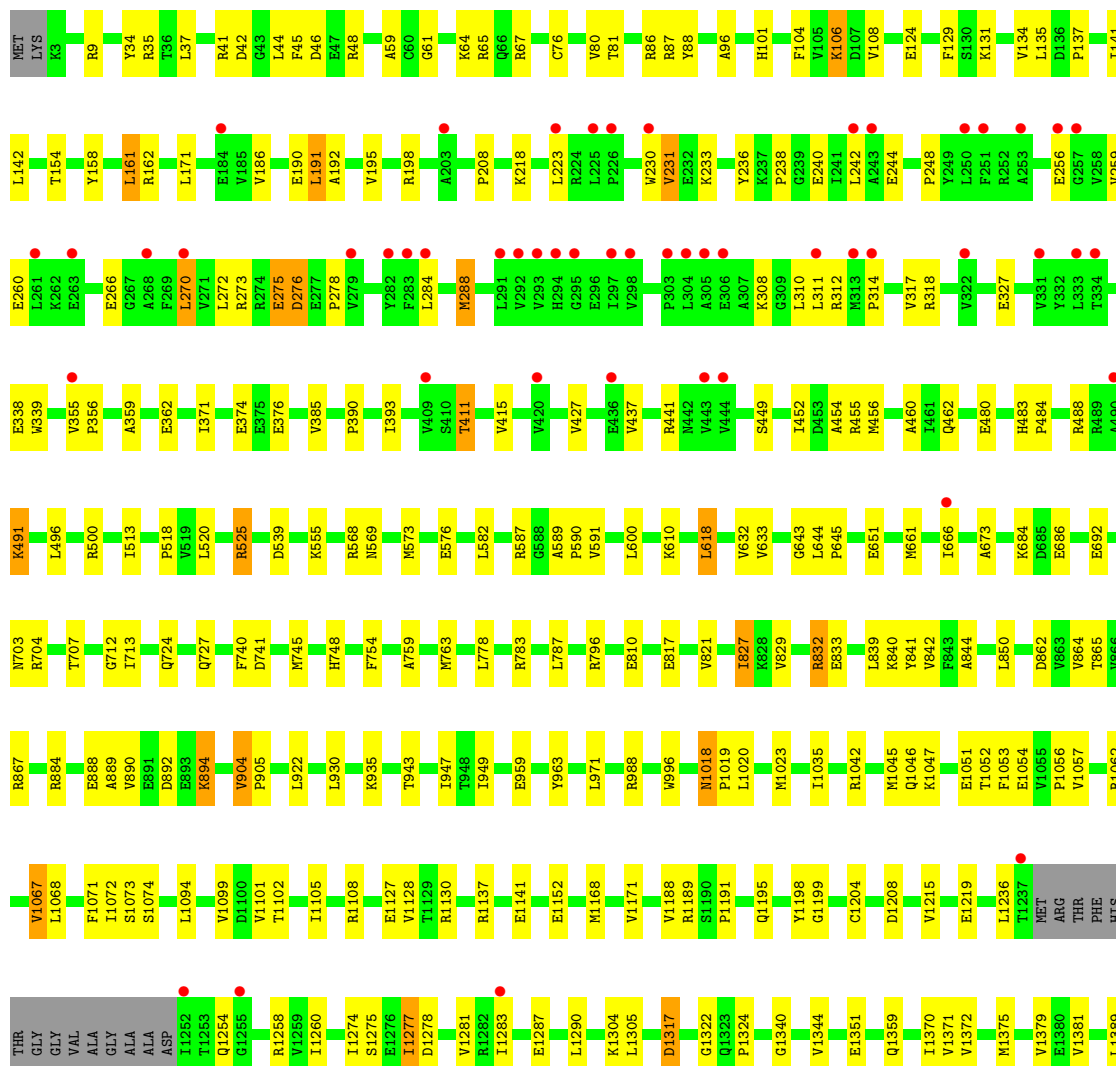
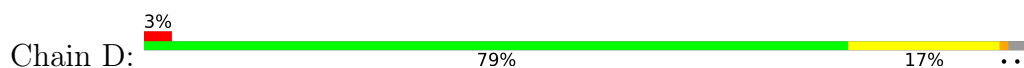


• Molecule 2: DNA-directed RNA polymerase subunit beta



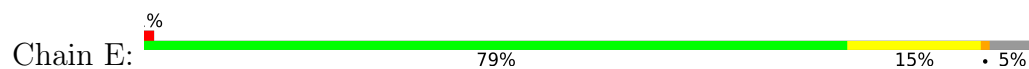


• Molecule 3: DNA-directed RNA polymerase subunit beta'

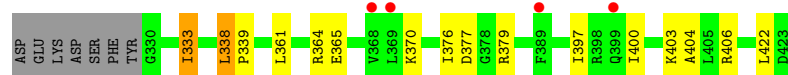
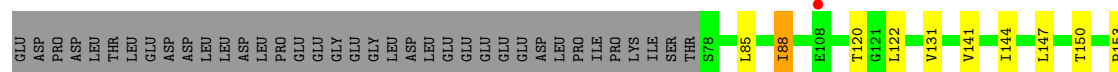
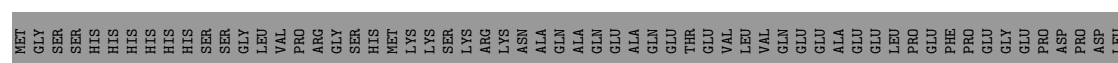




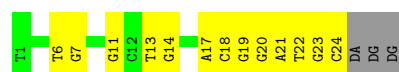
- Molecule 4: DNA-directed RNA polymerase subunit omega



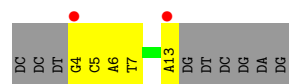
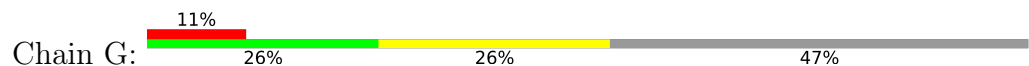
- Molecule 5: RNA polymerase sigma factor SigA



- Molecule 6: nontemplate DNA



- Molecule 7: template DNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.70Å 103.85Å 295.41Å 90.00° 98.61° 90.00°	Depositor
Resolution (Å)	44.23 – 3.45 44.23 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.23-3.45) 99.7 (44.23-3.45)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.220 , 0.258 0.219 , 0.256	Depositor DCC
R_{free} test set	1606 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å ²)	81.4	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	28227	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: ZN, MG

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	0.28	0/1814	0.81	2/2466 (0.1%)
1	B	0.28	0/1782	0.80	0/2424
2	C	0.29	0/8937	0.75	4/12087 (0.0%)
3	D	0.29	0/11944	0.75	5/16149 (0.0%)
4	E	0.27	0/772	0.70	0/1040
5	F	0.28	0/2766	0.74	5/3719 (0.1%)
6	H	0.30	0/556	0.63	0/858
7	G	0.28	0/226	0.42	0/347
All	All	0.29	0/28797	0.75	16/39090 (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
3	D	0	1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1340	GLY	CA-C-N	6.14	125.87	119.05
3	D	1340	GLY	C-N-CA	6.14	125.87	119.05
5	F	333	ILE	N-CA-C	5.68	113.17	107.55
1	A	8	ALA	CA-C-N	5.67	125.87	120.31
1	A	8	ALA	C-N-CA	5.67	125.87	120.31
2	C	35	PRO	CA-C-N	5.64	125.75	119.32
2	C	35	PRO	C-N-CA	5.64	125.75	119.32
5	F	262	VAL	N-CA-C	5.48	115.68	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	271	GLU	N-CA-C	-5.36	105.44	111.28
3	D	1018	ASN	CA-C-N	5.23	124.67	119.24
3	D	1018	ASN	C-N-CA	5.23	124.67	119.24
5	F	333	ILE	CA-C-N	5.16	125.14	120.03
5	F	333	ILE	C-N-CA	5.16	125.14	120.03
3	D	65	ARG	N-CA-C	5.16	116.50	109.18
5	F	191	ASN	N-CA-C	5.16	119.26	112.92
2	C	303	PHE	N-CA-C	5.04	117.43	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	108	VAL	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	1782	0	1834	25	0
1	B	1750	0	1797	27	0
2	C	8770	0	8874	114	0
3	D	11738	0	11972	151	0
4	E	758	0	770	10	0
5	F	2725	0	2810	30	0
6	H	495	0	272	17	0
7	G	202	0	114	6	0
8	B	1	0	0	0	0
8	D	3	0	0	0	0
8	F	1	0	0	0	0
9	D	2	0	0	0	0
All	All	28227	0	28443	337	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 (337) 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:H:22:DT:H2''	6:H:23:DG:H5'	1.58	0.83
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.67	0.77
2:C:628:PHE:H	2:C:638:ASP:HB2	1.51	0.76
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.69	0.75
1:B:206:THR:HG22	1:B:209:GLU:H	1.53	0.73
1:B:91:ASN:HB3	1:B:94:LEU:HB2	1.71	0.71
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.25	0.68
3:D:491:LYS:HD3	3:D:491:LYS:N	2.07	0.68
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.60	0.67
2:C:397:GLU:HB2	2:C:631:SER:HB2	1.78	0.66
6:H:21:DA:OP2	6:H:21:DA:H8	1.79	0.66
3:D:42:ASP:OD1	3:D:48:ARG:NH2	2.29	0.65
3:D:61:GLY:O	3:D:64:LYS:NZ	2.29	0.65
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.79	0.65
2:C:97:ARG:NH1	2:C:110:GLU:OE1	2.29	0.65
2:C:593:ALA:HB1	2:C:659:PRO:HD2	1.78	0.65
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.79	0.64
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.77	0.64
2:C:758:ARG:HH21	2:C:788:THR:HB	1.63	0.62
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.80	0.62
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.82	0.62
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.79	0.62
2:C:402:SER:HA	2:C:566:THR:HG23	1.80	0.62
2:C:221:LEU:HD11	2:C:307:LEU:HD21	1.82	0.62
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.82	0.62
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.82	0.62
3:D:371:ILE:HG23	5:F:230:LYS:HD2	1.82	0.62
3:D:569:ASN:ND2	5:F:214:GLN:OE1	2.31	0.61
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.83	0.61
2:C:905:ILE:HG23	2:C:906:PHE:HD2	1.65	0.61
3:D:610:LYS:HZ3	7:G:13:DA:H3'	1.66	0.61
3:D:223:LEU:HD11	3:D:288:MET:HE1	1.82	0.61
3:D:520:LEU:O	3:D:525:ARG:NH1	2.35	0.60
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.82	0.60
3:D:41:ARG:HG3	3:D:48:ARG:HE	1.67	0.60
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.84	0.60
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.84	0.60
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.83	0.60
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.84	0.60
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.82	0.59
2:C:1116:ALA:HB2	3:D:88:TYR:HB3	1.83	0.59
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:OE2	2:C:606:VAL:N	2.36	0.59
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.84	0.59
3:D:233:LYS:NZ	3:D:240:GLU:OE2	2.27	0.58
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.85	0.58
1:B:138:LEU:HD11	1:B:140:MET:HE3	1.86	0.58
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.85	0.58
2:C:418:LEU:HD11	6:H:14:DG:C8	2.40	0.56
3:D:520:LEU:HD23	3:D:525:ARG:HG2	1.87	0.56
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.87	0.56
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.87	0.56
2:C:1016:ILE:O	3:D:87:ARG:NH1	2.38	0.56
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.35	0.55
2:C:218:VAL:HG12	2:C:222:MET:HE2	1.87	0.55
3:D:661:MET:HG2	3:D:666:ILE:HD12	1.89	0.55
6:H:23:DG:OP2	6:H:23:DG:H3'	2.06	0.55
3:D:949:ILE:HD11	3:D:1023:MET:HE1	1.87	0.55
2:C:331:ARG:NH2	6:H:14:DG:O6	2.39	0.55
2:C:1083:GLU:OE2	3:D:87:ARG:NH2	2.38	0.55
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.40	0.55
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.88	0.55
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.88	0.54
5:F:188:ILE:HG12	5:F:224:VAL:HG21	1.89	0.54
1:A:53:VAL:HG22	1:A:144:VAL:HG22	1.89	0.54
3:D:1450:ALA:HA	3:D:1455:LYS:HD2	1.89	0.54
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.30	0.54
2:C:1019:GLN:HG2	2:C:1058:ASP:HB3	1.90	0.54
1:B:32:PHE:HA	1:B:35:THR:HB	1.90	0.53
5:F:144:ILE:HB	5:F:147:LEU:HD13	1.90	0.53
2:C:614:ARG:NH2	2:C:618:GLY:O	2.42	0.53
3:D:129:PHE:HD1	3:D:456:MET:HE3	1.74	0.53
2:C:170:PRO:HA	6:H:13:DT:O4	2.09	0.53
3:D:96:ALA:HB2	3:D:555:LYS:HG2	1.91	0.53
2:C:132:ALA:HB1	2:C:394:PHE:HE1	1.74	0.52
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.91	0.52
1:A:99:LEU:HD21	1:A:122:ILE:HD11	1.91	0.52
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.90	0.52
3:D:411:THR:HB	3:D:437:VAL:H	1.75	0.52
3:D:850:LEU:HD12	3:D:884:ARG:NH2	2.25	0.52
6:H:20:DG:H2''	6:H:21:DA:H5'	1.92	0.52
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.75	0.52
3:D:610:LYS:NZ	7:G:13:DA:H3'	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.92	0.52
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.92	0.52
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.92	0.52
2:C:937:ASP:OD2	2:C:939:ARG:NH1	2.43	0.51
3:D:496:LEU:HG	3:D:500:ARG:HD2	1.92	0.51
7:G:5:DC:H2''	7:G:6:DA:C8	2.45	0.51
1:B:175:ARG:N	1:B:200:TRP:O	2.43	0.51
1:B:220:GLU:O	1:B:223:THR:OG1	2.28	0.51
3:D:191:LEU:HB3	3:D:393:ILE:HD12	1.93	0.51
1:B:80:LEU:HD11	3:D:842:VAL:HG12	1.93	0.50
2:C:834:GLN:OE1	3:D:724:GLN:NE2	2.44	0.50
3:D:1105:ILE:HG23	3:D:1199:GLY:HA2	1.92	0.50
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.43	0.50
2:C:210:GLU:HB3	2:C:211:LEU:HD12	1.92	0.50
3:D:480:GLU:OE2	3:D:488:ARG:NH2	2.45	0.50
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.94	0.50
6:H:20:DG:H4'	6:H:20:DG:OP1	2.12	0.50
2:C:194:VAL:HG22	2:C:221:LEU:HD23	1.93	0.49
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	1.93	0.49
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.93	0.49
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.95	0.49
2:C:172:ILE:HG13	2:C:186:VAL:HG22	1.93	0.49
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.94	0.49
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.95	0.49
2:C:942:GLU:HG3	2:C:945:ARG:HH21	1.77	0.49
3:D:171:LEU:HD22	3:D:390:PRO:HG2	1.95	0.49
1:B:78:ILE:HG21	1:B:140:MET:HE1	1.92	0.49
3:D:284:LEU:HD22	3:D:288:MET:HE2	1.94	0.49
3:D:832:ARG:HD2	3:D:833:GLU:H	1.78	0.49
4:E:37:ASN:HD22	4:E:89:MET:HE1	1.78	0.49
5:F:193:ARG:HB2	6:H:6:DT:H1'	1.95	0.49
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.95	0.49
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.93	0.49
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.95	0.49
1:B:80:LEU:HG	3:D:844:ALA:HA	1.95	0.49
2:C:674:VAL:HG11	2:C:992:MET:HE3	1.95	0.49
3:D:106:LYS:HE3	3:D:587:ARG:HG3	1.95	0.49
6:H:23:DG:H1'	6:H:24:DC:C6	2.47	0.49
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.95	0.48
3:D:704:ARG:HB2	3:D:745:MET:HE2	1.96	0.48
2:C:503:LEU:HD23	2:C:508:ILE:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.96	0.48
3:D:248:PRO:HG3	3:D:308:LYS:HG3	1.96	0.48
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.96	0.48
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.96	0.48
3:D:45:PHE:O	3:D:86:ARG:NH2	2.46	0.48
3:D:959:GLU:OE1	3:D:959:GLU:N	2.45	0.48
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.48	0.48
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.13	0.48
1:A:32:PHE:HA	1:A:35:THR:HB	1.95	0.47
1:A:206:THR:HG22	1:A:208:LEU:H	1.78	0.47
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.96	0.47
3:D:67:ARG:CZ	5:F:379:ARG:HD3	2.44	0.47
3:D:142:LEU:HB2	3:D:161:LEU:HD11	1.95	0.47
3:D:1046:GLN:N	3:D:1046:GLN:OE1	2.47	0.47
2:C:884:GLN:O	2:C:888:THR:OG1	2.28	0.47
2:C:1022:GLY:O	2:C:1026:GLN:NE2	2.46	0.47
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.94	0.47
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.47	0.47
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.97	0.47
3:D:1191:PRO:HB3	3:D:1370:ILE:HD13	1.96	0.47
1:A:206:THR:HB	1:A:209:GLU:HG3	1.95	0.47
2:C:35:PRO:HG2	2:C:38:LYS:HD3	1.96	0.47
2:C:55:GLU:O	2:C:56:GLU:HB3	2.15	0.47
2:C:168:ARG:HE	2:C:168:ARG:HA	1.80	0.47
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.96	0.47
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.97	0.47
3:D:1275:SER:O	3:D:1322:GLY:N	2.39	0.47
2:C:144:PRO:HB2	2:C:273:GLY:HA3	1.96	0.46
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.96	0.46
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.14	0.46
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.97	0.46
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.49	0.46
3:D:1020:LEU:HB3	3:D:1035:ILE:HD12	1.97	0.46
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.69	0.46
2:C:168:ARG:O	2:C:267:TYR:HA	2.16	0.46
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.50	0.46
2:C:211:LEU:HD11	2:C:304:LEU:HD11	1.98	0.46
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.98	0.46
3:D:42:ASP:N	3:D:46:ASP:OD2	2.41	0.46
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.98	0.46
3:D:231:VAL:O	3:D:236:TYR:OH	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.48	0.45
3:D:759:ALA:HA	3:D:763:MET:HB2	1.96	0.45
4:E:13:VAL:HG21	4:E:19:LEU:HB2	1.98	0.45
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.98	0.45
3:D:162:ARG:O	3:D:449:SER:HB2	2.15	0.45
3:D:1168:MET:HE3	3:D:1171:VAL:HB	1.99	0.45
5:F:187:LEU:HD23	5:F:224:VAL:HG13	1.98	0.45
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.97	0.45
2:C:237:ARG:O	2:C:240:THR:OG1	2.27	0.45
2:C:428:ARG:NH2	2:C:447:ALA:O	2.34	0.45
3:D:842:VAL:HG22	3:D:865:THR:HB	1.97	0.45
1:A:70:GLY:N	2:C:607:ASP:OD1	2.50	0.45
2:C:422:ARG:HH22	6:H:13:DT:H4'	1.81	0.45
2:C:1094:ALA:HA	3:D:518:PRO:HB2	1.97	0.45
3:D:275:GLU:HB3	3:D:276:ASP:H	1.65	0.45
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.98	0.45
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.31	0.45
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.82	0.45
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.51	0.45
2:C:906:PHE:CG	3:D:1067:VAL:HG12	2.52	0.45
4:E:12:MET:HE1	4:E:69:LEU:HA	1.98	0.45
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.99	0.45
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.52	0.45
3:D:1045:MET:HE2	3:D:1073:SER:HA	1.99	0.45
4:E:33:HIS:CE1	4:E:89:MET:HB3	2.51	0.45
2:C:221:LEU:HD12	2:C:311:PHE:HE2	1.82	0.44
4:E:57:ASP:HB3	4:E:63:TRP:HE1	1.83	0.44
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.81	0.44
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.98	0.44
3:D:840:LYS:HE3	3:D:841:TYR:OH	2.16	0.44
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.99	0.44
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.99	0.44
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.51	0.44
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.52	0.44
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.53	0.44
5:F:194:LEU:HB2	6:H:6:DT:C2	2.53	0.44
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.71	0.44
2:C:471:TYR:HB2	2:C:486:MET:HE3	2.00	0.44
2:C:571:LEU:HD23	2:C:702:SER:HB3	2.00	0.44
2:C:716:LYS:HE3	3:D:37:LEU:HG	2.00	0.44
4:E:40:LEU:HG	4:E:67:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:HIS:ND1	1:B:158:ILE:HG12	2.33	0.44
3:D:573:MET:SD	5:F:210:LEU:HB3	2.58	0.44
4:E:83:ASP:OD1	4:E:83:ASP:N	2.50	0.44
2:C:966:LEU:HD13	2:C:986:PRO:HB3	2.00	0.44
3:D:1141:GLU:HG2	3:D:1168:MET:HE1	1.99	0.44
1:A:226:SER:O	1:A:228:PRO:HD3	2.18	0.43
2:C:224:GLU:H	2:C:224:GLU:CD	2.25	0.43
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.53	0.43
3:D:259:VAL:HG13	3:D:270:LEU:HD21	2.00	0.43
3:D:411:THR:HG23	5:F:178:ARG:HB2	2.00	0.43
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.53	0.43
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	2.00	0.43
6:H:17:DA:H2'	6:H:18:DC:C6	2.53	0.43
2:C:6:PHE:CD2	2:C:909:ALA:HB2	2.53	0.43
2:C:399:ASN:OD1	2:C:401:LEU:HB3	2.18	0.43
3:D:483:HIS:HA	3:D:484:PRO:HD3	1.91	0.43
6:H:18:DC:H2''	6:H:19:DG:C8	2.53	0.43
3:D:1047:LYS:N	3:D:1051:GLU:O	2.37	0.43
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.99	0.43
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.99	0.43
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.52	0.43
1:B:53:VAL:HG22	1:B:144:VAL:HG22	2.01	0.43
2:C:76:PRO:HG3	2:C:120:LEU:HD12	2.01	0.43
2:C:847:GLY:HA2	3:D:741:ASP:HA	1.99	0.43
3:D:456:MET:HE1	3:D:568:ARG:NE	2.34	0.43
3:D:796:ARG:NH1	3:D:862:ASP:OD2	2.52	0.43
1:A:94:LEU:O	1:A:146:ARG:NH1	2.51	0.43
3:D:889:ALA:HB1	3:D:930:LEU:HA	2.00	0.43
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	2.00	0.43
2:C:1009:SER:HB3	3:D:651:GLU:O	2.17	0.43
5:F:164:LYS:HA	5:F:171:LYS:HE3	2.01	0.43
2:C:259:GLY:HA2	2:C:263:ASP:HB2	2.01	0.43
2:C:740:GLU:HB3	2:C:805:ARG:NH1	2.33	0.43
2:C:937:ASP:OD1	2:C:938:LYS:N	2.52	0.43
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.88	0.43
3:D:9:ARG:HB2	3:D:1456:LYS:HG2	1.99	0.43
3:D:821:VAL:HG11	3:D:827:ILE:HD12	2.02	0.42
5:F:338:LEU:HD23	5:F:339:PRO:HD2	2.01	0.42
1:B:64:GLU:HA	1:B:165:ILE:HD13	2.00	0.42
1:B:111:ALA:HB3	1:B:125:PRO:HA	2.00	0.42
3:D:1381:VAL:HG21	3:D:1389:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:20:DG:H2'	6:H:21:DA:C8	2.54	0.42
1:B:8:ALA:HA	1:B:9:PRO:HD3	1.90	0.42
2:C:492:ASP:HB3	2:C:518:LYS:HG2	2.01	0.42
2:C:657:ASP:OD2	2:C:663:ASN:N	2.48	0.42
2:C:724:ARG:NH2	2:C:734:LEU:O	2.52	0.42
2:C:1088:LEU:HD22	3:D:618:LEU:HD21	2.01	0.42
3:D:244:GLU:HG3	3:D:310:LEU:HG	2.00	0.42
3:D:462:GLN:HB2	3:D:513:ILE:HG21	2.01	0.42
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.52	0.42
3:D:892:ASP:OD1	3:D:894:LYS:HD2	2.19	0.42
1:A:227:ASN:HA	1:A:228:PRO:HD3	1.86	0.42
1:B:185:ARG:NH2	3:D:692:GLU:HG3	2.35	0.42
2:C:580:MET:HE3	2:C:902:ILE:HG12	2.01	0.42
3:D:131:LYS:NZ	3:D:154:THR:HG22	2.34	0.42
3:D:633:VAL:HB	3:D:740:PHE:CZ	2.55	0.42
3:D:1018:ASN:HA	3:D:1019:PRO:HD3	1.87	0.42
4:E:49:GLN:NE2	4:E:50:THR:O	2.53	0.42
3:D:1071:PHE:O	3:D:1074:SER:OG	2.32	0.42
7:G:6:DA:H2''	7:G:7:DT:H5'	2.02	0.42
2:C:160:ALA:HB3	2:C:174:LEU:HB2	2.02	0.42
2:C:615:TYR:OH	2:C:623:TYR:OH	2.22	0.42
2:C:853:LEU:HB2	2:C:858:MET:HE1	2.01	0.42
5:F:85:LEU:HD22	6:H:7:DG:H1'	2.01	0.42
5:F:172:ARG:O	5:F:176:ILE:HG12	2.20	0.42
5:F:361:LEU:HB3	5:F:365:GLU:HG3	2.01	0.42
2:C:294:GLU:HB3	2:C:299:LYS:HD2	2.01	0.42
3:D:610:LYS:HZ3	7:G:13:DA:C3'	2.32	0.42
3:D:1344:VAL:HG11	3:D:1421:LEU:HD22	2.02	0.42
1:B:150:TYR:CE1	1:B:170:VAL:HG22	2.56	0.41
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.86	0.41
2:C:218:VAL:O	2:C:222:MET:HG2	2.19	0.41
2:C:266:ARG:NH1	6:H:11:DG:H1	2.18	0.41
2:C:711:GLU:O	2:C:758:ARG:NH1	2.53	0.41
3:D:270:LEU:HD12	3:D:284:LEU:HD11	2.02	0.41
3:D:539:ASP:HB3	3:D:600:LEU:HB3	2.02	0.41
3:D:589:ALA:HA	3:D:590:PRO:HD3	1.94	0.41
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.20	0.41
5:F:370:LYS:HB3	5:F:376:ILE:HG13	2.01	0.41
2:C:1052:MET:HE1	3:D:748:HIS:HB3	2.02	0.41
3:D:1281:VAL:HB	3:D:1317:ASP:H	1.85	0.41
1:A:153:ALA:HA	1:A:156:HIS:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:4:DG:H2"	7:G:5:DC:C6	2.55	0.41
2:C:501:THR:HA	2:C:502:PRO:HD3	1.89	0.41
2:C:766:GLU:HG3	3:D:64:LYS:HD2	2.02	0.41
2:C:936:VAL:HG11	2:C:959:PRO:HB2	2.02	0.41
3:D:1371:VAL:HG12	3:D:1375:MET:HE2	2.01	0.41
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.80	0.41
1:A:41:ARG:HA	1:A:177:VAL:HG11	2.02	0.41
1:B:51:THR:OG1	1:B:87:VAL:O	2.29	0.41
3:D:208:PRO:HA	3:D:390:PRO:HA	2.02	0.41
5:F:88:ILE:HG23	5:F:193:ARG:HG2	2.02	0.41
5:F:317:LEU:HD21	5:F:333:ILE:HD12	2.02	0.41
2:C:269:LEU:O	2:C:288:ARG:HD2	2.21	0.41
5:F:278:LEU:HA	5:F:281:GLU:HG2	2.01	0.41
2:C:10:ARG:NH2	2:C:12:VAL:HG12	2.36	0.41
5:F:163:LEU:HD13	5:F:174:LEU:HD13	2.02	0.41
2:C:12:VAL:HG23	2:C:13:ILE:HG23	2.03	0.41
2:C:270:GLY:O	2:C:274:ARG:N	2.45	0.41
2:C:456:ALA:HB3	2:C:459:ALA:HB2	2.03	0.41
3:D:374:GLU:C	3:D:376:GLU:H	2.28	0.41
2:C:13:ILE:HD13	2:C:483:VAL:HG11	2.02	0.41
2:C:226:VAL:HA	2:C:229:MET:HE2	2.02	0.41
2:C:423:ALA:O	2:C:428:ARG:NH1	2.54	0.41
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	2.03	0.41
3:D:661:MET:HE3	3:D:673:ALA:HB1	2.03	0.41
3:D:684:LYS:HE2	3:D:684:LYS:HB3	1.87	0.41
3:D:935:LYS:HB3	3:D:935:LYS:HE2	1.84	0.41
3:D:1462:LEU:HD22	3:D:1472:ILE:HB	2.03	0.41
3:D:59:ALA:HB3	3:D:76:CYS:HB2	2.02	0.41
2:C:87:ASP:HA	2:C:131:GLY:HA3	2.02	0.40
2:C:229:MET:HB2	2:C:233:GLU:HB2	2.02	0.40
2:C:774:LEU:HD22	2:C:774:LEU:HA	1.93	0.40
3:D:829:VAL:HG21	3:D:839:LEU:HD11	2.03	0.40
3:D:1274:ILE:HG22	3:D:1324:PRO:HA	2.03	0.40
1:A:36:LEU:HD11	1:B:221:HIS:HB3	2.04	0.40
2:C:874:LEU:HD13	3:D:783:ARG:HB3	2.03	0.40
3:D:988:ARG:NH2	3:D:1054:GLU:OE2	2.54	0.40
1:A:124:ASN:OD1	1:A:124:ASN:N	2.53	0.40
1:B:58:ILE:HB	1:B:61:VAL:HB	2.03	0.40
2:C:324:ASP:O	2:C:330:ASN:ND2	2.45	0.40
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.35	0.40
3:D:703:ASN:HB2	3:D:713:ILE:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1046:GLN:HA	3:D:1052:THR:HA	2.03	0.40
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.84	0.40
2:C:214:TYR:HE1	2:C:317:VAL:HG21	1.87	0.40
3:D:707:THR:HG23	3:D:712:GLY:HA3	2.04	0.40
3:D:1094:LEU:HD22	3:D:1260:ILE:HG12	2.02	0.40
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.85	0.40
3:D:633:VAL:HB	3:D:740:PHE:CE2	2.56	0.40
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	2.04	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	224/315 (71%)	221 (99%)	3 (1%)	0	100	100
1	B	220/315 (70%)	215 (98%)	5 (2%)	0	100	100
2	C	1107/1119 (99%)	1076 (97%)	31 (3%)	0	100	100
3	D	1482/1524 (97%)	1442 (97%)	40 (3%)	0	100	100
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
5	F	332/443 (75%)	328 (99%)	4 (1%)	0	100	100
All	All	3457/3815 (91%)	3372 (98%)	85 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	199/273 (73%)	193 (97%)	6 (3%)	36	61
1	B	195/273 (71%)	189 (97%)	6 (3%)	35	61
2	C	936/941 (100%)	893 (95%)	43 (5%)	24	51
3	D	1253/1279 (98%)	1189 (95%)	64 (5%)	21	49
4	E	82/88 (93%)	81 (99%)	1 (1%)	63	74
5	F	292/388 (75%)	280 (96%)	12 (4%)	27	54
All	All	2957/3242 (91%)	2825 (96%)	132 (4%)	24	52

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	80	LEU
1	A	134	GLU
1	A	142	VAL
1	A	189	ARG
1	A	229	GLN
1	B	34	VAL
1	B	80	LEU
1	B	94	LEU
1	B	186	LEU
1	B	190	THR
1	B	206	THR
2	C	11	GLU
2	C	42	VAL
2	C	56	GLU
2	C	81	ASP
2	C	97	ARG
2	C	103	LYS
2	C	177	GLU
2	C	194	VAL
2	C	221	LEU
2	C	232	GLU
2	C	342	ASP
2	C	358	ARG
2	C	397	GLU
2	C	418	LEU
2	C	421	GLU

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Mol	Chain	Res	Type
2	C	422	ARG
2	C	427	VAL
2	C	480	THR
2	C	524	VAL
2	C	583	LEU
2	C	584	GLU
2	C	617	ASP
2	C	633	GLN
2	C	638	ASP
2	C	648	ARG
2	C	657	ASP
2	C	715	THR
2	C	774	LEU
2	C	775	ARG
2	C	786	LYS
2	C	808	ARG
2	C	813	VAL
2	C	815	LEU
2	C	830	LYS
2	C	848	VAL
2	C	905	ILE
2	C	916	GLU
2	C	939	ARG
2	C	978	ARG
2	C	1001	VAL
2	C	1043	TYR
2	C	1058	ASP
2	C	1076	VAL
3	D	80	VAL
3	D	81	THR
3	D	106	LYS
3	D	135	LEU
3	D	141	ILE
3	D	161	LEU
3	D	186	VAL
3	D	190	GLU
3	D	191	LEU
3	D	198	ARG
3	D	230	TRP
3	D	231	VAL
3	D	256	GLU
3	D	270	LEU

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Mol	Chain	Res	Type
3	D	272	LEU
3	D	275	GLU
3	D	276	ASP
3	D	288	MET
3	D	312	ARG
3	D	327	GLU
3	D	362	GLU
3	D	411	THR
3	D	415	VAL
3	D	427	VAL
3	D	491	LYS
3	D	525	ARG
3	D	576	GLU
3	D	591	VAL
3	D	618	LEU
3	D	632	VAL
3	D	686	GLU
3	D	754	PHE
3	D	778	LEU
3	D	810	GLU
3	D	817	GLU
3	D	827	ILE
3	D	832	ARG
3	D	864	VAL
3	D	867	ARG
3	D	894	LYS
3	D	904	VAL
3	D	943	THR
3	D	971	LEU
3	D	1062	ARG
3	D	1067	VAL
3	D	1127	GLU
3	D	1128	VAL
3	D	1130	ARG
3	D	1152	GLU
3	D	1188	VAL
3	D	1195	GLN
3	D	1219	GLU
3	D	1277	ILE
3	D	1283	ILE
3	D	1287	GLU
3	D	1290	LEU

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Mol	Chain	Res	Type
3	D	1304	LYS
3	D	1305	LEU
3	D	1317	ASP
3	D	1408	ILE
3	D	1441	GLN
3	D	1493	LYS
3	D	1496	GLU
3	D	1501	GLU
4	E	50	THR
5	F	88	ILE
5	F	141	VAL
5	F	150	THR
5	F	205	ARG
5	F	287	THR
5	F	295	MET
5	F	310	ILE
5	F	338	LEU
5	F	364	ARG
5	F	377	ASP
5	F	406	ARG
5	F	422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	B	81	ASN
2	C	117	HIS
2	C	498	GLN
2	C	575	GLN
2	C	704	HIS
2	C	1026	GLN
3	D	386	HIS
3	D	569	ASN
3	D	703	ASN
3	D	714	GLN
3	D	994	GLN
3	D	1010	ASN
3	D	1018	ASN
3	D	1172	HIS
3	D	1195	GLN
3	D	1333	HIS

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Mol	Chain	Res	Type
3	D	1441	GLN
3	D	1442	ASN
4	E	33	HIS
5	F	191	ASN
5	F	214	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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 7 ligands modelled in this entry, 7 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	226/315 (71%)	-0.09	0 100 100	69, 93, 116, 124	0
1	B	222/315 (70%)	0.16	3 (1%) 73 49	72, 104, 134, 151	0
2	C	1111/1119 (99%)	-0.09	6 (0%) 87 70	57, 86, 156, 192	0
3	D	1486/1524 (97%)	0.12	52 (3%) 47 28	55, 89, 157, 186	1 (0%)
4	E	94/99 (94%)	-0.01	1 (1%) 78 54	62, 92, 133, 142	0
5	F	336/443 (75%)	0.24	5 (1%) 72 48	67, 108, 165, 181	0
6	H	24/27 (88%)	0.57	0 100 100	94, 158, 201, 220	0
7	G	10/19 (52%)	1.49	2 (20%) 3 3	145, 177, 201, 207	0
All	All	3509/3861 (90%)	0.06	69 (1%) 65 41	55, 93, 158, 220	1 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	268	ALA	5.2
3	D	304	LEU	4.9
3	D	284	LEU	4.8
3	D	223	LEU	4.5
3	D	250	LEU	4.2
3	D	243	ALA	4.2
3	D	242	LEU	4.1
3	D	257	GLY	3.7
3	D	297	ILE	3.6
3	D	298	VAL	3.4
3	D	230	TRP	3.3
3	D	292	VAL	3.2
3	D	282	TYR	3.0
3	D	322	VAL	3.0
7	G	13	DA	2.9
3	D	293	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
3	D	263	GLU	2.9
5	F	389	PHE	2.9
5	F	369	LEU	2.8
3	D	331	VAL	2.8
5	F	368	VAL	2.7
3	D	184	GLU	2.7
3	D	420	VAL	2.7
3	D	291	LEU	2.7
3	D	311	LEU	2.7
3	D	305	ALA	2.7
3	D	1237	THR	2.7
3	D	270	LEU	2.7
5	F	399	GLN	2.6
3	D	203	ALA	2.6
3	D	490	ALA	2.6
3	D	225	LEU	2.6
3	D	355	VAL	2.6
2	C	236	ILE	2.5
3	D	314	PRO	2.5
3	D	444	VAL	2.5
3	D	436	GLU	2.5
3	D	409	VAL	2.5
3	D	253	ALA	2.4
3	D	313	MET	2.4
3	D	306	GLU	2.4
3	D	261	LEU	2.4
3	D	279	VAL	2.4
3	D	251	PHE	2.3
3	D	1283	ILE	2.3
1	B	190	THR	2.3
3	D	294	HIS	2.3
3	D	333	LEU	2.3
2	C	207	LEU	2.2
3	D	295	GLY	2.2
3	D	303	PRO	2.2
2	C	275	TYR	2.2
3	D	226	PRO	2.2
5	F	108	GLU	2.2
1	B	228	PRO	2.2
3	D	283	PHE	2.2
4	E	95	VAL	2.1
3	D	1255	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
7	G	4	DG	2.1
3	D	666	ILE	2.1
3	D	1252	ILE	2.1
2	C	296	GLY	2.1
3	D	443	VAL	2.1
3	D	334	THR	2.1
3	D	1441	GLN	2.1
3	D	256	GLU	2.1
1	B	58	ILE	2.1
2	C	64	LEU	2.1
2	C	56	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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
8	MG	B	2001	1/1	0.47	0.12	120,120,120,120	0
8	MG	D	2005	1/1	0.72	0.12	91,91,91,91	0
8	MG	D	2004	1/1	0.86	0.24	62,62,62,62	0
8	MG	D	2003	1/1	0.96	0.14	53,53,53,53	0
8	MG	F	2001	1/1	0.97	0.04	91,91,91,91	0
9	ZN	D	2002	1/1	0.99	0.03	101,101,101,101	0
9	ZN	D	2001	1/1	1.00	0.04	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.