Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 05:36 PM JST

PDB ID	:	6LTS
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 (i) 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 (1)) were used in the production of this report:

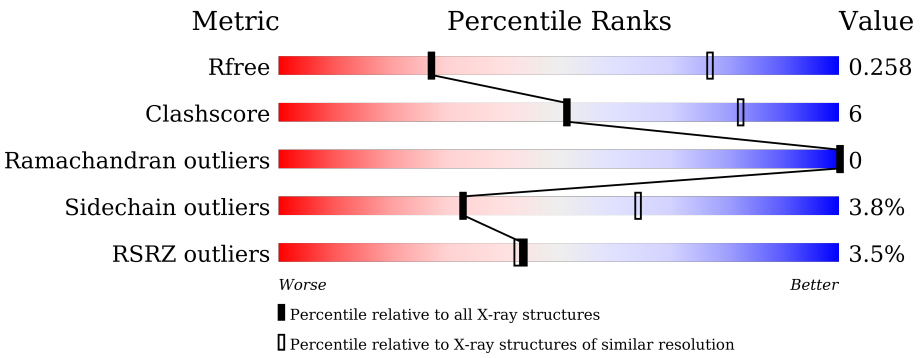
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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 <=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% 14% 28%
1	B	315	56% 13% • 30%
2	C	1119	2% 82% 16% ••
3	D	1524	5% 81% 16% • •
4	E	99	2% 82% 12% • 5%
5	F	443	3% 63% 12% 24%

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Mol	Chain	Length	Quality of chain
6	H	27	15% 41% 44% • 11%
7	G	19	5% 26% 26% 47%

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
8	MG	B	2001	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	226	1782	1138	310	332	2	0	0	0
1	B	222	1750	1118	304	326	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1111	8770	5548	1564	1634	24	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1486	11738	7441	2067	2195	35	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	94	758	483	132	139	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	336	2725	1717	498	506	4	0	0	0

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
			Total	C	N	O	P			
6	H	24	495	236	94	142	23	0	0	0

- Molecule 7 is a DNA chain called template DNA.

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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

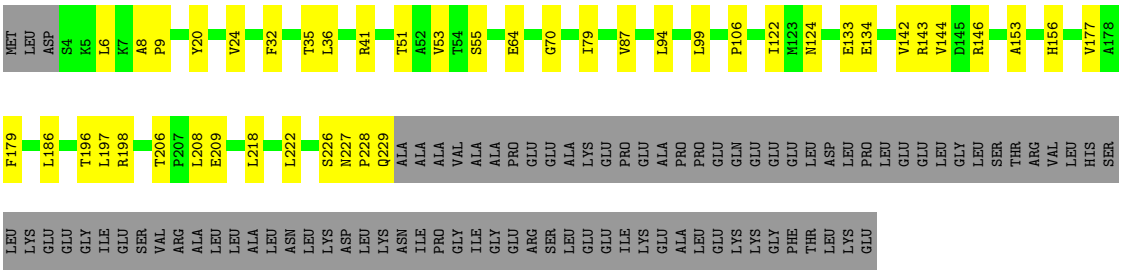
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
9	D	2	2	2	0	0

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.

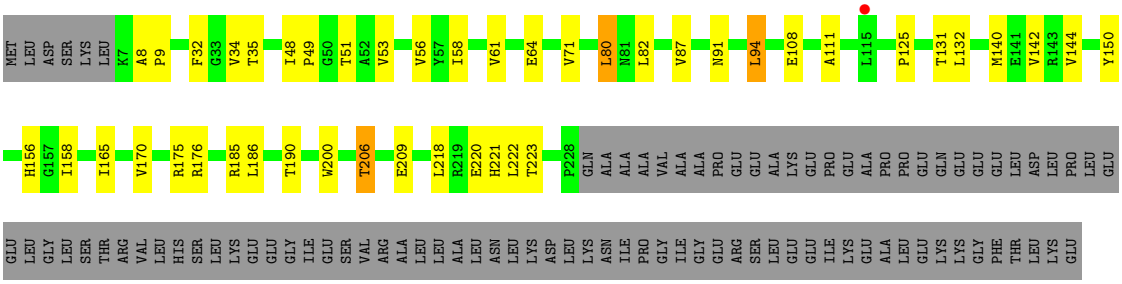
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



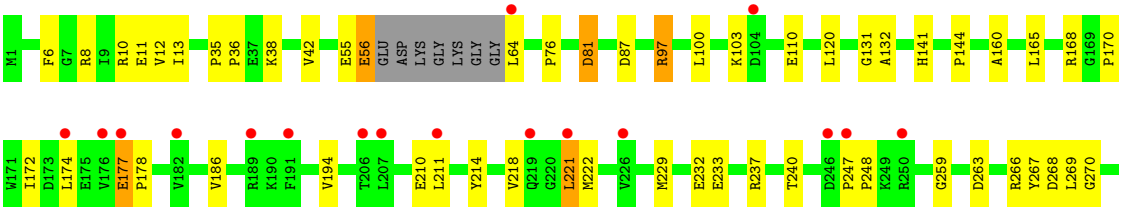
• Molecule 1: DNA-directed RNA polymerase subunit alpha

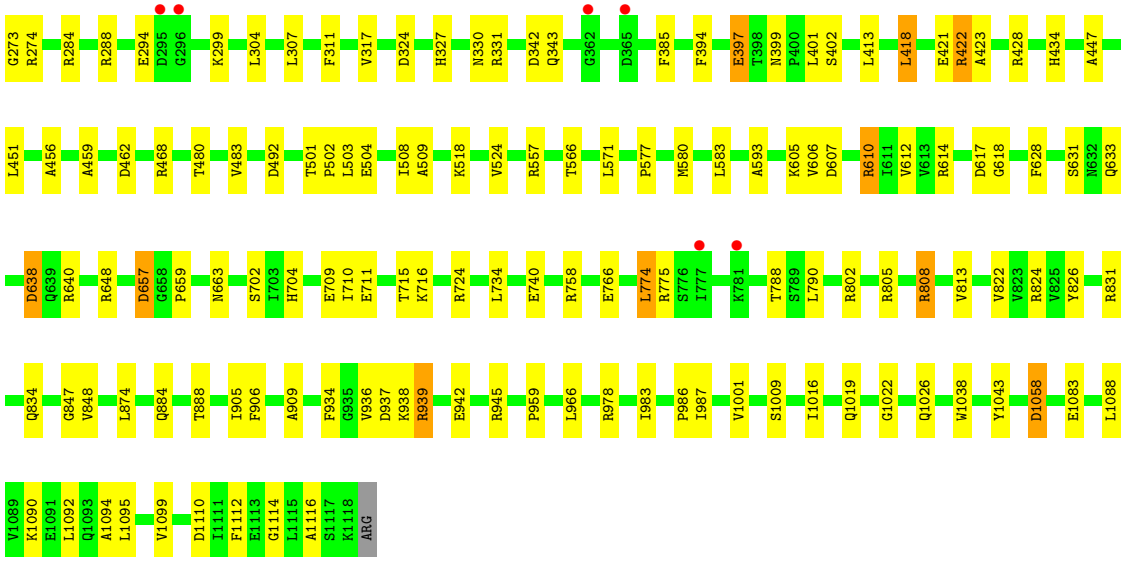
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

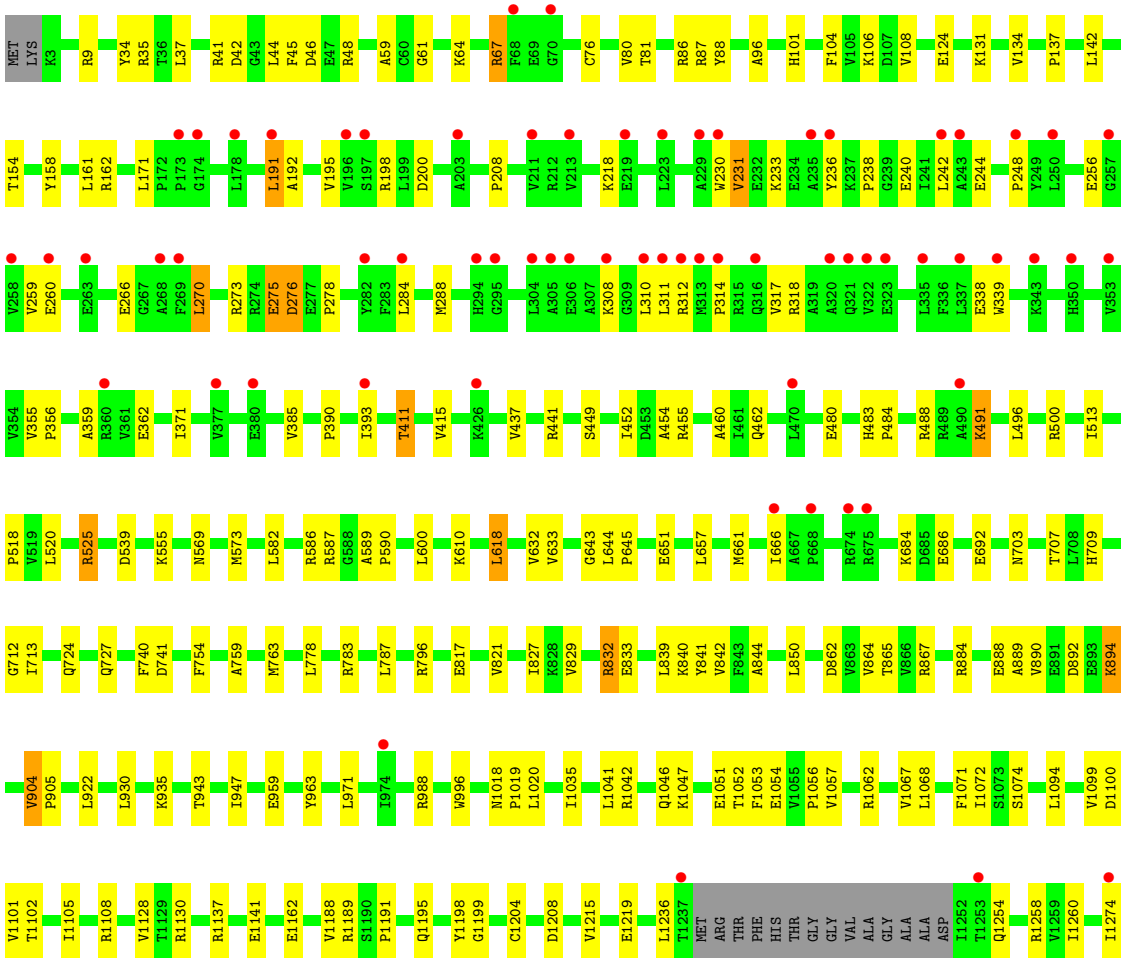
Chain C:

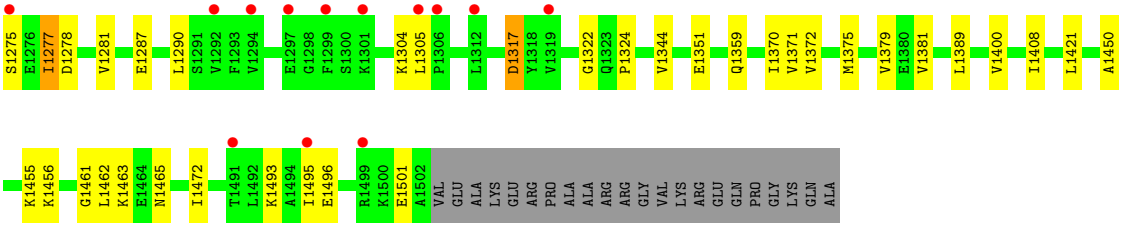




• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:



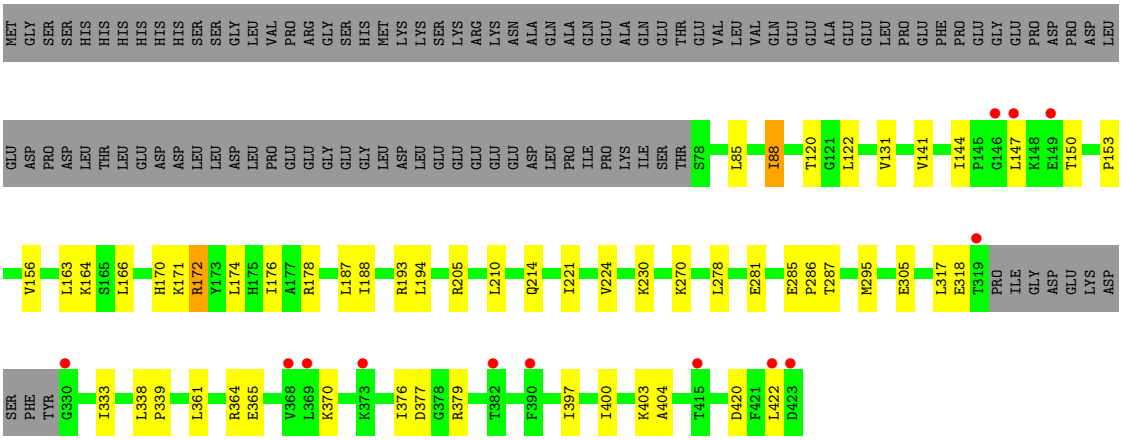


- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:

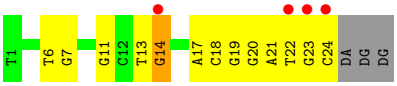
- Molecule 5: RNA polymerase sigma factor SigA

Chain F:



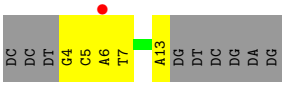
- Molecule 6: nontemplate DNA

Chain H:



- Molecule 7: template DNA

Chain G:



4 Data and refinement statistics (i)

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) 99.8 (44.23-3.45)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.220 , 0.258 0.220 , 0.258	Depositor DCC
R_{free} test set	1606 reflections (2.21%)	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)	0.28 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.22	0/1814	0.43	0/2466
1	B	0.22	0/1782	0.43	0/2424
2	C	0.22	0/8937	0.42	0/12087
3	D	0.22	0/11944	0.41	0/16149
4	E	0.21	0/772	0.38	0/1040
5	F	0.22	0/2766	0.38	0/3719
6	H	0.46	1/556 (0.2%)	0.95	1/858 (0.1%)
7	G	0.20	0/226	0.58	0/347
All	All	0.23	1/28797 (0.0%)	0.43	1/39090 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	14	DG	O3'-P	6.02	1.68	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	14	DG	P-O3'-C3'	6.46	127.45	119.70

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 (i)

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	26	0
1	B	1750	0	1797	26	0
2	C	8770	0	8874	106	0
3	D	11738	0	11972	140	0
4	E	758	0	770	8	0
5	F	2725	0	2810	31	0
6	H	495	0	272	17	0
7	G	202	0	114	5	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	318	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 (318) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.92	0.52
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.91	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
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
1:B:220:GLU:O	1:B:223:THR:OG1	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:832:ARG:HD2	3:D:833:GLU:H	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
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
2:C:503:LEU:HD23	2:C:508:ILE:HA	1.95	0.48
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:131:LYS:HZ2	3:D:154:THR:HG22	1.80	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
2:C:81:ASP:OD1	2:C:81:ASP:N	2.42	0.46
3:D:231:VAL:O	3:D:236:TYR:OH	2.34	0.46
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
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
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.52	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: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
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
1:A:226:SER:O	1:A:228:PRO:HD3	2.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:51:THR:OG1	1:A:87:VAL:O	2.26	0.43
3:D:821:VAL:HG11	3:D:827:ILE:HD12	2.02	0.42
5:F:270:LYS:HG2	5:F:295:MET:HE1	2.00	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
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
2:C:884:GLN:O	2:C:888:THR:OG1	2.28	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
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
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:1344:VAL:HG11	3:D:1421:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
1:B:140:MET:HB3	1:B:140:MET:HE2	1.97	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
3:D:657:LEU:HG	3:D:661:MET:HE2	2.01	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:610:LYS:HZ2	7:G:13:DA:H3'	1.86	0.41
2:C:13:ILE:HD13	2:C:483:VAL:HG11	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: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
3:D:1100:ASP:OD1	3:D:1463:LYS:NZ	2.45	0.41
2:C:87:ASP:HA	2:C:131:GLY:HA3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	196 (98%)	3 (2%)	65	84
1	B	195/273 (71%)	189 (97%)	6 (3%)	40	70
2	C	936/941 (100%)	896 (96%)	40 (4%)	29	61
3	D	1253/1279 (98%)	1201 (96%)	52 (4%)	30	61
4	E	82/88 (93%)	81 (99%)	1 (1%)	71	87
5	F	292/388 (75%)	281 (96%)	11 (4%)	33	64
All	All	2957/3242 (91%)	2844 (96%)	113 (4%)	33	64

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	142	VAL
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	8	ARG
2	C	11	GLU
2	C	42	VAL

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Mol	Chain	Res	Type
2	C	56	GLU
2	C	81	ASP
2	C	97	ARG
2	C	103	LYS
2	C	141	HIS
2	C	177	GLU
2	C	221	LEU
2	C	232	GLU
2	C	284	ARG
2	C	342	ASP
2	C	397	GLU
2	C	418	LEU
2	C	421	GLU
2	C	422	ARG
2	C	434	HIS
2	C	480	THR
2	C	524	VAL
2	C	557	ARG
2	C	583	LEU
2	C	610	ARG
2	C	617	ASP
2	C	633	GLN
2	C	638	ASP
2	C	640	ARG
2	C	648	ARG
2	C	657	ASP
2	C	715	THR
2	C	774	LEU
2	C	775	ARG
2	C	808	ARG
2	C	813	VAL
2	C	848	VAL
2	C	939	ARG
2	C	978	ARG
2	C	1001	VAL
2	C	1043	TYR
2	C	1058	ASP
3	D	67	ARG
3	D	80	VAL
3	D	81	THR
3	D	191	LEU
3	D	198	ARG

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Mol	Chain	Res	Type
3	D	200	ASP
3	D	230	TRP
3	D	231	VAL
3	D	256	GLU
3	D	270	LEU
3	D	275	GLU
3	D	276	ASP
3	D	288	MET
3	D	312	ARG
3	D	362	GLU
3	D	411	THR
3	D	415	VAL
3	D	491	LYS
3	D	525	ARG
3	D	586	ARG
3	D	618	LEU
3	D	632	VAL
3	D	686	GLU
3	D	709	HIS
3	D	754	PHE
3	D	778	LEU
3	D	817	GLU
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	1041	LEU
3	D	1062	ARG
3	D	1128	VAL
3	D	1130	ARG
3	D	1162	GLU
3	D	1188	VAL
3	D	1195	GLN
3	D	1219	GLU
3	D	1277	ILE
3	D	1287	GLU
3	D	1290	LEU
3	D	1304	LYS
3	D	1305	LEU

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Mol	Chain	Res	Type
3	D	1317	ASP
3	D	1408	ILE
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	172	ARG
5	F	205	ARG
5	F	287	THR
5	F	318	GLU
5	F	364	ARG
5	F	377	ASP
5	F	420	ASP
5	F	422	LEU

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	128	HIS
1	A	212	ASN
2	C	575	GLN
2	C	834	GLN
2	C	860	HIS
3	D	569	ASN
3	D	724	GLN
3	D	1195	GLN
3	D	1333	HIS
3	D	1441	GLN
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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.01	0	100	100	69, 93, 116, 124	0
1	B	222/315 (70%)	0.09	1 (0%)	91	89	72, 104, 134, 151	0
2	C	1111/1119 (99%)	0.01	23 (2%)	63	61	57, 86, 156, 192	0
3	D	1486/1524 (97%)	0.22	79 (5%)	26	26	55, 89, 157, 186	1 (0%)
4	E	94/99 (94%)	0.02	2 (2%)	63	61	62, 92, 133, 142	0
5	F	336/443 (75%)	0.21	13 (3%)	39	38	67, 108, 165, 181	0
6	H	24/27 (88%)	0.63	4 (16%)	1	2	94, 158, 201, 220	0
7	G	10/19 (52%)	1.06	1 (10%)	7	9	149, 177, 201, 207	0
All	All	3509/3861 (90%)	0.13	123 (3%)	44	42	55, 93, 158, 220	1 (0%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1237	THR	8.0
3	D	322	VAL	5.8
5	F	149	GLU	5.6
3	D	1297	GLU	5.3
2	C	219	GLN	4.6
5	F	423	ASP	4.5
2	C	296	GLY	4.5
3	D	321	GLN	4.5
3	D	1305	LEU	4.2
5	F	422	LEU	4.1
6	H	23	DG	4.0
3	D	337	LEU	4.0
6	H	24	DC	4.0
3	D	380	GLU	3.9
2	C	207	LEU	3.7
3	D	203	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
3	D	1294	VAL	3.7
5	F	146	GLY	3.6
4	E	95	VAL	3.6
6	H	22	DT	3.6
3	D	268	ALA	3.6
3	D	230	TRP	3.5
3	D	223	LEU	3.5
3	D	219	GLU	3.5
3	D	314	PRO	3.5
3	D	248	PRO	3.5
3	D	426	LYS	3.5
3	D	242	LEU	3.4
3	D	339	TRP	3.3
3	D	257	GLY	3.3
2	C	365	ASP	3.3
3	D	1275	SER	3.3
3	D	236	TYR	3.3
3	D	311	LEU	3.2
3	D	263	GLU	3.2
3	D	1499	ARG	3.1
3	D	295	GLY	3.1
3	D	360	ARG	3.1
3	D	675	ARG	3.0
2	C	104	ASP	3.0
3	D	196	VAL	3.0
3	D	70	GLY	2.9
2	C	189	ARG	2.9
3	D	308	LYS	2.8
2	C	182	VAL	2.8
3	D	1491	THR	2.8
3	D	173	PRO	2.7
3	D	490	ALA	2.7
2	C	295	ASP	2.7
3	D	213	VAL	2.7
5	F	319	THR	2.7
3	D	178	LEU	2.7
3	D	211	VAL	2.7
3	D	974	ILE	2.7
2	C	781	LYS	2.7
3	D	335	LEU	2.7
3	D	323	GLU	2.6
2	C	176	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
5	F	382	THR	2.6
5	F	147	LEU	2.6
3	D	235	ALA	2.6
3	D	393	ILE	2.6
3	D	1495	ILE	2.6
5	F	373	LYS	2.6
3	D	304	LEU	2.6
3	D	284	LEU	2.6
5	F	390	PHE	2.6
3	D	668	PRO	2.5
3	D	305	ALA	2.5
3	D	229	ALA	2.5
2	C	64	LEU	2.5
2	C	226	VAL	2.5
3	D	666	ILE	2.5
7	G	6	DA	2.5
3	D	313	MET	2.4
2	C	221	LEU	2.4
2	C	250	ARG	2.4
3	D	343	LYS	2.3
3	D	1306	PRO	2.3
4	E	94	PRO	2.3
3	D	68	PHE	2.3
3	D	174	GLY	2.3
3	D	294	HIS	2.3
2	C	206	THR	2.3
2	C	191	PHE	2.3
2	C	362	GLY	2.3
5	F	369	LEU	2.3
3	D	350	HIS	2.3
3	D	269	PHE	2.3
2	C	777	ILE	2.2
2	C	247	PRO	2.2
6	H	14	DG	2.2
3	D	310	LEU	2.2
3	D	250	LEU	2.2
3	D	306	GLU	2.2
3	D	316	GLN	2.2
3	D	1299	PHE	2.2
3	D	243	ALA	2.2
3	D	258	VAL	2.2
3	D	353	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	312	ARG	2.2
3	D	1301	LYS	2.2
3	D	377	VAL	2.2
2	C	211	LEU	2.1
2	C	174	LEU	2.1
3	D	260	GLU	2.1
5	F	330	GLY	2.1
3	D	1253	THR	2.1
2	C	246	ASP	2.1
3	D	282	TYR	2.1
3	D	470	LEU	2.1
5	F	415	THR	2.1
3	D	197	SER	2.1
3	D	674	ARG	2.1
1	B	115	LEU	2.1
3	D	320	ALA	2.1
3	D	1312	LEU	2.1
3	D	1274	ILE	2.1
2	C	177	GLU	2.0
3	D	1319	VAL	2.0
3	D	191	LEU	2.0
3	D	1292	VAL	2.0
5	F	368	VAL	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 monosaccharides 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MG	B	2001	1/1	0.70	0.79	120,120,120,120	0
8	MG	D	2005	1/1	0.86	0.14	91,91,91,91	0
8	MG	F	2001	1/1	0.91	0.24	91,91,91,91	0
8	MG	D	2004	1/1	0.97	0.46	62,62,62,62	0
8	MG	D	2003	1/1	0.98	0.34	53,53,53,53	0
9	ZN	D	2001	1/1	0.99	0.20	60,60,60,60	0
9	ZN	D	2002	1/1	0.99	0.10	101,101,101,101	0

6.5 Other polymers (i)

There are no such residues in this entry.