



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 06:42 PM BST

PDB ID : 6UTX
Title : E. coli sigma-S transcription initiation complex with an empty bubble ("Old" crystal)
Authors : Zuo, Y.; De, S.; Steitz, T.A.
Deposited on : 2019-10-30
Resolution : 4.05 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)	:	2.13

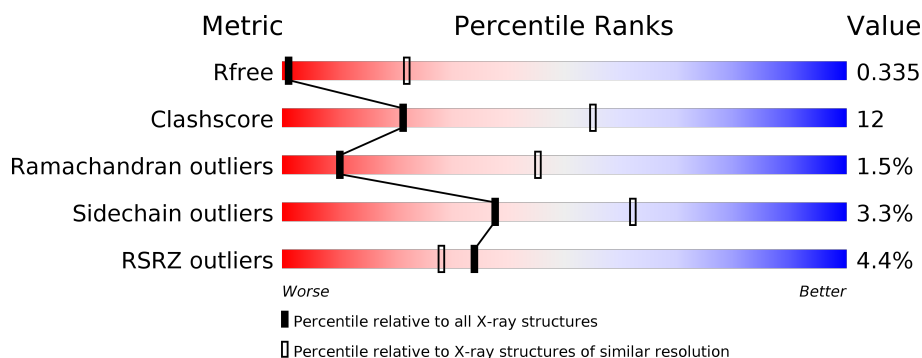
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.05 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	1127 (4.42-3.70)
Clashscore	141614	1033 (4.40-3.72)
Ramachandran outliers	138981	1145 (4.42-3.70)
Sidechain outliers	138945	1133 (4.42-3.70)
RSRZ outliers	127900	1005 (4.44-3.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	AAA	242	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>• 5%</div> </div> </div>
1	BBB	242	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>• 6%</div> </div> </div>
2	CCC	1342	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>•</div> </div> </div>
3	DDD	1407	<div> <div>7%</div> <div> <div></div> <div>71%</div> <div>22%</div> <div>• •</div> </div> </div>
4	EEE	90	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>12%</div> </div> </div>
5	FFF	336	<div> <div>5%</div> <div> <div></div> <div>62%</div> <div>19%</div> <div>• 18%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
6	111	50	
7	222	50	

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	ZN	DDD	1502	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28841 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	AAA	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	BBB	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-6	ALA	-	expression tag	UNP P0A7Z4
AAA	-5	HIS	-	expression tag	UNP P0A7Z4
AAA	-4	HIS	-	expression tag	UNP P0A7Z4
AAA	-3	HIS	-	expression tag	UNP P0A7Z4
AAA	-2	HIS	-	expression tag	UNP P0A7Z4
AAA	-1	HIS	-	expression tag	UNP P0A7Z4
AAA	0	HIS	-	expression tag	UNP P0A7Z4
BBB	-6	ALA	-	expression tag	UNP P0A7Z4
BBB	-5	HIS	-	expression tag	UNP P0A7Z4
BBB	-4	HIS	-	expression tag	UNP P0A7Z4
BBB	-3	HIS	-	expression tag	UNP P0A7Z4
BBB	-2	HIS	-	expression tag	UNP P0A7Z4
BBB	-1	HIS	-	expression tag	UNP P0A7Z4
BBB	0	HIS	-	expression tag	UNP P0A7Z4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CCC	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	DDD	1350	Total	C	N	O	S	0	0	0
			10478	6578	1867	1984	49			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	EEE	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	FFF	277	Total	C	N	O	S	0	0	0
			2253	1411	415	423	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FFF	2	GLY	SER	conflict	UNP P13445
FFF	33	GLU	GLN	conflict	UNP P13445
FFF	329	LEU	-	expression tag	UNP P13445
FFF	330	GLU	-	expression tag	UNP P13445
FFF	331	HIS	-	expression tag	UNP P13445
FFF	332	HIS	-	expression tag	UNP P13445
FFF	333	HIS	-	expression tag	UNP P13445
FFF	334	HIS	-	expression tag	UNP P13445
FFF	335	HIS	-	expression tag	UNP P13445
FFF	336	HIS	-	expression tag	UNP P13445

- Molecule 6 is a DNA chain called Synthetic DNA 50-MER (promoter non-template strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	111	32	Total	C	N	O	P	0	0	0
			661	314	121	194	32			

- Molecule 7 is a DNA chain called Synthetic DNA 50-MER (promoter template strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	222	34	Total	C	N	O	P	0	0	0
			695	332	127	203	33			

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	DDD	2	Total 2	Zn 2	0	0

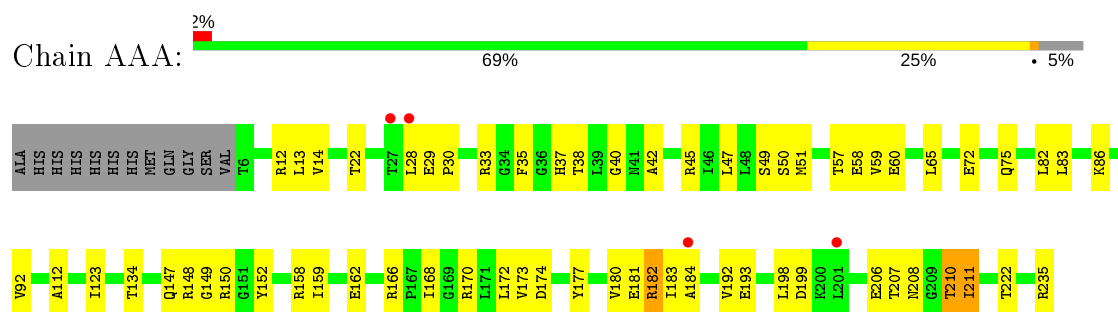
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	DDD	1	Total 1	Mg 1	0	0

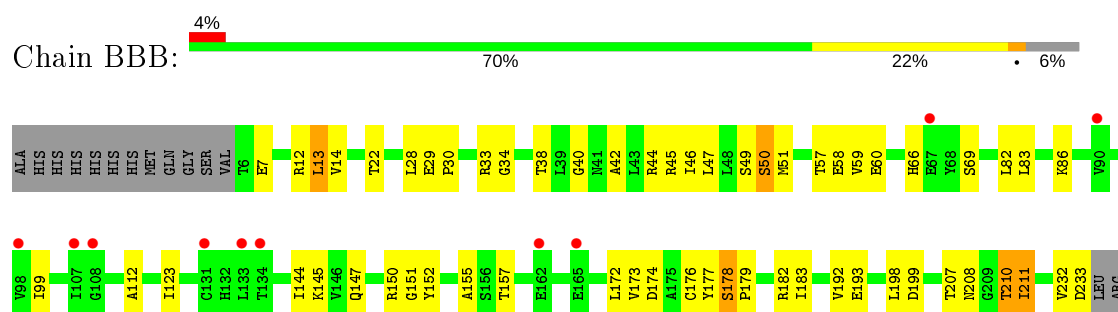
3 Residue-property plots [i](#)

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.

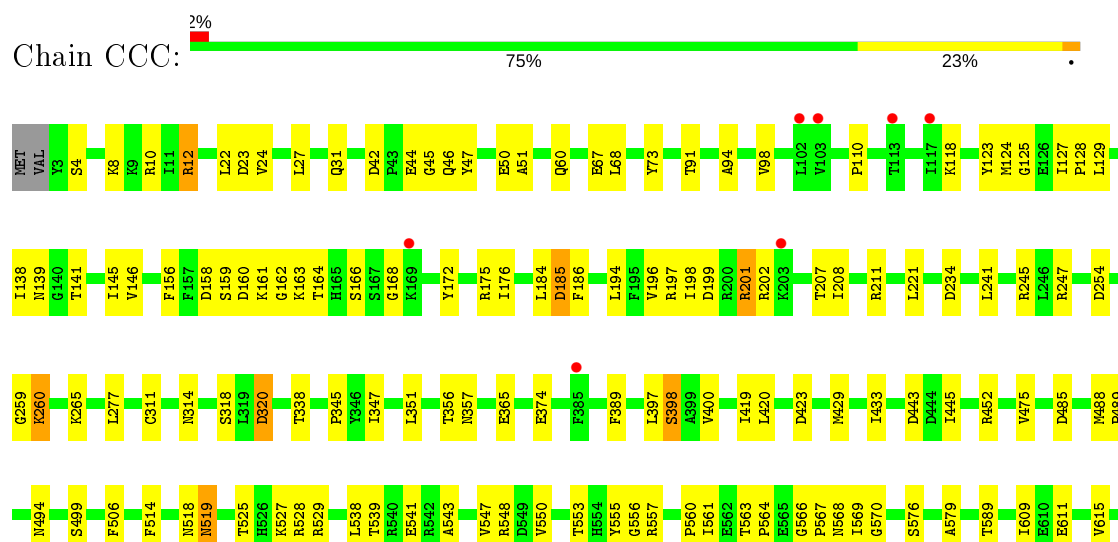
- Molecule 1: DNA-directed RNA polymerase subunit alpha

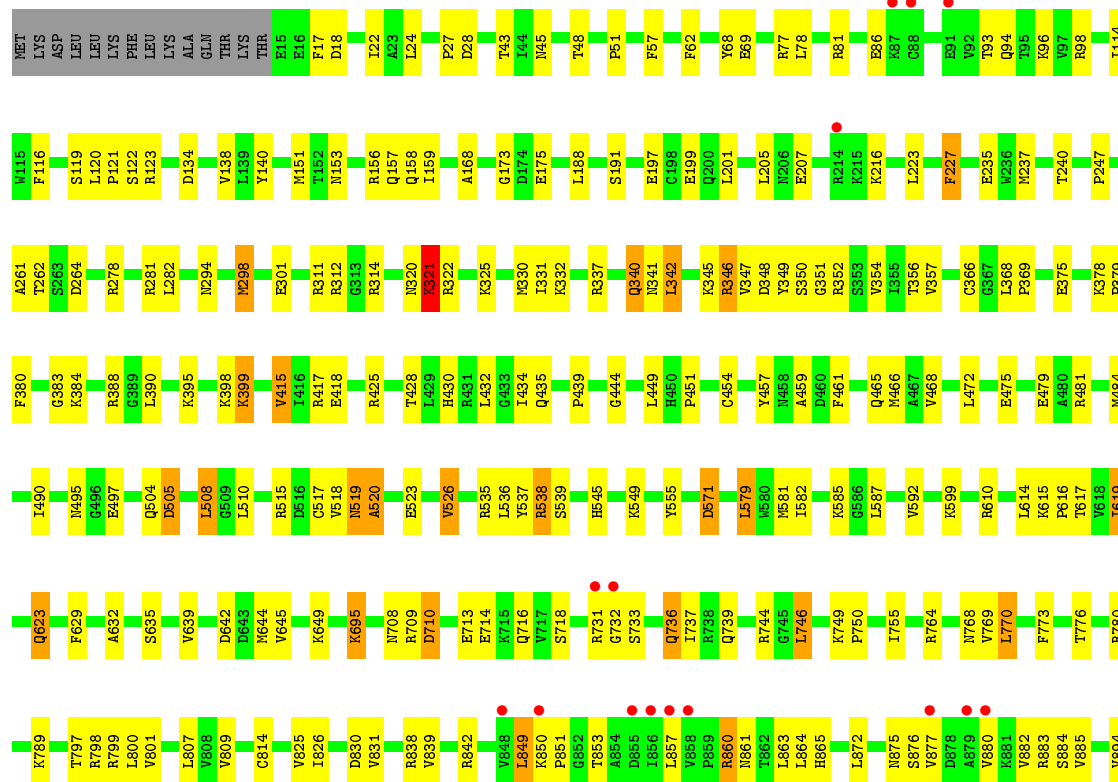


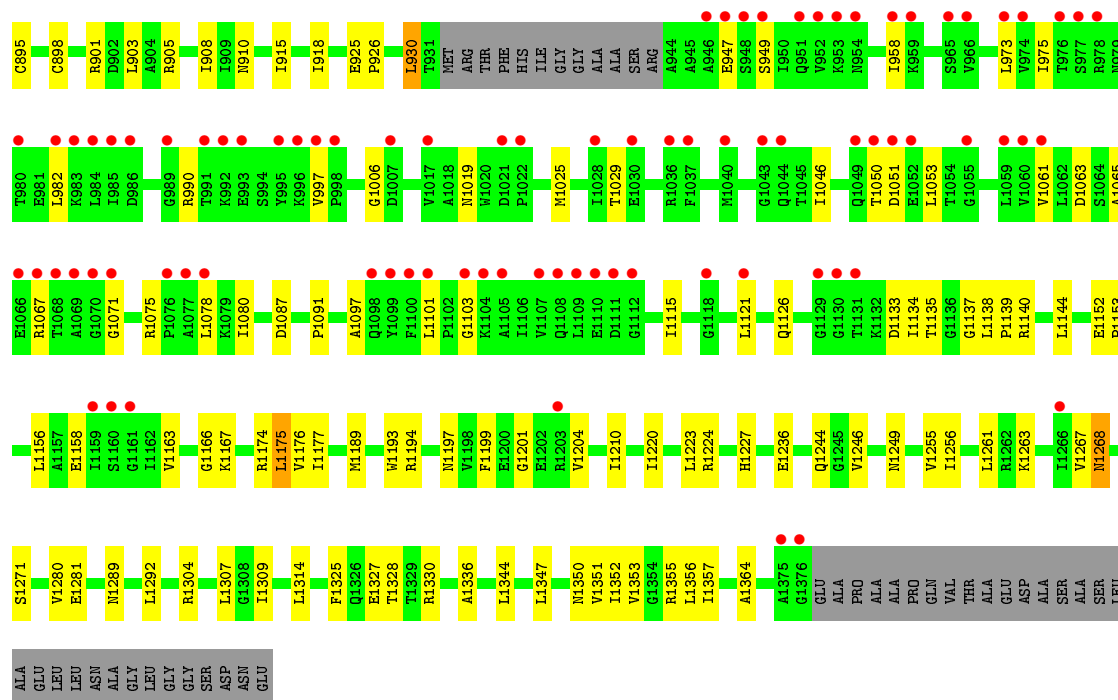
- Molecule 1: DNA-directed RNA polymerase subunit alpha



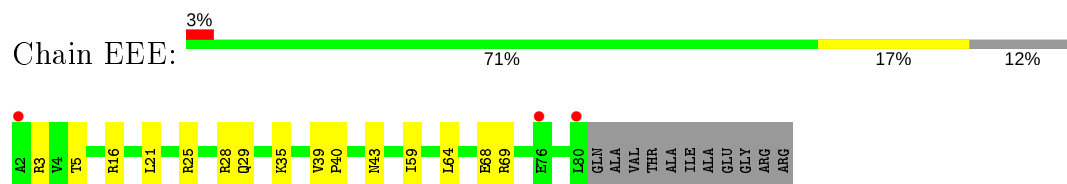
- Molecule 2: DNA-directed RNA polymerase subunit beta



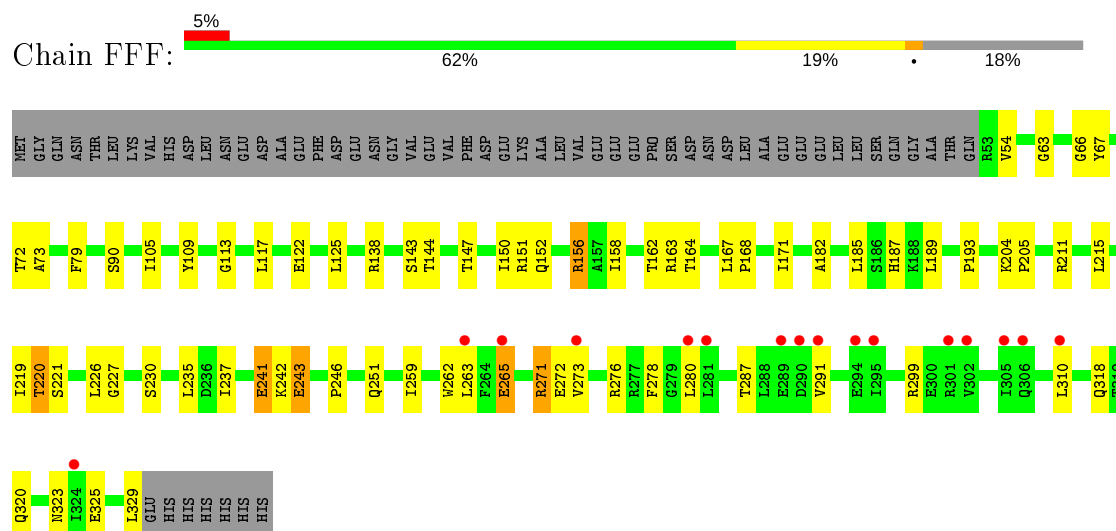




- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor RpoS

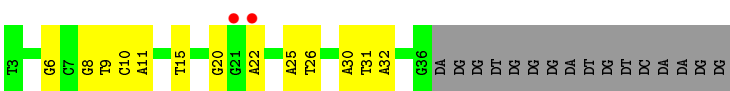


- Molecule 6: Synthetic DNA 50-MER (promoter non-template strand)





● Molecule 7: Synthetic DNA 50-MER (promoter template strand)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.07Å 153.30Å 230.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 4.05 48.89 – 4.05	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.90-4.05) 99.0 (48.89-4.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.279 , 0.349 0.274 , 0.335	Depositor DCC
R_{free} test set	1841 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	161.0	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 190.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28841	wwPDB-VP
Average B, all atoms (Å ²)	268.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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 [i](#)

5.1 Standard geometry [i](#)

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	AAA	0.64	0/1809	0.71	0/2450
1	BBB	0.64	0/1789	0.73	1/2425 (0.0%)
2	CCC	0.62	0/10739	0.74	0/14489
3	DDD	0.63	0/10636	0.74	0/14362
4	EEE	0.64	0/629	0.74	0/847
5	FFF	0.66	0/2282	0.65	0/3076
6	111	0.27	0/741	0.66	0/1143
7	222	0.30	0/779	0.63	0/1201
All	All	0.62	0/29404	0.73	1/39993 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	178	SER	N-CA-CB	6.02	119.53	110.50

There are no chirality outliers.

There are no planarity outliers.

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	AAA	1787	0	1813	70	0
1	BBB	1767	0	1789	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CCC	10570	0	10582	290	0
3	DDD	10478	0	10691	310	0
4	EEE	627	0	634	10	0
5	FFF	2253	0	2298	75	1
6	111	661	0	362	25	0
7	222	695	0	385	24	0
8	DDD	2	0	0	2	0
9	DDD	1	0	0	0	0
All	All	28841	0	28554	687	1

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 12.

All (687) 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)
3:DDD:898:CYS:SG	8:DDD:1502:ZN:ZN	1.16	1.32
2:CCC:894:GLN:NE2	3:DDD:69:GLU:OE2	1.85	1.08
2:CCC:563:THR:OG1	2:CCC:569:ILE:O	1.74	1.05
2:CCC:560:PRO:O	3:DDD:780:ARG:NH2	1.90	1.04
3:DDD:898:CYS:HG	8:DDD:1502:ZN:ZN	0.70	0.99
1:BBB:176:CYS:SG	3:DDD:535:ARG:NH2	2.35	0.99
5:FFF:273:VAL:HG13	5:FFF:291:VAL:HG11	1.45	0.97
2:CCC:891:GLY:O	2:CCC:892:GLU:C	2.04	0.95
1:AAA:72:GLU:OE2	2:CCC:726:TYR:OH	1.84	0.93
1:AAA:158:ARG:HB3	1:AAA:172:LEU:HD21	1.50	0.93
2:CCC:901:LEU:HD13	5:FFF:278:PHE:CE2	2.05	0.91
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:HD11	1.50	0.91
1:AAA:184:ALA:HB2	2:CCC:1091:GLY:HA3	1.53	0.91
2:CCC:550:VAL:HG21	3:DDD:776:THR:HG22	1.54	0.90
1:BBB:50:SER:O	1:BBB:150:ARG:HD2	1.71	0.89
5:FFF:241:GLU:HG3	5:FFF:242:LYS:H	1.36	0.89
2:CCC:890:LYS:HE3	2:CCC:893:THR:HG21	1.55	0.87
2:CCC:1284:ALA:HA	3:DDD:1357:ILE:HD12	1.57	0.87
3:DDD:615:LYS:HB2	3:DDD:616:PRO:HD3	1.59	0.85
5:FFF:241:GLU:HG3	5:FFF:242:LYS:N	1.91	0.85
2:CCC:550:VAL:HG21	3:DDD:776:THR:CG2	2.08	0.84
2:CCC:1281:TYR:OH	3:DDD:434:ILE:O	1.95	0.82
2:CCC:221:LEU:HD11	2:CCC:314:ASN:HB2	1.60	0.82
1:BBB:82:LEU:HD22	1:BBB:173:VAL:HG22	1.62	0.82
1:AAA:45:ARG:NE	1:BBB:38:THR:OG1	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:906:PHE:HZ	5:FFF:323:ASN:HA	1.46	0.80
2:CCC:1308:ILE:HG23	3:DDD:380:PHE:CE1	2.16	0.80
2:CCC:1342:GLU:HA	3:DDD:18:ASP:HB2	1.62	0.79
5:FFF:235:LEU:O	5:FFF:235:LEU:HD12	1.84	0.78
3:DDD:342:LEU:HD21	3:DDD:1352:ILE:HG23	1.66	0.78
3:DDD:481:ARG:NH1	4:EEE:3:ARG:O	2.17	0.77
3:DDD:850:LYS:HB2	3:DDD:851:PRO:HD2	1.66	0.77
3:DDD:1075:ARG:NH2	3:DDD:1193:TRP:CE3	2.53	0.76
1:BBB:82:LEU:HD22	1:BBB:173:VAL:CG2	2.15	0.75
1:AAA:152:TYR:OH	1:AAA:174:ASP:OD2	2.04	0.75
1:AAA:82:LEU:HD22	1:AAA:173:VAL:CG2	2.17	0.75
2:CCC:560:PRO:CB	3:DDD:776:THR:HG21	2.18	0.73
2:CCC:932:GLN:HE22	2:CCC:952:GLN:NE2	1.87	0.73
3:DDD:378:LYS:H	3:DDD:379:PRO:HD2	1.54	0.73
3:DDD:301:GLU:HG3	3:DDD:312:ARG:HH22	1.51	0.73
3:DDD:301:GLU:HG3	3:DDD:312:ARG:NH2	2.03	0.73
2:CCC:1222:GLU:OE2	3:DDD:537:TYR:HE1	1.71	0.73
2:CCC:1242:LYS:HD2	3:DDD:465:GLN:NE2	2.03	0.73
1:AAA:222:THR:OG1	1:BBB:233:ASP:HB3	1.89	0.73
3:DDD:857:LEU:CD2	3:DDD:875:ASN:HD22	2.02	0.72
1:AAA:92:VAL:O	1:AAA:148:ARG:NH2	2.22	0.72
3:DDD:134:ASP:HB3	3:DDD:159:ILE:HD11	1.69	0.72
3:DDD:849:LEU:HD11	3:DDD:853:THR:HA	1.72	0.72
5:FFF:242:LYS:HG3	5:FFF:243:GLU:H	1.54	0.72
3:DDD:1140:ARG:NH1	3:DDD:1144:LEU:HD11	2.05	0.71
3:DDD:378:LYS:N	3:DDD:379:PRO:HD2	2.05	0.71
1:AAA:159:ILE:HD11	2:CCC:876:GLU:OE1	1.90	0.71
1:AAA:158:ARG:HD2	1:AAA:172:LEU:HD11	1.73	0.71
2:CCC:397:LEU:O	2:CCC:398:SER:OG	2.08	0.71
5:FFF:259:ILE:CG2	5:FFF:280:LEU:HD21	2.20	0.71
3:DDD:857:LEU:HD22	3:DDD:875:ASN:HD22	1.55	0.70
2:CCC:139:ASN:ND2	7:222:22:DA:OP2	2.24	0.70
3:DDD:518:VAL:HG23	3:DDD:716:GLN:NE2	2.06	0.70
4:EEE:25:ARG:NH2	4:EEE:68:GLU:OE1	2.23	0.70
2:CCC:906:PHE:CZ	5:FFF:323:ASN:HA	2.26	0.70
3:DDD:857:LEU:HD22	3:DDD:875:ASN:ND2	2.07	0.70
2:CCC:560:PRO:HB2	3:DDD:776:THR:HG21	1.72	0.70
2:CCC:1242:LYS:HD2	3:DDD:465:GLN:HE22	1.56	0.69
1:AAA:57:THR:HG23	1:AAA:158:ARG:CZ	2.22	0.69
3:DDD:849:LEU:HA	3:DDD:857:LEU:HB3	1.73	0.69
1:AAA:235:ARG:HB2	1:BBB:13:LEU:HD23	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1103:VAL:HB	2:CCC:1104:PRO:HD3	1.75	0.68
2:CCC:118:LYS:NZ	2:CCC:485:ASP:O	2.27	0.68
3:DDD:809:VAL:CG2	3:DDD:915:ILE:HD11	2.24	0.68
2:CCC:1029:LEU:HG	2:CCC:1033:ARG:HD3	1.76	0.68
1:AAA:184:ALA:CB	2:CCC:1091:GLY:HA3	2.22	0.68
2:CCC:891:GLY:O	2:CCC:893:THR:N	2.26	0.68
2:CCC:1101:LEU:HD12	3:DDD:504:GLN:HG3	1.75	0.68
5:FFF:259:ILE:HG21	5:FFF:280:LEU:HD21	1.76	0.68
3:DDD:614:LEU:O	3:DDD:617:THR:OG1	2.10	0.67
2:CCC:259:GLY:O	2:CCC:260:LYS:HB2	1.94	0.67
2:CCC:168:GLY:O	3:DDD:1065:ALA:HB1	1.95	0.67
3:DDD:905:ARG:NH1	3:DDD:910:ASN:OD1	2.27	0.67
2:CCC:46:GLN:HB2	2:CCC:51:ALA:HA	1.75	0.66
3:DDD:504:GLN:HE22	3:DDD:731:ARG:NH2	1.92	0.66
3:DDD:863:LEU:HD22	3:DDD:908:ILE:HG13	1.78	0.66
1:AAA:158:ARG:HD2	1:AAA:172:LEU:HD21	1.78	0.66
2:CCC:1234:LYS:HE2	2:CCC:1238:LEU:HD21	1.78	0.66
3:DDD:839:VAL:HG12	3:DDD:839:VAL:O	1.96	0.66
3:DDD:850:LYS:HB2	3:DDD:851:PRO:CD	2.26	0.65
2:CCC:547:VAL:HG22	6:111:49:DG:N1	2.11	0.65
3:DDD:515:ARG:HH22	3:DDD:718:SER:C	1.99	0.65
2:CCC:932:GLN:HE22	2:CCC:952:GLN:HE22	1.44	0.65
3:DDD:140:TYR:OH	3:DDD:312:ARG:HD2	1.96	0.65
5:FFF:242:LYS:HG3	5:FFF:243:GLU:N	2.11	0.65
2:CCC:168:GLY:O	3:DDD:1065:ALA:CB	2.44	0.65
1:AAA:222:THR:OG1	1:BBB:233:ASP:CB	2.45	0.65
3:DDD:1140:ARG:HH12	3:DDD:1144:LEU:HD11	1.61	0.65
2:CCC:528:ARG:NH2	2:CCC:576:SER:O	2.30	0.65
5:FFF:105:ILE:O	5:FFF:109:TYR:HD2	1.80	0.65
3:DDD:789:LYS:HG3	3:DDD:1135:THR:HG23	1.79	0.64
2:CCC:12:ARG:HG3	2:CCC:1181:PRO:HB2	1.80	0.64
1:AAA:29:GLU:HB2	1:AAA:30:PRO:HA	1.80	0.64
2:CCC:576:SER:OG	2:CCC:659:GLN:O	2.16	0.63
2:CCC:1042:LEU:HD13	2:CCC:1046:VAL:HG12	1.80	0.63
2:CCC:1145:ILE:HG22	2:CCC:1161:LEU:HD11	1.81	0.63
2:CCC:992:LEU:HB3	2:CCC:993:PRO:HD2	1.81	0.63
3:DDD:1166:GLY:HA3	3:DDD:1176:VAL:HG23	1.80	0.63
1:BBB:29:GLU:HB2	1:BBB:30:PRO:HA	1.80	0.63
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:CD1	2.25	0.63
2:CCC:186:PHE:CD1	2:CCC:196:VAL:HG22	2.34	0.63
3:DDD:1133:ASP:O	3:DDD:1244:GLN:NE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:378:LYS:N	3:DDD:379:PRO:CD	2.62	0.63
5:FFF:156:ARG:NH2	6:111:34:DG:O6	2.32	0.62
3:DDD:332:LYS:HA	3:DDD:1328:THR:HG21	1.80	0.62
1:BBB:157:THR:O	1:BBB:157:THR:HG22	1.99	0.62
2:CCC:1318:GLY:O	2:CCC:1319:MET:HB2	1.99	0.62
3:DDD:1330:ARG:HH22	7:222:10:DC:H4'	1.64	0.62
2:CCC:804:PHE:O	2:CCC:1225:VAL:HG13	1.99	0.62
2:CCC:700:VAL:HG21	2:CCC:1114:GLU:HG3	1.82	0.62
1:BBB:44:ARG:HH12	3:DDD:538:ARG:HG2	1.65	0.62
1:AAA:181:GLU:O	2:CCC:821:ARG:NH2	2.33	0.62
2:CCC:821:ARG:HH11	2:CCC:1082:ILE:HD13	1.64	0.62
2:CCC:901:LEU:HD13	5:FFF:278:PHE:CD2	2.34	0.62
2:CCC:901:LEU:HD11	5:FFF:310:LEU:HD21	1.82	0.62
2:CCC:514:PHE:CZ	7:222:20:DG:C4'	2.83	0.61
2:CCC:1123:GLY:HA3	2:CCC:1204:LEU:HD11	1.82	0.61
2:CCC:514:PHE:CZ	7:222:20:DG:H4'	2.36	0.61
2:CCC:525:THR:HG21	2:CCC:687:ARG:CD	2.29	0.61
2:CCC:672:GLU:HG3	2:CCC:673:HIS:CD2	2.34	0.61
6:111:30:DG:H2'	6:111:31:DT:H71	1.82	0.61
5:FFF:220:THR:HG23	7:222:22:DA:N1	2.16	0.61
2:CCC:890:LYS:HE3	2:CCC:893:THR:CG2	2.28	0.60
5:FFF:227:GLY:N	7:222:20:DG:N2	2.49	0.60
2:CCC:1222:GLU:OE2	3:DDD:537:TYR:CE1	2.54	0.60
2:CCC:400:VAL:HG11	2:CCC:452:ARG:HD3	1.84	0.60
3:DDD:24:LEU:HD21	3:DDD:116:PHE:CZ	2.36	0.60
3:DDD:22:ILE:HG22	3:DDD:1336:ALA:HA	1.84	0.60
2:CCC:1294:LYS:HD3	3:DDD:347:VAL:HG13	1.82	0.60
3:DDD:644:MET:HB2	3:DDD:764:ARG:HD2	1.83	0.60
5:FFF:220:THR:CG2	7:222:22:DA:N1	2.65	0.59
2:CCC:548:ARG:HB3	2:CCC:570:GLY:HA3	1.85	0.59
2:CCC:514:PHE:CE1	7:222:20:DG:H4'	2.37	0.59
3:DDD:1314:LEU:HD11	3:DDD:1327:GLU:HG3	1.83	0.59
3:DDD:1063:ASP:HB3	3:DDD:1103:GLY:HA3	1.85	0.59
2:CCC:207:THR:HG21	2:CCC:351:LEU:HG	1.85	0.59
3:DDD:122:SER:O	3:DDD:123:ARG:HB2	2.02	0.58
1:AAA:38:THR:HG21	1:BBB:46:ILE:HD11	1.85	0.58
3:DDD:1263:LYS:HB2	3:DDD:1307:LEU:HD11	1.85	0.58
3:DDD:949:SER:HB3	3:DDD:1019:ASN:HD22	1.68	0.58
2:CCC:241:LEU:HD23	2:CCC:277:LEU:HD21	1.84	0.58
3:DDD:1140:ARG:HH12	3:DDD:1236:GLU:HG3	1.68	0.58
5:FFF:143:SER:HB3	6:111:41:DT:H73	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:82:LEU:HD22	1:AAA:173:VAL:HG21	1.85	0.58
3:DDD:1267:VAL:O	3:DDD:1268:ASN:CB	2.52	0.58
3:DDD:517:CYS:HB3	3:DDD:545:HIS:HB2	1.86	0.57
3:DDD:876:SER:HB3	3:DDD:990:ARG:NH1	2.19	0.57
1:AAA:45:ARG:NH2	1:BBB:34:GLY:O	2.34	0.57
2:CCC:758:ARG:HD3	2:CCC:835:GLU:HB2	1.86	0.57
3:DDD:1075:ARG:CZ	3:DDD:1193:TRP:HB3	2.34	0.57
3:DDD:399:LYS:NZ	5:FFF:329:LEU:HD21	2.19	0.57
3:DDD:842:ARG:HD3	3:DDD:882:VAL:HG21	1.86	0.57
2:CCC:564:PRO:HG2	2:CCC:568:ASN:O	2.04	0.57
3:DDD:351:GLY:O	3:DDD:468:VAL:N	2.23	0.57
3:DDD:518:VAL:N	3:DDD:716:GLN:HE22	2.00	0.57
2:CCC:635:THR:HG22	2:CCC:644:LEU:HD23	1.85	0.57
2:CCC:1301:ARG:HG3	2:CCC:1302:THR:N	2.20	0.57
2:CCC:160:ASP:O	2:CCC:162:GLY:N	2.34	0.57
2:CCC:185:ASP:HB2	2:CCC:197:ARG:HG3	1.87	0.57
3:DDD:1080:ILE:HB	3:DDD:1097:ALA:HB3	1.85	0.57
2:CCC:1120:ALA:HA	2:CCC:1204:LEU:HD12	1.86	0.57
2:CCC:797:GLY:HA3	2:CCC:1233:LEU:HD23	1.85	0.57
3:DDD:1167:LYS:HB2	3:DDD:1174:ARG:HD2	1.87	0.57
1:BBB:152:TYR:CE2	3:DDD:536:LEU:HD21	2.40	0.57
3:DDD:518:VAL:O	3:DDD:519:ASN:C	2.42	0.57
2:CCC:905:ILE:CG1	5:FFF:310:LEU:HD22	2.33	0.57
2:CCC:1291:LEU:HD11	3:DDD:1351:VAL:HG13	1.88	0.56
2:CCC:914:LYS:HD3	2:CCC:915:ASP:H	1.70	0.56
2:CCC:538:LEU:HD22	6:111:49:DG:N7	2.20	0.56
3:DDD:173:GLY:O	3:DDD:175:GLU:N	2.35	0.56
3:DDD:849:LEU:CD1	3:DDD:853:THR:HA	2.36	0.56
2:CCC:1269:ARG:HA	3:DDD:346:ARG:HA	1.87	0.56
2:CCC:68:LEU:HD12	2:CCC:475:VAL:HG13	1.88	0.56
2:CCC:1308:ILE:CG2	3:DDD:380:PHE:CE1	2.88	0.56
2:CCC:27:LEU:O	2:CCC:528:ARG:NH1	2.38	0.56
2:CCC:68:LEU:HD12	2:CCC:475:VAL:CG1	2.36	0.56
2:CCC:1290:MET:HG2	2:CCC:1294:LYS:HD2	1.86	0.56
2:CCC:905:ILE:HG12	5:FFF:310:LEU:HD22	1.86	0.56
2:CCC:374:GLU:OE1	6:111:44:DG:N2	2.29	0.56
2:CCC:638:SER:O	2:CCC:641:GLU:N	2.39	0.56
3:DDD:1267:VAL:O	3:DDD:1268:ASN:HB2	2.04	0.56
2:CCC:1302:THR:HG22	5:FFF:246:PRO:HA	1.88	0.56
3:DDD:134:ASP:CB	3:DDD:159:ILE:HD11	2.36	0.56
1:AAA:82:LEU:HD22	1:AAA:173:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:198:ILE:O	2:CCC:201:ARG:HG3	2.06	0.55
5:FFF:72:THR:HG22	5:FFF:73:ALA:H	1.71	0.55
2:CCC:525:THR:HG21	2:CCC:687:ARG:HD3	1.88	0.55
3:DDD:865:HIS:ND1	3:DDD:901:ARG:NH2	2.54	0.55
1:AAA:210:THR:HG22	1:AAA:211:ILE:N	2.22	0.55
3:DDD:508:LEU:HD12	3:DDD:508:LEU:O	2.07	0.55
3:DDD:1158:GLU:HA	3:DDD:1223:LEU:HD22	1.89	0.55
2:CCC:812:PHE:HB3	3:DDD:357:VAL:HG11	1.89	0.55
3:DDD:555:TYR:CE2	3:DDD:585:LYS:HD2	2.40	0.55
2:CCC:1296:ASP:O	2:CCC:1297:ASP:C	2.45	0.55
3:DDD:1261:LEU:HB3	3:DDD:1304:ARG:HD3	1.88	0.55
1:AAA:150:ARG:HH12	1:BBB:7:GLU:HB2	1.70	0.55
1:AAA:159:ILE:HG23	1:AAA:159:ILE:O	2.06	0.55
1:BBB:50:SER:O	1:BBB:150:ARG:HB2	2.06	0.55
2:CCC:560:PRO:HB2	3:DDD:776:THR:CG2	2.35	0.55
3:DDD:399:LYS:HZ1	5:FFF:329:LEU:HD21	1.70	0.55
3:DDD:807:LEU:HD22	3:DDD:1255:VAL:HG13	1.89	0.54
3:DDD:378:LYS:H	3:DDD:379:PRO:CD	2.20	0.54
3:DDD:62:PHE:CD1	3:DDD:247:PRO:HD3	2.42	0.54
3:DDD:262:THR:O	5:FFF:221:SER:HA	2.06	0.54
2:CCC:576:SER:HB3	2:CCC:579:ALA:HB2	1.90	0.54
6:111:32:DA:C2	7:222:32:DA:C6	2.95	0.54
1:AAA:75:GLN:NE2	2:CCC:772:SER:HA	2.23	0.54
2:CCC:1184:THR:HG23	2:CCC:1189:GLY:HA3	1.90	0.54
2:CCC:1268:GLN:NE2	3:DDD:352:ARG:HG2	2.22	0.54
1:BBB:83:LEU:HD11	3:DDD:526:VAL:O	2.07	0.54
2:CCC:894:GLN:HB3	3:DDD:77:ARG:HH21	1.71	0.54
1:BBB:83:LEU:HD21	3:DDD:526:VAL:CG2	2.38	0.54
2:CCC:547:VAL:HG22	6:111:49:DG:C6	2.43	0.54
3:DDD:800:LEU:HD22	3:DDD:1256:ILE:HG12	1.88	0.54
1:AAA:22:THR:OG1	1:AAA:207:THR:O	2.23	0.54
1:BBB:210:THR:HG22	1:BBB:211:ILE:N	2.23	0.54
2:CCC:1119:MET:HB2	2:CCC:1228:GLY:HA2	1.90	0.54
2:CCC:709:ALA:HB3	2:CCC:792:GLY:O	2.07	0.54
6:111:30:DG:C2'	6:111:31:DT:H71	2.37	0.53
3:DDD:857:LEU:CD2	3:DDD:875:ASN:ND2	2.68	0.53
2:CCC:967:LEU:HD21	2:CCC:1021:LEU:HD22	1.90	0.53
2:CCC:882:ILE:HG12	2:CCC:919:ARG:HB3	1.90	0.53
3:DDD:709:ARG:O	3:DDD:710:ASP:CB	2.56	0.53
1:AAA:158:ARG:CD	1:AAA:172:LEU:HD11	2.37	0.53
1:BBB:49:SER:O	1:BBB:151:GLY:CA	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:211:ARG:NH1	2:CCC:357:ASN:O	2.41	0.53
2:CCC:807:TRP:CD1	2:CCC:817:LEU:CD2	2.92	0.53
2:CCC:1077:SER:HA	3:DDD:356:THR:OG1	2.09	0.53
3:DDD:895:CYS:SG	3:DDD:898:CYS:SG	3.04	0.53
3:DDD:93:THR:HG22	3:DDD:94:GLN:H	1.73	0.53
3:DDD:451:PRO:HA	3:DDD:454:CYS:SG	2.49	0.53
2:CCC:1247:SER:O	3:DDD:348:ASP:HB3	2.08	0.53
3:DDD:930:LEU:HD12	3:DDD:1134:ILE:HD11	1.91	0.53
3:DDD:510:LEU:CD2	3:DDD:579:LEU:HD21	2.39	0.53
3:DDD:930:LEU:HD11	3:DDD:1246:VAL:CG2	2.39	0.53
2:CCC:1314:GLN:HA	4:EEE:28:ARG:NH2	2.24	0.53
5:FFF:72:THR:HG22	5:FFF:73:ALA:N	2.24	0.53
2:CCC:1212:LEU:HD21	2:CCC:1227:VAL:HG21	1.91	0.53
2:CCC:1063:GLY:O	3:DDD:354:VAL:HG11	2.09	0.53
2:CCC:1247:SER:HB3	3:DDD:375:GLU:O	2.08	0.53
5:FFF:152:GLN:HE21	5:FFF:156:ARG:HH11	1.57	0.53
6:111:32:DA:N3	7:222:32:DA:C2	2.76	0.52
1:AAA:199:ASP:OD1	1:AAA:199:ASP:N	2.43	0.52
2:CCC:494:ASN:ND2	7:222:25:DA:OP1	2.42	0.52
2:CCC:1210:ILE:HD12	2:CCC:1227:VAL:HB	1.90	0.52
1:AAA:83:LEU:HD12	2:CCC:694:ARG:NH2	2.24	0.52
1:AAA:134:THR:HA	2:CCC:773:LEU:HD22	1.91	0.52
3:DDD:157:GLN:HG2	3:DDD:188:LEU:HD21	1.90	0.52
3:DDD:582:ILE:HG23	3:DDD:623:GLN:CB	2.40	0.52
2:CCC:668:ILE:HD11	2:CCC:683:ALA:HB2	1.91	0.52
3:DDD:1197:ASN:N	3:DDD:1210:ILE:O	2.42	0.52
2:CCC:1313:HIS:CE1	3:DDD:380:PHE:HE1	2.28	0.52
2:CCC:519:ASN:HD21	2:CCC:796:LEU:HD22	1.75	0.52
2:CCC:890:LYS:CE	2:CCC:893:THR:HG21	2.35	0.52
5:FFF:182:ALA:HA	5:FFF:193:PRO:HG3	1.91	0.52
4:EEE:29:GLN:HB3	4:EEE:35:LYS:HG3	1.92	0.52
3:DDD:799:ARG:HB3	3:DDD:1309:ILE:HG21	1.92	0.52
1:AAA:37:HIS:HB2	1:BBB:45:ARG:NH2	2.24	0.52
2:CCC:4:SER:O	2:CCC:8:LYS:HG3	2.10	0.52
2:CCC:1196:LYS:NZ	3:DDD:642:ASP:OD1	2.37	0.52
5:FFF:263:LEU:HD22	5:FFF:271:ARG:HB2	1.91	0.52
1:BBB:199:ASP:N	1:BBB:199:ASP:OD1	2.43	0.52
2:CCC:821:ARG:NH1	2:CCC:1082:ILE:HD13	2.25	0.52
1:AAA:65:LEU:HB3	2:CCC:874:GLY:HA3	1.91	0.52
3:DDD:809:VAL:HG22	3:DDD:915:ILE:HD11	1.91	0.52
5:FFF:227:GLY:H	7:222:20:DG:N2	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:120:LEU:HA	3:DDD:121:PRO:C	2.31	0.51
3:DDD:322:ARG:NH2	5:FFF:221:SER:HB3	2.25	0.51
3:DDD:807:LEU:HD11	3:DDD:894:VAL:HG13	1.92	0.51
2:CCC:807:TRP:CD1	2:CCC:817:LEU:HD22	2.45	0.51
3:DDD:156:ARG:HH22	3:DDD:191:SER:HB2	1.75	0.51
3:DDD:57:PHE:O	3:DDD:98:ARG:NH2	2.43	0.51
3:DDD:839:VAL:HG13	3:DDD:882:VAL:CG1	2.41	0.51
2:CCC:539:THR:O	2:CCC:543:ALA:N	2.43	0.51
2:CCC:94:ALA:HB2	2:CCC:129:LEU:HD11	1.93	0.51
3:DDD:1347:LEU:HD22	3:DDD:1357:ILE:HG23	1.91	0.51
2:CCC:156:PHE:CZ	2:CCC:445:ILE:HG13	2.45	0.51
3:DDD:1075:ARG:HD2	3:DDD:1193:TRP:HB3	1.92	0.51
5:FFF:144:THR:HA	6:111:40:DA:N7	2.26	0.51
2:CCC:389:PHE:O	2:CCC:419:ILE:HG23	2.11	0.51
2:CCC:1284:ALA:CA	3:DDD:1357:ILE:HD12	2.37	0.51
6:111:30:DG:C8	6:111:31:DT:C7	2.94	0.51
1:AAA:83:LEU:HD12	2:CCC:694:ARG:HH21	1.74	0.51
2:CCC:878:THR:HG22	2:CCC:879:GLY:N	2.25	0.51
3:DDD:915:ILE:O	3:DDD:918:ILE:N	2.44	0.51
1:AAA:181:GLU:HB3	1:AAA:206:GLU:O	2.11	0.51
1:BBB:86:LYS:HE2	1:BBB:174:ASP:HB2	1.93	0.51
3:DDD:235:GLU:OE2	3:DDD:235:GLU:N	2.39	0.51
3:DDD:357:VAL:HG12	3:DDD:461:PHE:CE2	2.46	0.51
2:CCC:1101:LEU:CD1	3:DDD:504:GLN:HG3	2.40	0.51
3:DDD:395:LYS:HG3	5:FFF:251:GLN:NE2	2.26	0.51
3:DDD:582:ILE:HG23	3:DDD:623:GLN:HB2	1.92	0.50
3:DDD:619:ILE:O	3:DDD:623:GLN:HG2	2.10	0.50
3:DDD:826:ILE:HG12	3:DDD:831:VAL:HG13	1.92	0.50
2:CCC:1257:GLN:HB3	2:CCC:1296:ASP:OD1	2.11	0.50
2:CCC:1268:GLN:HE22	3:DDD:352:ARG:HG2	1.77	0.50
2:CCC:73:TYR:HB2	2:CCC:98:VAL:HG22	1.93	0.50
1:AAA:35:PHE:HZ	1:BBB:50:SER:CB	2.23	0.50
2:CCC:44:GLU:O	2:CCC:46:GLN:N	2.44	0.50
2:CCC:728:ASP:OD1	2:CCC:729:ALA:N	2.44	0.50
3:DDD:264:ASP:OD1	5:FFF:221:SER:OG	2.24	0.50
5:FFF:66:GLY:HA3	6:111:42:DG:C6	2.47	0.50
1:AAA:57:THR:HG22	1:AAA:58:GLU:HG3	1.94	0.50
1:AAA:75:GLN:HG2	2:CCC:727:VAL:HG11	1.94	0.50
5:FFF:262:TRP:HE1	5:FFF:320:GLN:HE22	1.57	0.50
3:DDD:347:VAL:O	3:DDD:350:SER:OG	2.15	0.50
3:DDD:615:LYS:HB2	3:DDD:616:PRO:CD	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:635:THR:CG2	2:CCC:644:LEU:HD23	2.42	0.50
3:DDD:321:LYS:O	3:DDD:321:LYS:HD2	2.11	0.50
1:AAA:192:VAL:CG2	1:AAA:198:LEU:HD12	2.41	0.50
2:CCC:1253:LEU:HB3	5:FFF:235:LEU:HD13	1.94	0.50
2:CCC:555:TYR:OH	2:CCC:654:ASP:OD1	2.22	0.50
5:FFF:226:LEU:HB3	7:222:20:DG:H1	1.77	0.49
1:AAA:49:SER:HB3	2:CCC:1083:GLU:OE2	2.12	0.49
2:CCC:842:ASP:N	2:CCC:1045:GLY:O	2.45	0.49
2:CCC:984:VAL:O	2:CCC:984:VAL:HG13	2.11	0.49
3:DDD:119:SER:HA	3:DDD:311:ARG:HH21	1.75	0.49
2:CCC:618:GLN:HE21	3:DDD:769:VAL:HG23	1.76	0.49
3:DDD:839:VAL:HG13	3:DDD:882:VAL:HG12	1.93	0.49
6:111:56:DG:O6	7:222:6:DG:O6	2.31	0.49
3:DDD:1080:ILE:HD12	3:DDD:1115:ILE:HD11	1.94	0.49
6:111:55:DC:H2"	6:111:56:DG:C8	2.47	0.49
3:DDD:1075:ARG:NH1	3:DDD:1193:TRP:HB3	2.27	0.49
2:CCC:347:ILE:HD11	2:CCC:433:ILE:HD11	1.94	0.49
2:CCC:557:ARG:NH1	2:CCC:611:GLU:OE1	2.45	0.49
3:DDD:1350:ASN:HA	3:DDD:1353:VAL:HG22	1.95	0.49
5:FFF:273:VAL:HG12	5:FFF:273:VAL:O	2.13	0.49
2:CCC:706:ARG:HA	2:CCC:793:GLU:HA	1.94	0.49
3:DDD:495:ASN:O	3:DDD:497:GLU:N	2.36	0.49
3:DDD:713:GLU:HG2	3:DDD:714:GLU:N	2.27	0.49
2:CCC:1004:ASP:OD1	2:CCC:1004:ASP:N	2.46	0.49
2:CCC:347:ILE:HD11	2:CCC:433:ILE:CD1	2.43	0.49
2:CCC:808:ASN:HA	3:DDD:629:PHE:HB3	1.95	0.49
2:CCC:1066:MET:HG2	2:CCC:1234:LYS:HA	1.94	0.49
2:CCC:397:LEU:O	2:CCC:398:SER:CB	2.60	0.49
3:DDD:1025:MET:CB	3:DDD:1126:GLN:HE21	2.25	0.49
3:DDD:134:ASP:O	3:DDD:138:VAL:HG23	2.12	0.49
3:DDD:1364:ALA:HB3	4:EEE:21:LEU:CD1	2.43	0.49
2:CCC:514:PHE:CZ	7:222:20:DG:C1'	2.96	0.49
1:BBB:44:ARG:HH12	3:DDD:538:ARG:CG	2.25	0.49
2:CCC:1105:SER:CB	3:DDD:731:ARG:HD2	2.41	0.49
1:AAA:158:ARG:HB3	1:AAA:172:LEU:CD2	2.35	0.48
2:CCC:518:ASN:O	2:CCC:519:ASN:HB2	2.13	0.48
2:CCC:1269:ARG:NH2	3:DDD:340:GLN:O	2.46	0.48
3:DDD:925:GLU:HB3	3:DDD:926:PRO:HD3	1.95	0.48
3:DDD:518:VAL:O	3:DDD:520:ALA:N	2.46	0.48
2:CCC:620:ASN:ND2	3:DDD:768:ASN:HB2	2.28	0.48
2:CCC:1105:SER:HB2	3:DDD:731:ARG:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:331:ILE:O	3:DDD:331:ILE:HG22	2.14	0.48
3:DDD:519:ASN:HA	3:DDD:523:GLU:CG	2.43	0.48
5:FFF:63:GLY:HA2	6:111:42:DG:N2	2.28	0.48
1:AAA:184:ALA:HB2	2:CCC:1091:GLY:CA	2.34	0.48
3:DDD:1025:MET:HB2	3:DDD:1126:GLN:HE21	1.78	0.48
3:DDD:1347:LEU:HD22	3:DDD:1357:ILE:CG2	2.43	0.48
3:DDD:380:PHE:HB3	3:DDD:415:VAL:HG11	1.95	0.48
3:DDD:592:VAL:O	3:DDD:592:VAL:HG22	2.12	0.48
1:AAA:38:THR:HG23	1:BBB:42:ALA:O	2.13	0.48
2:CCC:1308:ILE:HG23	3:DDD:380:PHE:CD1	2.47	0.48
3:DDD:504:GLN:HE22	3:DDD:731:ARG:HH21	1.57	0.48
2:CCC:1318:GLY:O	2:CCC:1319:MET:CB	2.62	0.48
1:BBB:47:LEU:HD13	1:BBB:183:ILE:HD12	1.95	0.48
2:CCC:615:VAL:HA	2:CCC:638:SER:HB3	1.96	0.48
3:DDD:223:LEU:O	3:DDD:227:PHE:HB2	2.14	0.48
3:DDD:430:HIS:CD2	3:DDD:432:LEU:HB2	2.49	0.48
2:CCC:620:ASN:HD21	3:DDD:768:ASN:HB2	1.78	0.48
5:FFF:263:LEU:HB3	5:FFF:271:ARG:HG3	1.94	0.48
1:BBB:49:SER:O	1:BBB:151:GLY:HA3	2.14	0.48
1:BBB:83:LEU:HD21	3:DDD:526:VAL:HB	1.95	0.48
2:CCC:127:ILE:O	2:CCC:127:ILE:HG13	2.13	0.48
2:CCC:1313:HIS:CE1	3:DDD:380:PHE:CE1	3.02	0.48
2:CCC:566:GLY:O	2:CCC:568:ASN:N	2.47	0.48
2:CCC:24:VAL:HG11	2:CCC:704:MET:SD	2.54	0.48
2:CCC:91:THR:HG21	2:CCC:128:PRO:HG3	1.96	0.48
3:DDD:349:TYR:CE1	3:DDD:472:LEU:HD11	2.48	0.48
2:CCC:1268:GLN:OE1	3:DDD:352:ARG:HD2	2.14	0.48
2:CCC:208:ILE:HD11	2:CCC:365:GLU:HB2	1.96	0.47
3:DDD:1256:ILE:HD12	3:DDD:1256:ILE:N	2.29	0.47
1:BBB:152:TYR:CD2	3:DDD:536:LEU:HD21	2.48	0.47
1:AAA:182:ARG:HD2	2:CCC:1092:THR:CG2	2.44	0.47
1:AAA:149:GLY:N	1:AAA:177:TYR:CD1	2.82	0.47
7:222:15:DT:H3'	7:222:15:DT:H6	1.78	0.47
2:CCC:757:THR:O	2:CCC:833:ILE:HD12	2.13	0.47
3:DDD:1078:LEU:HG	3:DDD:1101:LEU:HD11	1.96	0.47
3:DDD:930:LEU:CD1	3:DDD:1246:VAL:CG2	2.93	0.47
1:BBB:22:THR:OG1	1:BBB:207:THR:O	2.21	0.47
1:BBB:57:THR:HG22	1:BBB:58:GLU:HG3	1.96	0.47
3:DDD:1078:LEU:HD12	3:DDD:1121:LEU:HB3	1.97	0.47
5:FFF:318:GLN:HA	5:FFF:323:ASN:HB2	1.96	0.47
1:AAA:86:LYS:HE2	1:AAA:174:ASP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:488:MET:HB3	2:CCC:489:PRO:HD2	1.96	0.47
3:DDD:45:ASN:HB3	3:DDD:48:THR:HG1	1.79	0.47
3:DDD:294:ASN:O	3:DDD:298:MET:HG3	2.14	0.47
2:CCC:156:PHE:CE2	2:CCC:158:ASP:HB2	2.50	0.47
2:CCC:241:LEU:CD2	2:CCC:277:LEU:HD21	2.45	0.47
2:CCC:550:VAL:HG21	3:DDD:776:THR:HG21	1.93	0.47
2:CCC:1101:LEU:HD13	3:DDD:504:GLN:HA	1.96	0.47
3:DDD:519:ASN:O	3:DDD:520:ALA:HB3	2.15	0.47
3:DDD:926:PRO:O	3:DDD:930:LEU:N	2.48	0.47
5:FFF:144:THR:O	5:FFF:147:THR:OG1	2.32	0.47
3:DDD:825:VAL:HG23	3:DDD:838:ARG:CD	2.45	0.47
1:AAA:47:LEU:HD13	1:AAA:183:ILE:CD1	2.45	0.46
2:CCC:1257:GLN:HB2	2:CCC:1258:PRO:HD2	1.96	0.46
3:DDD:973:LEU:CD2	3:DDD:1006:GLY:HA2	2.45	0.46
3:DDD:197:GLU:O	3:DDD:201:LEU:HG	2.15	0.46
2:CCC:1111:GLN:HG3	2:CCC:1112:ILE:HD13	1.98	0.46
3:DDD:435:GLN:HB2	3:DDD:457:TYR:OH	2.15	0.46
2:CCC:514:PHE:CE2	7:222:20:DG:O4'	2.69	0.46
5:FFF:265:GLU:O	5:FFF:265:GLU:HG2	2.16	0.46
1:AAA:35:PHE:HZ	1:BBB:50:SER:HB3	1.80	0.46
2:CCC:1042:LEU:HD13	2:CCC:1046:VAL:CG1	2.44	0.46
2:CCC:259:GLY:O	2:CCC:260:LYS:CB	2.63	0.46
2:CCC:42:ASP:O	2:CCC:50:GLU:HG2	2.15	0.46
2:CCC:400:VAL:HG11	2:CCC:452:ARG:CD	2.45	0.46
6:111:44:DG:H5"	6:111:45:DT:OP1	2.16	0.46
2:CCC:159:SER:HB3	2:CCC:172:TYR:HA	1.98	0.46
2:CCC:548:ARG:CB	2:CCC:570:GLY:HA3	2.46	0.46
3:DDD:114:ILE:HD11	3:DDD:311:ARG:HB3	1.97	0.46
3:DDD:45:ASN:HB3	3:DDD:48:THR:OG1	2.16	0.46
5:FFF:204:LYS:HB3	5:FFF:205:PRO:HD2	1.97	0.46
2:CCC:1307:ASN:HB3	2:CCC:1312:ASN:O	2.15	0.46
1:BBB:145:LYS:O	1:BBB:145:LYS:HG2	2.15	0.46
2:CCC:834:GLN:HE21	2:CCC:836:LEU:HD21	1.80	0.46
2:CCC:800:MET:O	2:CCC:1229:TYR:HA	2.16	0.46
2:CCC:823:VAL:HG12	2:CCC:1059:ARG:NH2	2.30	0.46
2:CCC:1294:LYS:HB3	3:DDD:347:VAL:HG13	1.97	0.46
3:DDD:368:LEU:HD12	3:DDD:369:PRO:HD2	1.98	0.46
1:AAA:47:LEU:HA	1:AAA:51:MET:HG2	1.98	0.46
2:CCC:890:LYS:HE3	2:CCC:893:THR:CB	2.46	0.46
2:CCC:894:GLN:HE22	3:DDD:69:GLU:CD	2.16	0.46
3:DDD:1140:ARG:NH1	3:DDD:1236:GLU:HG3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1309:VAL:O	3:DDD:383:GLY:HA2	2.16	0.46
5:FFF:220:THR:HG21	7:222:22:DA:N1	2.31	0.46
1:BBB:157:THR:CG2	1:BBB:157:THR:O	2.64	0.45
2:CCC:868:SER:OG	2:CCC:944:ARG:N	2.49	0.45
3:DDD:839:VAL:O	3:DDD:839:VAL:CG1	2.63	0.45
1:AAA:112:ALA:HB1	1:AAA:123:ILE:HG21	1.97	0.45
3:DDD:1050:THR:HG22	3:DDD:1051:ASP:N	2.31	0.45
5:FFF:287:THR:O	5:FFF:291:VAL:HG23	2.16	0.45
1:BBB:86:LYS:CE	1:BBB:174:ASP:HB2	2.45	0.45
2:CCC:138:ILE:O	2:CCC:141:THR:OG1	2.32	0.45
2:CCC:311:CYS:O	2:CCC:311:CYS:SG	2.74	0.45
2:CCC:46:GLN:HB2	2:CCC:51:ALA:CA	2.45	0.45
2:CCC:635:THR:CG2	2:CCC:644:LEU:CD2	2.95	0.45
2:CCC:1101:LEU:O	3:DDD:731:ARG:HG2	2.16	0.45
1:BBB:192:VAL:HG23	1:BBB:198:LEU:HD12	1.97	0.45
1:BBB:47:LEU:HA	1:BBB:51:MET:HG2	1.98	0.45
2:CCC:1252:SER:OG	2:CCC:1257:GLN:N	2.50	0.45
2:CCC:1315:MET:HG3	2:CCC:1317:PRO:HD3	1.99	0.45
2:CCC:1286:THR:OG1	3:DDD:479:GLU:OE2	2.26	0.45
1:AAA:57:THR:HG23	1:AAA:158:ARG:NE	2.32	0.45
1:BBB:192:VAL:CG2	1:BBB:198:LEU:HD12	2.47	0.45
2:CCC:98:VAL:HB	2:CCC:124:MET:HE2	1.98	0.45
2:CCC:811:ASN:HA	2:CCC:815:SER:O	2.16	0.45
3:DDD:975:ILE:CD1	3:DDD:997:VAL:HG11	2.46	0.45
5:FFF:204:LYS:HB3	5:FFF:205:PRO:CD	2.46	0.45
2:CCC:1034:ARG:O	2:CCC:1038:GLN:N	2.44	0.45
2:CCC:1291:LEU:CD1	3:DDD:1351:VAL:HG13	2.47	0.45
2:CCC:60:GLN:HA	2:CCC:67:GLU:HA	1.98	0.45
2:CCC:1257:GLN:OE1	3:DDD:345:LYS:HG2	2.16	0.45
3:DDD:366:CYS:O	3:DDD:366:CYS:SG	2.75	0.45
3:DDD:490:ILE:HD11	3:DDD:614:LEU:HD13	1.98	0.45
2:CCC:1264:GLN:NE2	5:FFF:237:ILE:HD13	2.32	0.45
1:AAA:134:THR:CA	2:CCC:773:LEU:HD22	2.46	0.45
1:AAA:47:LEU:HD13	1:AAA:183:ILE:HD12	1.98	0.45
2:CCC:557:ARG:HH12	2:CCC:611:GLU:CD	2.20	0.45
3:DDD:1087:ASP:OD1	3:DDD:1087:ASP:N	2.50	0.44
3:DDD:1175:LEU:HD12	3:DDD:1177:ILE:HG12	1.99	0.44
3:DDD:320:ASN:O	3:DDD:321:LYS:HG3	2.17	0.44
3:DDD:320:ASN:O	3:DDD:322:ARG:N	2.50	0.44
2:CCC:1146:GLN:HB2	2:CCC:1161:LEU:HD12	1.99	0.44
3:DDD:1075:ARG:NH1	3:DDD:1193:TRP:CB	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:43:THR:HG21	5:FFF:164:THR:CG2	2.47	0.44
3:DDD:857:LEU:HD21	3:DDD:875:ASN:HD22	1.80	0.44
5:FFF:163:ARG:CD	5:FFF:167:LEU:HD12	2.47	0.44
3:DDD:884:SER:OG	3:DDD:885:VAL:N	2.51	0.44
2:CCC:168:GLY:C	3:DDD:1065:ALA:HA	2.38	0.44
3:DDD:1152:GLU:HG3	3:DDD:1194:ARG:HD3	1.98	0.44
3:DDD:261:ALA:HA	5:FFF:219:ILE:CG2	2.48	0.44
5:FFF:263:LEU:CD2	5:FFF:271:ARG:HB2	2.47	0.44
1:AAA:86:LYS:NZ	2:CCC:826:ASP:OD2	2.50	0.44
2:CCC:186:PHE:CE1	2:CCC:429:MET:HG2	2.53	0.44
2:CCC:989:LEU:HD13	2:CCC:1000:LEU:CD2	2.48	0.44
3:DDD:1075:ARG:CZ	3:DDD:1193:TRP:CE3	3.00	0.44
3:DDD:1156:LEU:HB2	3:DDD:1223:LEU:CD1	2.47	0.44
3:DDD:958:ILE:HG23	3:DDD:982:LEU:HD11	2.00	0.44
3:DDD:1364:ALA:HB3	4:EEE:21:LEU:HD11	1.99	0.44
1:BBB:50:SER:O	1:BBB:150:ARG:CD	2.56	0.44
2:CCC:208:ILE:HG13	2:CCC:356:THR:HG21	1.98	0.44
3:DDD:1271:SER:OG	3:DDD:1292:LEU:HD21	2.17	0.44
5:FFF:105:ILE:HG21	5:FFF:150:ILE:HG22	1.99	0.44
7:222:30:DA:C8	7:222:31:DT:H72	2.53	0.44
1:AAA:35:PHE:CZ	1:BBB:50:SER:OG	2.55	0.44
1:BBB:112:ALA:HB1	1:BBB:123:ILE:HG21	2.00	0.44
1:BBB:177:TYR:O	1:BBB:179:PRO:N	2.51	0.44
2:CCC:967:LEU:CD2	2:CCC:1021:LEU:HD22	2.47	0.44
2:CCC:199:ASP:HB2	2:CCC:201:ARG:HG3	1.98	0.44
2:CCC:254:ASP:HB2	2:CCC:265:LYS:HE3	2.00	0.44
2:CCC:1085:MET:HE1	2:CCC:1097:VAL:HG23	2.00	0.44
2:CCC:185:ASP:OD1	2:CCC:185:ASP:N	2.50	0.44
3:DDD:322:ARG:HH21	5:FFF:221:SER:HB3	1.83	0.44
2:CCC:1274:GLU:HA	3:DDD:428:THR:HG21	2.00	0.44
1:BBB:177:TYR:O	1:BBB:179:PRO:HD3	2.18	0.44
2:CCC:895:LEU:HD23	2:CCC:895:LEU:HA	1.90	0.44
3:DDD:733:SER:O	3:DDD:737:ILE:HG13	2.18	0.44
2:CCC:175:ARG:HB2	2:CCC:175:ARG:NH1	2.32	0.43
2:CCC:176:ILE:HD12	2:CCC:184:LEU:HD23	1.99	0.43
2:CCC:514:PHE:CZ	7:222:20:DG:O4'	2.71	0.43
1:BBB:47:LEU:HD13	1:BBB:183:ILE:CD1	2.47	0.43
3:DDD:1256:ILE:H	3:DDD:1256:ILE:HD12	1.84	0.43
1:BBB:99:ILE:HA	1:BBB:144:ILE:O	2.19	0.43
2:CCC:807:TRP:CD1	2:CCC:817:LEU:HD21	2.54	0.43
2:CCC:758:ARG:NE	2:CCC:835:GLU:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:65:LEU:HD13	2:CCC:873:ILE:O	2.19	0.43
5:FFF:158:ILE:O	5:FFF:162:THR:HB	2.19	0.43
6:111:30:DG:C4	6:111:31:DT:C5	3.06	0.43
2:CCC:1157:GLN:O	2:CCC:1157:GLN:HG3	2.19	0.43
2:CCC:1337:ILE:HG23	2:CCC:1337:ILE:O	2.19	0.43
2:CCC:156:PHE:CZ	2:CCC:445:ILE:CG1	3.02	0.43
3:DDD:1220:ILE:HG23	3:DDD:1224:ARG:NH1	2.33	0.43
3:DDD:903:LEU:HD21	3:DDD:1249:ASN:HD22	1.83	0.43
3:DDD:708:ASN:HD22	3:DDD:714:GLU:HB3	1.83	0.43
6:111:30:DG:C8	6:111:31:DT:H73	2.53	0.43
2:CCC:125:GLY:HA2	2:CCC:499:SER:HB2	1.99	0.43
3:DDD:1138:LEU:N	3:DDD:1139:PRO:CD	2.81	0.43
3:DDD:825:VAL:HG23	3:DDD:838:ARG:HD2	1.99	0.43
3:DDD:872:LEU:HD22	3:DDD:877:VAL:HG21	2.00	0.43
4:EEE:39:VAL:HG13	4:EEE:40:PRO:HD2	2.01	0.43
2:CCC:901:LEU:CD1	5:FFF:278:PHE:CE2	2.92	0.43
7:222:8:DG:H2'	7:222:9:DT:C6	2.53	0.43
1:BBB:44:ARG:HH12	3:DDD:538:ARG:CD	2.31	0.43
2:CCC:245:ARG:C	2:CCC:247:ARG:H	2.22	0.43
3:DDD:1280:VAL:HG12	3:DDD:1281:GLU:N	2.33	0.43
3:DDD:388:ARG:HB3	3:DDD:390:LEU:HD13	2.00	0.43
3:DDD:369:PRO:HB3	3:DDD:444:GLY:O	2.19	0.43
2:CCC:1103:VAL:HG11	3:DDD:639:VAL:HG11	2.00	0.43
3:DDD:770:LEU:O	3:DDD:773:PHE:N	2.51	0.43
6:111:30:DG:C5	6:111:31:DT:C4	3.07	0.43
1:AAA:192:VAL:HG23	1:AAA:198:LEU:HD12	2.01	0.43
1:BBB:50:SER:HA	1:BBB:150:ARG:HD2	2.00	0.43
3:DDD:1029:THR:HG22	3:DDD:1121:LEU:HD11	2.01	0.43
3:DDD:839:VAL:HG12	3:DDD:864:LEU:CD1	2.48	0.43
3:DDD:877:VAL:HG11	3:DDD:880:VAL:CG2	2.49	0.43
3:DDD:93:THR:HG22	3:DDD:94:GLN:N	2.34	0.43
5:FFF:241:GLU:CG	5:FFF:242:LYS:N	2.67	0.43
3:DDD:1330:ARG:NH2	7:222:10:DC:H4'	2.31	0.43
1:BBB:178:SER:HA	1:BBB:179:PRO:HD2	1.76	0.43
5:FFF:272:GLU:HG2	5:FFF:276:ARG:NH2	2.34	0.43
1:AAA:65:LEU:HD13	2:CCC:873:ILE:HB	2.01	0.43
4:EEE:59:ILE:HG23	4:EEE:64:LEU:HD11	2.01	0.43
2:CCC:127:ILE:CG1	2:CCC:127:ILE:O	2.67	0.42
2:CCC:555:TYR:HA	3:DDD:773:PHE:HE1	1.84	0.42
3:DDD:1175:LEU:HD12	3:DDD:1177:ILE:CG1	2.49	0.42
3:DDD:571:ASP:N	3:DDD:571:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:749:LYS:HB3	3:DDD:750:PRO:HD2	2.01	0.42
1:AAA:59:VAL:HG12	1:AAA:60:GLU:N	2.34	0.42
2:CCC:10:ARG:NH1	2:CCC:697:LYS:HD3	2.34	0.42
3:DDD:27:PRO:HB3	3:DDD:240:THR:OG1	2.19	0.42
3:DDD:632:ALA:O	3:DDD:635:SER:OG	2.31	0.42
3:DDD:807:LEU:CD2	3:DDD:1255:VAL:HG13	2.48	0.42
3:DDD:282:LEU:HD21	5:FFF:125:LEU:HD21	2.01	0.42
5:FFF:143:SER:CB	6:111:41:DT:H73	2.49	0.42
1:BBB:59:VAL:HG12	1:BBB:60:GLU:N	2.34	0.42
2:CCC:389:PHE:HB3	2:CCC:420:LEU:HD12	2.01	0.42
3:DDD:504:GLN:HB3	3:DDD:505:ASP:H	1.68	0.42
5:FFF:79:PHE:O	5:FFF:90:SER:OG	2.36	0.42
2:CCC:625:GLU:O	2:CCC:626:GLU:HB3	2.19	0.42
2:CCC:700:VAL:O	2:CCC:1069:ARG:NH2	2.52	0.42
3:DDD:342:LEU:HD11	3:DDD:1352:ILE:O	2.19	0.42
3:DDD:337:ARG:NH1	3:DDD:341:ASN:HD22	2.17	0.42
3:DDD:332:LYS:HA	3:DDD:1328:THR:CG2	2.47	0.42
3:DDD:732:GLY:HA2	3:DDD:736:GLN:HG3	2.00	0.42
3:DDD:926:PRO:O	3:DDD:930:LEU:HG	2.20	0.42
6:111:53:DG:N2	7:222:11:DA:C2	2.87	0.42
1:AAA:192:VAL:HG21	1:AAA:198:LEU:HD12	2.02	0.42
2:CCC:1072:ASN:OD1	2:CCC:1072:ASN:N	2.52	0.42
1:AAA:57:THR:HG21	1:AAA:147:GLN:NE2	2.34	0.42
3:DDD:1289:ASN:HA	3:DDD:1292:LEU:HD12	2.01	0.42
3:DDD:116:PHE:HB3	3:DDD:237:MET:SD	2.59	0.42
3:DDD:746:LEU:H	3:DDD:746:LEU:HD12	1.84	0.42
1:BBB:29:GLU:CB	1:BBB:30:PRO:HA	2.44	0.42
2:CCC:31:GLN:HG3	2:CCC:527:LYS:HB3	2.01	0.42
2:CCC:145:ILE:HD11	2:CCC:506:PHE:CD1	2.55	0.42
5:FFF:162:THR:HG23	5:FFF:163:ARG:N	2.35	0.42
5:FFF:185:LEU:HB3	5:FFF:189:LEU:HD12	2.02	0.42
3:DDD:1075:ARG:CD	3:DDD:1193:TRP:HB3	2.50	0.42
2:CCC:1322:SER:HB2	3:DDD:341:ASN:O	2.20	0.42
3:DDD:949:SER:HB3	3:DDD:1019:ASN:ND2	2.34	0.42
5:FFF:138:ARG:NH1	6:111:37:DA:N7	2.67	0.42
1:AAA:42:ALA:HA	1:BBB:38:THR:HG23	2.02	0.42
2:CCC:1112:ILE:HG22	2:CCC:1116:HIS:CD2	2.55	0.42
2:CCC:146:VAL:HG13	2:CCC:529:ARG:O	2.20	0.42
2:CCC:805:MET:HG2	2:CCC:1225:VAL:HG11	2.01	0.42
3:DDD:17:PHE:H	3:DDD:1355:ARG:NH1	2.18	0.42
3:DDD:68:TYR:CZ	3:DDD:78:LEU:HD21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:182:ARG:HD2	2:CCC:1092:THR:HG23	2.01	0.41
2:CCC:1285:TYR:O	2:CCC:1289:GLU:N	2.44	0.41
2:CCC:163:LYS:HG2	2:CCC:164:THR:N	2.35	0.41
2:CCC:194:LEU:HA	2:CCC:194:LEU:HD12	1.88	0.41
3:DDD:325:LYS:HE2	3:DDD:330:MET:HG2	2.02	0.41
3:DDD:425:ARG:HD2	3:DDD:459:ALA:HB2	2.02	0.41
3:DDD:839:VAL:HG12	3:DDD:864:LEU:HD12	2.01	0.41
1:AAA:47:LEU:O	1:AAA:180:VAL:HG21	2.20	0.41
2:CCC:686:GLN:HG2	2:CCC:796:LEU:HD13	2.02	0.41
2:CCC:806:PRO:HB3	3:DDD:505:ASP:OD2	2.20	0.41
3:DDD:709:ARG:HB3	3:DDD:710:ASP:H	1.71	0.41
1:BBB:192:VAL:O	1:BBB:193:GLU:C	2.58	0.41
2:CCC:1281:TYR:CD2	3:DDD:484:MET:HG2	2.55	0.41
2:CCC:618:GLN:HG2	2:CCC:619:ALA:H	1.86	0.41
1:AAA:159:ILE:CD1	2:CCC:876:GLU:OE1	2.63	0.41
3:DDD:1152:GLU:N	3:DDD:1153:PRO:HD3	2.35	0.41
3:DDD:368:LEU:HD23	3:DDD:439:PRO:HB3	2.02	0.41
3:DDD:736:GLN:HA	3:DDD:736:GLN:HE21	1.85	0.41
1:AAA:222:THR:OG1	1:BBB:233:ASP:HB2	2.18	0.41
2:CCC:799:ASN:HA	2:CCC:1231:TYR:HA	2.02	0.41
2:CCC:868:SER:HB2	2:CCC:944:ARG:HB2	2.03	0.41
2:CCC:967:LEU:HD21	2:CCC:1021:LEU:CD2	2.51	0.41
3:DDD:151:MET:C	3:DDD:153:ASN:H	2.23	0.41
3:DDD:755:ILE:H	3:DDD:755:ILE:HD12	1.84	0.41
5:FFF:171:ILE:HG21	5:FFF:215:LEU:HD13	2.03	0.41
2:CCC:1269:ARG:NH2	3:DDD:340:GLN:HA	2.35	0.41
3:DDD:449:LEU:HD22	3:DDD:466:MET:SD	2.60	0.41
3:DDD:517:CYS:SG	3:DDD:518:VAL:N	2.93	0.41
3:DDD:709:ARG:O	3:DDD:710:ASP:HB3	2.21	0.41
2:CCC:550:VAL:CG2	3:DDD:776:THR:HG22	2.38	0.41
3:DDD:797:THR:O	3:DDD:801:VAL:HG23	2.20	0.41
1:AAA:86:LYS:CE	1:AAA:174:ASP:HB2	2.50	0.41
1:BBB:155:ALA:HB1	1:BBB:172:LEU:HD23	2.01	0.41
1:BBB:33:ARG:HH22	2:CCC:1081:PRO:HB3	1.86	0.41
2:CCC:618:GLN:HG2	2:CCC:619:ALA:N	2.35	0.41
3:DDD:1067:ARG:HD3	3:DDD:1071:GLY:O	2.20	0.41
3:DDD:1156:LEU:HB2	3:DDD:1223:LEU:HD12	2.02	0.41
3:DDD:417:ARG:C	3:DDD:418:GLU:HG2	2.40	0.41
3:DDD:695:LYS:HA	3:DDD:695:LYS:HE3	2.02	0.41
3:DDD:298:MET:SD	5:FFF:117:LEU:HB3	2.60	0.41
2:CCC:635:THR:HG22	2:CCC:644:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:800:MET:HE2	2:CCC:800:MET:HB3	1.95	0.41
3:DDD:1046:ILE:HG22	3:DDD:1061:VAL:HA	2.03	0.41
3:DDD:1134:ILE:O	3:DDD:1138:LEU:HG	2.21	0.41
3:DDD:1158:GLU:N	3:DDD:1158:GLU:OE1	2.54	0.41
1:AAA:35:PHE:CZ	1:BBB:50:SER:CB	3.02	0.41
2:CCC:1210:ILE:HG22	2:CCC:1211:ARG:N	2.36	0.41
3:DDD:1163:VAL:HG23	3:DDD:1204:VAL:HG22	2.02	0.41
2:CCC:809:GLY:HA3	3:DDD:629:PHE:CD1	2.56	0.41
3:DDD:350:SER:HA	3:DDD:468:VAL:O	2.21	0.41
3:DDD:644:MET:O	3:DDD:764:ARG:NH1	2.54	0.41
3:DDD:910:ASN:HD21	4:EEE:16:ARG:HD2	1.85	0.41
1:BBB:182:ARG:HD3	3:DDD:581:MET:HE1	2.03	0.41
2:CCC:1119:MET:HB2	2:CCC:1228:GLY:CA	2.51	0.41
2:CCC:865:LEU:HD23	2:CCC:871:VAL:HG23	2.01	0.41
3:DDD:349:TYR:CG	3:DDD:472:LEU:HD21	2.56	0.41
3:DDD:51:PRO:HB3	3:DDD:57:PHE:O	2.20	0.41
5:FFF:168:PRO:HB3	6:111:32:DA:OP2	2.20	0.41
2:CCC:564:PRO:O	2:CCC:569:ILE:HA	2.21	0.41
2:CCC:660:VAL:HG11	3:DDD:769:VAL:CG1	2.51	0.41
5:FFF:158:ILE:CG2	7:222:26:DT:O2	2.69	0.41
1:AAA:192:VAL:O	1:AAA:193:GLU:C	2.59	0.40
2:CCC:12:ARG:NH2	2:CCC:698:PRO:O	2.44	0.40
2:CCC:758:ARG:HG2	2:CCC:759:SER:N	2.36	0.40
2:CCC:802:VAL:HG12	2:CCC:803:ALA:N	2.36	0.40
3:DDD:535:ARG:O	3:DDD:539:SER:OG	2.22	0.40
1:AAA:86:LYS:HG2	1:AAA:173:VAL:HG12	2.04	0.40
1:BBB:66:HIS:CE1	1:BBB:69:SER:HB3	2.56	0.40
2:CCC:556:GLY:HA3	2:CCC:589:THR:HG21	2.02	0.40
3:DDD:645:VAL:HG23	3:DDD:645:VAL:O	2.21	0.40
5:FFF:151:ARG:HG3	5:FFF:152:GLN:N	2.37	0.40
2:CCC:22:LEU:HB3	2:CCC:655:VAL:HG11	2.03	0.40
3:DDD:736:GLN:CA	3:DDD:736:GLN:HE21	2.34	0.40
5:FFF:66:GLY:HA3	6:111:42:DG:C5	2.56	0.40
1:AAA:35:PHE:CE1	1:BBB:46:ILE:HG12	2.57	0.40
1:BBB:57:THR:HG21	1:BBB:147:GLN:NE2	2.37	0.40
2:CCC:1061:GLN:NE2	2:CCC:1240:ASP:OD1	2.54	0.40
2:CCC:160:ASP:OD1	2:CCC:160:ASP:N	2.54	0.40
2:CCC:338:THR:HG23	2:CCC:345:PRO:HG3	2.03	0.40
3:DDD:814:CYS:SG	3:DDD:883:ARG:NH2	2.75	0.40
5:FFF:235:LEU:C	5:FFF:235:LEU:HD12	2.42	0.40
2:CCC:123:TYR:HB3	5:FFF:187:HIS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:318:SER:OG	2:CCC:320:ASP:OD1	2.37	0.40
3:DDD:168:ALA:O	3:DDD:173:GLY:N	2.54	0.40
3:DDD:278:ARG:HD3	5:FFF:122:GLU:CG	2.51	0.40
2:CCC:1309:VAL:HG13	3:DDD:383:GLY:N	2.37	0.40
3:DDD:739:GLN:HG2	3:DDD:744:ARG:HH11	1.86	0.40
3:DDD:475:GLU:OE2	4:EEE:28:ARG:NH2	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:67:TYR:O	5:FFF:299:ARG:NH2[3_644]	1.65	0.55

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	AAA	228/242 (94%)	202 (89%)	19 (8%)	7 (3%)	4	31
1	BBB	226/242 (93%)	204 (90%)	16 (7%)	6 (3%)	5	34
2	CCC	1338/1342 (100%)	1193 (89%)	124 (9%)	21 (2%)	9	44
3	DDD	1346/1407 (96%)	1210 (90%)	118 (9%)	18 (1%)	12	48
4	EEE	77/90 (86%)	70 (91%)	7 (9%)	0	100	100
5	FFF	275/336 (82%)	248 (90%)	25 (9%)	2 (1%)	22	61
All	All	3490/3659 (95%)	3127 (90%)	309 (9%)	54 (2%)	10	45

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	CCC	161	LYS
2	CCC	1319	MET

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Mol	Chain	Res	Type
3	DDD	519	ASN
3	DDD	710	ASP
3	DDD	861	ASN
3	DDD	1053	LEU
3	DDD	1268	ASN
1	AAA	168	ILE
1	BBB	232	VAL
2	CCC	45	GLY
2	CCC	398	SER
2	CCC	892	GLU
2	CCC	909	LYS
2	CCC	1004	ASP
2	CCC	1297	ASP
2	CCC	1318	GLY
3	DDD	207	GLU
5	FFF	230	SER
1	AAA	162	GLU
1	AAA	208	ASN
1	BBB	208	ASN
2	CCC	201	ARG
2	CCC	234	ASP
2	CCC	260	LYS
2	CCC	567	PRO
2	CCC	812	PHE
2	CCC	912	ASP
2	CCC	1103	VAL
3	DDD	342	LEU
3	DDD	1201	GLY
1	AAA	210	THR
1	AAA	211	ILE
2	CCC	1224	PRO
3	DDD	947	GLU
3	DDD	1344	LEU
1	BBB	210	THR
1	BBB	211	ILE
2	CCC	110	PRO
2	CCC	519	ASN
3	DDD	81	ARG
3	DDD	96	LYS
3	DDD	321	LYS
3	DDD	1325	PHE
5	FFF	113	GLY

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Mol	Chain	Res	Type
2	CCC	1153	ALA
3	DDD	520	ALA
3	DDD	860	ARG
3	DDD	1091	PRO
1	AAA	40	GLY
1	BBB	14	VAL
1	BBB	40	GLY
3	DDD	1137	GLY
1	AAA	14	VAL
2	CCC	939	VAL

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	AAA	198/208 (95%)	190 (96%)	8 (4%)	31	57
1	BBB	196/208 (94%)	192 (98%)	4 (2%)	55	73
2	CCC	1155/1157 (100%)	1124 (97%)	31 (3%)	44	66
3	DDD	1127/1168 (96%)	1083 (96%)	44 (4%)	32	58
4	EEE	67/74 (90%)	64 (96%)	3 (4%)	27	54
5	FFF	240/292 (82%)	231 (96%)	9 (4%)	33	59
All	All	2983/3107 (96%)	2884 (97%)	99 (3%)	38	62

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	12	ARG
1	AAA	13	LEU
1	AAA	28	LEU
1	AAA	33	ARG
1	AAA	50	SER
1	AAA	166	ARG
1	AAA	170	ARG
1	AAA	182	ARG

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Mol	Chain	Res	Type
1	BBB	12	ARG
1	BBB	13	LEU
1	BBB	28	LEU
1	BBB	50	SER
2	CCC	12	ARG
2	CCC	23	ASP
2	CCC	47	TYR
2	CCC	166	SER
2	CCC	185	ASP
2	CCC	202	ARG
2	CCC	320	ASP
2	CCC	423	ASP
2	CCC	443	ASP
2	CCC	541	GLU
2	CCC	553	THR
2	CCC	561	ILE
2	CCC	609	ILE
2	CCC	628	HIS
2	CCC	635	THR
2	CCC	660	VAL
2	CCC	694	ARG
2	CCC	700	VAL
2	CCC	764	CYS
2	CCC	788	SER
2	CCC	849	GLU
2	CCC	888	THR
2	CCC	913	VAL
2	CCC	914	LYS
2	CCC	994	ARG
2	CCC	1069	ARG
2	CCC	1089	GLU
2	CCC	1135	GLN
2	CCC	1224	PRO
2	CCC	1240	ASP
2	CCC	1272	GLU
3	DDD	28	ASP
3	DDD	86	GLU
3	DDD	158	GLN
3	DDD	199	GLU
3	DDD	205	LEU
3	DDD	216	LYS
3	DDD	227	PHE

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Mol	Chain	Res	Type
3	DDD	281	ARG
3	DDD	298	MET
3	DDD	314	ARG
3	DDD	321	LYS
3	DDD	340	GLN
3	DDD	346	ARG
3	DDD	384	LYS
3	DDD	398	LYS
3	DDD	399	LYS
3	DDD	415	VAL
3	DDD	505	ASP
3	DDD	508	LEU
3	DDD	526	VAL
3	DDD	538	ARG
3	DDD	549	LYS
3	DDD	571	ASP
3	DDD	579	LEU
3	DDD	587	LEU
3	DDD	599	LYS
3	DDD	610	ARG
3	DDD	619	ILE
3	DDD	623	GLN
3	DDD	649	LYS
3	DDD	695	LYS
3	DDD	736	GLN
3	DDD	746	LEU
3	DDD	770	LEU
3	DDD	798	ARG
3	DDD	830	ASP
3	DDD	849	LEU
3	DDD	860	ARG
3	DDD	930	LEU
3	DDD	1175	LEU
3	DDD	1189	MET
3	DDD	1199	PHE
3	DDD	1227	HIS
3	DDD	1356	LEU
4	EEE	5	THR
4	EEE	43	ASN
4	EEE	69	ARG
5	FFF	54	VAL
5	FFF	156	ARG

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Mol	Chain	Res	Type
5	FFF	211	ARG
5	FFF	220	THR
5	FFF	241	GLU
5	FFF	243	GLU
5	FFF	265	GLU
5	FFF	271	ARG
5	FFF	325	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	230/242 (95%)	-0.15	4 (1%) 70 61	207, 270, 374, 441	0
1	BBB	228/242 (94%)	0.00	10 (4%) 34 28	201, 298, 374, 400	0
2	CCC	1340/1342 (99%)	-0.26	22 (1%) 72 62	121, 230, 363, 462	0
3	DDD	1350/1407 (95%)	0.04	99 (7%) 15 12	127, 252, 425, 497	0
4	EEE	79/90 (87%)	-0.29	3 (3%) 40 32	221, 293, 450, 469	0
5	FFF	277/336 (82%)	0.19	16 (5%) 23 19	182, 279, 432, 486	0
6	111	32/50 (64%)	-0.07	0 100 100	251, 304, 379, 395	0
7	222	34/50 (68%)	-0.03	2 (5%) 22 18	224, 288, 383, 409	0
All	All	3570/3759 (94%)	-0.09	156 (4%) 34 28	121, 256, 410, 497	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	DDD	1068	THR	7.8
3	DDD	997	VAL	6.5
3	DDD	1101	LEU	6.4
3	DDD	1030	GLU	6.2
5	FFF	263	LEU	6.2
3	DDD	1076	PRO	5.7
3	DDD	857	LEU	5.5
3	DDD	1130	GLY	5.3
3	DDD	1078	LEU	5.3
3	DDD	1111	ASP	5.2
3	DDD	978	ARG	5.0
3	DDD	1069	ALA	5.0
3	DDD	976	THR	5.0
3	DDD	977	SER	4.9
3	DDD	982	LEU	4.8
3	DDD	1066	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
3	DDD	856	ILE	4.7
3	DDD	1112	GLY	4.7
2	CCC	912	ASP	4.7
3	DDD	1099	TYR	4.6
3	DDD	965	SER	4.6
3	DDD	1129	GLY	4.5
3	DDD	992	LYS	4.5
5	FFF	291	VAL	4.4
5	FFF	301	ARG	4.3
3	DDD	949	SER	4.2
5	FFF	310	LEU	4.0
3	DDD	1077	ALA	4.0
5	FFF	273	VAL	4.0
3	DDD	879	ALA	3.9
3	DDD	1110	GLU	3.9
3	DDD	1055	GLY	3.8
2	CCC	913	VAL	3.8
3	DDD	1051	ASP	3.8
3	DDD	998	PRO	3.7
5	FFF	265	GLU	3.7
1	AAA	27	THR	3.7
3	DDD	1104	LYS	3.7
1	BBB	134	THR	3.6
3	DDD	947	GLU	3.6
3	DDD	1052	GLU	3.6
3	DDD	1203	ARG	3.5
3	DDD	966	VAL	3.4
3	DDD	951	GLN	3.4
3	DDD	1059	LEU	3.4
3	DDD	1105	ALA	3.4
2	CCC	983	GLY	3.4
7	222	21	DG	3.4
3	DDD	1161	GLY	3.3
1	BBB	107	ILE	3.3
5	FFF	295	ILE	3.3
5	FFF	306	GLN	3.3
2	CCC	906	PHE	3.3
5	FFF	294	GLU	3.2
3	DDD	1376	GLY	3.2
5	FFF	302	VAL	3.1
5	FFF	305	ILE	3.1
3	DDD	858	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
5	FFF	289	GLU	3.1
3	DDD	1131	THR	3.0
3	DDD	996	LYS	3.0
3	DDD	731	ARG	3.0
3	DDD	732	GLY	3.0
2	CCC	883	LEU	3.0
1	BBB	133	LEU	3.0
3	DDD	1037	PHE	2.9
1	AAA	28	LEU	2.9
3	DDD	983	LYS	2.9
3	DDD	958	ILE	2.9
7	222	22	DA	2.9
3	DDD	959	LYS	2.9
3	DDD	1266	ILE	2.8
2	CCC	911	SER	2.8
3	DDD	1028	ILE	2.8
2	CCC	113	THR	2.8
3	DDD	989	GLY	2.8
3	DDD	1050	THR	2.8
2	CCC	169	LYS	2.8
3	DDD	880	VAL	2.8
3	DDD	1118	GLY	2.7
3	DDD	952	VAL	2.7
3	DDD	974	VAL	2.7
3	DDD	1109	LEU	2.7
3	DDD	1098	GLN	2.7
2	CCC	885	GLY	2.7
3	DDD	993	GLU	2.7
4	EEE	80	LEU	2.7
3	DDD	214	ARG	2.7
3	DDD	1071	GLY	2.7
2	CCC	905	ILE	2.7
3	DDD	948	SER	2.7
2	CCC	102	LEU	2.6
1	BBB	90	VAL	2.6
2	CCC	203	LYS	2.6
3	DDD	973	LEU	2.6
3	DDD	980	THR	2.6
1	BBB	165	GLU	2.5
5	FFF	324	ILE	2.5
3	DDD	1022	PRO	2.5
3	DDD	87	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
3	DDD	1067	ARG	2.5
3	DDD	88	CYS	2.5
5	FFF	290	ASP	2.5
3	DDD	91	GLU	2.4
3	DDD	1159	ILE	2.4
2	CCC	1001	GLY	2.4
3	DDD	1108	GLN	2.4
3	DDD	1160	SER	2.4
3	DDD	984	LEU	2.4
3	DDD	995	TYR	2.4
3	DDD	991	THR	2.4
3	DDD	1103	GLY	2.4
3	DDD	1044	GLN	2.3
2	CCC	994	ARG	2.3
2	CCC	850	ILE	2.3
3	DDD	1049	GLN	2.3
3	DDD	1036	ARG	2.3
3	DDD	1061	VAL	2.3
5	FFF	280	LEU	2.3
4	EEE	76	GLU	2.3
2	CCC	103	VAL	2.3
3	DDD	954	ASN	2.3
3	DDD	946	ALA	2.3
3	DDD	1100	PHE	2.3
3	DDD	1040	MET	2.3
3	DDD	1021	ASP	2.3
3	DDD	1070	GLY	2.2
3	DDD	877	VAL	2.2
5	FFF	281	LEU	2.2
1	BBB	162	GLU	2.2
3	DDD	953	LYS	2.2
3	DDD	986	ASP	2.2
3	DDD	848	VAL	2.2
3	DDD	1007	ASP	2.2
4	EEE	2	ALA	2.1
1	BBB	131	CYS	2.1
2	CCC	117	ILE	2.1
1	BBB	98	VAL	2.1
1	BBB	67	GLU	2.1
2	CCC	1003	THR	2.1
3	DDD	855	ASP	2.1
3	DDD	985	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
3	DDD	1121	LEU	2.1
3	DDD	1043	GLY	2.1
2	CCC	696	ASP	2.1
3	DDD	1017	VAL	2.1
3	DDD	1060	VAL	2.1
3	DDD	1375	ALA	2.1
1	BBB	108	GLY	2.1
2	CCC	385	PHE	2.1
2	CCC	703	GLY	2.1
3	DDD	850	LYS	2.0
1	AAA	201	LEU	2.0
1	AAA	184	ALA	2.0
2	CCC	984	VAL	2.0
3	DDD	1107	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	ZN	DDD	1501	1/1	0.98	0.13	332,332,332,332	0
8	ZN	DDD	1502	1/1	0.99	0.17	268,268,268,268	0
9	MG	DDD	1503	1/1	0.99	0.28	95,95,95,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.