Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:20 PM GMT

PDB ID	:	1A79
Title	:	CRYSTAL STRUCTURE OF THE TRNA SPLICING ENDONUCLEASE FROM METHANOCOCCUS JANNASCHII
Authors	:	Li, H.; Trotta, C.R.; Abelson, J.N.
Deposited on	:	1998-03-23
Resolution	:	2.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

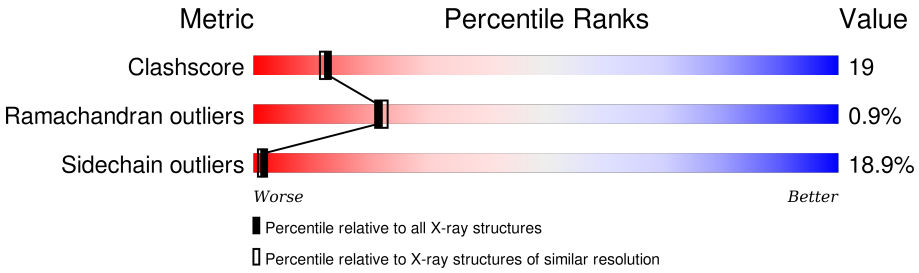
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.28 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))
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	171	53% 37% 10%
1	B	171	56% 35% 9%
1	C	171	50% 40% 10%
1	D	171	63% 27% 9%

2 Entry composition

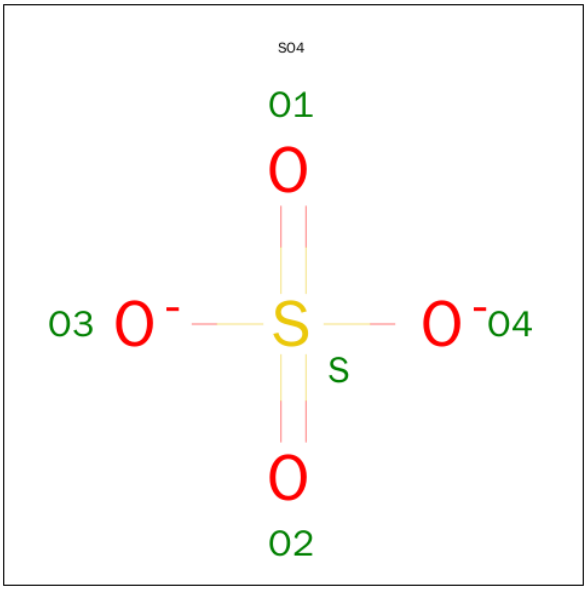
There are 4 unique types of molecules in this entry. The entry contains 5651 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRNA ENDONUCLEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1396	908	231	255	2			
1	B	171	Total	C	N	O	S	0	0	0
			1396	908	231	255	2			
1	C	171	Total	C	N	O	S	0	0	0
			1396	908	231	255	2			
1	D	171	Total	C	N	O	S	0	0	0
			1396	908	231	255	2			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	S		0	0
			5	4	1			
2	C	1	Total	O	S		0	0
			5	4	1			

- Molecule 3 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Au 1 1	0	0
3	A	1	Total Au 1 1	0	0
3	D	1	Total Au 1 1	0	0
3	C	1	Total Au 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	B	14	Total O 14 14	0	0
4	C	14	Total O 14 14	0	0
4	D	13	Total O 13 13	0	0

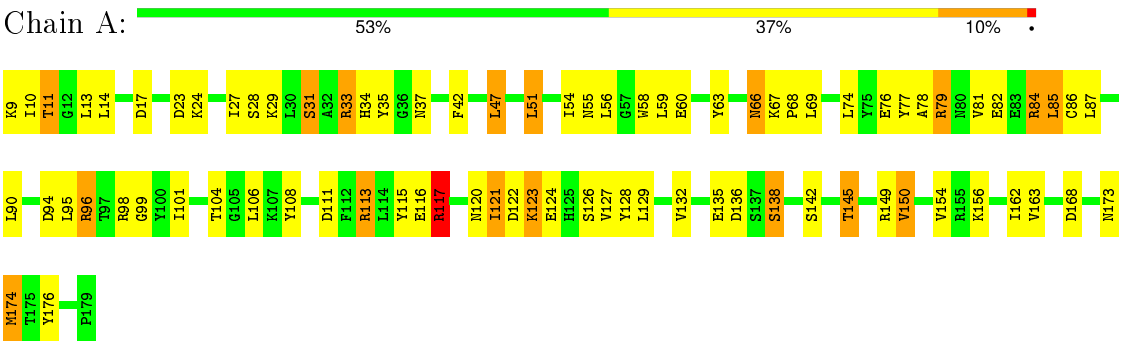
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

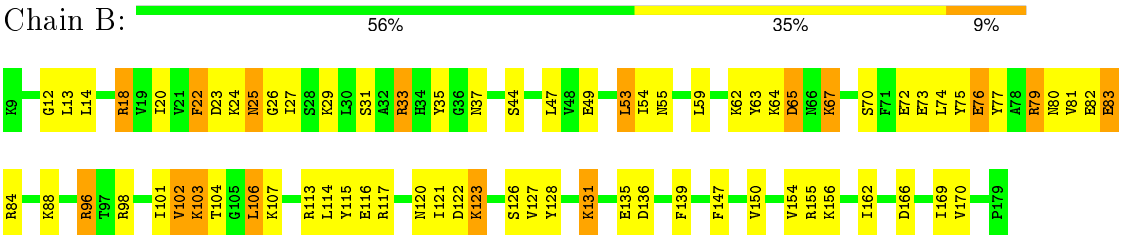
- Molecule 1: TRNA ENDONUCLEASE

Chain A:



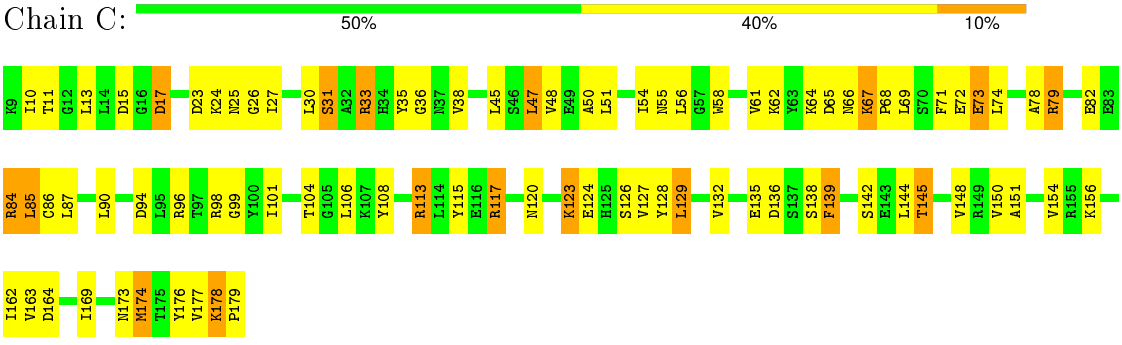
- Molecule 1: TRNA ENDONUCLEASE

Chain B:



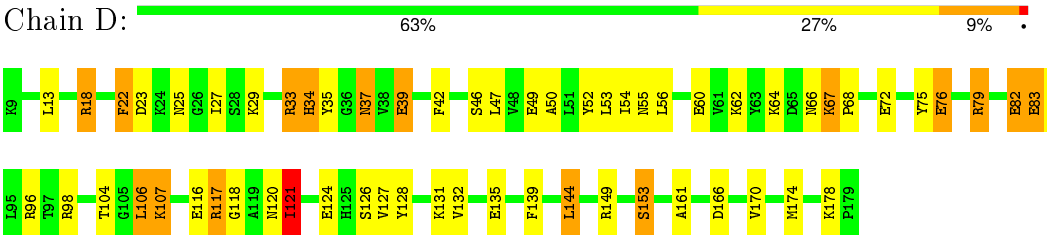
- Molecule 1: TRNA ENDONUCLEASE

Chain C:



- Molecule 1: TRNA ENDONUCLEASE

Chain D:


63%
27%
9%
K9
L13
R18
F22
D23
K24
N25
G26
I27
S28
K29
R33
H34
Y35
G36
N37
Y38
E39
F42
S46
L47
V48
E49
A50
L51
Y52
L53
I54
N55
L56
E60
V61
K62
Y63
K64
D65
N66
K67
P68
E72
Y75
E76
R79
E82
E83
R84
K93
D94
L95
R96
T97
R98
T104
G105
L106
K107
E116
R117
G118
A119
N120
I121
E124
H125
S126
V127
Y128
K131
V132
E135
F139
L144
R149
S153
A161
D166
V170
M174
K178
P179

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.95Å 80.04Å 193.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.28	Depositor
% Data completeness (in resolution range)	77.2 (50.00-2.28)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.857	Depositor
R, R_{free}	0.200 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5651	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AU, SO4

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	0.37	0/1424	0.65	0/1920
1	B	0.38	0/1424	0.62	0/1920
1	C	0.37	0/1424	0.66	0/1920
1	D	0.38	0/1424	0.63	1/1920 (0.1%)
All	All	0.37	0/5696	0.64	1/7680 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	118	GLY	N-CA-C	5.02	125.65	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1396	0	1419	71	0
1	B	1396	0	1419	55	0
1	C	1396	0	1419	74	0
1	D	1396	0	1419	42	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	0	0	0
4	B	14	0	0	1	0
4	C	14	0	0	0	0
4	D	13	0	0	0	0
All	All	5651	0	5676	217	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 19.

All (217) 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)
1:A:150:VAL:HG23	1:C:150:VAL:HG23	1.37	1.05
1:A:120:ASN:ND2	1:A:123:LYS:H	1.57	1.02
1:D:121:ILE:H	1:D:124:GLU:HG3	1.26	1.01
1:A:120:ASN:HD21	1:A:123:LYS:H	1.17	0.87
1:A:78:ALA:HB1	1:A:85:LEU:HD13	1.58	0.85
1:B:13:LEU:HG	1:B:22:PHE:HZ	1.43	0.84
1:C:178:LYS:HA	1:C:178:LYS:HE3	1.59	0.82
1:A:106:LEU:HD12	1:C:145:THR:HG21	1.62	0.82
1:A:101:ILE:HG21	1:A:121:ILE:HD11	1.62	0.81
1:A:33:ARG:HD2	1:A:58:TRP:HH2	1.47	0.80
1:C:84:ARG:HH11	1:C:84:ARG:HG3	1.48	0.79
1:B:65:ASP:HB2	1:B:67:LYS:HG2	1.62	0.79
1:B:101:ILE:HD12	1:B:121:ILE:HD11	1.64	0.78
1:B:80:ASN:HD21	1:C:64:LYS:HD2	1.48	0.78
1:C:108:TYR:HE2	1:C:154:VAL:HG21	1.47	0.78
1:C:178:LYS:HE2	1:D:98:ARG:HH22	1.49	0.76
1:C:27:ILE:O	1:C:31:SER:HB2	1.86	0.76
1:C:78:ALA:HB1	1:C:85:LEU:HD13	1.67	0.74
1:C:129:LEU:HD13	1:C:156:LYS:HD2	1.68	0.74
1:D:18:ARG:HH12	1:D:37:ASN:HD21	1.35	0.74
1:A:81:VAL:HG23	1:A:82:GLU:HG3	1.71	0.73
1:B:72:GLU:HG3	1:B:76:GLU:OE2	1.89	0.72
1:B:65:ASP:N	1:B:65:ASP:OD1	2.23	0.72
1:C:108:TYR:CE2	1:C:154:VAL:HG21	2.26	0.71
1:C:33:ARG:HD2	1:C:58:TRP:HH2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ASP:OD2	1:C:104:THR:HG22	1.93	0.69
1:B:13:LEU:HG	1:B:22:PHE:CZ	2.27	0.69
1:A:173:ASN:ND2	1:A:174:MET:H	1.91	0.69
1:A:108:TYR:CE2	1:A:154:VAL:HG21	2.27	0.68
1:B:127:VAL:HG13	1:B:128:TYR:CD1	2.30	0.67
1:A:27:ILE:O	1:A:31:SER:HB2	1.95	0.66
1:A:63:TYR:O	1:D:79:ARG:NH2	2.27	0.66
1:A:33:ARG:HD2	1:A:58:TRP:CH2	2.30	0.66
1:D:13:LEU:HG	1:D:22:PHE:HE1	1.62	0.65
1:B:120:ASN:OD1	1:B:122:ASP:HB2	1.97	0.65
1:C:23:ASP:O	1:C:27:ILE:HG13	1.97	0.65
1:B:127:VAL:HG13	1:B:128:TYR:HD1	1.61	0.65
1:A:106:LEU:O	1:C:145:THR:CG2	2.46	0.64
1:A:101:ILE:CG2	1:A:121:ILE:HD11	2.26	0.64
1:C:120:ASN:ND2	1:C:123:LYS:HD3	2.12	0.64
1:A:108:TYR:HE2	1:A:154:VAL:HG21	1.61	0.64
1:C:129:LEU:HD13	1:C:156:LYS:CD	2.28	0.63
1:B:83:GLU:HG2	1:B:84:ARG:HG3	1.81	0.62
1:B:18:ARG:HD3	1:B:44:SER:OG	1.98	0.62
1:D:18:ARG:NH1	1:D:37:ASN:HD21	1.98	0.62
1:D:62:LYS:HB3	1:D:68:PRO:HA	1.81	0.62
1:D:127:VAL:HG13	1:D:128:TYR:HD1	1.64	0.62
1:D:33:ARG:HB3	1:D:35:TYR:CE2	2.34	0.62
1:D:82:GLU:HG3	1:D:83:GLU:N	2.16	0.61
1:D:33:ARG:O	1:D:34:HIS:HB2	2.01	0.61
1:C:69:LEU:HB3	1:C:73:GLU:HB3	1.82	0.61
1:A:120:ASN:ND2	1:A:123:LYS:N	2.41	0.60
1:C:173:ASN:ND2	1:C:174:MET:H	1.98	0.60
1:C:178:LYS:HE2	1:D:98:ARG:NH2	2.17	0.60
1:C:101:ILE:HB	1:C:115:TYR:HB2	1.83	0.60
1:B:120:ASN:ND2	1:B:123:LYS:HG2	2.17	0.59
1:A:63:TYR:HB2	1:A:69:LEU:HD11	1.86	0.58
1:B:33:ARG:HB3	1:B:35:TYR:CE2	2.37	0.58
1:A:101:ILE:HB	1:A:115:TYR:HB2	1.86	0.57
1:A:106:LEU:O	1:C:145:THR:HG23	2.04	0.57
1:A:145:THR:CG2	1:C:106:LEU:O	2.52	0.57
1:D:94:ASP:O	1:D:98:ARG:HG3	2.05	0.57
1:A:104:THR:HG22	1:D:166:ASP:OD2	2.04	0.56
1:A:94:ASP:O	1:A:98:ARG:HG3	2.06	0.56
1:A:33:ARG:HB2	1:A:35:TYR:CE2	2.40	0.56
1:D:127:VAL:HG13	1:D:128:TYR:CD1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:NH1	1:B:96:ARG:HE	2.04	0.56
1:B:103:LYS:HG3	1:B:115:TYR:HE1	1.72	0.55
1:C:85:LEU:HG	1:C:85:LEU:O	2.07	0.54
1:D:104:THR:OG1	1:D:106:LEU:HB2	2.07	0.54
1:A:106:LEU:CD1	1:C:145:THR:HG21	2.36	0.54
1:D:72:GLU:HG3	1:D:76:GLU:OE1	2.07	0.54
1:B:136:ASP:HB3	1:C:82:GLU:HG2	1.88	0.54
1:C:33:ARG:HD2	1:C:58:TRP:CH2	2.40	0.54
1:C:84:ARG:HH11	1:C:84:ARG:CG	2.18	0.54
1:A:51:LEU:HD13	1:A:74:LEU:HG	1.89	0.54
1:B:18:ARG:CD	1:B:44:SER:OG	2.56	0.54
1:A:54:ILE:HD12	1:A:74:LEU:HD23	1.90	0.53
1:B:98:ARG:O	1:B:117:ARG:HD3	2.07	0.53
1:D:67:LYS:HD3	1:D:67:LYS:N	2.23	0.53
1:C:135:GLU:HG3	1:C:162:ILE:HG21	1.90	0.53
1:B:25:ASN:O	1:B:29:LYS:HG3	2.09	0.53
1:D:144:LEU:HD13	1:D:174:MET:SD	2.49	0.53
1:B:136:ASP:O	1:C:82:GLU:HG2	2.09	0.53
1:C:17:ASP:O	1:C:47:LEU:HD13	2.09	0.52
1:C:120:ASN:CG	1:C:123:LYS:HD3	2.30	0.52
1:A:78:ALA:HB1	1:A:85:LEU:CD1	2.36	0.52
1:A:145:THR:HG23	1:C:106:LEU:O	2.10	0.52
1:A:129:LEU:HD13	1:A:156:LYS:HD3	1.91	0.52
1:C:150:VAL:HG12	1:C:151:ALA:N	2.25	0.51
1:B:96:ARG:HD2	1:B:102:VAL:HG23	1.92	0.51
1:A:79:ARG:NH1	1:A:86:CYS:HB2	2.25	0.51
1:D:120:ASN:HB3	1:D:124:GLU:HB2	1.91	0.51
1:C:135:GLU:HG3	1:C:162:ILE:CG2	2.41	0.51
1:C:36:GLY:HA3	1:C:45:LEU:HD23	1.93	0.51
1:A:77:TYR:O	1:A:81:VAL:HG13	2.11	0.50
1:B:14:LEU:HD21	1:B:77:TYR:CD2	2.46	0.50
1:C:142:SER:HA	1:C:145:THR:CG2	2.42	0.50
1:A:99:GLY:O	1:A:117:ARG:HA	2.12	0.50
1:C:99:GLY:O	1:C:117:ARG:HB2	2.12	0.49
1:A:113:ARG:NH1	1:A:115:TYR:OH	2.45	0.49
1:B:75:TYR:O	1:B:79:ARG:HG2	2.12	0.49
1:A:120:ASN:ND2	1:A:123:LYS:HD2	2.26	0.49
1:C:139:PHE:HE1	1:D:139:PHE:CE2	2.31	0.49
1:D:149:ARG:O	1:D:153:SER:HB3	2.12	0.48
1:A:106:LEU:O	1:C:145:THR:HG21	2.12	0.48
1:B:53:LEU:HB3	1:B:59:LEU:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ASP:O	1:A:27:ILE:HG13	2.13	0.48
1:A:163:VAL:HA	1:A:168:ASP:O	2.14	0.48
1:A:142:SER:HA	1:A:145:THR:CG2	2.44	0.48
1:C:38:VAL:HG12	1:C:38:VAL:O	2.13	0.48
1:C:84:ARG:HG3	1:C:84:ARG:NH1	2.23	0.48
1:A:173:ASN:ND2	1:A:174:MET:N	2.61	0.48
1:C:163:VAL:HG22	1:C:169:ILE:HG12	1.95	0.48
1:B:53:LEU:HB3	1:B:59:LEU:HB3	1.95	0.47
1:D:50:ALA:O	1:D:54:ILE:HG13	2.14	0.47
1:C:94:ASP:O	1:C:98:ARG:HG3	2.14	0.47
1:B:22:PHE:O	1:B:23:ASP:C	2.52	0.47
1:B:154:VAL:HG23	1:B:156:LYS:HB2	1.96	0.47
1:C:177:VAL:HG12	1:C:179:PRO:HD3	1.96	0.47
1:B:150:VAL:O	1:B:154:VAL:HG22	2.14	0.47
1:C:87:LEU:HB3	1:C:132:VAL:HG11	1.97	0.47
1:A:78:ALA:CB	1:A:85:LEU:HD13	2.36	0.47
1:A:95:LEU:HA	1:A:98:ARG:HG3	1.97	0.47
1:B:131:LYS:HG3	1:B:147:PHE:CZ	2.50	0.46
1:C:178:LYS:HA	1:C:178:LYS:CE	2.39	0.46
1:A:127:VAL:HG13	1:A:128:TYR:CD2	2.50	0.46
1:C:176:TYR:HE1	1:D:170:VAL:HG13	1.80	0.46
1:B:23:ASP:OD2	1:B:26:GLY:N	2.49	0.46
1:D:75:TYR:O	1:D:79:ARG:HG2	2.15	0.46
1:A:79:ARG:NH2	1:A:86:CYS:SG	2.89	0.46
1:A:176:TYR:HE1	1:B:170:VAL:CG1	2.28	0.46
1:D:116:GLU:O	1:D:120:ASN:ND2	2.46	0.46
1:C:173:ASN:ND2	1:C:174:MET:N	2.63	0.46
1:D:18:ARG:HH12	1:D:37:ASN:ND2	2.09	0.45
1:D:56:LEU:HD23	1:D:56:LEU:HA	1.80	0.45
1:D:82:GLU:HG3	1:D:83:GLU:H	1.82	0.45
1:C:10:ILE:HG12	1:C:26:GLY:HA3	1.98	0.45
1:C:33:ARG:HB2	1:C:35:TYR:CE2	2.52	0.45
1:B:126:SER:OG	1:B:156:LYS:HE3	2.17	0.45
1:D:23:ASP:O	1:D:27:ILE:HG13	2.16	0.45
1:B:96:ARG:NH1	4:B:180:HOH:O	2.51	0.44
1:D:132:VAL:HA	1:D:161:ALA:O	2.18	0.44
1:A:84:ARG:HG2	1:A:84:ARG:H	1.60	0.44
1:B:80:ASN:ND2	1:C:64:LYS:HD2	2.26	0.44
1:C:113:ARG:HG3	1:C:126:SER:HB3	1.99	0.44
1:B:84:ARG:O	1:B:88:LYS:HG2	2.18	0.44
1:B:14:LEU:HD11	1:B:77:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:GLY:O	1:C:30:LEU:HG	2.17	0.44
1:A:135:GLU:HG3	1:A:162:ILE:HG21	1.98	0.44
1:C:84:ARG:CG	1:C:84:ARG:NH1	2.77	0.44
1:A:10:ILE:O	1:A:59:LEU:HD12	2.18	0.44
1:C:144:LEU:O	1:C:148:VAL:HG23	2.17	0.44
1:B:82:GLU:HG3	1:B:83:GLU:H	1.82	0.44
1:A:120:ASN:C	1:A:122:ASP:H	2.21	0.43
1:C:154:VAL:O	1:C:154:VAL:HG22	2.18	0.43
1:A:154:VAL:HG22	1:A:154:VAL:O	2.18	0.43
1:D:107:LYS:O	1:D:107:LYS:HE2	2.18	0.43
1:A:42:PHE:C	1:A:42:PHE:CD1	2.91	0.43
1:C:50:ALA:O	1:C:54:ILE:HG13	2.19	0.43
1:C:65:ASP:OD2	1:C:67:LYS:HB2	2.18	0.43
1:A:120:ASN:C	1:A:122:ASP:N	2.72	0.43
1:D:144:LEU:HA	1:D:144:LEU:HD23	1.86	0.43
1:C:139:PHE:HE1	1:D:139:PHE:CZ	2.37	0.43
1:B:70:SER:H	1:B:73:GLU:HB2	1.84	0.43
1:D:39:GLU:HG3	1:D:42:PHE:CE2	2.54	0.43
1:A:60:GLU:HG2	1:A:68:PRO:HB3	2.00	0.43
1:B:22:PHE:HA	1:B:27:ILE:HD11	2.00	0.43
1:C:15:ASP:OD1	1:C:15:ASP:O	2.36	0.43
1:C:127:VAL:HG13	1:C:128:TYR:CD2	2.53	0.43
1:D:121:ILE:N	1:D:124:GLU:HG3	2.11	0.43
1:C:72:GLU:H	1:C:72:GLU:CD	2.21	0.43
1:B:54:ILE:CD1	1:B:74:LEU:HD22	2.48	0.43
1:B:82:GLU:HG3	1:B:83:GLU:N	2.33	0.43
1:C:142:SER:HA	1:C:145:THR:HG22	2.02	0.42
1:A:84:ARG:NH1	1:A:111:ASP:OD1	2.51	0.42
1:B:104:THR:OG1	1:B:106:LEU:HB2	2.18	0.42
1:B:113:ARG:HA	1:B:128:TYR:O	2.19	0.42
1:A:173:ASN:HD22	1:A:174:MET:H	1.63	0.42
1:A:145:THR:HG21	1:C:106:LEU:O	2.20	0.42
1:A:14:LEU:HD11	1:A:77:TYR:CE2	2.54	0.42
1:B:162:ILE:O	1:B:169:ILE:HA	2.20	0.42
1:A:11:THR:HA	1:A:60:GLU:O	2.20	0.42
1:D:83:GLU:HG2	1:D:84:ARG:N	2.35	0.42
1:C:54:ILE:HD12	1:C:74:LEU:HD23	2.02	0.42
1:B:12:GLY:HA2	1:B:20:ILE:O	2.19	0.42
1:D:60:GLU:HG3	1:D:68:PRO:HB3	2.02	0.42
1:B:63:TYR:CZ	1:B:64:LYS:HE3	2.54	0.42
1:D:121:ILE:H	1:D:124:GLU:CG	2.13	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:GLU:O	1:B:53:LEU:HD22	2.20	0.42
1:A:96:ARG:HD3	1:A:96:ARG:HA	1.62	0.42
1:C:178:LYS:CE	1:D:98:ARG:HH22	2.26	0.41
1:B:83:GLU:HG2	1:B:84:ARG:CG	2.49	0.41
1:A:126:SER:O	1:A:156:LYS:NZ	2.53	0.41
1:B:77:TYR:O	1:B:81:VAL:HG23	2.19	0.41
1:A:116:GLU:O	1:A:117:ARG:C	2.58	0.41
1:A:135:GLU:HB2	1:A:162:ILE:HG22	2.02	0.41
1:A:120:ASN:O	1:A:122:ASP:N	2.53	0.41
1:B:33:ARG:O	1:B:96:ARG:NH2	2.53	0.41
1:A:47:LEU:HD22	1:A:82:GLU:OE2	2.20	0.41
1:C:10:ILE:HG12	1:C:26:GLY:CA	2.49	0.41
1:C:79:ARG:NH1	1:C:86:CYS:HB2	2.36	0.41
1:C:164:ASP:OD1	1:C:164:ASP:C	2.59	0.41
1:C:61:VAL:O	1:C:68:PRO:HA	2.20	0.41
1:A:149:ARG:NH2	1:C:108:TYR:CE2	2.89	0.41
1:A:142:SER:HA	1:A:145:THR:HG22	2.02	0.41
1:C:55:ASN:HB2	1:C:71:PHE:CE2	2.55	0.41
1:A:120:ASN:HD21	1:A:123:LYS:N	1.99	0.41
1:A:87:LEU:HB3	1:A:132:VAL:HG11	2.03	0.41
1:A:66:ASN:O	1:A:67:LYS:C	2.60	0.41
1:C:62:LYS:HE3	1:C:62:LYS:HB2	1.89	0.41
1:D:46:SER:OG	1:D:49:GLU:HB2	2.21	0.41
1:A:138:SER:HA	1:B:139:PHE:O	2.21	0.41
1:A:33:ARG:O	1:A:34:HIS:HB2	2.20	0.40
1:B:67:LYS:HG2	1:B:67:LYS:H	1.43	0.40
1:B:23:ASP:O	1:B:27:ILE:HG13	2.21	0.40
1:D:52:TYR:CE1	1:D:93:LYS:HG3	2.55	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	169/171 (99%)	155 (92%)	12 (7%)	2 (1%)	16 15
1	B	169/171 (99%)	158 (94%)	11 (6%)	0	100 100
1	C	169/171 (99%)	156 (92%)	13 (8%)	0	100 100
1	D	169/171 (99%)	155 (92%)	10 (6%)	4 (2%)	7 5
All	All	676/684 (99%)	624 (92%)	46 (7%)	6 (1%)	21 22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	117	ARG
1	A	117	ARG
1	D	121	ILE
1	D	34	HIS
1	D	66	ASN
1	A	121	ILE

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	151/151 (100%)	121 (80%)	30 (20%)	1 1
1	B	151/151 (100%)	124 (82%)	27 (18%)	2 1
1	C	151/151 (100%)	121 (80%)	30 (20%)	1 1
1	D	151/151 (100%)	124 (82%)	27 (18%)	2 1
All	All	604/604 (100%)	490 (81%)	114 (19%)	2 1

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	11	THR
1	A	13	LEU
1	A	17	ASP
1	A	24	LYS

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Mol	Chain	Res	Type
1	A	28	SER
1	A	29	LYS
1	A	31	SER
1	A	33	ARG
1	A	37	ASN
1	A	47	LEU
1	A	51	LEU
1	A	55	ASN
1	A	56	LEU
1	A	66	ASN
1	A	76	GLU
1	A	79	ARG
1	A	84	ARG
1	A	85	LEU
1	A	90	LEU
1	A	96	ARG
1	A	113	ARG
1	A	117	ARG
1	A	123	LYS
1	A	124	GLU
1	A	136	ASP
1	A	138	SER
1	A	145	THR
1	A	150	VAL
1	A	174	MET
1	B	18	ARG
1	B	22	PHE
1	B	24	LYS
1	B	25	ASN
1	B	31	SER
1	B	33	ARG
1	B	37	ASN
1	B	47	LEU
1	B	53	LEU
1	B	55	ASN
1	B	62	LYS
1	B	65	ASP
1	B	67	LYS
1	B	76	GLU
1	B	79	ARG
1	B	83	GLU
1	B	96	ARG

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Mol	Chain	Res	Type
1	B	102	VAL
1	B	103	LYS
1	B	106	LEU
1	B	107	LYS
1	B	114	LEU
1	B	116	GLU
1	B	123	LYS
1	B	131	LYS
1	B	135	GLU
1	B	155	ARG
1	C	11	THR
1	C	13	LEU
1	C	17	ASP
1	C	24	LYS
1	C	25	ASN
1	C	31	SER
1	C	33	ARG
1	C	47	LEU
1	C	48	VAL
1	C	51	LEU
1	C	56	LEU
1	C	66	ASN
1	C	67	LYS
1	C	73	GLU
1	C	79	ARG
1	C	84	ARG
1	C	85	LEU
1	C	90	LEU
1	C	96	ARG
1	C	113	ARG
1	C	117	ARG
1	C	123	LYS
1	C	124	GLU
1	C	129	LEU
1	C	136	ASP
1	C	138	SER
1	C	139	PHE
1	C	145	THR
1	C	174	MET
1	C	178	LYS
1	D	18	ARG
1	D	22	PHE

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Mol	Chain	Res	Type
1	D	25	ASN
1	D	29	LYS
1	D	33	ARG
1	D	37	ASN
1	D	39	GLU
1	D	47	LEU
1	D	53	LEU
1	D	55	ASN
1	D	64	LYS
1	D	67	LYS
1	D	76	GLU
1	D	79	ARG
1	D	82	GLU
1	D	83	GLU
1	D	96	ARG
1	D	106	LEU
1	D	107	LYS
1	D	117	ARG
1	D	121	ILE
1	D	126	SER
1	D	131	LYS
1	D	135	GLU
1	D	144	LEU
1	D	153	SER
1	D	178	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	120	ASN
1	A	173	ASN
1	B	66	ASN
1	B	80	ASN
1	C	25	ASN
1	C	34	HIS
1	C	173	ASN
1	D	37	ASN
1	D	66	ASN
1	D	80	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	1	-	4,4,4	0.08	0	6,6,6	0.14	0
2	SO4	C	2	-	4,4,4	0.08	0	6,6,6	0.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1	-	-	0/0/0/0	0/0/0/0
2	SO4	C	2	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.