Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 01:07 AM EDT

PDB ID	:	1I8D
Title	:	CRYSTAL STRUCTURE OF RIBOFLAVIN SYNTHASE
Authors	:	Liao, D.-I.; Wawrzak, Z.; Calabrese, J.C.; Viitanen, P.V.; Jordan, D.B.
Deposited on	:	2001-03-13
Resolution	:	2.00 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 (i)) were used in the production of this report:

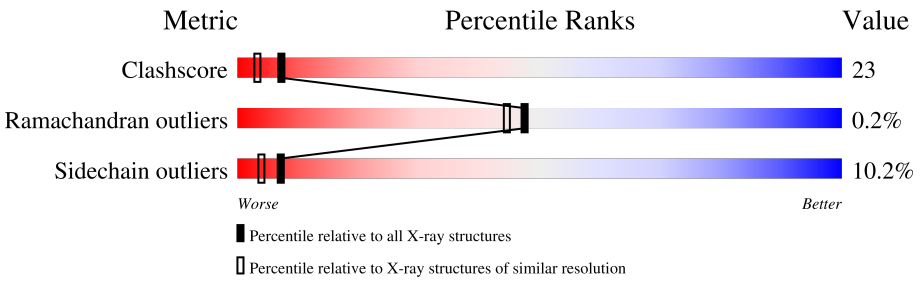
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	213	54% 37% 6% • •
1	B	213	51% 33% 8% • 6%
1	C	213	48% 29% 8% • 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4807 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 RIBOFLAVIN SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	206	1593	1003	277	303	10	0	0	0
1	B	201	1555	983	270	292	10	0	0	0
1	C	185	1430	909	245	267	9	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	101	101	101	0	0
2	B	54	54	54	0	0
2	C	74	74	74	0	0

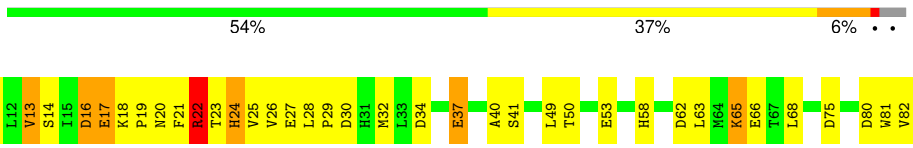
3 Residue-property plots (i)

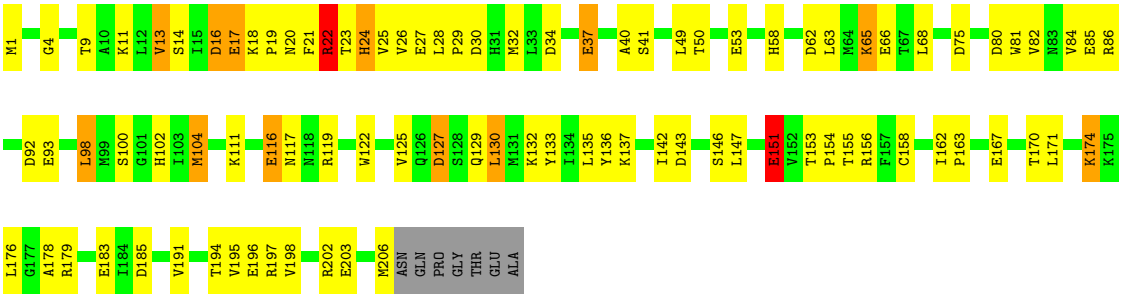
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: RIBOFLAVIN SYNTHASE

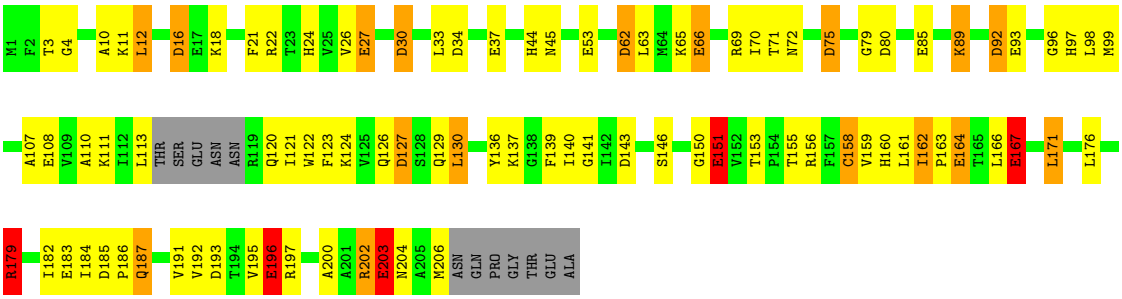
Chain A:





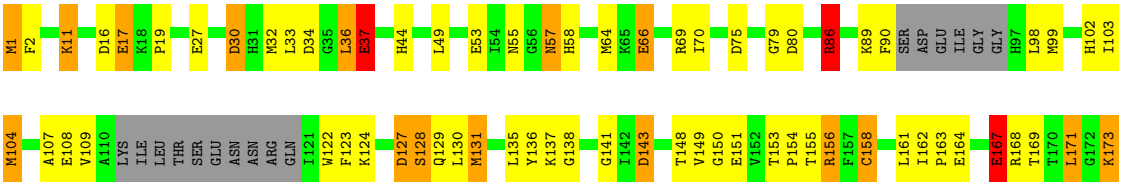
• Molecule 1: RIBOFLAVIN SYNTHASE

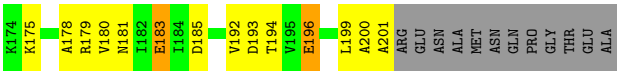
Chain B:



• Molecule 1: RIBOFLAVIN SYNTHASE

Chain C:




K174
K175
A178
R179
V180
N181
I182
E183
I184
D185
V192
D193
T194
V195
E196
L199
A200
A201
ARG
GLU
ASN
ALA
MET
ASN
GLN
PRO
GLY
THR
GLU
ALA

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.08Å 61.70Å 219.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.239 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4807	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	0.94	13/1617 (0.8%)	1.26	19/2188 (0.9%)
1	B	0.92	13/1578 (0.8%)	1.27	16/2133 (0.8%)
1	C	0.92	11/1452 (0.8%)	1.25	17/1965 (0.9%)
All	All	0.93	37/4647 (0.8%)	1.26	52/6286 (0.8%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	GLU	CD-OE2	9.20	1.35	1.25
1	C	164	GLU	CD-OE1	-8.52	1.16	1.25
1	B	53	GLU	CD-OE2	8.41	1.34	1.25
1	A	167	GLU	CD-OE2	7.90	1.34	1.25
1	C	167	GLU	CD-OE2	7.84	1.34	1.25
1	B	66	GLU	CD-OE2	7.82	1.34	1.25
1	B	167	GLU	CD-OE2	7.65	1.34	1.25
1	C	164	GLU	CD-OE2	7.52	1.33	1.25
1	C	17	GLU	CD-OE2	7.19	1.33	1.25
1	C	196	GLU	CD-OE2	7.19	1.33	1.25
1	A	53	GLU	CD-OE2	7.09	1.33	1.25
1	B	37	GLU	CD-OE2	6.53	1.32	1.25
1	B	183	GLU	CD-OE2	6.33	1.32	1.25
1	A	27	GLU	CD-OE2	6.30	1.32	1.25
1	A	37	GLU	CD-OE2	6.27	1.32	1.25
1	B	203	GLU	CD-OE2	6.23	1.32	1.25
1	A	93	GLU	CD-OE2	6.16	1.32	1.25
1	A	183	GLU	CD-OE2	5.99	1.32	1.25
1	B	151	GLU	CD-OE2	5.97	1.32	1.25
1	B	108	GLU	CD-OE2	5.87	1.32	1.25
1	A	151	GLU	CD-OE2	5.86	1.32	1.25
1	C	37	GLU	CD-OE2	5.86	1.32	1.25
1	A	196	GLU	CD-OE2	5.81	1.32	1.25
1	B	27	GLU	CD-OE2	5.76	1.31	1.25
1	C	183	GLU	CD-OE2	5.72	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	GLU	CD-OE2	5.71	1.31	1.25
1	B	196	GLU	CD-OE2	5.63	1.31	1.25
1	B	85	GLU	CD-OE2	5.54	1.31	1.25
1	A	66	GLU	CD-OE2	5.52	1.31	1.25
1	C	108	GLU	CD-OE2	5.52	1.31	1.25
1	B	93	GLU	CD-OE2	5.30	1.31	1.25
1	C	66	GLU	CD-OE2	5.17	1.31	1.25
1	C	53	GLU	CD-OE2	5.15	1.31	1.25
1	A	85	GLU	CD-OE2	5.12	1.31	1.25
1	A	17	GLU	CD-OE2	5.09	1.31	1.25
1	C	27	GLU	CD-OE1	-5.07	1.20	1.25
1	A	116	GLU	CD-OE2	5.05	1.31	1.25

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	127	ASP	CB-CG-OD2	-9.75	109.53	118.30
1	A	75	ASP	CB-CG-OD2	-8.84	110.34	118.30
1	A	143	ASP	CB-CG-OD1	8.08	125.58	118.30
1	C	30	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	B	143	ASP	CB-CG-OD2	-7.87	111.22	118.30
1	C	127	ASP	CB-CG-OD1	7.75	125.27	118.30
1	B	16	ASP	CB-CG-OD1	7.61	125.15	118.30
1	B	179	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	B	143	ASP	CB-CG-OD1	7.42	124.97	118.30
1	A	34	ASP	CB-CG-OD1	7.40	124.96	118.30
1	B	127	ASP	CB-CG-OD2	-7.29	111.73	118.30
1	A	143	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	A	30	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	C	80	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	B	16	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	A	34	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	B	92	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	A	16	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	C	143	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	C	193	ASP	CB-CG-OD2	-6.61	112.36	118.30
1	C	185	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	C	30	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	16	ASP	CB-CG-OD1	6.25	123.92	118.30
1	B	75	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	C	143	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	185	ASP	CB-CG-OD2	-6.18	112.74	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	30	ASP	CB-CG-OD1	6.17	123.85	118.30
1	C	34	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	A	127	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	80	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	B	80	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	B	127	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	127	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	C	75	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	C	16	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	C	16	ASP	CB-CG-OD1	5.74	123.47	118.30
1	C	34	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	62	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	B	92	ASP	CB-CG-OD1	5.56	123.30	118.30
1	C	86	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	75	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	22	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	80	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	193	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	A	80	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	75	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	92	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	C	75	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	193	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	156	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	34	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	A	119	ARG	NE-CZ-NH1	5.06	122.83	120.30

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	A	1593	0	1618	65	0
1	B	1555	0	1587	93	0
1	C	1430	0	1459	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	101	0	0	4	0
2	B	54	0	0	1	0
2	C	74	0	0	1	0
All	All	4807	0	4664	208	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 23.

All (208) 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:22:ARG:HD3	1:A:24:HIS:HE1	1.19	1.06
1:B:187:GLN:HE21	1:B:187:GLN:H	1.03	1.01
1:A:22:ARG:HD3	1:A:24:HIS:CE1	1.96	1.00
1:B:162:ILE:HD13	1:B:162:ILE:H	1.31	0.94
1:A:22:ARG:HH11	1:A:24:HIS:CE1	1.98	0.81
1:B:120:GLN:NE2	1:B:122:TRP:NE1	2.30	0.80
1:C:104:MET:CE	1:C:130:LEU:HD22	2.11	0.79
1:C:161:LEU:HD11	1:C:171:LEU:HD13	1.64	0.79
1:B:89:LYS:HD3	1:B:92:ASP:OD2	1.83	0.79
1:A:18:LYS:HB3	1:A:19:PRO:HD2	1.65	0.78
1:B:136:TYR:CD1	1:B:137:LYS:HG3	2.18	0.78
1:B:187:GLN:H	1:B:187:GLN:NE2	1.82	0.77
1:B:155:THR:HB	1:B:156:ARG:NH1	2.01	0.76
1:C:104:MET:HE3	1:C:130:LEU:HD22	1.66	0.76
1:B:18:LYS:HG3	1:B:21:PHE:CZ	2.21	0.75
1:B:185:ASP:OD1	1:B:187:GLN:NE2	2.18	0.75
1:A:22:ARG:HH11	1:A:24:HIS:HE1	1.34	0.75
1:A:13:VAL:HG12	1:A:25:VAL:O	1.87	0.74
1:A:153:THR:HB	1:A:154:PRO:HD2	1.69	0.71
1:B:136:TYR:HE1	1:B:137:LYS:HE2	1.56	0.71
1:B:89:LYS:HD3	1:B:89:LYS:N	2.08	0.69
1:B:192:VAL:O	1:B:196:GLU:HG2	1.93	0.69
1:A:122:TRP:CD2	1:A:158:CYS:HB3	2.28	0.69
1:B:120:GLN:NE2	1:B:122:TRP:HE1	1.89	0.68
1:B:187:GLN:HE21	1:B:187:GLN:N	1.86	0.68
1:B:187:GLN:O	1:B:191:VAL:HG23	1.93	0.68
1:A:202:ARG:NH1	1:B:196:GLU:OE2	2.27	0.68
1:B:18:LYS:HG3	1:B:21:PHE:CE2	2.29	0.67
1:B:186:PRO:HD2	1:B:187:GLN:NE2	2.10	0.67
1:B:120:GLN:HE22	1:B:122:TRP:HE1	1.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:GLN:HG3	1:B:160:HIS:CE1	2.31	0.66
1:A:142:ILE:HG13	1:A:147:LEU:HD12	1.78	0.66
1:C:90:PHE:N	2:C:265:HOH:O	2.29	0.66
1:B:3:THR:HB	1:B:96:GLY:HA3	1.76	0.66
1:B:151:GLU:CD	1:B:151:GLU:H	2.00	0.65
1:A:1:MET:CE	1:A:100:SER:HA	2.27	0.65
1:B:136:TYR:HE1	1:B:137:LYS:CE	2.10	0.65
1:B:186:PRO:HD2	1:B:187:GLN:HE22	1.62	0.64
1:C:69:ARG:NH2	1:C:70:ILE:HD12	2.11	0.64
1:A:28:LEU:HB2	1:A:29:PRO:HD2	1.77	0.64
1:B:163:PRO:HA	1:B:166:LEU:HD12	1.78	0.64
1:B:203:GLU:O	1:B:206:MET:HB3	1.97	0.64
1:C:135:LEU:O	1:C:149:VAL:HB	1.98	0.63
1:C:161:LEU:CD1	1:C:171:LEU:HD13	2.26	0.63
1:B:71:THR:O	1:B:179:ARG:NH2	2.31	0.63
1:B:98:LEU:N	1:B:98:LEU:HD23	2.12	0.63
1:C:143:ASP:OD2	1:C:180:VAL:HG12	2.00	0.62
1:A:197:ARG:NH1	2:A:271:HOH:O	2.28	0.62
1:B:136:TYR:HD1	1:B:137:LYS:HG3	1.62	0.62
1:C:2:PHE:O	1:C:98:LEU:HD12	2.00	0.61
1:C:127:ASP:O	1:C:129:GLN:N	2.34	0.61
1:A:16:ASP:HB3	1:A:23:THR:HB	1.83	0.61
1:B:121:ILE:HD12	1:B:161:LEU:HD11	1.82	0.61
1:B:66:GLU:O	1:B:70:ILE:HD12	2.02	0.60
1:A:18:LYS:HB3	1:A:19:PRO:CD	2.32	0.60
1:C:69:ARG:HH22	1:C:70:ILE:HD12	1.67	0.59
1:A:153:THR:HB	1:A:154:PRO:CD	2.32	0.59
1:A:1:MET:HE1	1:A:100:SER:HA	1.84	0.58
1:C:104:MET:HG2	1:C:130:LEU:HD13	1.85	0.58
1:B:72:ASN:HA	1:B:179:ARG:HH21	1.68	0.58
1:B:11:LYS:HE2	1:B:79:GLY:HA2	1.85	0.58
1:B:136:TYR:CD1	1:B:137:LYS:CG	2.86	0.58
1:A:125:VAL:HG22	1:A:155:THR:O	2.03	0.57
1:A:191:VAL:O	1:A:195:VAL:HG23	2.04	0.57
1:C:30:ASP:HA	1:C:33:LEU:HD12	1.84	0.57
1:B:162:ILE:H	1:B:162:ILE:CD1	2.11	0.57
1:A:65:LYS:HA	1:A:68:LEU:HD12	1.85	0.57
1:B:72:ASN:HA	1:B:179:ARG:NH2	2.19	0.57
1:C:11:LYS:HD3	1:C:79:GLY:HA2	1.86	0.56
1:B:97:HIS:O	1:B:99:MET:HG3	2.05	0.56
1:C:122:TRP:CE2	1:C:158:CYS:HB3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:MET:HE2	1:C:130:LEU:HD22	1.87	0.56
1:C:99:MET:HE3	1:C:141:GLY:HA3	1.89	0.55
1:B:156:ARG:HG3	1:B:156:ARG:HH11	1.71	0.55
1:A:17:GLU:OE1	1:A:22:ARG:HB2	2.05	0.55
1:C:122:TRP:CZ2	1:C:151:GLU:HB3	2.42	0.55
1:B:110:ALA:C	1:B:176:LEU:HD11	2.27	0.55
1:A:102:HIS:NE2	1:A:104:MET:HG3	2.22	0.55
2:A:309:HOH:O	1:C:1:MET:HE2	2.07	0.54
1:C:167:GLU:HG2	1:C:168:ARG:HG2	1.88	0.54
1:A:111:LYS:HA	1:A:176:LEU:HD21	1.90	0.54
1:B:12:LEU:HD21	1:B:24:HIS:HB3	1.88	0.54
1:A:32:MET:O	1:A:86:ARG:NH1	2.41	0.53
1:B:4:GLY:HA3	1:B:146:SER:HB2	1.90	0.53
1:C:162:ILE:HB	1:C:163:PRO:HD2	1.90	0.53
1:A:127:ASP:OD2	1:A:129:GLN:HB2	2.09	0.53
1:C:66:GLU:OE2	1:C:69:ARG:NH2	2.27	0.53
1:B:179:ARG:NH2	2:B:251:HOH:O	2.40	0.53
1:A:136:TYR:O	1:A:137:LYS:HB2	2.09	0.52
1:B:89:LYS:HD3	1:B:89:LYS:H	1.74	0.52
1:C:107:ALA:O	1:C:179:ARG:HA	2.09	0.52
1:C:124:LYS:HD3	1:C:156:ARG:CZ	2.40	0.52
1:A:65:LYS:HE3	1:A:68:LEU:CD1	2.40	0.52
1:A:4:GLY:HA3	1:A:146:SER:HB2	1.91	0.52
1:B:89:LYS:N	1:B:89:LYS:CD	2.72	0.52
1:B:22:ARG:NE	1:B:24:HIS:NE2	2.58	0.51
1:B:136:TYR:CE1	1:B:137:LYS:CG	2.93	0.51
1:B:121:ILE:HD11	1:B:161:LEU:HD12	1.92	0.51
1:A:28:LEU:HB2	1:A:29:PRO:CD	2.40	0.51
1:C:103:ILE:HD12	1:C:181:ASN:HB3	1.92	0.51
1:B:111:LYS:N	1:B:176:LEU:HD11	2.26	0.51
1:B:162:ILE:HD13	1:B:162:ILE:N	2.13	0.51
1:C:136:TYR:O	1:C:137:LYS:HB2	2.11	0.51
1:B:69:ARG:NH1	1:B:70:ILE:HG13	2.26	0.50
1:A:22:ARG:NH2	2:A:285:HOH:O	2.44	0.50
1:B:129:GLN:HG2	1:B:130:LEU:HD13	1.93	0.50
1:B:136:TYR:CD2	1:B:151:GLU:HA	2.46	0.50
1:A:26:VAL:CG2	1:A:28:LEU:HD23	2.42	0.50
1:B:136:TYR:HD2	1:B:151:GLU:HA	1.77	0.50
1:B:111:LYS:HE2	1:B:113:LEU:HD21	1.93	0.49
1:C:104:MET:HE3	1:C:130:LEU:CD2	2.40	0.49
1:A:127:ASP:HB3	1:A:130:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:PHE:HE1	1:B:159:VAL:HG22	1.78	0.49
1:B:10:ALA:HB1	1:B:27:GLU:O	2.13	0.48
1:A:11:LYS:HB2	1:A:81:TRP:CE2	2.48	0.48
1:B:12:LEU:HD23	1:B:26:VAL:HG12	1.95	0.48
1:A:162:ILE:HB	1:A:163:PRO:HD2	1.96	0.48
1:A:1:MET:HE2	1:A:100:SER:HA	1.93	0.47
1:B:136:TYR:CE1	1:B:137:LYS:HG2	2.49	0.47
1:C:55:ASN:O	1:C:58:HIS:HB2	2.13	0.47
1:C:123:PHE:O	1:C:156:ARG:HB2	2.14	0.47
1:C:138:GLY:O	1:C:148:THR:HA	2.14	0.47
1:B:153:THR:C	1:B:155:THR:H	2.18	0.47
1:A:151:GLU:HG2	1:A:158:CYS:SG	2.55	0.46
1:B:121:ILE:CD1	1:B:161:LEU:CD1	2.94	0.46
1:B:122:TRP:CD2	1:B:158:CYS:HB3	2.51	0.46
1:A:40:ALA:O	1:A:50:THR:HA	2.15	0.46
1:B:127:ASP:HB3	1:B:129:GLN:NE2	2.31	0.46
1:B:202:ARG:HH12	1:C:199:LEU:HD13	1.81	0.46
1:A:194:THR:O	1:A:198:VAL:HG23	2.16	0.46
1:C:36:LEU:C	1:C:37:GLU:HG2	2.36	0.46
1:A:1:MET:SD	1:A:98:LEU:HD23	2.56	0.45
1:A:65:LYS:HE3	1:A:68:LEU:HD13	1.98	0.45
1:C:138:GLY:O	1:C:149:VAL:N	2.38	0.45
1:A:50:THR:O	1:A:50:THR:OG1	2.34	0.45
1:B:30:ASP:HA	1:B:33:LEU:CD1	2.47	0.45
1:A:41:SER:HA	1:A:49:LEU:O	2.17	0.45
1:B:171:LEU:HA	1:B:171:LEU:HD23	1.57	0.45
1:B:121:ILE:CD1	1:B:161:LEU:HD11	2.45	0.45
1:A:195:VAL:HB	1:C:194:THR:HG21	1.98	0.44
1:B:62:ASP:C	1:B:63:LEU:HD12	2.37	0.44
1:B:89:LYS:O	1:B:92:ASP:HB2	2.16	0.44
1:C:155:THR:OG1	1:C:156:ARG:HD2	2.17	0.44
1:B:66:GLU:C	1:B:70:ILE:HD12	2.37	0.44
1:B:72:ASN:O	1:B:75:ASP:HB2	2.17	0.44
1:B:120:GLN:CG	1:B:160:HIS:CE1	3.00	0.44
1:B:184:ILE:HD13	1:B:184:ILE:HA	1.70	0.44
1:C:44:HIS:CD2	1:C:49:LEU:HD12	2.52	0.44
1:C:200:ALA:O	1:C:201:ALA:O	2.35	0.44
1:A:174:LYS:HG2	1:A:178:ALA:HB1	2.00	0.44
1:B:63:LEU:HD12	1:B:63:LEU:N	2.32	0.44
1:C:104:MET:HG2	1:C:130:LEU:CD1	2.47	0.44
1:C:192:VAL:O	1:C:196:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ASN:O	1:A:21:PHE:HB3	2.18	0.44
1:A:151:GLU:HG2	1:A:151:GLU:H	1.47	0.44
1:A:11:LYS:HB2	1:A:81:TRP:CD2	2.53	0.43
1:A:116:GLU:O	1:A:117:ASN:HB2	2.18	0.43
1:B:155:THR:HB	1:B:156:ARG:HH11	1.78	0.43
1:B:164:GLU:O	1:B:167:GLU:N	2.41	0.43
1:B:65:LYS:HD3	1:B:65:LYS:HA	1.83	0.43
1:A:130:LEU:HD12	1:A:130:LEU:HA	1.50	0.43
1:B:136:TYR:CD2	1:B:150:GLY:O	2.72	0.43
1:C:109:VAL:HG23	1:C:178:ALA:O	2.19	0.43
1:B:44:HIS:O	1:B:45:ASN:HB2	2.18	0.43
1:B:111:LYS:HE2	1:B:113:LEU:HD11	2.01	0.43
1:A:122:TRP:CE2	1:A:158:CYS:HB3	2.54	0.43
1:A:130:LEU:HD12	1:A:133:TYR:CE1	2.53	0.43
1:B:196:GLU:HG2	1:B:196:GLU:H	1.50	0.43
1:A:63:LEU:HD12	1:A:63:LEU:N	2.34	0.42
1:C:32:MET:O	1:C:86:ARG:HD3	2.18	0.42
1:C:57:ASN:HD22	1:C:57:ASN:H	1.66	0.42
1:C:128:SER:O	1:C:131:MET:HB2	2.18	0.42
1:A:170:THR:OG1	2:A:273:HOH:O	2.22	0.42
1:B:155:THR:HB	1:B:156:ARG:HH12	1.82	0.42
1:A:21:PHE:HB2	1:A:63:LEU:O	2.19	0.42
1:A:153:THR:CB	1:A:154:PRO:CD	2.94	0.42
1:C:86:ARG:HE	1:C:86:ARG:HB3	1.68	0.42
1:B:204:ASN:C	1:B:206:MET:H	2.23	0.42
1:A:127:ASP:O	1:A:130:LEU:HB2	2.20	0.42
1:B:140:ILE:HD11	1:B:182:ILE:HG23	2.01	0.42
1:A:22:ARG:NH1	1:A:24:HIS:HE1	2.11	0.41
1:C:102:HIS:O	1:C:183:GLU:HG3	2.20	0.41
1:C:169:THR:OG1	1:C:171:LEU:HB2	2.20	0.41
1:B:66:GLU:OE1	1:B:69:ARG:NH2	2.50	0.41
1:B:197:ARG:O	1:B:200:ALA:HB3	2.20	0.41
1:C:136:TYR:HD1	1:C:150:GLY:O	2.02	0.41
1:A:82:VAL:HG23	1:A:84:VAL:HG13	2.01	0.41
1:C:36:LEU:HD23	1:C:36:LEU:HA	1.92	0.41
1:C:44:HIS:CG	1:C:49:LEU:HD12	2.56	0.41
1:B:136:TYR:CD2	1:B:150:GLY:C	2.93	0.41
1:B:140:ILE:HD12	1:B:141:GLY:H	1.86	0.41
1:A:22:ARG:HD2	1:A:68:LEU:CD2	2.51	0.41
1:B:191:VAL:O	1:B:195:VAL:HG23	2.21	0.41
1:A:13:VAL:HG12	1:A:25:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ILE:HD11	1:B:161:LEU:CD1	2.50	0.41
1:A:62:ASP:C	1:A:63:LEU:HD12	2.41	0.41
1:B:30:ASP:HA	1:B:33:LEU:HD12	2.03	0.41
1:C:173:LYS:HB2	1:C:173:LYS:HE3	1.89	0.41
1:B:12:LEU:HD23	1:B:12:LEU:HA	1.83	0.41
1:C:104:MET:HE2	1:C:130:LEU:HD13	2.03	0.41
1:C:153:THR:HB	1:C:154:PRO:HD2	2.03	0.41
1:A:117:ASN:ND2	1:C:19:PRO:O	2.43	0.41
1:C:32:MET:HE3	1:C:86:ARG:CG	2.51	0.41
1:A:9:THR:HA	1:A:82:VAL:O	2.20	0.40
1:A:26:VAL:HG23	1:A:28:LEU:HD23	2.03	0.40
1:B:107:ALA:HB3	1:B:182:ILE:HD11	2.04	0.40
1:B:107:ALA:HB2	1:B:182:ILE:CD1	2.50	0.40
1:A:28:LEU:CB	1:A:29:PRO:CD	3.00	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	204/213 (96%)	202 (99%)	2 (1%)	0	100	100
1	B	197/213 (92%)	190 (96%)	7 (4%)	0	100	100
1	C	179/213 (84%)	172 (96%)	6 (3%)	1 (1%)	25	19
All	All	580/639 (91%)	564 (97%)	15 (3%)	1 (0%)	47	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	128	SER

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	177/182 (97%)	160 (90%)	17 (10%)	8 5
1	B	172/182 (94%)	154 (90%)	18 (10%)	7 4
1	C	159/182 (87%)	142 (89%)	17 (11%)	6 3
All	All	508/546 (93%)	456 (90%)	52 (10%)	7 4

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	14	SER
1	A	22	ARG
1	A	24	HIS
1	A	37	GLU
1	A	58	HIS
1	A	65	LYS
1	A	98	LEU
1	A	104	MET
1	A	130	LEU
1	A	132	LYS
1	A	135	LEU
1	A	151	GLU
1	A	171	LEU
1	A	174	LYS
1	A	179	ARG
1	A	206	MET
1	B	12	LEU
1	B	16	ASP
1	B	30	ASP
1	B	89	LYS
1	B	124	LYS
1	B	126	GLN
1	B	130	LEU
1	B	139	PHE
1	B	151	GLU

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Mol	Chain	Res	Type
1	B	158	CYS
1	B	162	ILE
1	B	167	GLU
1	B	171	LEU
1	B	179	ARG
1	B	187	GLN
1	B	196	GLU
1	B	202	ARG
1	B	203	GLU
1	C	1	MET
1	C	11	LYS
1	C	17	GLU
1	C	36	LEU
1	C	37	GLU
1	C	57	ASN
1	C	64	MET
1	C	86	ARG
1	C	89	LYS
1	C	104	MET
1	C	131	MET
1	C	156	ARG
1	C	158	CYS
1	C	167	GLU
1	C	171	LEU
1	C	173	LYS
1	C	175	LYS

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

Mol	Chain	Res	Type
1	A	24	HIS
1	A	31	HIS
1	A	126	GLN
1	B	31	HIS
1	B	97	HIS
1	B	120	GLN
1	B	187	GLN
1	B	204	ASN
1	C	57	ASN
1	C	97	HIS
1	C	187	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)

There are no ligands in this entry.

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.