Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 07:57 PM EDT

PDB ID	:	2G6V
Title	:	The crystal structure of ribD from Escherichia coli
Authors	:	Stenmark, P.; Moche, M.; Gurmu, D.; Nordlund, P.; Structural Proteomics in Europe (SPINE)
Deposited on	:	2006-02-25
Resolution	:	2.60 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:

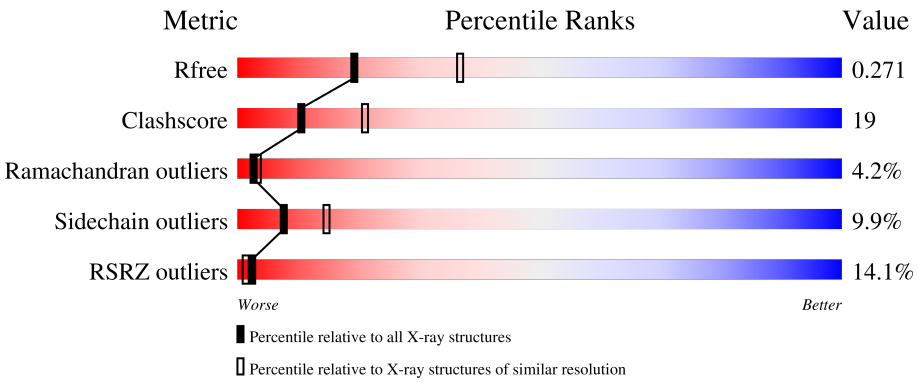
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	402	12% 54% 28% 5% 12%
1	B	402	12% 59% 25% 6% 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5530 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 biosynthesis protein ribD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	355	2709	1708	488	498	6	9	0	0	0
1	B	363	2756	1730	503	511	3	9	0	0	0

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	EXPRESSION TAG	UNP P25539
A	-25	ASP	-	EXPRESSION TAG	UNP P25539
A	-24	TYR	-	EXPRESSION TAG	UNP P25539
A	-23	LYS	-	EXPRESSION TAG	UNP P25539
A	-22	ASP	-	EXPRESSION TAG	UNP P25539
A	-21	ASP	-	EXPRESSION TAG	UNP P25539
A	-20	ASP	-	EXPRESSION TAG	UNP P25539
A	-19	ASP	-	EXPRESSION TAG	UNP P25539
A	-18	LYS	-	EXPRESSION TAG	UNP P25539
A	-17	GLY	-	EXPRESSION TAG	UNP P25539
A	-16	SER	-	EXPRESSION TAG	UNP P25539
A	-15	SER	-	EXPRESSION TAG	UNP P25539
A	-14	THR	-	EXPRESSION TAG	UNP P25539
A	-13	SER	-	EXPRESSION TAG	UNP P25539
A	-12	LEU	-	EXPRESSION TAG	UNP P25539
A	-11	TYR	-	EXPRESSION TAG	UNP P25539
A	-10	LYS	-	EXPRESSION TAG	UNP P25539
A	-9	LYS	-	EXPRESSION TAG	UNP P25539
A	-8	ALA	-	EXPRESSION TAG	UNP P25539
A	-7	GLY	-	EXPRESSION TAG	UNP P25539
A	-6	SER	-	EXPRESSION TAG	UNP P25539
A	-5	GLU	-	EXPRESSION TAG	UNP P25539
A	-4	THR	-	EXPRESSION TAG	UNP P25539
A	-3	LEU	-	EXPRESSION TAG	UNP P25539
A	-2	TYR	-	EXPRESSION TAG	UNP P25539

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ILE	-	EXPRESSION TAG	UNP P25539
A	0	GLN	-	EXPRESSION TAG	UNP P25539
A	1	GLY	-	EXPRESSION TAG	UNP P25539
A	7	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	58	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	100	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	127	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	128	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	142	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	163	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	285	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	286	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	368	SER	-	EXPRESSION TAG	UNP P25539
A	369	THR	-	EXPRESSION TAG	UNP P25539
A	370	HIS	-	EXPRESSION TAG	UNP P25539
A	371	HIS	-	EXPRESSION TAG	UNP P25539
A	372	HIS	-	EXPRESSION TAG	UNP P25539
A	373	HIS	-	EXPRESSION TAG	UNP P25539
A	374	HIS	-	EXPRESSION TAG	UNP P25539
A	375	HIS	-	EXPRESSION TAG	UNP P25539
B	-26	MET	-	EXPRESSION TAG	UNP P25539
B	-25	ASP	-	EXPRESSION TAG	UNP P25539
B	-24	TYR	-	EXPRESSION TAG	UNP P25539
B	-23	LYS	-	EXPRESSION TAG	UNP P25539
B	-22	ASP	-	EXPRESSION TAG	UNP P25539
B	-21	ASP	-	EXPRESSION TAG	UNP P25539
B	-20	ASP	-	EXPRESSION TAG	UNP P25539
B	-19	ASP	-	EXPRESSION TAG	UNP P25539
B	-18	LYS	-	EXPRESSION TAG	UNP P25539
B	-17	GLY	-	EXPRESSION TAG	UNP P25539
B	-16	SER	-	EXPRESSION TAG	UNP P25539
B	-15	SER	-	EXPRESSION TAG	UNP P25539
B	-14	THR	-	EXPRESSION TAG	UNP P25539
B	-13	SER	-	EXPRESSION TAG	UNP P25539
B	-12	LEU	-	EXPRESSION TAG	UNP P25539
B	-11	TYR	-	EXPRESSION TAG	UNP P25539
B	-10	LYS	-	EXPRESSION TAG	UNP P25539
B	-9	LYS	-	EXPRESSION TAG	UNP P25539
B	-8	ALA	-	EXPRESSION TAG	UNP P25539
B	-7	GLY	-	EXPRESSION TAG	UNP P25539
B	-6	SER	-	EXPRESSION TAG	UNP P25539
B	-5	GLU	-	EXPRESSION TAG	UNP P25539

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	THR	-	EXPRESSION TAG	UNP P25539
B	-3	LEU	-	EXPRESSION TAG	UNP P25539
B	-2	TYR	-	EXPRESSION TAG	UNP P25539
B	-1	ILE	-	EXPRESSION TAG	UNP P25539
B	0	GLN	-	EXPRESSION TAG	UNP P25539
B	1	GLY	-	EXPRESSION TAG	UNP P25539
B	7	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	58	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	100	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	127	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	128	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	142	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	163	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	285	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	286	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	368	SER	-	EXPRESSION TAG	UNP P25539
B	369	THR	-	EXPRESSION TAG	UNP P25539
B	370	HIS	-	EXPRESSION TAG	UNP P25539
B	371	HIS	-	EXPRESSION TAG	UNP P25539
B	372	HIS	-	EXPRESSION TAG	UNP P25539
B	373	HIS	-	EXPRESSION TAG	UNP P25539
B	374	HIS	-	EXPRESSION TAG	UNP P25539
B	375	HIS	-	EXPRESSION TAG	UNP P25539

- Molecule 2 is water.

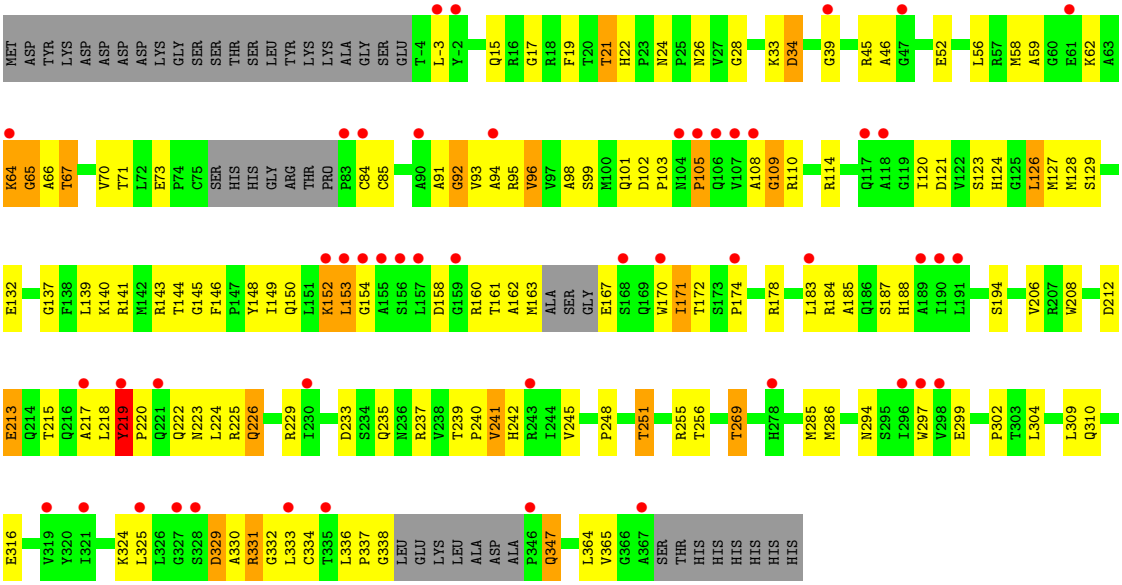
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	42	42	42	0	0
			Total	O		
2	B	23	23	23	0	0

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.

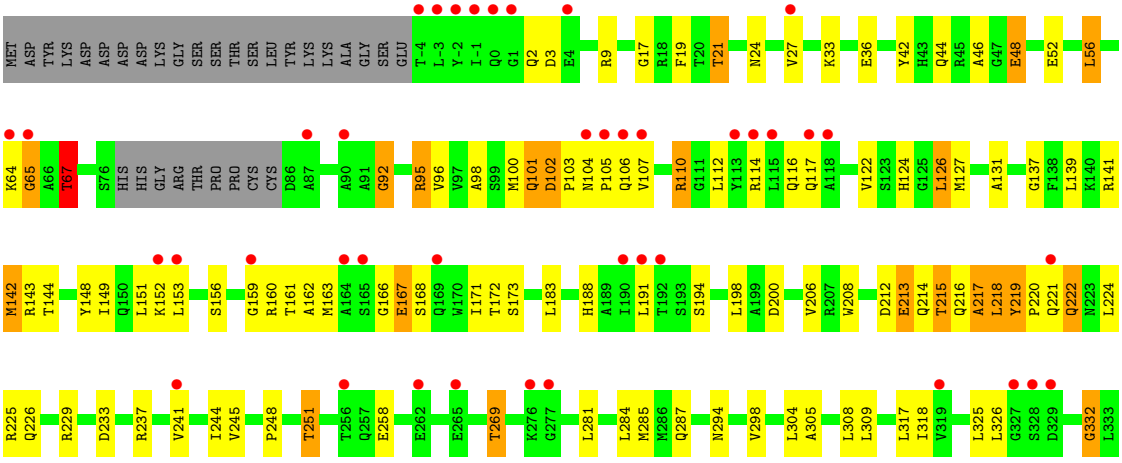
• Molecule 1: Riboflavin biosynthesis protein ribD

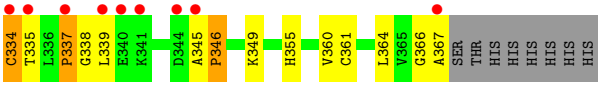
Chain A:



• Molecule 1: Riboflavin biosynthesis protein ribD

Chain B:




C334
T335
L336
P337
G338
L339
E340
K341
D344
A345
P346
K349
H355
V360
C361
L364
V365
G366
A367
SER
THR
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	172.60Å 172.60Å 76.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.25 – 2.60 28.25 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.25-2.60) 100.0 (28.25-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.244 , 0.285 0.237 , 0.271	Depositor DCC
R_{free} test set	2010 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	71.0	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 82.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5530	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.47	0/2753	0.66	2/3723 (0.1%)
1	B	0.41	0/2800	0.62	0/3790
All	All	0.44	0/5553	0.64	2/7513 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	153	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	67	THR	N-CA-C	5.20	125.04	111.00

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	2709	0	2698	111	0
1	B	2756	0	2735	97	0
2	A	42	0	0	6	0
2	B	23	0	0	6	0
All	All	5530	0	5433	202	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 (202) 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:B:213:GLU:HA	2:B:395:HOH:O	1.32	1.25
1:B:194:SER:HB3	1:B:233:ASP:HB3	1.14	1.11
1:B:206:VAL:H	1:B:226:GLN:HE22	1.04	1.00
1:B:194:SER:CB	1:B:233:ASP:HB3	1.99	0.91
1:B:141:ARG:HH11	1:B:294:ASN:HD21	1.20	0.87
1:B:160:ARG:HA	1:B:332:GLY:HA3	1.59	0.85
1:A:194:SER:HB3	1:A:233:ASP:HB3	1.58	0.84
1:A:152:LYS:HE3	1:A:163:MSE:SE	2.28	0.83
1:A:141:ARG:HH11	1:A:294:ASN:HD21	1.26	0.82
1:A:206:VAL:H	1:A:226:GLN:NE2	1.77	0.81
1:A:229:ARG:NH2	1:A:248:PRO:O	2.15	0.78
1:A:39:GLY:HA2	1:A:58:MSE:HE2	1.63	0.78
1:A:33:LYS:HE3	1:A:65:GLY:HA3	1.65	0.78
1:A:218:LEU:HG	1:A:219:TYR:N	1.98	0.77
1:A:24:ASN:ND2	1:A:46:ALA:HA	1.98	0.77
1:A:206:VAL:H	1:A:226:GLN:HE22	1.31	0.77
1:B:160:ARG:HA	1:B:332:GLY:CA	2.15	0.77
1:B:142:MSE:HA	1:B:142:MSE:HE2	1.67	0.77
1:A:332:GLY:HA3	1:B:335:THR:HG22	1.65	0.76
1:A:208:TRP:CZ2	1:A:215:THR:HG23	2.20	0.76
1:A:28:GLY:H	1:A:71:THR:CG2	2.00	0.75
1:B:21:THR:HG23	1:B:24:ASN:O	1.88	0.74
1:B:215:THR:OG1	2:B:387:HOH:O	2.05	0.74
1:B:33:LYS:HD3	1:B:65:GLY:HA3	1.68	0.73
1:B:137:GLY:HA2	1:B:148:TYR:HB2	1.72	0.71
1:A:21:THR:HG23	1:A:24:ASN:O	1.90	0.71
1:B:168:SER:HB2	1:B:200:ASP:OD2	1.90	0.71
1:A:208:TRP:CH2	1:A:215:THR:HG23	2.25	0.70
1:A:269:THR:HG21	2:A:408:HOH:O	1.91	0.70
1:A:218:LEU:HB3	2:A:415:HOH:O	1.92	0.70
1:B:212:ASP:OD2	1:B:214:GLN:OE1	2.09	0.69
1:A:19:PHE:O	1:A:225:ARG:NH1	2.23	0.69
1:B:206:VAL:N	1:B:226:GLN:HE22	1.85	0.69
1:B:194:SER:HB3	1:B:233:ASP:CB	2.08	0.69
1:A:144:THR:O	1:A:146:PHE:N	2.24	0.69
1:A:45:ARG:NH1	1:A:223:ASN:O	2.27	0.67
1:B:141:ARG:HH11	1:B:294:ASN:ND2	1.92	0.67
1:A:239:THR:HG22	1:A:241:VAL:H	1.58	0.67
1:A:194:SER:CB	1:A:233:ASP:HB3	2.25	0.67
1:B:206:VAL:H	1:B:226:GLN:NE2	1.85	0.67
1:A:347:GLN:HA	1:A:347:GLN:OE1	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:GLN:OE1	1:B:214:GLN:N	2.24	0.65
1:A:28:GLY:H	1:A:71:THR:HG22	1.62	0.64
1:A:99:SER:O	1:A:128:MSE:HB2	1.97	0.64
1:A:162:ALA:HB1	1:A:171:ILE:HD12	1.78	0.64
1:B:24:ASN:ND2	1:B:46:ALA:HA	2.13	0.64
1:B:105:PRO:O	1:B:107:VAL:N	2.28	0.62
1:B:161:THR:O	1:B:163:MSE:N	2.31	0.62
1:A:239:THR:HG23	1:A:240:PRO:HD2	1.82	0.61
1:A:39:GLY:CA	1:A:58:MSE:HE2	2.29	0.61
1:A:108:ALA:O	1:A:110:ARG:N	2.32	0.61
1:A:128:MSE:SE	1:A:128:MSE:O	2.68	0.60
1:A:17:GLY:O	1:A:21:THR:HB	2.00	0.60
1:A:28:GLY:H	1:A:71:THR:HG21	1.66	0.60
1:A:132:GLU:OE2	1:A:143:ARG:NH2	2.35	0.60
1:B:208:TRP:CH2	1:B:215:THR:HG23	2.37	0.59
1:A:71:THR:HG23	2:A:402:HOH:O	2.01	0.59
1:A:219:TYR:N	1:A:220:PRO:HD2	2.18	0.59
1:B:64:LYS:HA	1:B:92:GLY:O	2.02	0.59
1:A:178:ARG:HH11	1:A:178:ARG:HB3	1.67	0.59
1:B:245:VAL:HA	1:B:251:THR:HG21	1.85	0.58
1:B:141:ARG:NH1	1:B:294:ASN:HD21	1.97	0.58
1:A:302:PRO:HG3	1:A:332:GLY:O	2.04	0.58
1:A:141:ARG:HE	1:A:294:ASN:HD22	1.51	0.58
1:A:21:THR:CG2	2:A:376:HOH:O	2.52	0.58
1:A:229:ARG:NH1	1:A:251:THR:HG22	2.19	0.58
1:A:95:ARG:HA	1:A:121:ASP:O	2.04	0.57
1:B:229:ARG:NH2	1:B:248:PRO:O	2.37	0.57
1:A:332:GLY:CA	1:B:335:THR:HG22	2.34	0.57
1:B:110:ARG:O	1:B:110:ARG:HG2	2.04	0.57
1:A:33:LYS:CE	1:A:65:GLY:HA3	2.35	0.57
1:B:142:MSE:HA	1:B:142:MSE:CE	2.35	0.57
1:B:217:ALA:O	1:B:218:LEU:O	2.23	0.56
1:B:96:VAL:HG22	1:B:122:VAL:HG12	1.87	0.56
1:B:104:ASN:O	1:B:105:PRO:C	2.43	0.56
1:A:137:GLY:HA2	1:A:148:TYR:HB2	1.88	0.56
1:B:98:ALA:O	1:B:124:HIS:HA	2.06	0.56
1:B:116:GLN:OE1	1:B:122:VAL:HG22	2.06	0.55
1:A:154:GLY:HA3	1:A:163:MSE:HB3	1.88	0.55
1:B:42:TYR:CE1	1:B:44:GLN:HG2	2.42	0.55
1:B:141:ARG:HE	1:B:294:ASN:HD22	1.53	0.54
1:A:66:ALA:HA	1:A:94:ALA:H	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ALA:O	1:A:62:LYS:HE3	2.08	0.54
1:A:187:SER:OG	1:A:297:TRP:HB2	2.08	0.53
1:B:17:GLY:O	1:B:21:THR:HB	2.08	0.53
1:B:52:GLU:O	1:B:56:LEU:HB2	2.07	0.53
1:A:98:ALA:O	1:A:124:HIS:HA	2.08	0.53
1:A:45:ARG:HH22	1:A:223:ASN:HD22	1.57	0.53
1:B:149:ILE:HD11	1:B:285:MSE:SE	2.59	0.53
1:B:258:GLU:OE1	1:B:269:THR:HG21	2.09	0.53
1:A:141:ARG:HH11	1:A:294:ASN:ND2	2.03	0.52
1:B:139:LEU:O	1:B:143:ARG:HG3	2.08	0.52
1:B:222:GLN:NE2	1:B:222:GLN:H	2.08	0.52
1:A:149:ILE:HD11	1:A:285:MSE:SE	2.59	0.52
1:B:198:LEU:HD11	1:B:237:ARG:HB3	1.92	0.52
1:A:188:HIS:HD2	1:A:294:ASN:H	1.57	0.52
1:A:64:LYS:O	1:A:92:GLY:O	2.27	0.52
1:A:108:ALA:C	1:A:110:ARG:H	2.11	0.52
1:A:309:LEU:HD13	1:B:325:LEU:HD13	1.90	0.52
1:A:67:THR:HG23	1:A:95:ARG:HG2	1.92	0.51
1:B:188:HIS:HA	1:B:225:ARG:NH2	2.25	0.51
1:A:245:VAL:HA	1:A:251:THR:HG21	1.92	0.51
1:A:144:THR:C	1:A:146:PHE:H	2.13	0.51
1:A:150:GLN:HG2	1:A:316:GLU:HG2	1.92	0.51
1:A:188:HIS:CD2	1:A:294:ASN:H	2.28	0.51
1:B:100:MSE:HE2	1:B:131:ALA:HB1	1.92	0.51
1:B:212:ASP:CG	1:B:214:GLN:OE1	2.49	0.51
1:A:21:THR:HG21	1:A:26:ASN:OD1	2.11	0.51
1:A:158:ASP:O	1:B:334:CYS:HA	2.11	0.51
1:B:218:LEU:HG	1:B:219:TYR:H	1.75	0.51
1:B:141:ARG:O	1:B:144:THR:O	2.29	0.50
1:A:235:GLN:HB2	1:A:237:ARG:HD2	1.94	0.50
1:A:239:THR:HB	1:A:242:HIS:ND1	2.27	0.50
1:A:139:LEU:O	1:A:143:ARG:HG3	2.12	0.50
1:A:185:ALA:HA	1:A:206:VAL:HG21	1.94	0.50
1:A:126:LEU:HD22	1:A:127:MSE:HG3	1.93	0.50
1:A:141:ARG:HE	1:A:294:ASN:ND2	2.10	0.49
1:B:101:GLN:O	1:B:102:ASP:HB3	2.11	0.49
1:A:160:ARG:HA	1:A:331:ARG:O	2.12	0.49
1:A:310:GLN:OE1	1:A:337:PRO:HD2	2.12	0.48
1:A:255:ARG:HD2	1:A:269:THR:HB	1.95	0.48
1:B:355:HIS:HD2	2:B:377:HOH:O	1.96	0.48
1:A:150:GLN:HG2	1:A:316:GLU:CG	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:HE	1:B:294:ASN:ND2	2.10	0.48
1:B:156:SER:OG	1:B:159:GLY:O	2.22	0.48
1:B:332:GLY:C	1:B:334:CYS:N	2.66	0.48
1:B:222:GLN:H	1:B:222:GLN:HE21	1.62	0.48
1:A:206:VAL:N	1:A:226:GLN:HE22	2.05	0.48
1:A:212:ASP:C	1:A:212:ASP:OD2	2.52	0.48
1:B:191:LEU:HB3	1:B:298:VAL:HG22	1.96	0.48
1:A:144:THR:O	1:A:144:THR:OG1	2.32	0.47
1:B:9:ARG:HG3	2:B:392:HOH:O	2.14	0.47
1:B:317:LEU:HB2	1:B:364:LEU:HB2	1.97	0.47
1:B:3:ASP:HB3	1:B:126:LEU:HD11	1.97	0.46
1:A:66:ALA:HB3	2:A:399:HOH:O	2.14	0.46
1:B:160:ARG:NH1	1:B:326:LEU:O	2.49	0.46
1:B:349:LYS:HE2	1:B:367:ALA:CB	2.45	0.46
1:B:67:THR:HA	1:B:95:ARG:O	2.15	0.46
1:B:220:PRO:HB2	1:B:222:GLN:NE2	2.31	0.46
1:A:218:LEU:HG	1:A:219:TYR:H	1.77	0.46
1:B:212:ASP:OD1	1:B:214:GLN:NE2	2.42	0.46
1:B:126:LEU:HD22	1:B:127:MSE:HG3	1.98	0.46
1:B:366:GLY:O	1:B:367:ALA:C	2.55	0.45
1:B:332:GLY:C	1:B:334:CYS:H	2.18	0.45
1:B:345:ALA:O	1:B:346:PRO:C	2.55	0.45
1:B:171:ILE:O	1:B:173:SER:N	2.46	0.45
1:A:219:TYR:N	1:A:220:PRO:CD	2.79	0.45
1:A:137:GLY:HA2	1:A:148:TYR:CB	2.47	0.45
1:B:229:ARG:NH1	1:B:244:ILE:O	2.50	0.45
1:A:316:GLU:HB2	1:A:364:LEU:O	2.17	0.44
1:A:161:THR:HG22	1:A:330:ALA:O	2.18	0.44
1:A:219:TYR:H	1:A:220:PRO:HD2	1.82	0.44
1:B:188:HIS:CD2	1:B:294:ASN:H	2.35	0.44
1:B:166:GLY:C	1:B:168:SER:H	2.21	0.44
1:A:24:ASN:HD22	1:A:46:ALA:HA	1.82	0.44
1:A:96:VAL:HG13	1:A:120:ILE:HG21	2.00	0.44
1:B:48:GLU:HB3	2:B:381:HOH:O	2.18	0.44
1:B:318:ILE:HG23	1:B:361:CYS:SG	2.58	0.44
1:B:19:PHE:HB3	1:B:219:TYR:CZ	2.53	0.43
1:A:45:ARG:HH12	1:A:223:ASN:HB3	1.84	0.43
1:B:216:GLN:C	1:B:217:ALA:O	2.54	0.43
1:B:218:LEU:HG	1:B:219:TYR:N	2.32	0.43
1:B:218:LEU:CG	1:B:219:TYR:H	2.30	0.43
1:B:284:LEU:HG	1:B:285:MSE:HE2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:PRO:HA	1:A:333:LEU:O	2.17	0.43
1:B:281:LEU:HD13	1:B:308:LEU:HD23	2.00	0.43
1:A:332:GLY:HA3	1:B:335:THR:CG2	2.43	0.43
1:B:172:THR:N	2:B:397:HOH:O	2.51	0.43
1:A:146:PHE:CZ	1:A:286:MSE:HG3	2.54	0.43
1:B:188:HIS:HD2	1:B:294:ASN:H	1.67	0.43
1:A:34:ASP:HA	2:A:410:HOH:O	2.18	0.42
1:A:174:PRO:O	1:A:178:ARG:HG3	2.20	0.42
1:A:212:ASP:OD2	1:A:213:GLU:N	2.53	0.42
1:A:22:HIS:HB3	1:A:188:HIS:CD2	2.53	0.42
1:A:73:GLU:CB	1:A:101:GLN:OE1	2.67	0.42
1:A:226:GLN:NE2	1:A:226:GLN:HA	2.34	0.42
1:B:151:LEU:HD21	1:B:305:ALA:HB1	2.00	0.42
1:A:103:PRO:O	1:A:105:PRO:HA	2.19	0.42
1:B:194:SER:CB	1:B:233:ASP:CB	2.84	0.42
1:B:219:TYR:HD1	1:B:219:TYR:HA	1.71	0.42
1:B:337:PRO:HB2	1:B:338:GLY:H	1.61	0.42
1:A:184:ARG:NE	1:A:299:GLU:OE1	2.46	0.42
1:B:27:VAL:O	1:B:42:TYR:HA	2.20	0.42
1:A:101:GLN:HG3	1:A:109:GLY:HA2	2.00	0.42
1:A:310:GLN:HE22	1:A:338:GLY:H	1.66	0.42
1:B:219:TYR:N	1:B:220:PRO:CD	2.82	0.42
1:A:218:LEU:CG	1:A:219:TYR:N	2.76	0.42
1:A:220:PRO:HG2	1:A:223:ASN:OD1	2.20	0.42
1:A:178:ARG:HB3	1:A:178:ARG:NH1	2.34	0.41
1:A:52:GLU:OE2	1:A:84:CYS:SG	2.70	0.41
1:A:70:VAL:O	1:A:98:ALA:HA	2.19	0.41
1:A:101:GLN:CG	1:A:109:GLY:HA2	2.50	0.41
1:B:110:ARG:C	1:B:112:LEU:N	2.73	0.41
1:B:334:CYS:O	1:B:335:THR:C	2.59	0.41
1:A:33:LYS:CD	1:A:65:GLY:HA3	2.51	0.41
1:A:140:LYS:O	1:A:144:THR:O	2.39	0.41
1:A:91:ALA:O	1:A:93:VAL:N	2.53	0.41
1:B:217:ALA:O	1:B:218:LEU:C	2.57	0.41
1:A:167:GLU:HB3	1:A:170:TRP:HE1	1.86	0.41
1:A:102:ASP:HA	1:A:103:PRO:HD3	1.89	0.40
1:A:325:LEU:HD21	1:B:309:LEU:HD22	2.03	0.40
1:B:159:GLY:HA3	1:B:334:CYS:CB	2.52	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	347/402 (86%)	310 (89%)	24 (7%)	13 (4%)	3 4
1	B	359/402 (89%)	319 (89%)	23 (6%)	17 (5%)	2 2
All	All	706/804 (88%)	629 (89%)	47 (7%)	30 (4%)	3 3

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	GLY
1	A	105	PRO
1	A	172	THR
1	A	213	GLU
1	A	217	ALA
1	A	331	ARG
1	B	103	PRO
1	B	162	ALA
1	B	213	GLU
1	B	217	ALA
1	B	332	GLY
1	B	334	CYS
1	B	337	PRO
1	A	65	GLY
1	A	109	GLY
1	A	129	SER
1	A	145	GLY
1	B	65	GLY
1	B	67	THR
1	B	92	GLY
1	B	95	ARG
1	B	167	GLU
1	B	218	LEU
1	B	221	GLN
1	B	106	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	34	ASP
1	A	329	ASP
1	B	102	ASP
1	B	346	PRO
1	A	219	TYR

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	281/321 (88%)	252 (90%)	29 (10%)	7 13
1	B	282/321 (88%)	255 (90%)	27 (10%)	8 16
All	All	563/642 (88%)	507 (90%)	56 (10%)	8 15

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	LEU
1	A	15	GLN
1	A	21	THR
1	A	56	LEU
1	A	64	LYS
1	A	85	CYS
1	A	96	VAL
1	A	114	ARG
1	A	123	SER
1	A	126	LEU
1	A	152	LYS
1	A	153	LEU
1	A	171	ILE
1	A	183	LEU
1	A	219	TYR
1	A	222	GLN
1	A	224	LEU
1	A	226	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	241	VAL
1	A	251	THR
1	A	256	THR
1	A	269	THR
1	A	304	LEU
1	A	324	LYS
1	A	329	ASP
1	A	334	CYS
1	A	336	LEU
1	A	347	GLN
1	A	365	VAL
1	B	2	GLN
1	B	21	THR
1	B	36	GLU
1	B	48	GLU
1	B	56	LEU
1	B	67	THR
1	B	101	GLN
1	B	110	ARG
1	B	114	ARG
1	B	117	GLN
1	B	126	LEU
1	B	142	MSE
1	B	152	LYS
1	B	153	LEU
1	B	167	GLU
1	B	183	LEU
1	B	215	THR
1	B	219	TYR
1	B	222	GLN
1	B	224	LEU
1	B	241	VAL
1	B	251	THR
1	B	269	THR
1	B	287	GLN
1	B	304	LEU
1	B	339	LEU
1	B	360	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	44	GLN
1	A	117	GLN
1	A	188	HIS
1	A	221	GLN
1	A	222	GLN
1	A	223	ASN
1	A	226	GLN
1	A	291	GLN
1	A	294	ASN
1	B	15	GLN
1	B	101	GLN
1	B	133	GLN
1	B	186	GLN
1	B	188	HIS
1	B	222	GLN
1	B	226	GLN
1	B	257	GLN
1	B	294	ASN
1	B	310	GLN
1	B	363	HIS

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)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	346/402 (86%)	0.82	49 (14%)	2	1	74, 86, 100, 111	0
1	B	354/402 (88%)	0.91	50 (14%)	2	1	75, 87, 99, 106	0
All	All	700/804 (87%)	0.86	99 (14%)	2	1	74, 86, 100, 111	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	CYS	8.5
1	B	-4	THR	8.0
1	B	327	GLY	7.7
1	B	328	SER	6.3
1	A	108	ALA	5.4
1	B	165	SER	5.0
1	A	105	PRO	5.0
1	A	104	ASN	4.7
1	B	113	TYR	4.6
1	B	367	ALA	4.6
1	B	329	ASP	4.5
1	B	90	ALA	4.5
1	A	346	PRO	4.5
1	B	164	ALA	4.5
1	B	-2	TYR	4.4
1	A	106	GLN	4.3
1	B	-1	ILE	4.1
1	B	-3	LEU	3.9
1	B	277	GLY	3.9
1	B	241	VAL	3.8
1	A	367	ALA	3.8
1	B	153	LEU	3.8
1	B	337	PRO	3.7
1	A	168	SER	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	104	ASN	3.6
1	B	345	ALA	3.6
1	A	83	PRO	3.5
1	A	298	VAL	3.5
1	A	107	VAL	3.5
1	A	328	SER	3.4
1	A	325	LEU	3.4
1	A	159	GLY	3.4
1	B	117	GLN	3.4
1	A	117	GLN	3.4
1	B	114	ARG	3.4
1	A	153	LEU	3.4
1	B	191	LEU	3.3
1	A	118	ALA	3.3
1	B	107	VAL	3.2
1	A	335	THR	3.1
1	B	192	THR	3.1
1	B	221	GLN	3.1
1	A	321	ILE	3.1
1	B	276	LYS	3.1
1	A	156	SER	3.0
1	B	115	LEU	3.0
1	A	183	LEU	3.0
1	B	27	VAL	3.0
1	A	319	VAL	3.0
1	A	64	LYS	2.9
1	A	190	ILE	2.9
1	B	335	THR	2.9
1	B	105	PRO	2.9
1	B	118	ALA	2.9
1	B	0	GLN	2.8
1	A	94	ALA	2.8
1	A	170	TRP	2.8
1	A	191	LEU	2.8
1	B	344	ASP	2.8
1	A	152	LYS	2.8
1	A	-2	TYR	2.7
1	A	-3	LEU	2.7
1	A	157	LEU	2.7
1	B	106	GLN	2.7
1	B	1	GLY	2.7
1	B	152	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	65	GLY	2.7
1	A	278	HIS	2.7
1	B	340	GLU	2.7
1	A	221	GLN	2.6
1	B	262	GLU	2.5
1	A	189	ALA	2.5
1	B	190	ILE	2.5
1	A	174	PRO	2.5
1	A	154	GLY	2.4
1	A	47	GLY	2.4
1	B	169	GLN	2.4
1	A	155	ALA	2.4
1	B	4	GLU	2.4
1	A	333	LEU	2.4
1	A	39	GLY	2.4
1	A	230	ILE	2.4
1	B	339	LEU	2.3
1	A	327	GLY	2.3
1	B	87	ALA	2.3
1	A	296	ILE	2.3
1	A	243	ARG	2.2
1	A	219	TYR	2.2
1	B	64	LYS	2.2
1	A	297	TRP	2.2
1	B	256	THR	2.2
1	B	265	GLU	2.1
1	B	159	GLY	2.1
1	B	341	LYS	2.1
1	A	61	GLU	2.1
1	A	90	ALA	2.1
1	A	217	ALA	2.1
1	A	84	CYS	2.0
1	B	319	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.