Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:39 AM GMT

PDB ID : 2I1L
Title : Crystal structure of the C2 form of FAD synthetase from Thermotoga maritima
Authors : Wang, W.; Shin, D.H.; Yokota, H.; Kim, R.; Kim, S.-H.; Berkeley Structural Genomics Center (BSGC)
Deposited on : 2006-08-14
Resolution : 2.50 Å(reported)

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)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
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 2.50 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	Percentile Ranks	Value
Rfree		0.286
Clashscore		21
Ramachandran outliers		2.7%
Sidechain outliers		6.8%
RSRZ outliers		6.1%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
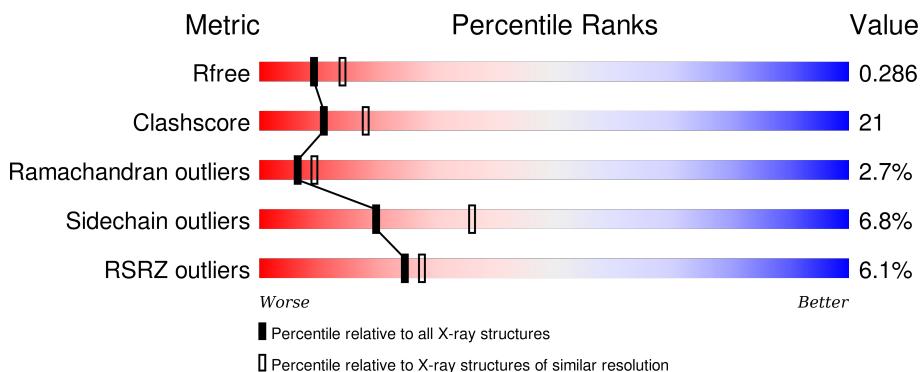
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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.

Mol	Chain	Length	Quality of chain
1	A	293	5% / 50% / 35% / 5% / 9%
1	B	293	6% / 59% / 27% / 6% / 8%
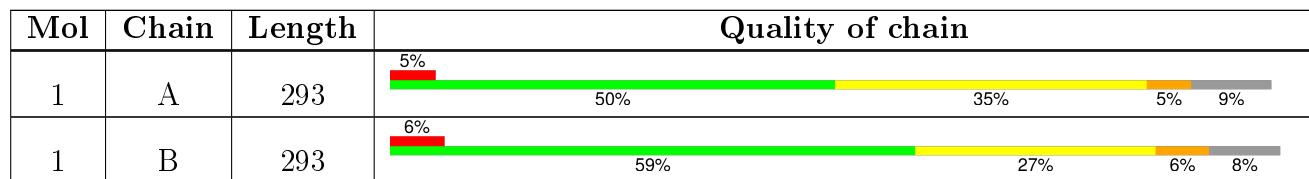
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4427 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 kinase/FMN adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total 2166	C 1396	N 371	O 393	Se 6	0	0	0
1	B	269	Total 2178	C 1404	N 372	O 396	Se 6	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WZW1
A	22	MSE	MET	MODIFIED RESIDUE	UNP Q9WZW1
A	54	MSE	MET	MODIFIED RESIDUE	UNP Q9WZW1
A	62	MSE	MET	MODIFIED RESIDUE	UNP Q9WZW1
A	214	MSE	MET	MODIFIED RESIDUE	UNP Q9WZW1
A	254	MSE	MET	MODIFIED RESIDUE	UNP Q9WZW1
A	280	MSE	MET	MODIFIED RESIDUE	UNP Q9WZW1
B	301	MSE	MET	MODIFIED RESIDUE	UNP Q9WZW1
B	322	MSE	MET	MODIFIED RESIDUE	UNP Q9WZW1
B	354	MSE	MET	MODIFIED RESIDUE	UNP Q9WZW1
B	362	MSE	MET	MODIFIED RESIDUE	UNP Q9WZW1
B	514	MSE	MET	MODIFIED RESIDUE	UNP Q9WZW1
B	554	MSE	MET	MODIFIED RESIDUE	UNP Q9WZW1
B	580	MSE	MET	MODIFIED RESIDUE	UNP Q9WZW1

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	39	Total 39	O 39	0	0
2	B	44	Total 44	O 44	0	0

3 Residue-property plots ⓘ

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.

- Molecule 1: Riboflavin kinase/FMN adenylyltransferase
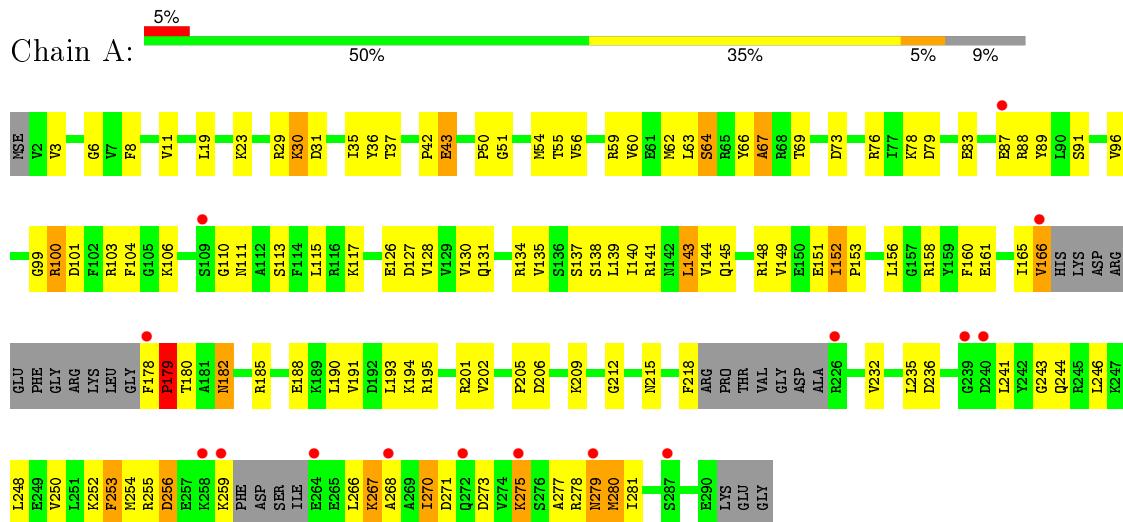
- Molecule 1: Riboflavin kinase/FMN adenylyltransferase
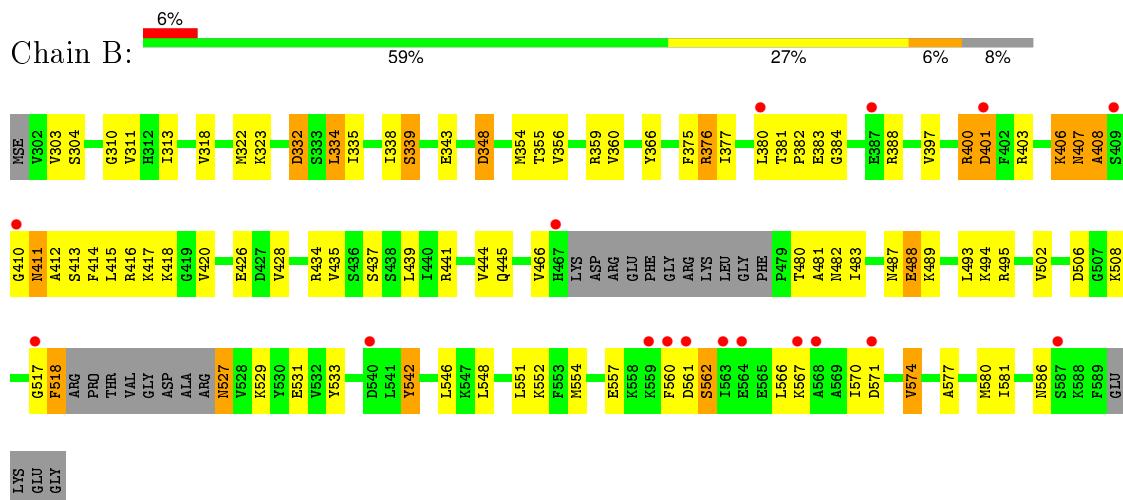
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	95.19Å 117.65Å 79.27Å 90.00° 126.79° 90.00°	Depositor
Resolution (Å)	14.58 – 2.50 19.91 – 2.49	Depositor EDS
% Data completeness (in resolution range)	88.3 (14.58-2.50) 97.6 (19.91-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.45 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.281 0.250 , 0.286	Depositor DCC
R_{free} test set	1166 reflections (4.93%)	DCC
Wilson B-factor (Å^2)	41.4	Xtriage
Anisotropy	0.895	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 30.6	EDS
Estimated twinning fraction	0.478 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	0 of 47246 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4427	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1/2197 (0.0%)	0.76	1/2938 (0.0%)
1	B	0.43	0/2211	0.73	2/2959 (0.1%)
All	All	0.45	1/4408 (0.0%)	0.74	3/5897 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	MSE	N-CA	8.02	1.62	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	481	ALA	N-CA-CB	10.13	124.28	110.10
1	B	481	ALA	N-CA-C	-6.85	92.51	111.00
1	A	180	THR	N-CA-C	5.94	127.05	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	2166	0	2203	106	0
1	B	2178	0	2213	79	0
2	A	39	0	0	0	0
2	B	44	0	0	1	0
All	All	4427	0	4416	184	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 21.

All (184) 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:495:ARG:HH21	1:B:557:GLU:HG2	0.94	1.08
1:A:201:ARG:NH2	1:A:209:LYS:HZ3	1.58	1.00
1:A:35:ILE:HB	1:A:69:THR:HG22	1.43	0.99
1:B:495:ARG:NH2	1:B:557:GLU:HG2	1.78	0.96
1:A:278:ARG:O	1:A:279:ASN:HB2	1.71	0.90
1:A:201:ARG:HH22	1:A:209:LYS:HZ3	1.12	0.88
1:B:310:GLY:H	1:B:354:MSE:HE2	1.36	0.88
1:A:201:ARG:HH22	1:A:209:LYS:NZ	1.74	0.86
1:B:383:GLU:HG3	1:B:414:PHE:HZ	1.45	0.82
1:B:495:ARG:HH21	1:B:557:GLU:CG	1.87	0.82
1:B:411:ASN:N	1:B:411:ASN:HD22	1.75	0.82
1:A:100:ARG:HD3	1:A:126:GLU:OE2	1.80	0.80
1:B:437:SER:O	1:B:441:ARG:HG3	1.82	0.78
1:A:212:GLY:HA2	1:A:235:LEU:HD13	1.65	0.78
1:A:145:GLN:O	1:A:194:LYS:HB2	1.84	0.78
1:A:201:ARG:NH2	1:A:209:LYS:NZ	2.32	0.76
1:B:310:GLY:N	1:B:354:MSE:HE2	2.01	0.75
1:A:254:MSE:HG2	1:A:280:MSE:HE1	1.69	0.75
1:A:149:VAL:HA	1:A:152:ILE:HG13	1.69	0.74
1:A:144:VAL:HG13	1:A:193:LEU:HD23	1.70	0.73
1:A:270:ILE:HG13	1:A:271:ASP:N	2.03	0.73
1:A:130:VAL:HG12	1:A:131:GLN:HG3	1.74	0.69
1:B:354:MSE:HE3	1:B:359:ARG:HG3	1.72	0.68
1:A:166:VAL:HG23	1:A:243:GLY:H	1.57	0.68
1:B:482:ASN:OD1	1:B:531:GLU:HG2	1.94	0.68
1:A:277:ALA:HA	1:A:280:MSE:HE3	1.77	0.67
1:B:483:ILE:HD11	1:B:546:LEU:HD12	1.75	0.66
1:A:63:LEU:HB3	1:A:69:THR:HG21	1.77	0.66
1:A:79:ASP:O	1:A:106:LYS:HE3	1.95	0.66
1:B:413:SER:O	1:B:417:LYS:HG3	1.96	0.66
1:B:466:VAL:O	1:B:542:TYR:O	2.14	0.65
1:B:480:THR:HG22	1:B:533:TYR:HB2	1.79	0.65
1:A:236:ASP:OD1	1:A:278:ARG:NH2	2.29	0.65
1:A:241:LEU:HD13	1:A:246:LEU:HD11	1.80	0.64
1:A:140:ILE:O	1:A:144:VAL:HG23	1.98	0.64
1:A:128:VAL:O	1:A:135:VAL:HG23	1.97	0.64
1:A:37:THR:O	1:A:37:THR:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:THR:HA	1:B:488:GLU:OE2	1.97	0.64
1:A:195:ARG:HD3	1:A:218:PHE:CE2	2.32	0.64
1:A:3:VAL:O	1:A:96:VAL:HA	1.97	0.64
1:A:43:GLU:CD	1:A:43:GLU:H	2.02	0.63
1:A:278:ARG:O	1:A:279:ASN:CB	2.45	0.63
1:B:428:VAL:O	1:B:435:VAL:HG23	1.98	0.62
1:A:73:ASP:HB2	1:A:76:ARG:CZ	2.30	0.62
1:B:567:LYS:O	1:B:571:ASP:HB2	1.98	0.62
1:A:8:PHE:O	1:A:59:ARG:HD2	1.99	0.62
1:B:348:ASP:N	1:B:348:ASP:OD2	2.28	0.62
1:B:444:VAL:HG13	1:B:493:LEU:HD23	1.83	0.61
1:A:103:ARG:HA	1:A:110:GLY:O	2.01	0.61
1:A:254:MSE:SE	1:A:280:MSE:HE1	2.51	0.61
1:B:411:ASN:N	1:B:411:ASN:ND2	2.48	0.61
1:A:83:GLU:O	1:A:87:GLU:HB2	2.01	0.61
1:B:375:PHE:O	1:B:376:ARG:CB	2.49	0.60
1:B:313:ILE:HD11	1:B:428:VAL:HG11	1.84	0.60
1:A:205:PRO:HG2	1:A:244:GLN:NE2	2.17	0.60
1:A:254:MSE:CG	1:A:280:MSE:HE1	2.32	0.60
1:A:29:ARG:O	1:A:30:LYS:HD2	2.03	0.59
1:B:415:LEU:O	1:B:420:VAL:HB	2.04	0.58
1:B:518:PHE:CD2	1:B:529:LYS:HE3	2.38	0.58
1:B:323:LYS:HD3	1:B:366:TYR:O	2.05	0.57
1:B:561:ASP:O	1:B:562:SER:HB2	2.05	0.56
1:B:332:ASP:OD2	1:B:332:ASP:N	2.31	0.56
1:B:527:ASN:N	1:B:527:ASN:HD22	2.04	0.56
1:B:577:ALA:O	1:B:581:ILE:HG13	2.06	0.55
1:B:502:VAL:HG22	1:B:548:LEU:HD22	1.88	0.55
1:A:23:LYS:HE2	1:A:66:TYR:O	2.07	0.55
1:B:334:LEU:HD23	1:B:335:ILE:H	1.70	0.55
1:A:42:PRO:HG2	1:A:43:GLU:OE2	2.07	0.55
1:A:148:ARG:HD2	1:A:151:GLU:OE1	2.06	0.55
1:B:311:VAL:HG23	1:B:354:MSE:HE1	1.87	0.55
1:A:209:LYS:NZ	1:B:586:ASN:OD1	2.38	0.55
1:B:401:ASP:O	1:B:401:ASP:CG	2.44	0.55
1:B:554:MSE:HG2	1:B:580:MSE:SE	2.56	0.54
1:A:56:VAL:O	1:A:60:VAL:HG23	2.07	0.54
1:A:73:ASP:CG	1:A:76:ARG:HG3	2.28	0.54
1:B:383:GLU:HG3	1:B:414:PHE:CZ	2.35	0.54
1:A:66:TYR:O	1:A:67:ALA:HB2	2.06	0.54
1:A:275:LYS:O	1:A:275:LYS:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:GLY:HA2	1:A:235:LEU:CD1	2.36	0.54
1:B:445:GLN:O	1:B:494:LYS:HB2	2.08	0.54
1:B:406:LYS:O	1:B:407:ASN:C	2.46	0.53
1:A:139:LEU:HD23	1:A:143:LEU:HD22	1.90	0.53
1:A:165:ILE:HG22	1:A:166:VAL:N	2.23	0.53
1:B:343:GLU:CD	1:B:343:GLU:H	2.12	0.53
1:B:356:VAL:HG23	1:B:488:GLU:OE1	2.09	0.53
1:B:354:MSE:HE3	1:B:359:ARG:CG	2.39	0.53
1:A:73:ASP:HB3	1:A:76:ARG:HG3	1.91	0.52
1:B:483:ILE:CD1	1:B:546:LEU:HD12	2.40	0.52
1:B:570:ILE:O	1:B:574:VAL:HG13	2.09	0.52
1:A:202:VAL:HG22	1:A:248:LEU:CD2	2.39	0.52
1:A:202:VAL:HA	1:A:248:LEU:HD23	1.90	0.52
1:B:310:GLY:CA	1:B:354:MSE:HE2	2.40	0.51
1:A:166:VAL:HG12	1:A:182:ASN:O	2.10	0.51
1:A:152:ILE:HD12	1:A:160:PHE:HB2	1.93	0.51
1:B:375:PHE:O	1:B:376:ARG:HB3	2.10	0.51
1:A:202:VAL:HG22	1:A:248:LEU:HD22	1.93	0.51
1:A:194:LYS:HD3	1:A:253:PHE:HE1	1.75	0.51
1:A:55:THR:HA	1:A:188:GLU:OE2	2.11	0.51
1:A:19:LEU:HD11	1:A:63:LEU:HD23	1.94	0.50
1:B:303:VAL:HG12	1:B:304:SER:N	2.25	0.50
1:A:165:ILE:CG2	1:A:166:VAL:N	2.74	0.50
1:A:255:ARG:HH11	1:A:255:ARG:HG3	1.77	0.50
1:A:73:ASP:OD1	1:A:76:ARG:NH1	2.45	0.49
1:B:334:LEU:HD23	1:B:335:ILE:N	2.26	0.49
1:B:400:ARG:O	1:B:401:ASP:OD2	2.30	0.49
1:B:412:ALA:HB1	1:B:416:ARG:NH1	2.27	0.49
1:A:96:VAL:HG21	1:A:115:LEU:HD13	1.95	0.49
1:B:489:LYS:NZ	2:B:665:HOH:O	2.46	0.49
1:A:266:LEU:C	1:A:268:ALA:H	2.17	0.49
1:A:36:TYR:CZ	1:A:89:TYR:HB3	2.48	0.49
1:A:152:ILE:HB	1:A:153:PRO:HD3	1.94	0.48
1:A:73:ASP:CB	1:A:76:ARG:CZ	2.91	0.48
1:A:127:ASP:OD1	1:A:134:ARG:HD3	2.13	0.48
1:B:506:ASP:OD2	1:B:508:LYS:HG2	2.14	0.48
1:B:376:ARG:HG3	1:B:376:ARG:O	2.14	0.47
1:A:252:LYS:HB3	1:A:252:LYS:HE2	1.58	0.47
1:B:334:LEU:CD2	1:B:335:ILE:N	2.78	0.47
1:A:29:ARG:O	1:A:30:LYS:C	2.53	0.47
1:A:113:SER:O	1:A:117:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLU:O	1:A:87:GLU:CB	2.63	0.46
1:B:401:ASP:OD2	1:B:401:ASP:O	2.33	0.46
1:A:195:ARG:HD3	1:A:218:PHE:CZ	2.49	0.46
1:B:313:ILE:CD1	1:B:428:VAL:HG11	2.46	0.46
1:A:232:VAL:HG13	1:A:232:VAL:O	2.16	0.46
1:A:11:VAL:HB	1:A:62:MSE:HE2	1.97	0.46
1:B:517:GLY:O	1:B:518:PHE:HB2	2.15	0.46
1:A:51:GLY:O	1:A:141:ARG:HD2	2.15	0.46
1:A:11:VAL:HB	1:A:62:MSE:CE	2.45	0.45
1:A:88:ARG:HG2	1:A:88:ARG:O	2.15	0.45
1:B:355:THR:CA	1:B:488:GLU:OE2	2.63	0.45
1:A:149:VAL:O	1:A:152:ILE:HG13	2.15	0.45
1:A:43:GLU:CD	1:A:43:GLU:N	2.69	0.45
1:B:354:MSE:HE3	1:B:359:ARG:CB	2.47	0.45
1:A:73:ASP:CB	1:A:76:ARG:HG3	2.46	0.45
1:A:63:LEU:CB	1:A:69:THR:HG21	2.47	0.45
1:A:158:ARG:HH11	1:A:158:ARG:HG2	1.81	0.45
1:A:137:SER:O	1:A:141:ARG:HB2	2.17	0.45
1:B:560:PHE:CD1	1:B:566:LEU:HD13	2.52	0.45
1:B:338:ILE:O	1:B:339:SER:C	2.55	0.44
1:A:277:ALA:O	1:A:281:ILE:HG13	2.17	0.44
1:B:561:ASP:O	1:B:562:SER:CB	2.66	0.44
1:A:255:ARG:HE	1:A:273:ASP:CG	2.20	0.44
1:B:303:VAL:CG1	1:B:304:SER:N	2.81	0.44
1:B:487:ASN:O	1:B:488:GLU:O	2.35	0.44
1:A:202:VAL:HG13	1:A:248:LEU:HD21	2.00	0.44
1:A:254:MSE:HG2	1:A:280:MSE:CE	2.44	0.44
1:A:166:VAL:CG1	1:A:182:ASN:O	2.66	0.44
1:A:64:SER:C	1:A:66:TYR:H	2.22	0.44
1:B:343:GLU:N	1:B:343:GLU:CD	2.71	0.44
1:A:50:PRO:HB2	1:A:141:ARG:HG2	2.00	0.43
1:A:194:LYS:HE2	1:A:256:ASP:OD2	2.19	0.43
1:B:527:ASN:ND2	1:B:527:ASN:O	2.51	0.43
1:A:111:ASN:N	1:A:111:ASN:OD1	2.51	0.43
1:B:406:LYS:O	1:B:408:ALA:N	2.50	0.43
1:B:410:GLY:O	1:B:411:ASN:HB3	2.17	0.43
1:B:356:VAL:O	1:B:360:VAL:HG23	2.18	0.43
1:A:178:PHE:HB3	1:A:179:PRO:HD2	2.00	0.43
1:A:50:PRO:O	1:A:191:VAL:HA	2.19	0.43
1:A:185:ARG:HB3	1:A:190:LEU:HD12	2.01	0.43
1:A:73:ASP:C	1:A:73:ASP:OD2	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:ARG:HE	1:B:557:GLU:CB	2.31	0.43
1:B:376:ARG:HE	1:B:388:ARG:NH1	2.17	0.42
1:A:35:ILE:CB	1:A:69:THR:HG22	2.31	0.42
1:A:99:GLY:O	1:A:100:ARG:C	2.58	0.42
1:B:551:LEU:O	1:B:552:LYS:HG2	2.19	0.42
1:B:322:MSE:HB3	1:B:322:MSE:HE2	1.99	0.42
1:B:403:ARG:HG2	1:B:403:ARG:HH11	1.84	0.42
1:B:318:VAL:HG13	1:B:397:VAL:HG12	2.00	0.42
1:B:414:PHE:CZ	1:B:418:LYS:HE2	2.54	0.42
1:A:160:PHE:HD2	1:A:250:VAL:HG11	1.85	0.42
1:A:73:ASP:HB2	1:A:76:ARG:NH2	2.35	0.42
1:B:381:THR:O	1:B:384:GLY:N	2.53	0.41
1:A:29:ARG:C	1:A:30:LYS:HD2	2.39	0.41
1:A:267:LYS:HG2	1:A:267:LYS:O	2.20	0.41
1:A:29:ARG:C	1:A:31:ASP:N	2.72	0.41
1:B:377:ILE:HA	1:B:380:LEU:HG	2.02	0.41
1:B:400:ARG:CZ	1:B:426:GLU:OE2	2.69	0.41
1:B:382:PRO:O	1:B:414:PHE:CE2	2.74	0.41
1:A:266:LEU:C	1:A:268:ALA:N	2.74	0.41
1:A:100:ARG:HD2	1:A:100:ARG:HA	1.76	0.40
1:A:202:VAL:HG13	1:A:248:LEU:CD2	2.51	0.40
1:A:156:LEU:HD12	1:A:156:LEU:HA	1.91	0.40
1:A:6:GLY:O	1:A:37:THR:HA	2.22	0.40
1:A:62:MSE:SE	1:A:158:ARG:NH2	3.05	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	259/293 (88%)	231 (89%)	22 (8%)	6 (2%)	8	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	263/293 (90%)	241 (92%)	14 (5%)	8 (3%)	5 7
All	All	522/586 (89%)	472 (90%)	36 (7%)	14 (3%)	6 9

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	179	PRO
1	B	488	GLU
1	A	279	ASN
1	B	376	ARG
1	B	407	ASN
1	B	408	ALA
1	B	562	SER
1	A	67	ALA
1	A	267	LYS
1	B	339	SER
1	B	406	LYS
1	B	542	TYR
1	A	104	PHE

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	236/250 (94%)	215 (91%)	21 (9%)	12 23
1	B	238/250 (95%)	227 (95%)	11 (5%)	33 57
All	All	474/500 (95%)	442 (93%)	32 (7%)	20 36

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	43	GLU

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Mol	Chain	Res	Type
1	A	54	MSE
1	A	64	SER
1	A	78	LYS
1	A	91	SER
1	A	101	ASP
1	A	138	SER
1	A	143	LEU
1	A	152	ILE
1	A	161	GLU
1	A	166	VAL
1	A	179	PRO
1	A	182	ASN
1	A	206	ASP
1	A	215	ASN
1	A	253	PHE
1	A	256	ASP
1	A	259	LYS
1	A	270	ILE
1	A	275	LYS
1	B	332	ASP
1	B	334	LEU
1	B	348	ASP
1	B	400	ARG
1	B	401	ASP
1	B	411	ASN
1	B	434	ARG
1	B	439	LEU
1	B	518	PHE
1	B	527	ASN
1	B	574	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	107	ASN
1	A	182	ASN
1	A	244	GLN
1	A	272	GLN
1	A	279	ASN
1	B	411	ASN
1	B	442	ASN

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Mol	Chain	Res	Type
1	B	515	ASN

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 carbohydrates 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	261/293 (89%)	0.09	15 (5%)	27	31	16, 43, 81, 116	0
1	B	263/293 (89%)	0.21	17 (6%)	22	25	14, 43, 89, 128	0
All	All	524/586 (89%)	0.15	32 (6%)	25	27	14, 43, 86, 128	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	568	ALA	6.8
1	B	560	PHE	6.5
1	A	259	LYS	6.1
1	A	240	ASP	5.7
1	B	410	GLY	5.0
1	A	287	SER	4.6
1	A	226	ARG	4.0
1	B	559	LYS	3.9
1	B	380	LEU	3.7
1	B	517	GLY	3.6
1	B	587	SER	3.6
1	A	87	GLU	3.5
1	B	401	ASP	3.4
1	B	387	GLU	3.2
1	A	268	ALA	3.2
1	B	563	ILE	3.1
1	A	166	VAL	2.9
1	A	109	SER	2.9
1	B	540	ASP	2.8
1	A	279	ASN	2.8
1	B	467	HIS	2.5
1	B	561	ASP	2.5
1	B	409	SER	2.4
1	A	239	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	258	LYS	2.3
1	B	564	GLU	2.2
1	A	178	PHE	2.2
1	A	264	GLU	2.1
1	B	567	LYS	2.1
1	A	272	GLN	2.1
1	B	571	ASP	2.0
1	A	275	LYS	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 carbohydrates 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.