Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2016 – 10:32 PM EDT

PDB ID	:	5DMX
Title	:	Crystal structure of D-alanine-D-alanine ligase from Acinetobacter baumannii, space group p212121
Authors	:	Huynh, K.H.; Hong, M.K.; Kang, L.W.
Deposited on	:	2015-09-09
Resolution	:	2.81 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 (1)) were used in the production of this report:

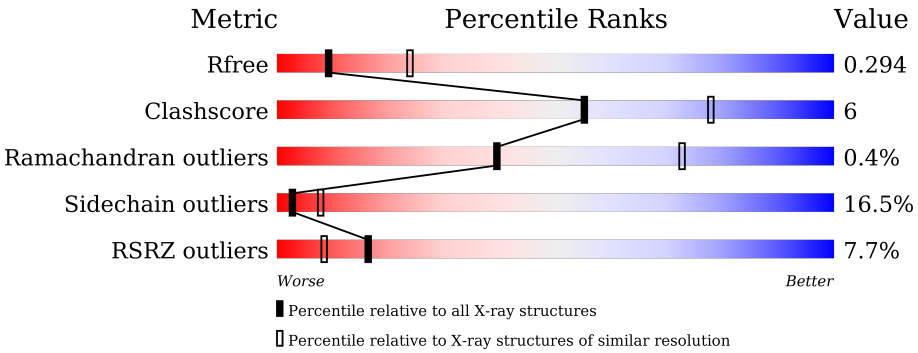
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.81 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}	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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	308	58% 15% 24%
1	B	308	4% 65% 16% 16%
1	C	308	7% 67% 10% 18%
1	D	308	10% 66% 19% 5% 10%
1	E	308	9% 48% 12% 36%
1	F	308	5% 63% 11% 22%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11162 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 D-alanine–D-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1786	1134	305	339	8			
1	B	259	Total	C	N	O	S	0	0	0
			1970	1252	334	377	7			
1	C	253	Total	C	N	O	S	0	0	0
			1926	1225	327	366	8			
1	D	276	Total	C	N	O	S	0	0	0
			2094	1330	355	401	8			
1	E	197	Total	C	N	O	S	0	0	0
			1483	943	254	281	5			
1	F	241	Total	C	N	O	S	0	0	0
			1834	1164	312	351	7			

- Molecule 2 is water.

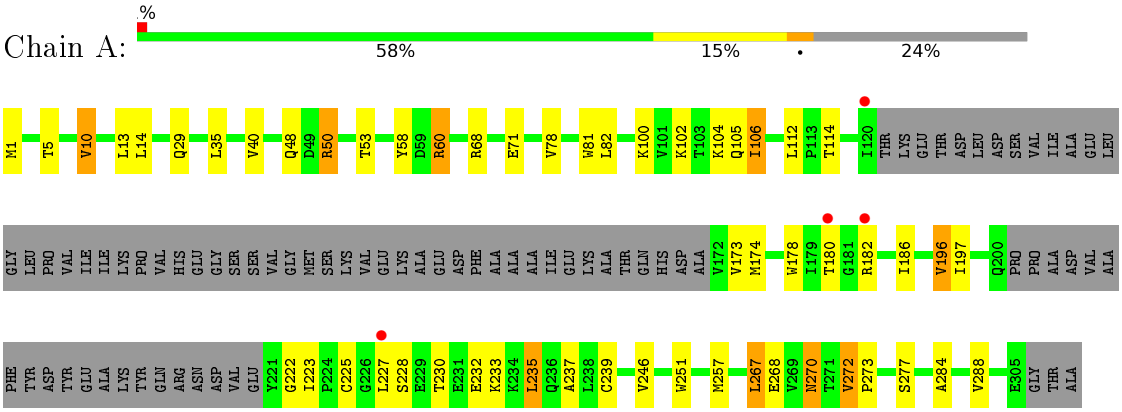
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total	O	0	0
			14	14		
2	B	14	Total	O	0	0
			14	14		
2	C	13	Total	O	0	0
			13	13		
2	D	8	Total	O	0	0
			8	8		
2	E	10	Total	O	0	0
			10	10		
2	F	10	Total	O	0	0
			10	10		

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.

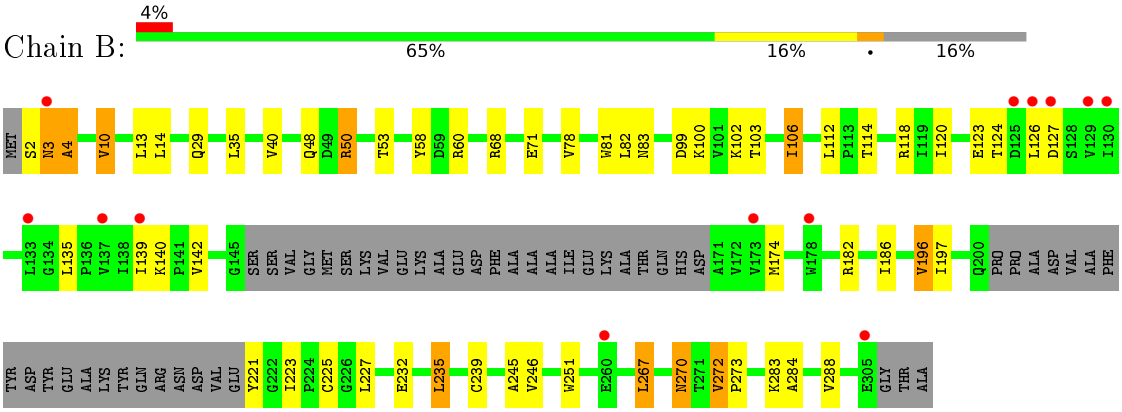
- Molecule 1: D-alanine–D-alanine ligase

Chain A:



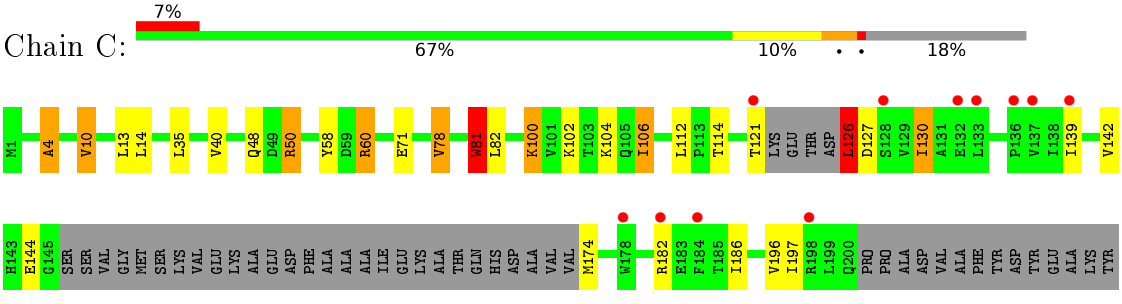
- Molecule 1: D-alanine–D-alanine ligase

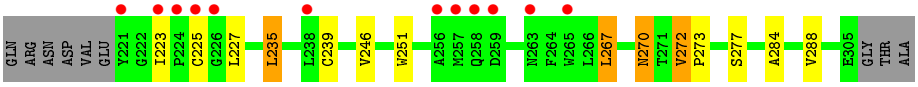
Chain B:



- Molecule 1: D-alanine–D-alanine ligase

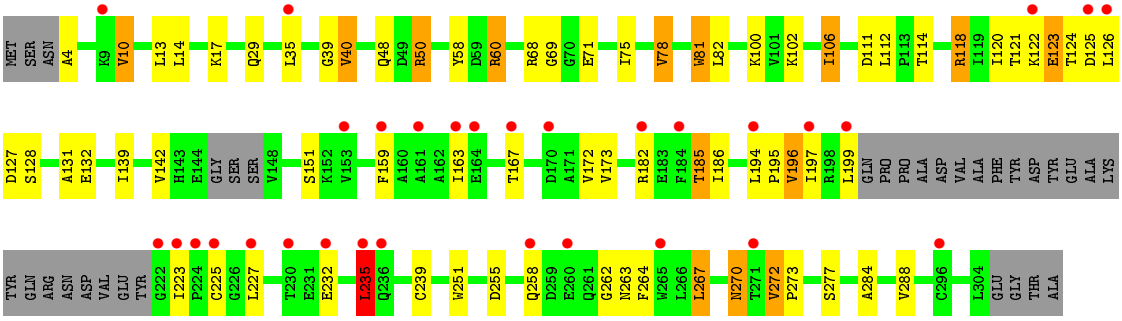
Chain C:





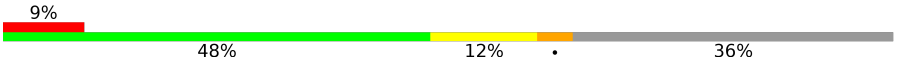
• Molecule 1: D-alanine–D-alanine ligase

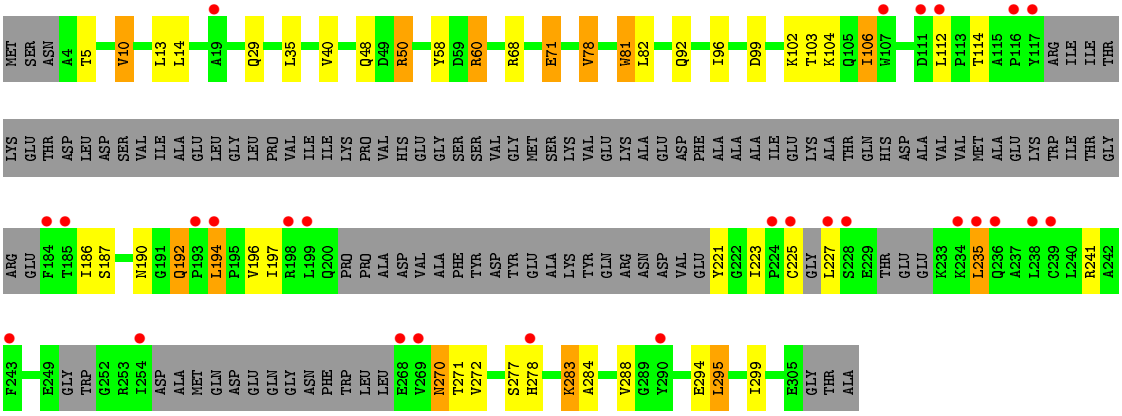
Chain D:



• Molecule 1: D-alanine–D-alanine ligase

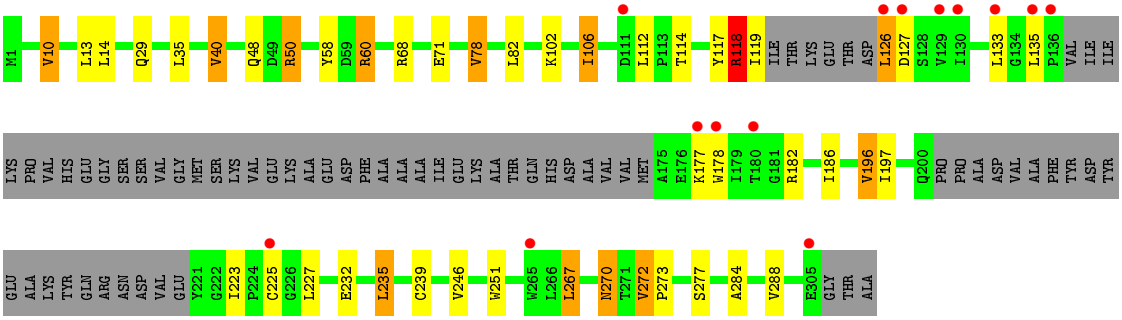
Chain E:





• Molecule 1: D-alanine–D-alanine ligase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.68Å 116.78Å 177.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.82 – 2.81 44.82 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.82-2.81) 99.2 (44.82-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.248 , 0.293 0.251 , 0.294	Depositor DCC
R_{free} test set	2915 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	74.7	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 69.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11162	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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

5.1 Standard geometry

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	0.60	0/1817	0.85	2/2459 (0.1%)
1	B	0.63	0/2004	0.87	2/2716 (0.1%)
1	C	0.64	1/1959 (0.1%)	0.84	3/2652 (0.1%)
1	D	0.61	0/2129	0.84	2/2883 (0.1%)
1	E	0.68	0/1503	0.95	5/2028 (0.2%)
1	F	0.61	0/1865	0.89	5/2524 (0.2%)
All	All	0.63	1/11277 (0.0%)	0.87	19/15262 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	81	TRP	CB-CG	-5.01	1.41	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	118	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	E	81	TRP	CA-CB-CG	-6.73	100.92	113.70
1	C	4	ALA	CB-CA-C	6.55	119.92	110.10
1	F	126	LEU	CA-CB-CG	6.46	130.16	115.30
1	D	235	LEU	CA-CB-CG	6.43	130.08	115.30
1	F	118	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	126	LEU	CA-CB-CG	5.82	128.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	71	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	C	267	LEU	CA-CB-CG	5.60	128.19	115.30
1	E	294	GLU	CA-CB-CG	5.43	125.35	113.40
1	F	267	LEU	CA-CB-CG	5.31	127.51	115.30
1	E	241	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	267	LEU	CA-CB-CG	5.23	127.33	115.30
1	B	267	LEU	CA-CB-CG	5.23	127.32	115.30
1	F	126	LEU	CB-CG-CD1	5.16	119.78	111.00
1	D	81	TRP	CA-CB-CG	-5.08	104.04	113.70
1	E	192	GLN	CA-CB-CG	5.07	124.55	113.40
1	B	10	VAL	CA-CB-CG1	5.06	118.50	110.90
1	A	173	VAL	C-N-CA	5.05	134.32	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	ILE	Peptide
1	B	4	ALA	Peptide
1	C	4	ALA	Peptide

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	1786	0	1789	25	0
1	B	1970	0	1978	22	0
1	C	1926	0	1936	20	0
1	D	2094	0	2108	48	0
1	E	1483	0	1497	25	0
1	F	1834	0	1833	16	0
2	A	14	0	0	0	0
2	B	14	0	0	0	1
2	C	13	0	0	0	1
2	D	8	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11162	0	11141	140	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (140) 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:E:187:SER:HB2	1:E:194:LEU:HD22	1.19	1.15
1:E:194:LEU:HD21	1:E:284:ALA:CB	1.84	1.07
1:E:194:LEU:HD21	1:E:284:ALA:HB3	1.35	1.07
1:E:187:SER:HB2	1:E:194:LEU:CD2	1.91	1.00
1:D:235:LEU:CD2	1:D:264:PHE:CE1	2.61	0.84
1:D:258:GLN:OE1	1:D:264:PHE:CD1	2.34	0.81
1:A:233:LYS:HD3	1:D:132:GLU:HG3	1.63	0.80
1:A:106:ILE:HG22	1:B:106:ILE:HG22	1.64	0.80
1:D:258:GLN:HE22	1:D:263:ASN:C	1.87	0.78
1:D:235:LEU:HD22	1:D:264:PHE:CE1	2.18	0.77
1:E:194:LEU:HD21	1:E:284:ALA:HB1	1.66	0.77
1:A:53:THR:HG22	1:B:53:THR:HG22	1.67	0.75
1:D:258:GLN:NE2	1:D:263:ASN:O	2.23	0.71
1:D:258:GLN:OE1	1:D:264:PHE:CE1	2.45	0.69
1:E:78:VAL:HG12	1:F:78:VAL:HA	1.76	0.68
1:D:255:ASP:HB3	1:D:267:LEU:CD1	2.24	0.67
1:E:187:SER:O	1:E:194:LEU:HB3	1.95	0.66
1:A:288:VAL:HG12	1:A:288:VAL:O	1.96	0.66
1:C:288:VAL:O	1:C:288:VAL:HG12	1.95	0.66
1:A:100:LYS:NZ	1:A:268:GLU:OE1	2.27	0.65
1:B:71:GLU:HG3	1:B:272:VAL:HG13	1.80	0.63
1:C:71:GLU:HG3	1:C:272:VAL:HG13	1.81	0.63
1:E:288:VAL:O	1:E:288:VAL:HG12	1.97	0.63
1:E:78:VAL:HA	1:F:78:VAL:HG12	1.81	0.63
1:F:71:GLU:HG3	1:F:272:VAL:HG13	1.80	0.62
1:D:125:ASP:HB3	1:D:128:SER:OG	1.99	0.62
1:D:142:VAL:HG23	1:D:172:VAL:O	1.99	0.62
1:A:71:GLU:HG3	1:A:272:VAL:HG13	1.81	0.61
1:C:126:LEU:O	1:C:130:ILE:HD12	1.99	0.61
1:D:255:ASP:HB3	1:D:267:LEU:HD11	1.83	0.61
1:E:92:GLN:O	1:E:96:ILE:HG12	2.00	0.61
1:E:194:LEU:CD2	1:E:284:ALA:HB1	2.30	0.60
1:A:230:THR:HB	1:D:128:SER:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:GLU:HG3	1:D:272:VAL:HG13	1.83	0.59
1:B:106:ILE:HD11	1:B:245:ALA:O	2.03	0.58
1:D:17:LYS:HB3	1:D:48:GLN:NE2	2.18	0.58
1:A:71:GLU:OE1	1:A:270:ASN:OD1	2.23	0.57
1:E:71:GLU:OE1	1:E:270:ASN:OD1	2.22	0.57
1:F:71:GLU:OE1	1:F:270:ASN:OD1	2.23	0.56
1:B:71:GLU:OE1	1:B:270:ASN:OD1	2.23	0.56
1:E:221:TYR:CZ	1:E:283:LYS:HE3	2.40	0.56
1:F:117:TYR:O	1:F:118:ARG:HD2	2.06	0.56
1:D:186:ILE:HD12	1:D:186:ILE:N	2.21	0.56
1:E:295:LEU:C	1:E:295:LEU:HD12	2.27	0.56
1:D:120:ILE:HG22	1:D:173:VAL:O	2.06	0.55
1:D:71:GLU:OE1	1:D:270:ASN:OD1	2.24	0.55
1:C:78:VAL:HA	1:D:78:VAL:HG12	1.87	0.54
1:C:71:GLU:OE1	1:C:270:ASN:OD1	2.25	0.54
1:C:100:LYS:HG3	1:C:142:VAL:O	2.07	0.54
1:B:100:LYS:HG3	1:B:142:VAL:O	2.07	0.54
1:C:78:VAL:HG12	1:D:78:VAL:HA	1.88	0.54
1:E:102:LYS:O	1:E:106:ILE:HG23	2.08	0.53
1:F:102:LYS:O	1:F:106:ILE:HG23	2.08	0.53
1:D:102:LYS:O	1:D:106:ILE:HG23	2.09	0.53
1:A:102:LYS:O	1:A:106:ILE:HG23	2.09	0.52
1:E:194:LEU:CD2	1:E:284:ALA:CB	2.72	0.52
1:B:186:ILE:HD12	1:B:186:ILE:N	2.25	0.52
1:C:102:LYS:O	1:C:106:ILE:HG23	2.09	0.52
1:A:233:LYS:CD	1:D:132:GLU:HG3	2.36	0.52
1:D:255:ASP:CB	1:D:267:LEU:CD1	2.88	0.52
1:D:251:TRP:CZ3	1:D:273:PRO:HG2	2.46	0.51
1:A:105:GLN:NE2	1:B:106:ILE:HD12	2.26	0.51
1:A:186:ILE:HD12	1:A:186:ILE:N	2.26	0.51
1:C:10:VAL:HB	1:C:60:ARG:HG3	1.93	0.51
1:D:10:VAL:HB	1:D:60:ARG:HG3	1.94	0.50
1:E:186:ILE:N	1:E:186:ILE:HD12	2.27	0.50
1:F:186:ILE:N	1:F:186:ILE:HD12	2.27	0.49
1:B:2:SER:O	1:B:3:ASN:HB2	2.13	0.49
1:D:100:LYS:HD3	1:D:142:VAL:O	2.13	0.49
1:A:10:VAL:HB	1:A:60:ARG:HG3	1.94	0.49
1:E:10:VAL:HB	1:E:60:ARG:HG3	1.95	0.49
1:E:197:ILE:HD11	1:E:284:ALA:HB2	1.95	0.48
1:F:251:TRP:CZ3	1:F:273:PRO:HG2	2.49	0.48
1:B:50:ARG:NH2	1:B:58:TYR:OH	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:TRP:CZ3	1:C:273:PRO:HG2	2.49	0.47
1:E:190:ASN:O	1:E:192:GLN:OE1	2.32	0.47
1:B:106:ILE:HD11	1:B:246:VAL:HA	1.97	0.47
1:B:251:TRP:CZ3	1:B:273:PRO:HG2	2.50	0.47
1:D:235:LEU:HD21	1:D:264:PHE:CE1	2.47	0.47
1:F:10:VAL:HB	1:F:60:ARG:HG3	1.96	0.47
1:E:35:LEU:HB3	1:E:40:VAL:HG22	1.97	0.47
1:B:102:LYS:O	1:B:106:ILE:HG23	2.15	0.47
1:D:50:ARG:NH2	1:D:58:TYR:OH	2.48	0.47
1:A:35:LEU:HB3	1:A:40:VAL:HG22	1.97	0.46
1:D:185:THR:CG2	1:D:199:LEU:HD21	2.45	0.46
1:C:50:ARG:NH2	1:C:58:TYR:OH	2.49	0.46
1:A:251:TRP:CZ3	1:A:273:PRO:HG2	2.50	0.46
1:D:258:GLN:NE2	1:D:258:GLN:HA	2.31	0.46
1:F:186:ILE:HD13	1:F:239:CYS:SG	2.56	0.46
1:F:35:LEU:HB3	1:F:40:VAL:HG22	1.98	0.46
1:B:186:ILE:HD13	1:B:239:CYS:SG	2.56	0.45
1:D:186:ILE:HD13	1:D:239:CYS:SG	2.56	0.45
1:C:186:ILE:N	1:C:186:ILE:HD12	2.31	0.45
1:A:186:ILE:HD13	1:A:239:CYS:SG	2.56	0.45
1:B:196:VAL:HG13	1:B:232:GLU:HG3	1.98	0.45
1:D:197:ILE:HD11	1:D:284:ALA:HB2	1.99	0.45
1:D:35:LEU:HB3	1:D:40:VAL:HG22	1.98	0.45
1:B:35:LEU:HB3	1:B:40:VAL:HG22	1.98	0.45
1:F:50:ARG:NH2	1:F:58:TYR:OH	2.50	0.45
1:C:288:VAL:CG1	1:C:288:VAL:O	2.64	0.44
1:C:35:LEU:HB3	1:C:40:VAL:HG22	1.99	0.44
1:D:235:LEU:CD2	1:D:264:PHE:CD1	2.99	0.44
1:A:237:ALA:HB2	1:D:131:ALA:O	2.17	0.44
1:F:196:VAL:HG13	1:F:232:GLU:HG3	2.00	0.44
1:A:104:LYS:HD2	1:A:174:MET:HE1	1.99	0.44
1:A:50:ARG:NH2	1:A:58:TYR:OH	2.50	0.44
1:A:53:THR:CG2	1:B:53:THR:HG22	2.42	0.44
1:D:235:LEU:HD22	1:D:264:PHE:CZ	2.52	0.44
1:E:50:ARG:NH2	1:E:58:TYR:OH	2.49	0.44
1:D:118:ARG:NE	1:D:132:GLU:OE2	2.50	0.44
1:C:81:TRP:HZ3	1:D:69:GLY:O	2.01	0.44
1:B:100:LYS:HE3	1:B:140:LYS:HD3	2.00	0.43
1:C:81:TRP:CZ3	1:D:75:ILE:HB	2.52	0.43
1:C:186:ILE:HD13	1:C:239:CYS:SG	2.58	0.43
1:A:196:VAL:HG13	1:A:232:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ILE:HD11	1:B:235:LEU:HD13	2.01	0.43
1:A:230:THR:HB	1:D:128:SER:CB	2.47	0.43
1:D:100:LYS:HE2	1:D:142:VAL:O	2.19	0.42
1:D:235:LEU:HD22	1:D:264:PHE:CD1	2.52	0.42
1:F:133:LEU:HD23	1:F:177:LYS:HB3	2.01	0.42
1:D:255:ASP:CB	1:D:267:LEU:HD12	2.49	0.42
1:C:197:ILE:HD11	1:C:284:ALA:HB2	2.00	0.42
1:A:186:ILE:HD11	1:A:235:LEU:HD13	2.02	0.42
1:C:186:ILE:HD11	1:C:235:LEU:HD13	2.03	0.41
1:F:186:ILE:HD11	1:F:235:LEU:HD13	2.03	0.41
1:B:221:TYR:CZ	1:B:283:LYS:HE3	2.55	0.41
1:D:185:THR:HG22	1:D:199:LEU:HD21	2.01	0.41
1:F:197:ILE:HD11	1:F:284:ALA:HB2	2.01	0.41
1:D:4:ALA:HB1	1:D:39:GLY:O	2.21	0.41
1:E:295:LEU:CD1	1:E:299:ILE:CD1	2.99	0.41
1:D:196:VAL:HG13	1:D:232:GLU:HG3	2.03	0.41
1:C:104:LYS:HD2	1:C:174:MET:HE1	2.03	0.40
1:B:197:ILE:HD11	1:B:284:ALA:HB2	2.01	0.40
1:D:258:GLN:NE2	1:D:262:GLY:C	2.75	0.40
1:E:186:ILE:HD11	1:E:235:LEU:HD13	2.03	0.40
1:A:233:LYS:HD3	1:D:132:GLU:CG	2.43	0.40
1:A:197:ILE:HD11	1:A:284:ALA:HB2	2.03	0.40
1:B:99:ASP:O	1:B:103:THR:OG1	2.30	0.40
1:D:194:LEU:HB3	1:D:195:PRO:HD2	2.04	0.40
1:E:99:ASP:O	1:E:103:THR:HG23	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:HOH:O	2:C:409:HOH:O[1_655]	1.91	0.29

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	228/308 (74%)	222 (97%)	5 (2%)	1 (0%)	39 73
1	B	253/308 (82%)	244 (96%)	6 (2%)	3 (1%)	16 45
1	C	245/308 (80%)	238 (97%)	7 (3%)	0	100 100
1	D	270/308 (88%)	262 (97%)	7 (3%)	1 (0%)	39 73
1	E	183/308 (59%)	175 (96%)	8 (4%)	0	100 100
1	F	233/308 (76%)	227 (97%)	6 (3%)	0	100 100
All	All	1412/1848 (76%)	1368 (97%)	39 (3%)	5 (0%)	39 73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	ALA
1	B	123	GLU
1	D	123	GLU
1	A	222	GLY
1	B	3	ASN

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	188/247 (76%)	157 (84%)	31 (16%)	3 8
1	B	209/247 (85%)	177 (85%)	32 (15%)	3 10
1	C	204/247 (83%)	174 (85%)	30 (15%)	4 11
1	D	221/247 (90%)	182 (82%)	39 (18%)	2 6
1	E	157/247 (64%)	128 (82%)	29 (18%)	2 5
1	F	193/247 (78%)	161 (83%)	32 (17%)	3 8
All	All	1172/1482 (79%)	979 (84%)	193 (16%)	3 8

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	THR
1	A	10	VAL
1	A	13	LEU
1	A	14	LEU
1	A	29	GLN
1	A	48	GLN
1	A	50	ARG
1	A	60	ARG
1	A	68	ARG
1	A	78	VAL
1	A	81	TRP
1	A	82	LEU
1	A	106	ILE
1	A	112	LEU
1	A	114	THR
1	A	178	TRP
1	A	180	THR
1	A	182	ARG
1	A	196	VAL
1	A	223	ILE
1	A	225	CYS
1	A	227	LEU
1	A	228	SER
1	A	235	LEU
1	A	246	VAL
1	A	257	MET
1	A	267	LEU
1	A	270	ASN
1	A	272	VAL
1	A	277	SER
1	B	10	VAL
1	B	13	LEU
1	B	14	LEU
1	B	29	GLN
1	B	48	GLN
1	B	50	ARG
1	B	60	ARG
1	B	68	ARG
1	B	78	VAL
1	B	81	TRP
1	B	82	LEU
1	B	83	ASN

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Mol	Chain	Res	Type
1	B	106	ILE
1	B	112	LEU
1	B	114	THR
1	B	118	ARG
1	B	124	THR
1	B	126	LEU
1	B	127	ASP
1	B	135	LEU
1	B	139	ILE
1	B	174	MET
1	B	182	ARG
1	B	196	VAL
1	B	223	ILE
1	B	225	CYS
1	B	227	LEU
1	B	235	LEU
1	B	267	LEU
1	B	270	ASN
1	B	272	VAL
1	B	288	VAL
1	C	10	VAL
1	C	13	LEU
1	C	14	LEU
1	C	48	GLN
1	C	50	ARG
1	C	60	ARG
1	C	78	VAL
1	C	81	TRP
1	C	82	LEU
1	C	100	LYS
1	C	106	ILE
1	C	112	LEU
1	C	114	THR
1	C	121	THR
1	C	126	LEU
1	C	127	ASP
1	C	130	ILE
1	C	139	ILE
1	C	144	GLU
1	C	182	ARG
1	C	196	VAL
1	C	223	ILE

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Mol	Chain	Res	Type
1	C	225	CYS
1	C	227	LEU
1	C	235	LEU
1	C	246	VAL
1	C	267	LEU
1	C	270	ASN
1	C	272	VAL
1	C	277	SER
1	D	10	VAL
1	D	13	LEU
1	D	14	LEU
1	D	29	GLN
1	D	40	VAL
1	D	50	ARG
1	D	60	ARG
1	D	68	ARG
1	D	78	VAL
1	D	81	TRP
1	D	82	LEU
1	D	106	ILE
1	D	111	ASP
1	D	112	LEU
1	D	114	THR
1	D	118	ARG
1	D	121	THR
1	D	122	LYS
1	D	123	GLU
1	D	124	THR
1	D	126	LEU
1	D	127	ASP
1	D	139	ILE
1	D	151	SER
1	D	159	PHE
1	D	163	ILE
1	D	167	THR
1	D	182	ARG
1	D	185	THR
1	D	196	VAL
1	D	223	ILE
1	D	225	CYS
1	D	227	LEU
1	D	235	LEU

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Mol	Chain	Res	Type
1	D	267	LEU
1	D	270	ASN
1	D	272	VAL
1	D	277	SER
1	D	288	VAL
1	E	5	THR
1	E	10	VAL
1	E	13	LEU
1	E	14	LEU
1	E	29	GLN
1	E	48	GLN
1	E	50	ARG
1	E	60	ARG
1	E	68	ARG
1	E	78	VAL
1	E	81	TRP
1	E	82	LEU
1	E	104	LYS
1	E	106	ILE
1	E	112	LEU
1	E	114	THR
1	E	194	LEU
1	E	196	VAL
1	E	223	ILE
1	E	225	CYS
1	E	227	LEU
1	E	235	LEU
1	E	270	ASN
1	E	271	THR
1	E	272	VAL
1	E	277	SER
1	E	278	HIS
1	E	283	LYS
1	E	295	LEU
1	F	10	VAL
1	F	13	LEU
1	F	14	LEU
1	F	29	GLN
1	F	40	VAL
1	F	48	GLN
1	F	50	ARG
1	F	60	ARG

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Mol	Chain	Res	Type
1	F	68	ARG
1	F	78	VAL
1	F	82	LEU
1	F	106	ILE
1	F	112	LEU
1	F	114	THR
1	F	118	ARG
1	F	119	ILE
1	F	126	LEU
1	F	127	ASP
1	F	135	LEU
1	F	178	TRP
1	F	182	ARG
1	F	196	VAL
1	F	223	ILE
1	F	225	CYS
1	F	227	LEU
1	F	235	LEU
1	F	246	VAL
1	F	267	LEU
1	F	270	ASN
1	F	272	VAL
1	F	277	SER
1	F	288	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	244	GLN
1	B	105	GLN
1	D	48	GLN
1	D	258	GLN
1	F	3	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	234/308 (75%)	0.26	4 (1%) 73 63	53, 75, 117, 147	0
1	B	259/308 (84%)	0.31	13 (5%) 32 21	50, 75, 135, 174	0
1	C	253/308 (82%)	0.46	23 (9%) 11 6	47, 74, 127, 161	0
1	D	276/308 (89%)	0.82	31 (11%) 7 3	62, 102, 148, 159	0
1	E	197/308 (63%)	0.82	27 (13%) 4 2	61, 100, 139, 179	0
1	F	241/308 (78%)	0.39	14 (5%) 26 17	49, 76, 138, 188	0
All	All	1460/1848 (79%)	0.51	112 (7%) 16 8	47, 82, 139, 188	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	184	PHE	6.7
1	F	129	VAL	6.2
1	D	163	ILE	6.0
1	C	137	VAL	5.4
1	E	239	CYS	5.2
1	E	269	VAL	5.2
1	C	182	ARG	5.1
1	E	236	GLN	5.0
1	D	199	LEU	4.9
1	E	268	GLU	4.7
1	F	130	ILE	4.7
1	E	193	PRO	4.6
1	E	225	CYS	4.5
1	E	278	HIS	4.4
1	E	198	ARG	4.4
1	D	258	GLN	4.3
1	D	184	PHE	4.2
1	E	243	PHE	4.2
1	E	107	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	159	PHE	4.1
1	E	235	LEU	4.1
1	C	221	TYR	4.1
1	D	182	ARG	4.0
1	D	225	CYS	4.0
1	B	178	TRP	4.0
1	F	136	PRO	3.9
1	F	265	TRP	3.9
1	D	224	PRO	3.8
1	B	139	ILE	3.8
1	D	170	ASP	3.8
1	D	236	GLN	3.8
1	D	230	THR	3.8
1	E	254	ILE	3.8
1	B	125	ASP	3.7
1	B	130	ILE	3.7
1	F	127	ASP	3.6
1	E	194	LEU	3.6
1	C	132	GLU	3.6
1	E	227	LEU	3.6
1	E	228	SER	3.6
1	E	224	PRO	3.5
1	B	3	ASN	3.5
1	E	234	LYS	3.4
1	B	137	VAL	3.4
1	B	127	ASP	3.4
1	E	290	TYR	3.3
1	C	136	PRO	3.3
1	D	260	GLU	3.2
1	D	167	THR	3.2
1	A	120	ILE	3.2
1	E	111	ASP	3.2
1	D	227	LEU	3.1
1	F	178	TRP	3.1
1	C	258	GLN	3.0
1	D	164	GLU	3.0
1	E	199	LEU	3.0
1	D	35	LEU	3.0
1	E	238	LEU	2.9
1	C	226	GLY	2.9
1	E	116	PRO	2.8
1	C	178	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	227	LEU	2.8
1	C	128	SER	2.7
1	E	112	LEU	2.7
1	F	111	ASP	2.6
1	F	225	CYS	2.6
1	E	185	THR	2.6
1	D	222	GLY	2.6
1	F	133	LEU	2.6
1	B	305	GLU	2.6
1	D	265	TRP	2.5
1	F	305	GLU	2.5
1	C	184	PHE	2.5
1	F	180	THR	2.5
1	D	125	ASP	2.5
1	B	129	VAL	2.4
1	C	121	THR	2.4
1	E	117	TYR	2.4
1	E	19	ALA	2.4
1	B	126	LEU	2.4
1	B	133	LEU	2.4
1	D	9	LYS	2.4
1	C	224	PRO	2.3
1	D	161	ALA	2.3
1	C	257	MET	2.3
1	B	173	VAL	2.3
1	F	135	LEU	2.3
1	C	139	ILE	2.3
1	C	256	ALA	2.2
1	F	177	LYS	2.2
1	D	126	LEU	2.2
1	D	271	THR	2.2
1	C	223	ILE	2.2
1	D	197	ILE	2.2
1	D	223	ILE	2.2
1	C	225	CYS	2.2
1	D	296	CYS	2.2
1	C	238	LEU	2.1
1	C	133	LEU	2.1
1	D	232	GLU	2.1
1	C	259	ASP	2.1
1	A	180	THR	2.1
1	A	182	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	153	VAL	2.1
1	D	194	LEU	2.1
1	C	265	TRP	2.0
1	D	235	LEU	2.0
1	F	126	LEU	2.0
1	B	260	GLU	2.0
1	D	122	LYS	2.0
1	C	263	ASN	2.0
1	C	198	ARG	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.