Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2016 – 10:52 PM EDT

PDB ID	:	5D8D
Title	:	Crystal structure of D-alanine-D-alanine ligase from Acinetobacter baumannii
Authors	:	Huynh, K.H.; Hong, M.K.; Kang, L.W.
Deposited on	:	2015-08-17
Resolution	:	2.19 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 ⓘ symbol.

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

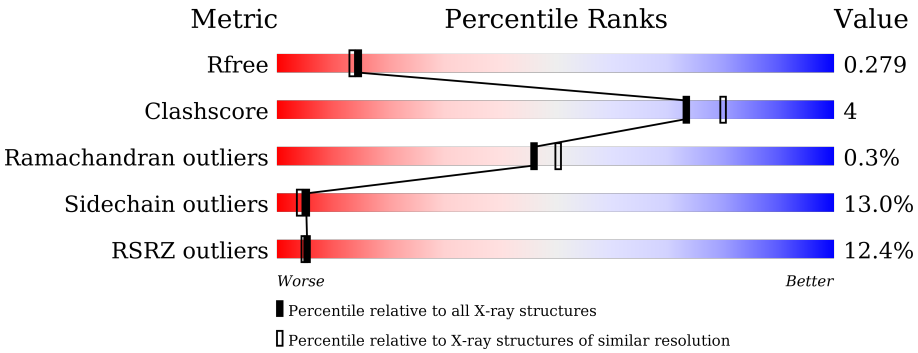
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.19 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	7% 77% 12% • 8%
1	B	308	5% 74% 13% 5% 8%
1	C	308	16% 74% 12% • 11%
1	D	308	8% 74% 16% •• 8%
1	E	308	10% 75% 12% • 10%
1	F	308	21% 74% 14% •• 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12910 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	282	Total	C	N	O	S	0	0	0
			2139	1356	363	412	8			
1	B	282	Total	C	N	O	S	0	0	0
			2141	1357	363	413	8			
1	C	274	Total	C	N	O	S	0	0	0
			2082	1323	354	397	8			
1	D	284	Total	C	N	O	S	0	0	0
			2154	1364	365	417	8			
1	E	276	Total	C	N	O	S	0	0	0
			2083	1322	353	400	8			
1	F	278	Total	C	N	O	S	0	0	0
			2112	1336	358	410	8			

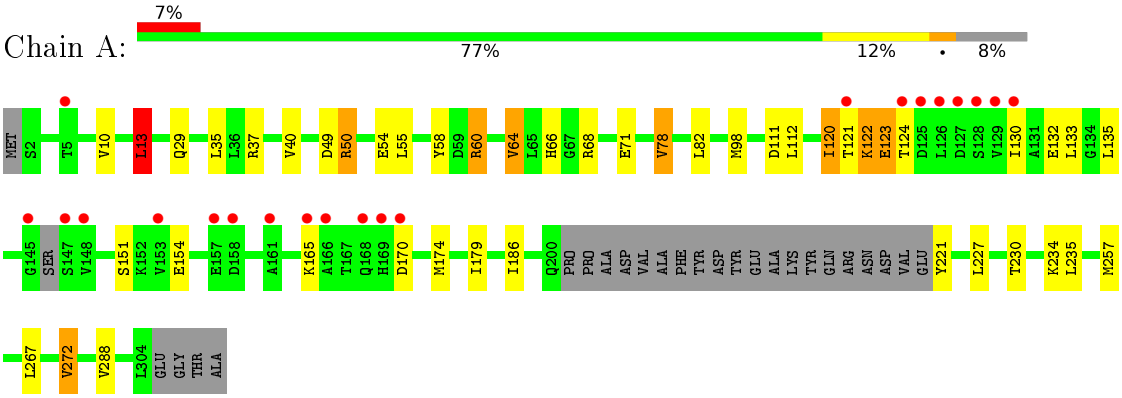
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	33	Total	O	0	0
			33	33		
2	B	30	Total	O	0	0
			30	30		
2	C	29	Total	O	0	0
			29	29		
2	D	36	Total	O	0	0
			36	36		
2	E	37	Total	O	0	0
			37	37		
2	F	34	Total	O	0	0
			34	34		

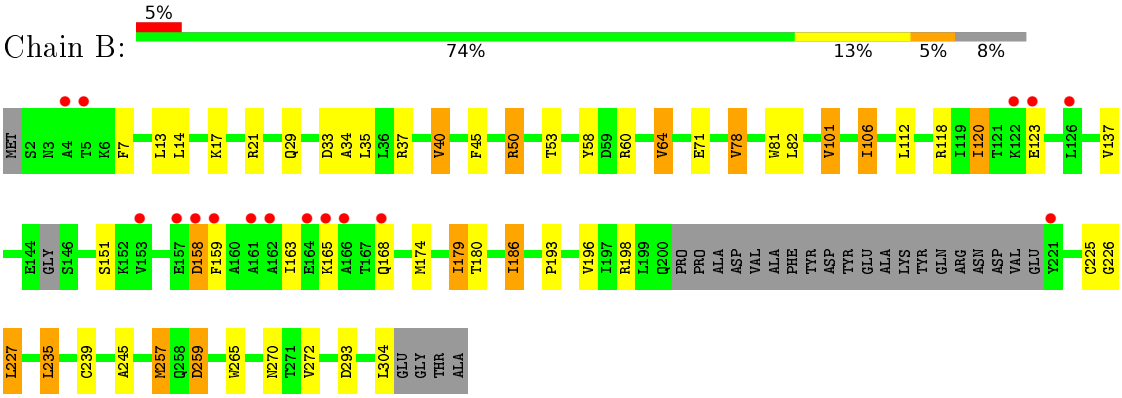
3 Residue-property plots (i)

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.

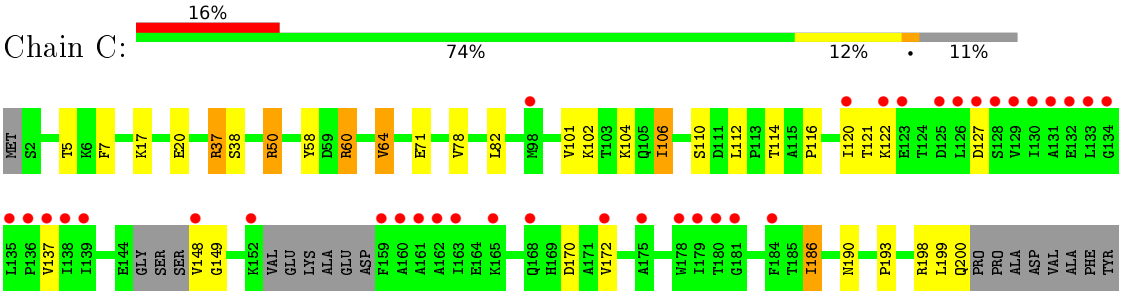
- Molecule 1: D-alanine–D-alanine ligase

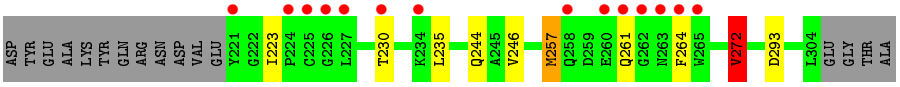


- Molecule 1: D-alanine–D-alanine ligase



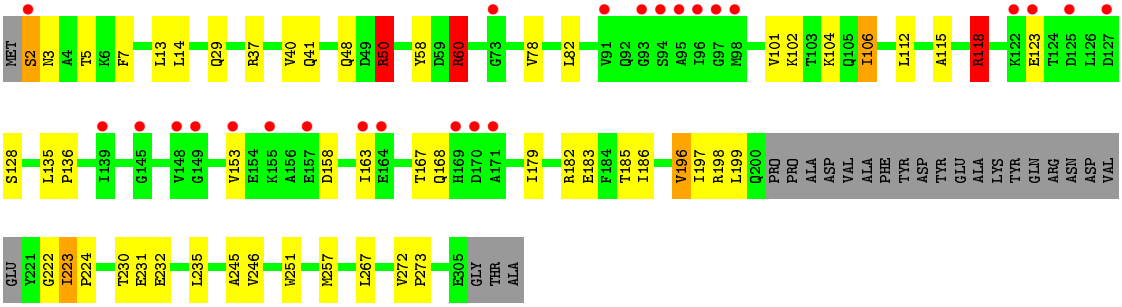
- Molecule 1: D-alanine–D-alanine ligase





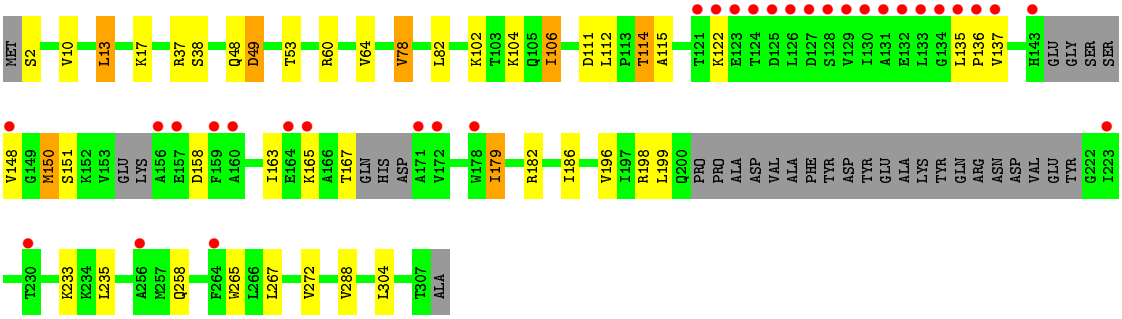
- Molecule 1: D-alanine–D-alanine ligase

Chain D:



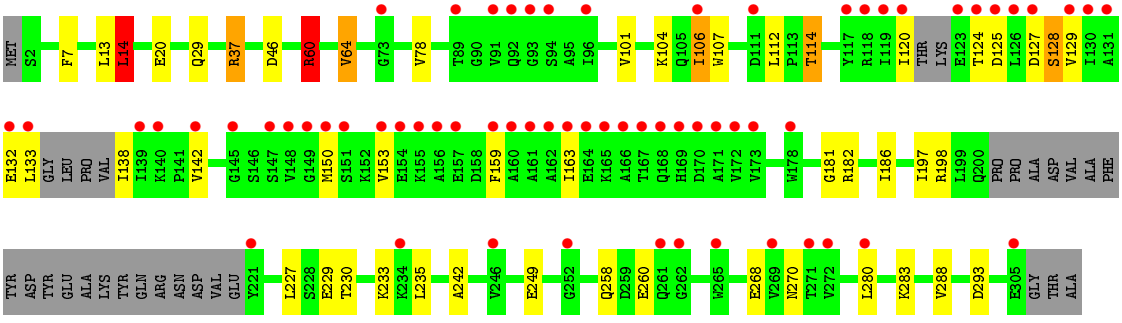
- Molecule 1: D-alanine–D-alanine ligase

Chain E:



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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	221.62Å 74.77Å 143.12Å 90.00° 103.27° 90.00°	Depositor
Resolution (Å)	36.05 – 2.19 36.05 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.4 (36.05-2.19) 98.5 (36.05-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.221 , 0.281 0.224 , 0.279	Depositor DCC
R_{free} test set	5778 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	45.2	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12910	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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	0.68	0/2175	0.86	4/2945 (0.1%)
1	B	0.70	0/2177	0.93	4/2948 (0.1%)
1	C	0.68	0/2117	0.86	5/2866 (0.2%)
1	D	0.68	0/2191	0.90	7/2968 (0.2%)
1	E	0.68	0/2115	0.87	4/2862 (0.1%)
1	F	0.68	0/2146	0.89	6/2903 (0.2%)
All	All	0.68	0/12921	0.89	30/17492 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	37	ARG	NE-CZ-NH2	-12.91	113.84	120.30
1	C	37	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	F	37	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	D	60	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	D	37	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	D	37	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	D	60	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	F	60	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	E	13	LEU	CA-CB-CG	6.16	129.47	115.30
1	B	259	ASP	CB-CG-OD1	6.15	123.83	118.30
1	E	37	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	50	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	C	37	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	D	118	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	F	60	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	118	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	D	50	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	49	ASP	CB-CG-OD1	5.33	123.10	118.30
1	E	37	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	64	VAL	CB-CA-C	5.24	121.35	111.40
1	F	14	LEU	CA-CB-CG	5.22	127.30	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	64	VAL	CB-CA-C	5.22	121.31	111.40
1	F	64	VAL	CB-CA-C	5.17	121.23	111.40
1	D	118	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	37	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	E	60	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	C	272	VAL	CB-CA-C	5.14	121.16	111.40
1	A	13	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	60	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	B	21	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2139	0	2144	21	0
1	B	2141	0	2146	23	0
1	C	2082	0	2092	13	0
1	D	2154	0	2156	21	0
1	E	2083	0	2097	15	0
1	F	2112	0	2104	16	0
2	A	33	0	0	1	0
2	B	30	0	0	0	0
2	C	29	0	0	0	0
2	D	36	0	0	0	0
2	E	37	0	0	0	0
2	F	34	0	0	0	0
All	All	12910	0	12739	103	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 4.

All (103) 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:179:ILE:HD11	1:E:265:TRP:CD1	2.20	0.76
1:A:122:LYS:HA	1:A:122:LYS:HE3	1.67	0.74
1:A:120:ILE:HA	1:A:124:THR:HG21	1.71	0.73
1:F:125:ASP:O	1:F:128:SER:OG	2.09	0.70
1:C:104:LYS:NZ	1:C:114:THR:OG1	2.25	0.69
1:B:50:ARG:NH2	1:B:58:TYR:OH	2.26	0.68
1:B:226:GLY:HA2	1:D:5:THR:HG21	1.76	0.67
1:B:186:ILE:HD11	1:B:193:PRO:HB3	1.76	0.67
1:A:121:THR:H	1:A:124:THR:HG23	1.60	0.67
1:F:129:VAL:HG12	1:F:133:LEU:HD12	1.77	0.67
1:F:7:PHE:O	1:F:60:ARG:HD2	1.95	0.66
1:E:150:MET:HG2	1:E:151:SER:N	2.12	0.65
1:A:122:LYS:HA	1:A:122:LYS:CE	2.30	0.62
1:D:183:GLU:HG2	1:D:199:LEU:HD12	1.83	0.61
1:E:104:LYS:NZ	1:E:114:THR:OG1	2.34	0.61
1:F:104:LYS:NZ	1:F:114:THR:OG1	2.32	0.60
1:A:123:GLU:O	1:A:123:GLU:HG3	2.02	0.59
1:E:135:LEU:HD12	1:E:136:PRO:HA	1.85	0.59
1:A:121:THR:O	1:A:123:GLU:N	2.30	0.59
1:A:13:LEU:HD11	1:A:55:LEU:HD21	1.86	0.57
1:D:7:PHE:O	1:D:60:ARG:HD2	2.04	0.57
1:F:181:GLY:HA3	1:F:258:GLN:O	2.06	0.56
1:C:20:GLU:OE2	1:C:20:GLU:N	2.39	0.56
1:C:71:GLU:HG3	1:C:272:VAL:HG13	1.88	0.56
1:D:118:ARG:NH2	1:D:128:SER:OG	2.40	0.55
1:A:121:THR:H	1:A:124:THR:CG2	2.20	0.55
1:D:115:ALA:HB2	1:D:179:ILE:HD11	1.87	0.55
1:A:122:LYS:CA	1:A:122:LYS:HE3	2.37	0.54
1:D:197:ILE:HG23	1:D:222:GLY:HA3	1.89	0.54
1:A:130:ILE:HG23	1:A:135:LEU:HD12	1.89	0.54
1:C:102:LYS:O	1:C:106:ILE:HG23	2.08	0.54
1:B:71:GLU:OE1	1:B:270:ASN:ND2	2.42	0.53
1:E:102:LYS:O	1:E:106:ILE:HG23	2.08	0.53
1:A:50:ARG:NH2	1:A:58:TYR:OH	2.42	0.53
1:F:20:GLU:OE2	1:F:20:GLU:N	2.42	0.52
1:B:186:ILE:C	1:B:186:ILE:HD12	2.30	0.52
1:D:186:ILE:HD12	1:D:186:ILE:N	2.25	0.52
1:D:106:ILE:HD11	1:D:245:ALA:HB1	1.92	0.51
1:A:71:GLU:HG3	1:A:272:VAL:HG13	1.92	0.51
1:C:121:THR:HG22	1:C:172:VAL:HA	1.92	0.51
1:A:66:HIS:HD1	1:A:272:VAL:HG22	1.75	0.51
1:D:102:LYS:O	1:D:106:ILE:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ILE:HD11	1:B:163:ILE:HG21	1.92	0.50
1:B:81:TRP:CH2	1:E:17:LYS:HD3	2.47	0.50
1:F:101:VAL:HG13	1:F:142:VAL:CG2	2.41	0.49
1:D:106:ILE:HG22	1:F:106:ILE:HG22	1.93	0.49
1:F:129:VAL:CG1	1:F:133:LEU:HD12	2.41	0.49
1:F:138:ILE:HD11	1:F:150:MET:CE	2.42	0.49
1:A:130:ILE:HG23	1:A:135:LEU:CD1	2.42	0.49
1:C:186:ILE:HD11	1:C:193:PRO:HB3	1.94	0.49
1:F:14:LEU:O	1:F:46:ASP:HA	2.14	0.47
1:D:185:THR:C	1:D:186:ILE:HD12	2.35	0.47
1:D:153:VAL:HG13	1:D:158:ASP:HB2	1.96	0.47
1:D:2:SER:O	1:D:5:THR:HG22	2.15	0.47
1:C:148:VAL:HG12	1:C:149:GLY:N	2.30	0.47
1:C:7:PHE:O	1:C:60:ARG:HD2	2.14	0.47
1:F:197:ILE:HG21	1:F:280:LEU:CD2	2.45	0.47
1:A:78:VAL:HG12	1:C:78:VAL:HA	1.96	0.46
1:E:198:ARG:NH1	1:E:199:LEU:O	2.49	0.46
1:F:153:VAL:HG11	1:F:159:PHE:CZ	2.50	0.46
1:E:182:ARG:HH21	1:E:258:GLN:HE22	1.63	0.46
1:B:179:ILE:HD13	1:B:265:TRP:CD1	2.51	0.46
1:B:35:LEU:HB3	1:B:40:VAL:HG22	1.99	0.45
1:F:107:TRP:NE1	1:F:242:ALA:HB1	2.31	0.45
1:B:179:ILE:HD12	1:B:259:ASP:HB3	1.99	0.44
1:A:64:VAL:O	1:A:64:VAL:HG13	2.16	0.44
1:B:179:ILE:HD11	1:B:257:MET:HB3	2.00	0.44
1:F:138:ILE:HD11	1:F:150:MET:HE1	2.00	0.44
1:C:257:MET:O	1:C:264:PHE:HA	2.18	0.44
1:A:35:LEU:HB3	1:A:40:VAL:HG22	1.99	0.43
1:B:7:PHE:HB3	1:B:60:ARG:HD2	2.01	0.43
1:E:182:ARG:NH2	1:E:258:GLN:HE22	2.15	0.43
1:C:37:ARG:HD2	1:C:293:ASP:OD2	2.18	0.43
1:D:135:LEU:HA	1:D:136:PRO:C	2.38	0.43
1:B:106:ILE:HD11	1:B:245:ALA:HB1	2.01	0.43
1:B:34:ALA:HB1	1:B:293:ASP:HA	2.01	0.43
1:D:106:ILE:HD11	1:D:245:ALA:C	2.39	0.43
1:A:186:ILE:HD12	1:A:186:ILE:N	2.33	0.43
1:B:33:ASP:HB3	1:B:37:ARG:NH2	2.34	0.42
1:D:104:LYS:NZ	1:D:115:ALA:O	2.51	0.42
1:B:53:THR:HG22	1:E:53:THR:HG22	2.00	0.42
1:B:179:ILE:CD1	1:B:265:TRP:CD1	3.02	0.42
1:E:114:THR:O	1:E:115:ALA:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:ARG:NH2	1:C:58:TYR:OH	2.45	0.42
1:E:49:ASP:OD1	1:E:49:ASP:N	2.52	0.42
1:A:121:THR:OG1	1:A:121:THR:O	2.34	0.42
1:B:101:VAL:HG12	1:B:174:MET:HE3	2.01	0.42
1:C:148:VAL:HG12	1:C:149:GLY:H	1.85	0.42
1:D:223:ILE:HA	1:D:224:PRO:C	2.39	0.42
1:B:235:LEU:HD22	1:B:239:CYS:SG	2.60	0.42
1:D:196:VAL:HG13	1:D:232:GLU:CG	2.50	0.42
1:B:78:VAL:HA	1:E:78:VAL:HG12	2.02	0.42
1:F:37:ARG:HD2	1:F:293:ASP:OD2	2.20	0.42
1:E:106:ILE:O	1:E:106:ILE:HD12	2.20	0.41
1:B:225:CYS:SG	1:B:227:LEU:HB2	2.61	0.41
1:B:45:PHE:CE1	1:B:50:ARG:HB2	2.54	0.41
1:D:106:ILE:HD12	1:D:106:ILE:O	2.20	0.41
1:D:50:ARG:NH2	1:D:58:TYR:OH	2.51	0.41
1:B:158:ASP:N	1:B:158:ASP:OD1	2.54	0.41
1:A:98:MET:HB3	2:A:426:HOH:O	2.20	0.41
1:D:251:TRP:CH2	1:D:273:PRO:HD2	2.56	0.41
1:E:150:MET:HG2	1:E:151:SER:H	1.85	0.40
1:A:50:ARG:HD3	1:A:54:GLU:OE1	2.21	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	276/308 (90%)	265 (96%)	11 (4%)	0	100	100
1	B	276/308 (90%)	264 (96%)	12 (4%)	0	100	100
1	C	266/308 (86%)	252 (95%)	12 (4%)	2 (1%)	24	22
1	D	280/308 (91%)	266 (95%)	13 (5%)	1 (0%)	39	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	266/308 (86%)	255 (96%)	10 (4%)	1 (0%)	39 42
1	F	270/308 (88%)	253 (94%)	16 (6%)	1 (0%)	39 42
All	All	1634/1848 (88%)	1555 (95%)	74 (4%)	5 (0%)	46 50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	123	GLU
1	E	111	ASP
1	F	260	GLU
1	C	116	PRO
1	C	190	ASN

5.3.2 Protein sidechains

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	226/247 (92%)	195 (86%)	31 (14%)	4 3
1	B	227/247 (92%)	197 (87%)	30 (13%)	5 4
1	C	220/247 (89%)	193 (88%)	27 (12%)	6 5
1	D	228/247 (92%)	198 (87%)	30 (13%)	5 4
1	E	220/247 (89%)	191 (87%)	29 (13%)	5 4
1	F	223/247 (90%)	195 (87%)	28 (13%)	5 4
All	All	1344/1482 (91%)	1169 (87%)	175 (13%)	5 4

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	13	LEU
1	A	29	GLN
1	A	50	ARG
1	A	60	ARG

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Mol	Chain	Res	Type
1	A	64	VAL
1	A	68	ARG
1	A	78	VAL
1	A	82	LEU
1	A	111	ASP
1	A	112	LEU
1	A	120	ILE
1	A	122	LYS
1	A	123	GLU
1	A	132	GLU
1	A	133	LEU
1	A	151	SER
1	A	154	GLU
1	A	165	LYS
1	A	170	ASP
1	A	174	MET
1	A	179	ILE
1	A	221	TYR
1	A	227	LEU
1	A	230	THR
1	A	234	LYS
1	A	235	LEU
1	A	257	MET
1	A	267	LEU
1	A	272	VAL
1	A	288	VAL
1	B	13	LEU
1	B	14	LEU
1	B	17	LYS
1	B	29	GLN
1	B	40	VAL
1	B	50	ARG
1	B	64	VAL
1	B	78	VAL
1	B	82	LEU
1	B	101	VAL
1	B	106	ILE
1	B	112	LEU
1	B	120	ILE
1	B	123	GLU
1	B	137	VAL
1	B	151	SER

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Mol	Chain	Res	Type
1	B	158	ASP
1	B	159	PHE
1	B	165	LYS
1	B	168	GLN
1	B	179	ILE
1	B	180	THR
1	B	186	ILE
1	B	196	VAL
1	B	198	ARG
1	B	227	LEU
1	B	235	LEU
1	B	257	MET
1	B	272	VAL
1	B	304	LEU
1	C	5	THR
1	C	17	LYS
1	C	38	SER
1	C	60	ARG
1	C	64	VAL
1	C	82	LEU
1	C	101	VAL
1	C	106	ILE
1	C	110	SER
1	C	112	LEU
1	C	120	ILE
1	C	122	LYS
1	C	127	ASP
1	C	137	VAL
1	C	170	ASP
1	C	186	ILE
1	C	198	ARG
1	C	199	LEU
1	C	200	GLN
1	C	223	ILE
1	C	230	THR
1	C	235	LEU
1	C	244	GLN
1	C	246	VAL
1	C	257	MET
1	C	261	GLN
1	C	272	VAL
1	D	2	SER

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Mol	Chain	Res	Type
1	D	3	ASN
1	D	13	LEU
1	D	14	LEU
1	D	29	GLN
1	D	40	VAL
1	D	41	GLN
1	D	48	GLN
1	D	50	ARG
1	D	60	ARG
1	D	78	VAL
1	D	82	LEU
1	D	101	VAL
1	D	106	ILE
1	D	112	LEU
1	D	118	ARG
1	D	163	ILE
1	D	167	THR
1	D	168	GLN
1	D	182	ARG
1	D	196	VAL
1	D	198	ARG
1	D	223	ILE
1	D	230	THR
1	D	231	GLU
1	D	235	LEU
1	D	246	VAL
1	D	257	MET
1	D	267	LEU
1	D	272	VAL
1	E	2	SER
1	E	10	VAL
1	E	13	LEU
1	E	38	SER
1	E	48	GLN
1	E	49	ASP
1	E	64	VAL
1	E	78	VAL
1	E	82	LEU
1	E	106	ILE
1	E	112	LEU
1	E	114	THR
1	E	122	LYS

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Mol	Chain	Res	Type
1	E	137	VAL
1	E	148	VAL
1	E	150	MET
1	E	158	ASP
1	E	163	ILE
1	E	165	LYS
1	E	167	THR
1	E	179	ILE
1	E	186	ILE
1	E	196	VAL
1	E	233	LYS
1	E	235	LEU
1	E	267	LEU
1	E	272	VAL
1	E	288	VAL
1	E	304	LEU
1	F	13	LEU
1	F	14	LEU
1	F	29	GLN
1	F	60	ARG
1	F	64	VAL
1	F	78	VAL
1	F	106	ILE
1	F	112	LEU
1	F	114	THR
1	F	120	ILE
1	F	124	THR
1	F	127	ASP
1	F	128	SER
1	F	132	GLU
1	F	163	ILE
1	F	182	ARG
1	F	186	ILE
1	F	198	ARG
1	F	227	LEU
1	F	229	GLU
1	F	230	THR
1	F	233	LYS
1	F	235	LEU
1	F	249	GLU
1	F	268	GLU
1	F	270	ASN

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Mol	Chain	Res	Type
1	F	283	LYS
1	F	288	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	92	GLN
1	A	105	GLN
1	A	244	GLN
1	A	258	GLN
1	B	244	GLN
1	B	261	GLN
1	C	244	GLN
1	D	244	GLN
1	E	190	ASN
1	E	244	GLN
1	E	258	GLN
1	F	244	GLN
1	F	270	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

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	282/308 (91%)	0.36	21 (7%) 17 17	32, 49, 106, 133	0
1	B	282/308 (91%)	0.33	16 (5%) 27 27	31, 52, 98, 125	0
1	C	274/308 (88%)	0.91	49 (17%) 2 2	33, 57, 133, 163	0
1	D	284/308 (92%)	0.46	25 (8%) 12 11	32, 51, 106, 147	0
1	E	276/308 (89%)	0.56	32 (11%) 6 6	35, 57, 111, 131	0
1	F	278/308 (90%)	1.22	65 (23%) 1 1	34, 64, 143, 170	0
All	All	1676/1848 (90%)	0.64	208 (12%) 5 5	31, 54, 120, 170	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	159	PHE	12.0
1	F	126	LEU	9.6
1	D	148	VAL	9.3
1	F	148	VAL	8.3
1	F	172	VAL	8.1
1	F	160	ALA	7.9
1	C	133	LEU	6.9
1	C	178	TRP	6.8
1	F	159	PHE	6.8
1	A	169	HIS	6.8
1	F	123	GLU	6.5
1	C	129	VAL	6.4
1	F	154	GLU	6.3
1	F	124	THR	6.3
1	F	131	ALA	6.3
1	D	122	LYS	6.1
1	F	157	GLU	6.0
1	F	169	HIS	6.0
1	F	133	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	126	LEU	5.7
1	F	120	ILE	5.3
1	C	135	LEU	5.3
1	F	178	TRP	5.3
1	F	173	VAL	5.1
1	C	130	ILE	5.1
1	C	221	TYR	5.0
1	F	155	LYS	4.9
1	F	119	ILE	4.9
1	C	134	GLY	4.9
1	B	161	ALA	4.8
1	C	131	ALA	4.7
1	F	166	ALA	4.7
1	F	125	ASP	4.7
1	C	180	THR	4.7
1	E	122	LYS	4.6
1	F	171	ALA	4.6
1	E	131	ALA	4.6
1	C	132	GLU	4.6
1	F	153	VAL	4.6
1	F	156	ALA	4.5
1	D	169	HIS	4.5
1	F	129	VAL	4.5
1	A	129	VAL	4.5
1	F	305	GLU	4.5
1	E	132	GLU	4.5
1	E	148	VAL	4.4
1	E	264	PHE	4.4
1	E	135	LEU	4.4
1	D	163	ILE	4.3
1	E	128	SER	4.3
1	E	156	ALA	4.3
1	F	161	ALA	4.2
1	C	152	LYS	4.2
1	F	96	ILE	4.2
1	C	136	PRO	4.1
1	F	164	GLU	4.1
1	C	162	ALA	4.1
1	A	168	GLN	4.1
1	B	126	LEU	4.1
1	F	127	ASP	4.0
1	E	136	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	163	ILE	4.0
1	C	160	ALA	3.9
1	C	125	ASP	3.9
1	F	162	ALA	3.9
1	C	137	VAL	3.9
1	E	130	ILE	3.9
1	B	165	LYS	3.9
1	D	95	ALA	3.8
1	F	139	ILE	3.8
1	F	118	ARG	3.7
1	E	143	HIS	3.7
1	E	157	GLU	3.7
1	B	221	TYR	3.7
1	F	147	SER	3.7
1	E	129	VAL	3.7
1	E	127	ASP	3.6
1	F	167	THR	3.6
1	E	165	LYS	3.6
1	C	120	ILE	3.6
1	E	126	LEU	3.6
1	D	171	ALA	3.5
1	A	148	VAL	3.5
1	C	161	ALA	3.5
1	E	160	ALA	3.5
1	F	165	LYS	3.5
1	C	165	LYS	3.5
1	B	158	ASP	3.5
1	C	260	GLU	3.4
1	A	126	LEU	3.4
1	E	134	GLY	3.4
1	F	168	GLN	3.4
1	A	147	SER	3.4
1	D	164	GLU	3.4
1	A	165	LYS	3.3
1	B	123	GLU	3.3
1	E	159	PHE	3.3
1	F	221	TYR	3.2
1	D	2	SER	3.2
1	E	230	THR	3.2
1	C	168	GLN	3.2
1	F	150	MET	3.2
1	B	162	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	121	THR	3.2
1	C	224	PRO	3.2
1	E	133	LEU	3.2
1	E	172	VAL	3.2
1	F	132	GLU	3.1
1	B	159	PHE	3.1
1	F	94	SER	3.1
1	F	91	VAL	3.1
1	C	122	LYS	3.1
1	F	145	GLY	3.1
1	D	153	VAL	3.1
1	D	123	GLU	3.1
1	C	226	GLY	3.1
1	F	271	THR	3.1
1	C	265	TRP	3.0
1	C	227	LEU	3.0
1	D	94	SER	3.0
1	F	265	TRP	3.0
1	C	179	ILE	3.0
1	E	256	ALA	3.0
1	E	171	ALA	3.0
1	D	98	MET	2.9
1	D	96	ILE	2.9
1	E	137	VAL	2.9
1	C	163	ILE	2.9
1	D	170	ASP	2.9
1	C	138	ILE	2.9
1	C	181	GLY	2.9
1	A	153	VAL	2.8
1	C	261	GLN	2.8
1	F	93	GLY	2.8
1	F	170	ASP	2.8
1	F	269	VAL	2.8
1	A	124	THR	2.8
1	B	166	ALA	2.7
1	C	172	VAL	2.7
1	F	92	GLN	2.7
1	A	121	THR	2.7
1	B	122	LYS	2.7
1	C	262	GLY	2.7
1	E	178	TRP	2.6
1	D	139	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	151	SER	2.6
1	C	225	CYS	2.6
1	C	128	SER	2.6
1	D	97	GLY	2.6
1	A	130	ILE	2.5
1	E	164	GLU	2.5
1	B	168	GLN	2.5
1	D	145	GLY	2.5
1	C	258	GLN	2.5
1	B	157	GLU	2.5
1	E	223	ILE	2.5
1	C	230	THR	2.4
1	D	91	VAL	2.4
1	A	166	ALA	2.4
1	B	164	GLU	2.4
1	C	123	GLU	2.4
1	D	127	ASP	2.4
1	E	123	GLU	2.3
1	F	140	LYS	2.3
1	B	4	ALA	2.3
1	D	93	GLY	2.3
1	F	130	ILE	2.3
1	C	184	PHE	2.3
1	D	73	GLY	2.3
1	F	261	GLN	2.3
1	D	155	LYS	2.3
1	F	149	GLY	2.3
1	A	157	GLU	2.3
1	C	234	LYS	2.3
1	A	125	ASP	2.3
1	A	158	ASP	2.3
1	F	262	GLY	2.3
1	C	139	ILE	2.3
1	C	127	ASP	2.2
1	F	142	VAL	2.2
1	A	127	ASP	2.2
1	B	153	VAL	2.2
1	C	264	PHE	2.2
1	F	272	VAL	2.2
1	F	280	LEU	2.2
1	C	98	MET	2.2
1	D	157	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	234	LYS	2.2
1	C	263	ASN	2.1
1	A	145	GLY	2.1
1	A	128	SER	2.1
1	E	124	THR	2.1
1	C	148	VAL	2.1
1	D	125	ASP	2.1
1	C	175	ALA	2.1
1	A	170	ASP	2.1
1	F	106	ILE	2.1
1	F	111	ASP	2.1
1	D	149	GLY	2.1
1	F	117	TYR	2.1
1	F	89	THR	2.1
1	E	125	ASP	2.1
1	A	5	THR	2.1
1	B	5	THR	2.1
1	F	73	GLY	2.0
1	F	246	VAL	2.0
1	F	252	GLY	2.0
1	A	161	ALA	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.