



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:09 PM UTC

PDB ID : 5D8D / pdb_00005d8d
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

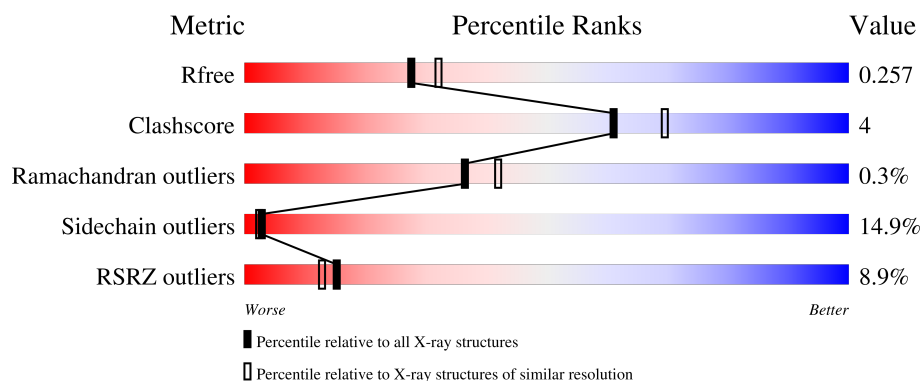
1 Overall quality at a glance

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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 $\leq 5\%$. 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	6% 76% 12% • 8%
1	B	308	4% 73% 14% • 8%
1	C	308	10% 72% 15% •• 11%
1	D	308	4% 72% 17% • 8%
1	E	308	9% 73% 15% • 10%

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Mol	Chain	Length	Quality of chain
1	F	308	15% 72% 16% • 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			

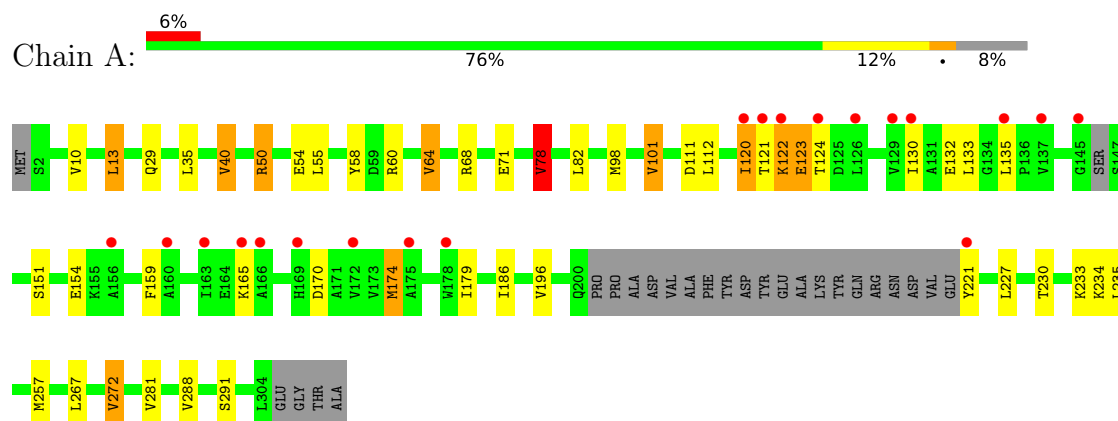
- Molecule 2 is water.

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		

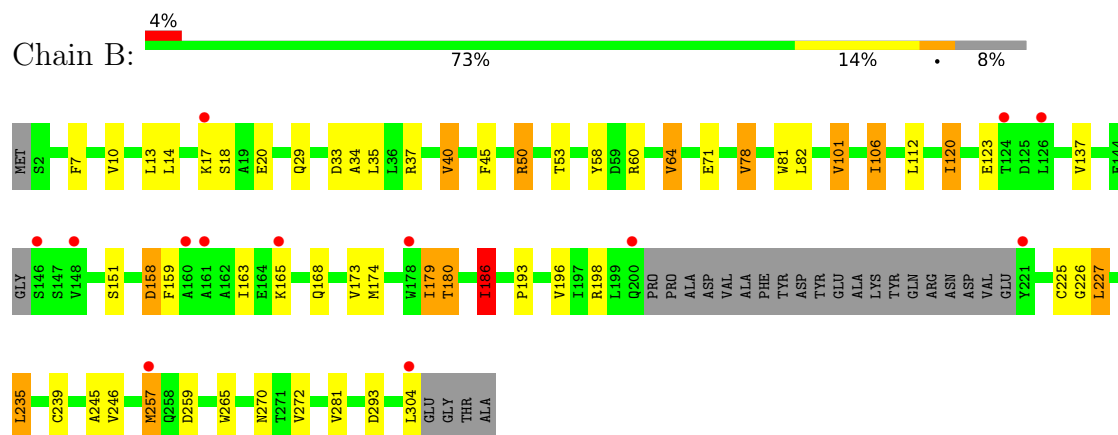
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

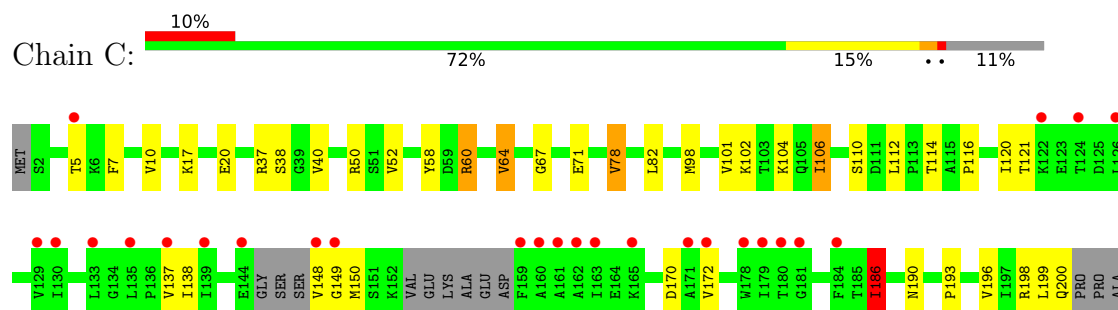
- Molecule 1: D-alanine–D-alanine ligase

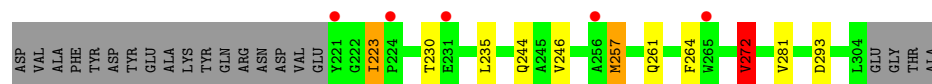


- Molecule 1: D-alanine–D-alanine ligase

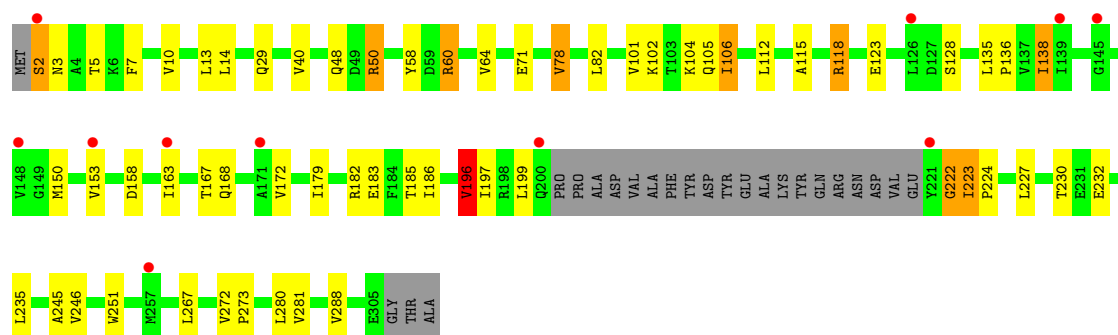
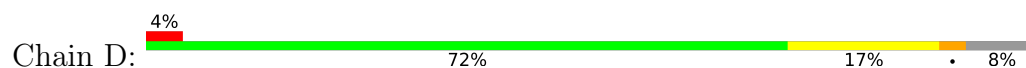


- Molecule 1: D-alanine–D-alanine ligase

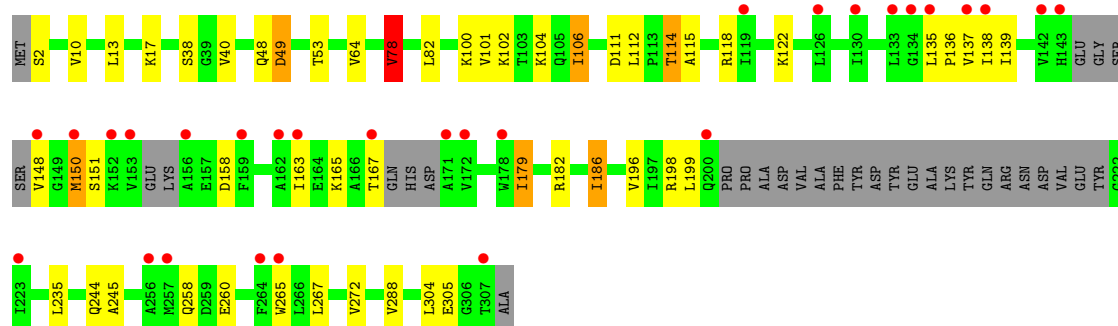
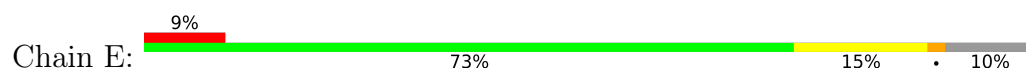




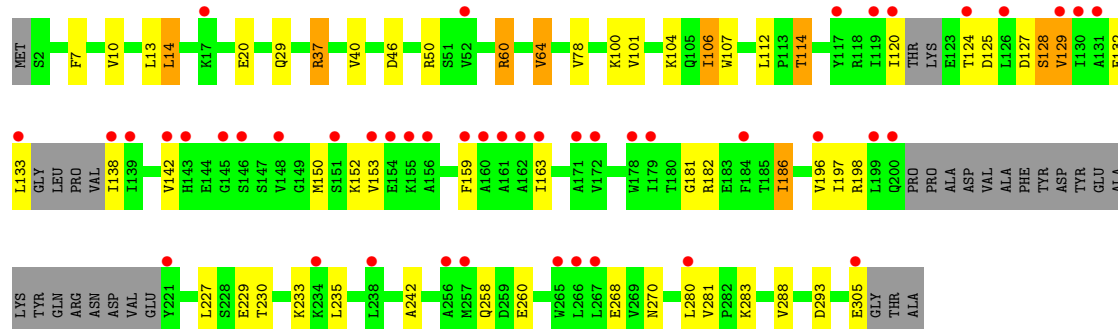
• Molecule 1: D-alanine–D-alanine ligase



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



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



4 Data and refinement statistics

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) 98.4 (36.05-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.221 , 0.281 (Not available) , 0.257	Depositor DCC
R_{free} test set	5778 reflections (4.94%)	wwPDB-VP
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 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.98	1/2175 (0.0%)	1.05	3/2945 (0.1%)
1	B	1.00	0/2177	1.12	5/2948 (0.2%)
1	C	0.98	2/2117 (0.1%)	1.08	5/2866 (0.2%)
1	D	0.96	1/2191 (0.0%)	1.09	7/2968 (0.2%)
1	E	0.95	0/2115	1.06	2/2862 (0.1%)
1	F	0.99	0/2146	1.05	5/2903 (0.2%)
All	All	0.98	4/12921 (0.0%)	1.08	27/17492 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	223	ILE	CA-CB	6.83	1.59	1.54
1	A	281	VAL	CA-CB	5.59	1.57	1.53
1	D	281	VAL	CA-CB	5.41	1.57	1.54
1	C	281	VAL	CA-CB	5.17	1.57	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	186	ILE	CB-CA-C	7.48	120.72	110.99
1	E	186	ILE	CB-CA-C	6.94	119.79	110.42
1	C	223	ILE	CB-CA-C	6.82	117.05	110.16
1	C	186	ILE	CB-CA-C	6.67	118.66	110.73
1	B	18	SER	N-CA-C	6.56	118.79	110.33
1	D	222	GLY	N-CA-C	6.53	120.39	112.49
1	B	186	ILE	CB-CA-C	6.39	119.29	110.99
1	B	180	THR	CB-CA-C	6.33	120.19	109.75
1	B	64	VAL	CB-CA-C	6.13	121.35	111.29
1	C	64	VAL	CB-CA-C	6.11	121.31	111.29
1	F	64	VAL	CB-CA-C	6.06	121.23	111.29
1	F	129	VAL	CB-CA-C	-6.03	104.26	111.97
1	F	37	ARG	NE-CZ-NH2	-5.95	113.84	119.20
1	D	280	LEU	N-CA-C	5.92	117.81	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	VAL	N-CA-CB	5.70	114.09	110.50
1	A	78	VAL	N-CA-CB	5.52	118.05	110.54
1	E	78	VAL	N-CA-CB	5.46	117.97	110.54
1	D	78	VAL	N-CA-CB	5.45	117.95	110.54
1	C	272	VAL	CB-CA-C	5.38	121.16	111.36
1	D	196	VAL	N-CA-CB	5.19	117.37	110.26
1	D	71	GLU	N-CA-CB	-5.18	103.08	110.80
1	D	138	ILE	CB-CA-C	-5.16	104.51	110.91
1	A	291	SER	N-CA-C	-5.13	104.10	110.41
1	C	52	VAL	CB-CA-C	-5.13	102.88	111.29
1	F	281	VAL	O-C-N	5.05	123.65	120.42
1	A	159	PHE	N-CA-C	5.03	116.46	110.97
1	D	64	VAL	CB-CA-C	5.01	119.51	111.29

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	24	0
1	C	2082	0	2092	15	0
1	D	2154	0	2156	21	0
1	E	2083	0	2097	17	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	108	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 (108) 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:HE3	1:A:122:LYS:HA	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:B:101:VAL:HG12	1:B:174:MET:HE3	1.80	0.63
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:HG3	1:A:123:GLU:O	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:B:186:ILE:C	1:B:186:ILE:HD12	2.30	0.56
1:F:181:GLY:HA3	1:F:258:GLN:O	2.06	0.56
1:C:20:GLU:N	1:C:20:GLU:OE2	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:HE3	1:A:122:LYS:CA	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:N	1:F:20:GLU:OE2	2.42	0.52
1:D:185:THR:C	1:D:186:ILE:HD12	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:102:LYS:O	1:D:106:ILE:HG23	2.12	0.50
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:D:106:ILE:HG22	1:F:106:ILE:HG22	1.93	0.49
1:F:101:VAL:HG13	1:F:142:VAL:CG2	2.41	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:D:135:LEU:HA	1:D:136:PRO:C	2.38	0.48
1:D:223:ILE:HA	1:D:224:PRO:C	2.39	0.48
1:F:14:LEU:O	1:F:46:ASP:HA	2.14	0.47
1:D:106:ILE:HD11	1:D:245:ALA:C	2.39	0.47
1:D:153:VAL:HG13	1:D:158:ASP:HB2	1.96	0.47
1:E:114:THR:O	1:E:115:ALA:C	2.57	0.47
1:D:2:SER:O	1:D:5:THR:HG22	2.15	0.47
1:C:7:PHE:O	1:C:60:ARG:HD2	2.14	0.47
1:C:148:VAL:HG12	1:C:149:GLY:N	2.30	0.47
1:F:138:ILE:HD11	1:F:150:MET:HE2	1.96	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:138:ILE:HD12	1:E:150:MET:HE3	1.97	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:C:138:ILE:HD11	1:C:150:MET:HE3	1.99	0.44
1:A:64:VAL:HG13	1:A:64:VAL:O	2.16	0.44
1:B:179:ILE:HD11	1:B:257:MET:HB3	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:B:106:ILE:HD11	1:B:245:ALA:C	2.44	0.43
1:B:34:ALA:HB1	1:B:293:ASP:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ILE:HD11	1:B:245:ALA:HB1	2.01	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: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:O	1:A:121:THR:OG1	2.34	0.42
1:C:148:VAL:HG12	1:C:149:GLY:H	1.85	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:HD12	1:E:106:ILE:O	2.20	0.41
1:B:45:PHE:CE1	1:B:50:ARG:HB2	2.54	0.41
1:B:225:CYS:SG	1:B:227:LEU:HB2	2.61	0.41
1:D:50:ARG:NH2	1:D:58:TYR:OH	2.51	0.41
1:D:106:ILE:O	1:D:106:ILE:HD12	2.20	0.41
1:B:158:ASP:N	1:B:158:ASP:OD1	2.54	0.41
1:E:244:GLN:O	1:E:245:ALA:C	2.63	0.41
1:A:98:MET:HB3	2:A:426:HOH:O	2.20	0.41
1:A:101:VAL:HG12	1:A:174:MET:HE3	2.03	0.41
1:D:251:TRP:CH2	1:D:273:PRO:HD2	2.56	0.41
1:C:67:GLY:HA2	1:C:98:MET:HE1	2.04	0.40
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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	16	16
1	D	280/308 (91%)	266 (95%)	13 (5%)	1 (0%)	30	34
1	E	266/308 (86%)	255 (96%)	10 (4%)	1 (0%)	30	34
1	F	270/308 (88%)	253 (94%)	16 (6%)	1 (0%)	30	34
All	All	1634/1848 (88%)	1555 (95%)	74 (4%)	5 (0%)	36	42

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%)	191 (84%)	35 (16%)	2	2
1	B	227/247 (92%)	193 (85%)	34 (15%)	3	2
1	C	220/247 (89%)	191 (87%)	29 (13%)	4	3
1	D	228/247 (92%)	195 (86%)	33 (14%)	3	2
1	E	220/247 (89%)	185 (84%)	35 (16%)	2	2
1	F	223/247 (90%)	189 (85%)	34 (15%)	3	2
All	All	1344/1482 (91%)	1144 (85%)	200 (15%)	3	2

All (200) 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	40	VAL
1	A	50	ARG
1	A	60	ARG
1	A	64	VAL
1	A	68	ARG
1	A	78	VAL
1	A	82	LEU
1	A	101	VAL
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	196	VAL
1	A	221	TYR
1	A	227	LEU
1	A	230	THR
1	A	233	LYS
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	10	VAL
1	B	13	LEU
1	B	14	LEU
1	B	17	LYS
1	B	20	GLU
1	B	29	GLN
1	B	40	VAL
1	B	50	ARG

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Mol	Chain	Res	Type
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
1	B	158	ASP
1	B	159	PHE
1	B	165	LYS
1	B	168	GLN
1	B	173	VAL
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	246	VAL
1	B	257	MET
1	B	272	VAL
1	B	304	LEU
1	C	5	THR
1	C	10	VAL
1	C	17	LYS
1	C	38	SER
1	C	40	VAL
1	C	60	ARG
1	C	64	VAL
1	C	78	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	137	VAL
1	C	170	ASP

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Mol	Chain	Res	Type
1	C	186	ILE
1	C	196	VAL
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
1	D	3	ASN
1	D	10	VAL
1	D	13	LEU
1	D	14	LEU
1	D	29	GLN
1	D	40	VAL
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	105	GLN
1	D	106	ILE
1	D	112	LEU
1	D	118	ARG
1	D	138	ILE
1	D	150	MET
1	D	163	ILE
1	D	167	THR
1	D	168	GLN
1	D	172	VAL
1	D	182	ARG
1	D	196	VAL
1	D	223	ILE
1	D	227	LEU
1	D	230	THR
1	D	235	LEU

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Mol	Chain	Res	Type
1	D	246	VAL
1	D	267	LEU
1	D	272	VAL
1	D	288	VAL
1	E	2	SER
1	E	10	VAL
1	E	13	LEU
1	E	38	SER
1	E	40	VAL
1	E	48	GLN
1	E	49	ASP
1	E	64	VAL
1	E	78	VAL
1	E	82	LEU
1	E	100	LYS
1	E	101	VAL
1	E	106	ILE
1	E	112	LEU
1	E	114	THR
1	E	118	ARG
1	E	122	LYS
1	E	137	VAL
1	E	139	ILE
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	235	LEU
1	E	260	GLU
1	E	267	LEU
1	E	272	VAL
1	E	288	VAL
1	E	304	LEU
1	E	305	GLU
1	F	10	VAL
1	F	13	LEU
1	F	14	LEU

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Mol	Chain	Res	Type
1	F	29	GLN
1	F	40	VAL
1	F	50	ARG
1	F	60	ARG
1	F	64	VAL
1	F	78	VAL
1	F	100	LYS
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	152	LYS
1	F	163	ILE
1	F	182	ARG
1	F	186	ILE
1	F	196	VAL
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	268	GLU
1	F	270	ASN
1	F	283	LYS
1	F	288	VAL
1	F	305	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	108	GLN
1	A	169	HIS
1	A	244	GLN
1	A	258	GLN
1	B	57	ASN
1	B	74	GLN

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Mol	Chain	Res	Type
1	B	190	ASN
1	B	244	GLN
1	B	261	GLN
1	C	169	HIS
1	C	190	ASN
1	C	192	GLN
1	C	244	GLN
1	C	258	GLN
1	C	302	GLN
1	D	169	HIS
1	D	244	GLN
1	E	143	HIS
1	E	190	ASN
1	E	244	GLN
1	E	258	GLN
1	F	190	ASN
1	F	192	GLN
1	F	244	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 ⓘ

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, 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	282/308 (91%)	0.18	20 (7%)	22 19	32, 49, 106, 133	0
1	B	282/308 (91%)	0.23	13 (4%)	37 34	31, 52, 98, 125	0
1	C	274/308 (88%)	0.54	31 (11%)	10 8	33, 57, 133, 163	0
1	D	284/308 (92%)	0.16	11 (3%)	43 40	32, 51, 106, 147	0
1	E	276/308 (89%)	0.50	29 (10%)	11 9	35, 57, 111, 131	0
1	F	278/308 (90%)	0.83	46 (16%)	4 3	34, 64, 143, 170	0
All	All	1676/1848 (90%)	0.40	150 (8%)	15 13	31, 54, 120, 170	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	159	PHE	6.2
1	E	153	VAL	5.8
1	D	148	VAL	5.4
1	C	148	VAL	5.3
1	F	178	TRP	5.2
1	F	133	LEU	5.0
1	F	17	LYS	4.9
1	E	143	HIS	4.9
1	C	135	LEU	4.8
1	C	179	ILE	4.8
1	F	305	GLU	4.8
1	F	148	VAL	4.7
1	A	145	GLY	4.6
1	F	179	ILE	4.4
1	B	221	TYR	4.3
1	E	148	VAL	4.3
1	F	221	TYR	4.2
1	F	138	ILE	4.2
1	B	148	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	163	ILE	4.1
1	E	178	TRP	4.0
1	C	221	TYR	3.9
1	F	156	ALA	3.9
1	E	256	ALA	3.9
1	E	264	PHE	3.8
1	F	139	ILE	3.8
1	C	149	GLY	3.8
1	A	129	VAL	3.6
1	C	265	TRP	3.6
1	E	172	VAL	3.6
1	F	145	GLY	3.6
1	A	221	TYR	3.5
1	F	265	TRP	3.5
1	E	142	VAL	3.4
1	A	172	VAL	3.4
1	C	172	VAL	3.4
1	A	135	LEU	3.4
1	A	126	LEU	3.3
1	D	171	ALA	3.3
1	E	171	ALA	3.3
1	E	162	ALA	3.2
1	F	160	ALA	3.2
1	D	200	GLN	3.2
1	E	167	THR	3.1
1	B	160	ALA	3.1
1	C	139	ILE	3.1
1	A	156	ALA	3.1
1	F	117	TYR	3.0
1	F	266	LEU	3.0
1	F	130	ILE	3.0
1	C	178	TRP	3.0
1	F	172	VAL	3.0
1	F	119	ILE	3.0
1	F	126	LEU	3.0
1	F	129	VAL	3.0
1	D	145	GLY	3.0
1	F	171	ALA	2.9
1	F	257	MET	2.9
1	E	223	ILE	2.9
1	A	120	ILE	2.8
1	C	184	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	156	ALA	2.8
1	C	163	ILE	2.8
1	F	159	PHE	2.8
1	A	163	ILE	2.8
1	E	126	LEU	2.8
1	F	267	LEU	2.8
1	F	184	PHE	2.7
1	C	171	ALA	2.7
1	F	153	VAL	2.7
1	C	161	ALA	2.7
1	F	161	ALA	2.7
1	B	257	MET	2.7
1	F	120	ILE	2.7
1	C	122	LYS	2.7
1	F	131	ALA	2.7
1	B	200	GLN	2.7
1	E	307	THR	2.7
1	C	129	VAL	2.7
1	C	144	GLU	2.6
1	E	133	LEU	2.6
1	E	138	ILE	2.6
1	C	133	LEU	2.6
1	C	181	GLY	2.6
1	C	5	THR	2.6
1	C	160	ALA	2.6
1	F	124	THR	2.6
1	E	200	GLN	2.6
1	F	142	VAL	2.6
1	B	17	LYS	2.5
1	B	161	ALA	2.5
1	C	137	VAL	2.5
1	A	124	THR	2.5
1	F	162	ALA	2.5
1	F	234	LYS	2.5
1	A	175	ALA	2.4
1	D	2	SER	2.4
1	A	122	LYS	2.4
1	E	152	LYS	2.4
1	D	139	ILE	2.4
1	E	150	MET	2.4
1	C	180	THR	2.4
1	F	200	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	153	VAL	2.4
1	C	124	THR	2.4
1	B	304	LEU	2.3
1	B	165	LYS	2.3
1	A	130	ILE	2.3
1	A	121	THR	2.3
1	C	162	ALA	2.3
1	D	221	TYR	2.3
1	F	280	LEU	2.3
1	E	257	MET	2.3
1	C	224	PRO	2.3
1	D	257	MET	2.3
1	E	135	LEU	2.3
1	F	238	LEU	2.3
1	E	159	PHE	2.2
1	F	154	GLU	2.2
1	B	178	TRP	2.2
1	B	124	THR	2.2
1	C	126	LEU	2.2
1	C	130	ILE	2.2
1	F	143	HIS	2.2
1	C	165	LYS	2.2
1	A	178	TRP	2.2
1	E	265	TRP	2.2
1	D	163	ILE	2.1
1	E	137	VAL	2.1
1	F	196	VAL	2.1
1	A	169	HIS	2.1
1	C	256	ALA	2.1
1	F	256	ALA	2.1
1	D	126	LEU	2.1
1	F	199	LEU	2.1
1	A	160	ALA	2.1
1	E	119	ILE	2.1
1	A	137	VAL	2.1
1	F	52	VAL	2.1
1	C	231	GLU	2.0
1	F	146	SER	2.1
1	F	151	SER	2.1
1	A	165	LYS	2.0
1	E	134	GLY	2.0
1	E	130	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	163	ILE	2.0
1	B	146	SER	2.0
1	A	166	ALA	2.0
1	B	126	LEU	2.0
1	F	155	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 oligosaccharides 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.