



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:27 PM GMT

PDB ID : 1AUG
Title : CRYSTAL STRUCTURE OF THE PYROGLUTAMYL PEPTIDASE I
FROM BACILLUS AMYLOLIQUEFACIENS
Authors : Odagaki, Y.; Hayashi, A.; Okada, K.; Hirotsu, K.; Kabashima, T.; Ito, K.;
Yoshimoto, T.; Tsuru, D.; Sato, M.; Clardy, J.
Deposited on : 1997-08-26
Resolution : 2.00 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 : 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

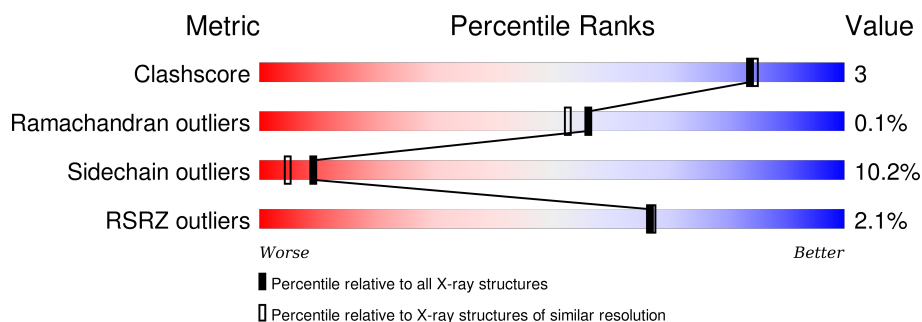
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 $\leq 5\%$. 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	215	<div> <div>2%</div> <div>79%16% . .</div> </div>
1	B	215	<div> <div>4%</div> <div>76%17%5% .</div> </div>
1	C	215	<div> <div>%</div> <div>80%14% . .</div> </div>
1	D	215	<div> <div>2%</div> <div>80%14% . .</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8095 atoms, of which 1388 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 PYROGLUTAMYL PEPTIDASE-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	210	Total	C	H	N	O	S	0	0	0
			1945	1017	347	279	297	5			
1	B	210	Total	C	H	N	O	S	0	0	0
			1945	1017	347	279	297	5			
1	C	210	Total	C	H	N	O	S	0	0	0
			1945	1017	347	279	297	5			
1	D	210	Total	C	H	N	O	S	0	0	0
			1945	1017	347	279	297	5			

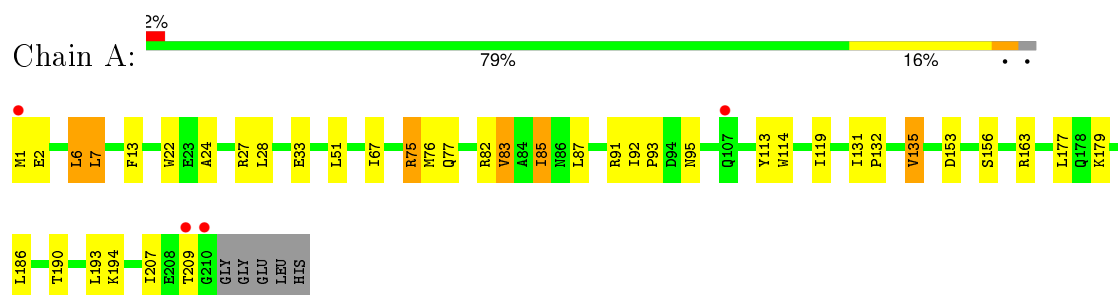
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	82	Total	O	0	0
			82	82		
2	B	83	Total	O	0	0
			83	83		
2	C	87	Total	O	0	0
			87	87		
2	D	63	Total	O	0	0
			63	63		

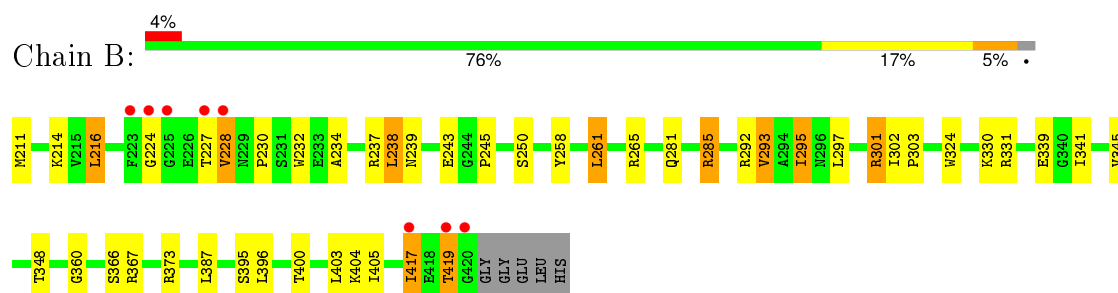
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

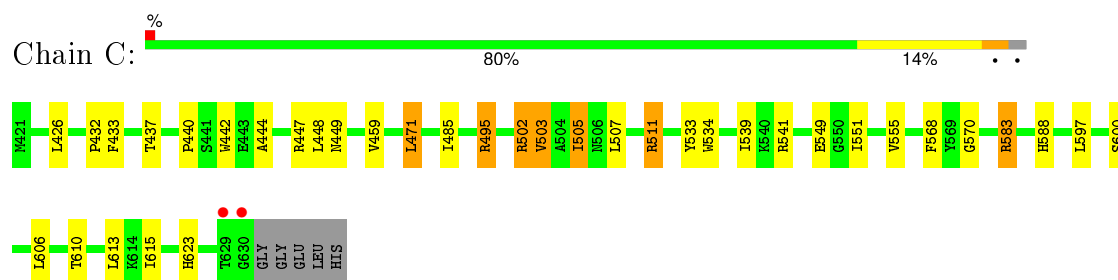
• Molecule 1: PYROGLUTAMYL PEPTIDASE-1



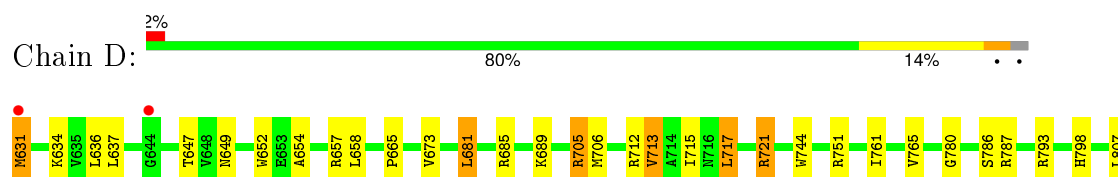
• Molecule 1: PYROGLUTAMYL PEPTIDASE-1

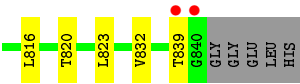


• Molecule 1: PYROGLUTAMYL PEPTIDASE-1



• Molecule 1: PYROGLUTAMYL PEPTIDASE-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.71Å 80.80Å 69.16Å 90.00° 92.75° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 25.78 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 79.0 (25.78-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.95Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.197 , 0.259 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.3	EDS
Estimated twinning fraction	0.001 for -k,-h,-l 0.004 for k,h,-l 0.031 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 50037 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8095	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.94	1/1635 (0.1%)	1.70	25/2222 (1.1%)
1	B	0.94	0/1635	1.58	25/2222 (1.1%)
1	C	0.96	0/1635	1.57	21/2222 (0.9%)
1	D	0.92	0/1635	1.55	26/2222 (1.2%)
All	All	0.94	1/6540 (0.0%)	1.60	97/8888 (1.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	VAL	CA-CB	5.40	1.66	1.54

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ARG	NE-CZ-NH1	26.18	133.39	120.30
1	A	75	ARG	NE-CZ-NH2	-20.91	109.84	120.30
1	D	705	ARG	NE-CZ-NH1	19.01	129.80	120.30
1	B	285	ARG	NE-CZ-NH1	18.23	129.41	120.30
1	C	495	ARG	NE-CZ-NH1	16.01	128.31	120.30
1	C	495	ARG	NE-CZ-NH2	-15.31	112.65	120.30
1	B	285	ARG	NE-CZ-NH2	-14.44	113.08	120.30
1	A	82	ARG	NE-CZ-NH1	11.83	126.21	120.30
1	C	502	ARG	NE-CZ-NH1	10.81	125.71	120.30
1	D	705	ARG	NE-CZ-NH2	-9.97	115.31	120.30
1	A	22	TRP	CD1-CG-CD2	9.37	113.79	106.30
1	B	292	ARG	NE-CZ-NH1	8.81	124.71	120.30
1	D	712	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	C	534	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	B	324	TRP	CE2-CD2-CG	-8.52	100.48	107.30
1	A	22	TRP	CE2-CD2-CG	-8.32	100.64	107.30
1	D	793	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	C	442	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	B	324	TRP	CD1-CG-CD2	8.08	112.76	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	TRP	CE2-CD2-CG	-8.00	100.90	107.30
1	D	652	TRP	CD1-CG-CD2	7.94	112.65	106.30
1	C	534	TRP	CE2-CD2-CG	-7.92	100.97	107.30
1	D	751	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	C	442	TRP	CE2-CD2-CG	-7.72	101.13	107.30
1	A	114	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	B	232	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	D	744	TRP	CD1-CG-CD2	7.44	112.25	106.30
1	A	6	LEU	CA-CB-CG	7.42	132.36	115.30
1	D	652	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	C	583	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	D	744	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	A	75	ARG	CB-CG-CD	7.13	130.14	111.60
1	A	114	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	D	721	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	B	373	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	D	793	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	C	541	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	27	ARG	CA-CB-CG	6.55	127.81	113.40
1	D	649	ASN	N-CA-C	-6.52	93.39	111.00
1	D	685	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	B	301	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	C	533	TYR	CB-CG-CD2	-6.42	117.15	121.00
1	B	419	THR	CA-C-N	6.38	128.97	116.20
1	C	511	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	209	THR	CA-C-N	6.26	128.72	116.20
1	D	839	THR	CA-C-N	6.24	128.67	116.20
1	A	163	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	83	VAL	CB-CA-C	-6.09	99.83	111.40
1	D	705	ARG	CB-CG-CD	6.04	127.31	111.60
1	A	114	TRP	CG-CD2-CE3	6.02	139.32	133.90
1	B	293	VAL	CB-CA-C	-6.02	99.97	111.40
1	A	22	TRP	CB-CG-CD1	-6.00	119.20	127.00
1	D	673	VAL	CG1-CB-CG2	-5.93	101.41	110.90
1	B	237	ARG	CA-CB-CG	5.89	126.36	113.40
1	D	787	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	D	657	ARG	CA-CB-CG	5.85	126.27	113.40
1	D	744	TRP	CB-CG-CD1	-5.83	119.42	127.00
1	C	503	VAL	CB-CA-C	-5.76	100.46	111.40
1	B	228	VAL	CA-CB-CG2	-5.74	102.29	110.90
1	A	114	TRP	CB-CG-CD1	-5.73	119.55	127.00
1	A	85	ILE	CA-CB-CG2	5.71	122.32	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	744	TRP	CG-CD2-CE3	5.69	139.02	133.90
1	A	22	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	A	153	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	367	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	D	631	MET	CA-CB-CG	5.45	122.56	113.30
1	A	76	MET	CG-SD-CE	-5.41	91.54	100.20
1	A	22	TRP	CG-CD2-CE3	5.41	138.77	133.90
1	C	623	HIS	CA-C-N	-5.39	105.33	117.20
1	B	232	TRP	CB-CG-CD1	-5.38	120.00	127.00
1	B	216	LEU	CA-CB-CG	5.38	127.66	115.30
1	C	583	ARG	CA-CB-CG	-5.37	101.58	113.40
1	D	713	VAL	CB-CA-C	-5.36	101.22	111.40
1	C	442	TRP	CB-CG-CD1	-5.34	120.05	127.00
1	B	295	ILE	CA-CB-CG1	-5.34	100.86	111.00
1	C	534	TRP	CG-CD1-NE1	-5.33	104.77	110.10
1	C	534	TRP	CB-CG-CD1	-5.33	120.07	127.00
1	A	85	ILE	CA-CB-CG1	-5.33	100.88	111.00
1	B	324	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	D	652	TRP	CB-CG-CD1	-5.32	120.08	127.00
1	B	265	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	C	534	TRP	CG-CD2-CE3	5.27	138.65	133.90
1	A	113	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	B	373	ARG	CA-CB-CG	-5.26	101.83	113.40
1	B	238	LEU	CA-CB-CG	5.25	127.37	115.30
1	C	568	PHE	CB-CG-CD2	-5.23	117.14	120.80
1	B	295	ILE	CA-CB-CG2	5.18	121.26	110.90
1	D	717	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	114	TRP	CG-CD1-NE1	-5.14	104.96	110.10
1	B	324	TRP	CB-CG-CD1	-5.09	120.39	127.00
1	D	793	ARG	CA-CB-CG	-5.07	102.25	113.40
1	A	82	ARG	CG-CD-NE	5.06	122.42	111.80
1	C	505	ILE	CA-CB-CG1	-5.05	101.41	111.00
1	C	505	ILE	CA-CB-CG2	5.03	120.96	110.90
1	B	265	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	B	324	TRP	CG-CD1-NE1	-5.01	105.09	110.10
1	D	706	MET	CG-SD-CE	-5.00	92.20	100.20

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	1598	347	1605	10	0
1	B	1598	347	1602	13	0
1	C	1598	347	1602	11	0
1	D	1598	347	1602	4	0
2	A	82	0	0	1	0
2	B	83	0	0	2	0
2	C	87	0	0	2	0
2	D	63	0	0	0	0
All	All	6707	1388	6411	38	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 3.

All (38) 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:A:186:LEU:O	1:A:190:THR:HG23	1.98	0.64
1:B:396:LEU:O	1:B:400:THR:HG23	2.01	0.60
1:C:606:LEU:O	1:C:610:THR:HG23	2.04	0.57
1:C:502:ARG:HD3	1:C:539:ILE:HD11	1.87	0.56
1:D:816:LEU:O	1:D:820:THR:HG23	2.04	0.56
1:B:331:ARG:CZ	1:B:417:ILE:HD13	2.38	0.54
1:B:261:LEU:HD11	1:B:360:GLY:HA3	1.93	0.51
1:B:234:ALA:HA	1:B:400:THR:HG22	1.94	0.49
1:C:444:ALA:HA	1:C:610:THR:HG22	1.93	0.49
1:B:395:SER:HB2	2:B:998:HOH:O	2.11	0.49
1:B:302:ILE:HG13	1:B:303:PRO:HD2	1.94	0.49
1:D:681:LEU:HD11	1:D:780:GLY:HA3	1.95	0.49
1:B:339:GLU:HG3	1:B:405:ILE:HD11	1.96	0.48
1:B:230:PRO:HG2	1:B:281:GLN:HE22	1.78	0.47
1:A:179:LYS:HG2	2:A:952:HOH:O	2.15	0.47
1:C:549:GLU:HG3	1:C:615:ILE:HD11	1.97	0.46
1:C:471:LEU:HD11	1:C:570:GLY:HA3	1.97	0.46
1:D:654:ALA:HA	1:D:820:THR:HG22	1.97	0.46
1:A:24:ALA:HA	1:A:190:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:665:PRO:HG2	1:D:832:VAL:HG22	1.99	0.45
1:C:432:PRO:HA	2:C:912:HOH:O	2.16	0.45
1:A:207:ILE:HA	1:A:207:ILE:HD12	1.84	0.44
1:A:13:PHE:HD1	1:A:95:ASN:OD1	2.01	0.44
1:A:33:GLU:HG3	1:A:194:LYS:HD2	2.00	0.44
1:B:330:LYS:HD3	1:B:419:THR:H	1.84	0.43
1:C:600:SER:HA	2:C:897:HOH:O	2.19	0.43
1:B:211:MET:O	1:B:245:PRO:HB3	2.18	0.43
1:C:447:ARG:HD2	1:C:610:THR:HG21	2.01	0.42
1:A:77:GLN:HG2	1:A:132:PRO:HB2	2.00	0.42
1:B:258:TYR:HD1	2:B:1079:HOH:O	2.02	0.42
1:A:119:ILE:HG21	1:A:119:ILE:HD13	1.88	0.42
1:C:502:ARG:CD	1:C:539:ILE:HD11	2.49	0.41
1:C:449:ASN:HD22	1:C:459:VAL:HA	1.83	0.41
1:C:485:ILE:HA	1:C:583:ARG:O	2.21	0.41
1:A:7:LEU:HA	1:A:67:ILE:O	2.21	0.41
1:B:243:GLU:HG3	1:B:404:LYS:HD2	2.02	0.41
1:B:239:ASN:ND2	1:B:250:SER:H	2.19	0.41
1:A:92:ILE:HG13	1:A:93:PRO:HD2	2.03	0.41

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	208/215 (97%)	203 (98%)	5 (2%)	0	100	100
1	B	208/215 (97%)	202 (97%)	5 (2%)	1 (0%)	34	26
1	C	208/215 (97%)	202 (97%)	6 (3%)	0	100	100
1	D	208/215 (97%)	201 (97%)	7 (3%)	0	100	100
All	All	832/860 (97%)	808 (97%)	23 (3%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	224	GLY

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	169/174 (97%)	153 (90%)	16 (10%)	11	6
1	B	169/174 (97%)	151 (89%)	18 (11%)	8	4
1	C	169/174 (97%)	153 (90%)	16 (10%)	11	6
1	D	169/174 (97%)	150 (89%)	19 (11%)	7	4
All	All	676/696 (97%)	607 (90%)	69 (10%)	9	5

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
1	A	6	LEU
1	A	7	LEU
1	A	28	LEU
1	A	51	LEU
1	A	75	ARG
1	A	83	VAL
1	A	85	ILE
1	A	87	LEU
1	A	91	ARG
1	A	131	ILE
1	A	135	VAL
1	A	156	SER
1	A	177	LEU
1	A	193	LEU
1	B	214	LYS
1	B	216	LEU
1	B	227	THR

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Mol	Chain	Res	Type
1	B	228	VAL
1	B	238	LEU
1	B	261	LEU
1	B	285	ARG
1	B	293	VAL
1	B	295	ILE
1	B	297	LEU
1	B	301	ARG
1	B	341	ILE
1	B	345	VAL
1	B	348	THR
1	B	366	SER
1	B	387	LEU
1	B	403	LEU
1	B	417	ILE
1	C	426	LEU
1	C	433	PHE
1	C	437	THR
1	C	440	PRO
1	C	448	LEU
1	C	471	LEU
1	C	495	ARG
1	C	503	VAL
1	C	505	ILE
1	C	507	LEU
1	C	511	ARG
1	C	551	ILE
1	C	555	VAL
1	C	588	HIS
1	C	597	LEU
1	C	613	LEU
1	D	631	MET
1	D	634	LYS
1	D	636	LEU
1	D	637	LEU
1	D	647	THR
1	D	658	LEU
1	D	681	LEU
1	D	689	LYS
1	D	705	ARG
1	D	713	VAL
1	D	715	ILE

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Mol	Chain	Res	Type
1	D	717	LEU
1	D	721	ARG
1	D	761	ILE
1	D	765	VAL
1	D	786	SER
1	D	798	HIS
1	D	807	LEU
1	D	823	LEU

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	29	ASN
1	A	77	GLN
1	A	159	HIS
1	B	239	ASN
1	B	371	HIS
1	C	449	ASN
1	C	527	GLN
1	D	659	ASN
1	D	737	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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, 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	210/215 (97%)	-0.35	4 (1%) 70 70	3, 12, 32, 62	0
1	B	210/215 (97%)	-0.22	8 (3%) 44 45	3, 13, 41, 62	0
1	C	210/215 (97%)	-0.35	2 (0%) 84 84	4, 12, 40, 60	0
1	D	210/215 (97%)	-0.23	4 (1%) 70 70	4, 13, 44, 74	0
All	All	840/860 (97%)	-0.28	18 (2%) 67 67	3, 12, 40, 74	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	840	GLY	12.1
1	B	224	GLY	5.7
1	D	631	MET	5.6
1	D	839	THR	5.5
1	B	419	THR	5.2
1	C	629	THR	4.4
1	A	209	THR	4.3
1	B	227	THR	4.2
1	C	630	GLY	3.8
1	A	210	GLY	3.7
1	D	644	GLY	3.7
1	B	420	GLY	3.6
1	B	225	GLY	3.6
1	A	1	MET	3.0
1	B	223	PHE	2.8
1	B	417	ILE	2.2
1	B	228	VAL	2.1
1	A	107	GLN	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.