



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:55 PM UTC

PDB ID : 1MT1 / pdb_00001mt1
Title : The Crystal Structure of Pyruvoyl-dependent Arginine Decarboxylase from Methanococcus jannaschii
Authors : Tolbert, W.D.; Graham, D.E.; White, R.H.; Ealick, S.E.
Deposited on : 2002-09-20
Resolution : 2.20 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
Mogul : 2022.3.0, CSD as543be (2022)
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

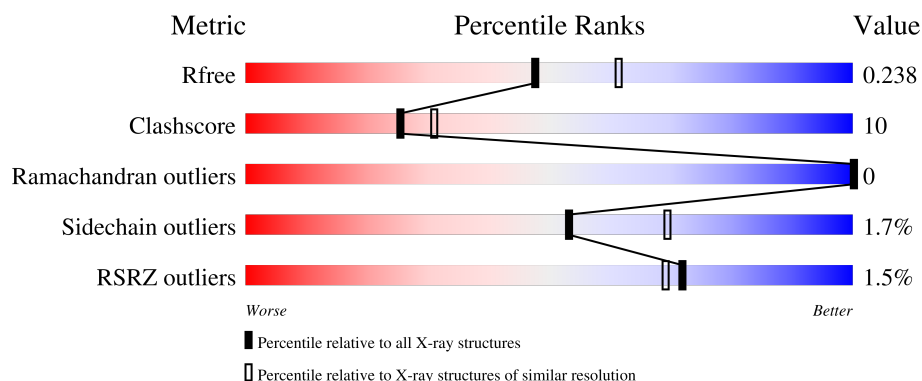
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	52	4% 77% 12% 12%
1	C	52	2% 83% 10% 8%
1	E	52	69% 25% • •
1	G	52	4% 62% 17% 21%
1	I	52	71% 19% • 6%

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Mol	Chain	Length	Quality of chain
1	K	52	10% 58% 27% 13%
2	B	113	85% 15%
2	D	113	81% 19%
2	F	113	% 74% 22%
2	H	113	% 81% 19%
2	J	113	% 84% 16%
2	L	113	% 78% 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7968 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 PYRUVOYL-DEPENDENT ARGININE DECARBOXYLASE BETA CHAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	46	Total	C	N	O	0	3	0
			364	235	60	69			
1	C	48	Total	C	N	O	0	1	0
			360	230	61	69			
1	E	50	Total	C	N	O	0	4	0
			397	253	66	78			
1	G	41	Total	C	N	O	0	2	0
			309	196	52	61			
1	I	49	Total	C	N	O	0	2	0
			377	241	63	73			
1	K	45	Total	C	N	O	0	2	0
			344	220	58	66			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q57764
C	1	MSE	MET	modified residue	UNP Q57764
E	1	MSE	MET	modified residue	UNP Q57764
G	1	MSE	MET	modified residue	UNP Q57764
I	1	MSE	MET	modified residue	UNP Q57764
K	1	MSE	MET	modified residue	UNP Q57764

- Molecule 2 is a protein called PYRUVOYL-DEPENDENT ARGININE DECARBOXYLASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	113	Total	C	N	O	S	Se	0	2	0
			872	562	137	165	3	5			
2	D	113	Total	C	N	O	S	Se	0	7	0
			911	586	142	174	4	5			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	F	113	Total	C	N	O	S	Se	0	4	0
			887	573	139	167	3	5			
2	H	113	Total	C	N	O	S	Se	0	5	0
			899	581	141	169	3	5			
2	J	113	Total	C	N	O	S	Se	0	3	0
			882	569	138	167	3	5			
2	L	113	Total	C	N	O	S	Se	0	1	0
			867	561	136	162	3	5			

There are 36 discrepancies between the modelled and reference sequences:

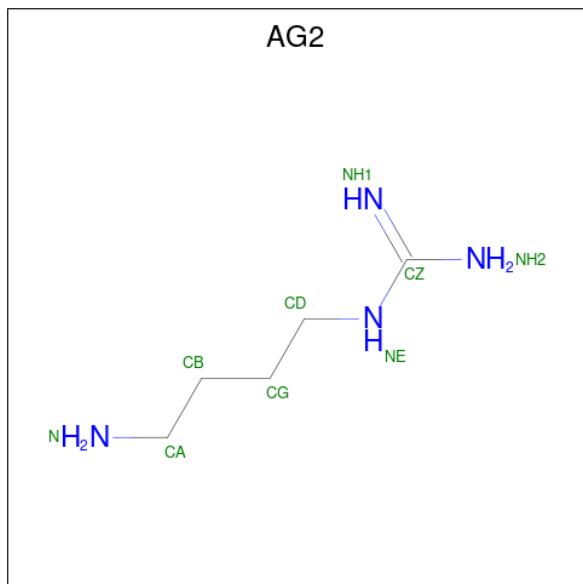
Chain	Residue	Modelled	Actual	Comment	Reference
B	53	PYR	SER	SEE REMARK 999	UNP Q57764
B	55	MSE	MET	modified residue	UNP Q57764
B	69	MSE	MET	modified residue	UNP Q57764
B	108	MSE	MET	modified residue	UNP Q57764
B	126	MSE	MET	modified residue	UNP Q57764
B	133	MSE	MET	modified residue	UNP Q57764
D	53	PYR	SER	SEE REMARK 999	UNP Q57764
D	55	MSE	MET	modified residue	UNP Q57764
D	69	MSE	MET	modified residue	UNP Q57764
D	108	MSE	MET	modified residue	UNP Q57764
D	126	MSE	MET	modified residue	UNP Q57764
D	133	MSE	MET	modified residue	UNP Q57764
F	53	PYR	SER	SEE REMARK 999	UNP Q57764
F	55	MSE	MET	modified residue	UNP Q57764
F	69	MSE	MET	modified residue	UNP Q57764
F	108	MSE	MET	modified residue	UNP Q57764
F	126	MSE	MET	modified residue	UNP Q57764
F	133	MSE	MET	modified residue	UNP Q57764
H	53	PYR	SER	SEE REMARK 999	UNP Q57764
H	55	MSE	MET	modified residue	UNP Q57764
H	69	MSE	MET	modified residue	UNP Q57764
H	108	MSE	MET	modified residue	UNP Q57764
H	126	MSE	MET	modified residue	UNP Q57764
H	133	MSE	MET	modified residue	UNP Q57764
J	53	PYR	SER	SEE REMARK 999	UNP Q57764
J	55	MSE	MET	modified residue	UNP Q57764
J	69	MSE	MET	modified residue	UNP Q57764
J	108	MSE	MET	modified residue	UNP Q57764
J	126	MSE	MET	modified residue	UNP Q57764
J	133	MSE	MET	modified residue	UNP Q57764
L	53	PYR	SER	SEE REMARK 999	UNP Q57764

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Chain	Residue	Modelled	Actual	Comment	Reference
L	55	MSE	MET	modified residue	UNP Q57764
L	69	MSE	MET	modified residue	UNP Q57764
L	108	MSE	MET	modified residue	UNP Q57764
L	126	MSE	MET	modified residue	UNP Q57764
L	133	MSE	MET	modified residue	UNP Q57764

- Molecule 3 is AGMATINE (CCD ID: AG2) (formula: C₅H₁₄N₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 9 5 4	0	0
3	B	1	Total C N 9 5 4	0	0
3	C	1	Total C N 9 5 4	0	0
3	G	1	Total C N 9 5 4	0	0
3	K	1	Total C N 9 5 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	25	Total O 25 25	0	0
4	B	52	Total O 52 52	0	0

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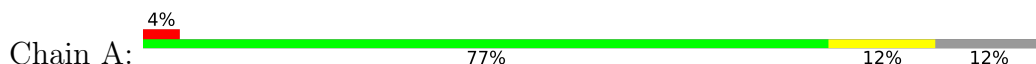
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	26	Total 26	O 26	0	0
4	D	56	Total 56	O 56	0	0
4	E	31	Total 31	O 31	0	0
4	F	60	Total 60	O 60	0	0
4	G	21	Total 21	O 21	0	0
4	H	47	Total 47	O 47	0	0
4	I	28	Total 28	O 28	0	0
4	J	39	Total 39	O 39	0	0
4	K	26	Total 26	O 26	0	0
4	L	43	Total 43	O 43	0	0

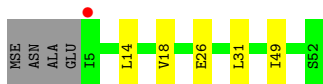
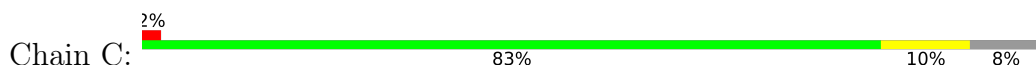
3 Residue-property plots [i](#)

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.

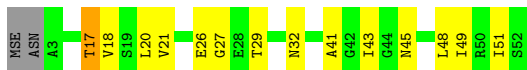
- Molecule 1: PYRUVOL-DEPENDENT ARGININE DECARBOXYLASE BETA CHAIN



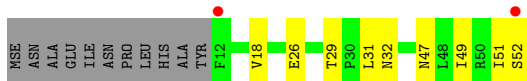
- Molecule 1: PYRUVOL-DEPENDENT ARGININE DECARBOXYLASE BETA CHAIN



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- Molecule 1: PYRUVOL-DEPENDENT ARGININE DECARBOXYLASE BETA CHAIN





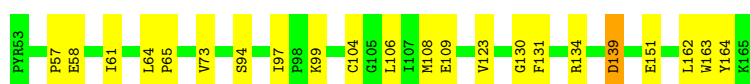
● Molecule 2: PYRUVYL-DEPENDENT ARGININE DECARBOXYLASE ALPHA CHAIN

Chain B: 85% 15%



● Molecule 2: PYRUVYL-DEPENDENT ARGININE DECARBOXYLASE ALPHA CHAIN

Chain D: 81% 19%



● Molecule 2: PYRUVYL-DEPENDENT ARGININE DECARBOXYLASE ALPHA CHAIN

Chain F: 74% 22%



● Molecule 2: PYRUVYL-DEPENDENT ARGININE DECARBOXYLASE ALPHA CHAIN

Chain H: 81% 19%



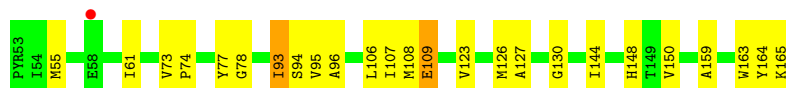
● Molecule 2: PYRUVYL-DEPENDENT ARGININE DECARBOXYLASE ALPHA CHAIN

Chain J: 84% 16%



● Molecule 2: PYRUVYL-DEPENDENT ARGININE DECARBOXYLASE ALPHA CHAIN

Chain L: 78% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.77Å 92.99Å 87.23Å 90.00° 94.84° 90.00°	Depositor
Resolution (Å)	63.50 – 2.20 63.50 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (63.50-2.20) 99.8 (63.50-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.190 , 0.229 0.203 , 0.238	Depositor DCC
R_{free} test set	8839 reflections (7.37%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7968	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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

Bond lengths and bond angles in the following residue types are not validated in this section: AG2, PYR

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	0.38	0/371	0.79	1/504 (0.2%)
1	C	0.40	0/366	0.85	1/498 (0.2%)
1	E	0.43	0/403	0.87	0/549
1	G	0.38	0/312	0.81	1/423 (0.2%)
1	I	0.40	0/383	0.88	1/521 (0.2%)
1	K	0.44	0/349	0.83	1/474 (0.2%)
2	B	0.44	0/880	0.91	1/1181 (0.1%)
2	D	0.42	0/918	0.94	3/1231 (0.2%)
2	F	0.42	0/895	0.91	4/1203 (0.3%)
2	H	0.42	0/906	0.91	1/1213 (0.1%)
2	J	0.40	0/889	0.86	1/1191 (0.1%)
2	L	0.42	0/875	0.92	2/1174 (0.2%)
All	All	0.42	0/7547	0.89	17/10162 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	73	VAL	N-CA-C	7.78	115.62	107.76
2	J	73	VAL	N-CA-C	6.85	115.44	107.77
2	H	73	VAL	N-CA-C	6.79	115.38	107.77
2	L	73	VAL	N-CA-C	6.70	115.28	107.77
2	B	73	VAL	N-CA-C	6.37	114.90	107.77
1	I	44	GLY	N-CA-C	6.21	123.45	115.32
2	F	73[A]	VAL	N-CA-C	5.82	114.36	107.73
2	F	73[B]	VAL	N-CA-C	5.82	114.36	107.73
2	F	151	GLU	N-CA-C	-5.69	105.11	112.68
1	A	26	GLU	N-CA-C	-5.69	102.10	110.52
2	F	76	ALA	N-CA-C	-5.53	100.17	109.07
1	G	26	GLU	N-CA-C	-5.50	102.61	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	26	GLU	N-CA-C	-5.45	102.69	110.59
2	D	139	ASP	N-CA-C	-5.33	103.41	111.56
2	D	151	GLU	N-CA-C	-5.15	105.83	112.68
1	K	26	GLU	N-CA-C	-5.04	103.06	110.52
2	L	150	VAL	N-CA-C	5.04	115.60	109.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	364	0	366	7	0
1	C	360	0	364	4	0
1	E	397	0	396	17	0
1	G	309	0	316	17	0
1	I	377	0	380	15	0
1	K	344	0	348	20	0
2	B	872	0	890	16	0
2	D	911	0	922	22	0
2	F	887	0	909	22	0
2	H	899	0	921	26	0
2	J	882	0	899	15	0
2	L	867	0	890	20	0
3	A	9	0	13	1	0
3	B	9	0	13	1	0
3	C	9	0	13	0	0
3	G	9	0	13	2	0
3	K	9	0	13	2	0
4	A	25	0	0	0	0
4	B	52	0	0	0	0
4	C	26	0	0	0	0
4	D	56	0	0	0	0
4	E	31	0	0	0	0
4	F	60	0	0	2	0
4	G	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	47	0	0	0	0
4	I	28	0	0	0	0
4	J	39	0	0	0	0
4	K	26	0	0	0	0
4	L	43	0	0	0	0
All	All	7968	0	7666	147	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 10.

All (147) 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)
2:D:104[B]:CYS:SG	2:F:69:MSE:HB3	1.81	1.21
2:D:134:ARG:HE	1:E:45:ASN:HD21	1.14	0.93
2:D:104[B]:CYS:HG	2:F:69:MSE:HB3	1.26	0.93
2:H:134:ARG:HE	1:K:45:ASN:HD21	1.17	0.91
1:E:21[B]:VAL:HG12	1:E:41:ALA:HB1	1.69	0.75
1:I:16:ASN:HD21	2:J:165:LYS:H	1.35	0.74
2:F:106[A]:LEU:HD21	2:F:108:MSE:HE2	1.69	0.73
1:E:21[B]:VAL:CG1	1:E:41:ALA:HB1	2.18	0.72
2:J:108:MSE:HE3	2:J:126:MSE:HE2	1.72	0.71
2:B:107:ILE:O	2:B:108:MSE:HE2	1.91	0.70
2:B:57:PRO:O	2:B:58:GLU:HG2	1.92	0.68
2:D:57:PRO:O	2:D:58:GLU:HG2	1.94	0.68
1:E:17:THR:HG21	4:F:213:HOH:O	1.92	0.68
2:D:106[A]:LEU:HD21	2:D:108:MSE:HE2	1.75	0.66
2:D:104[B]:CYS:SG	2:F:69:MSE:CB	2.74	0.65
1:E:18[B]:VAL:HG12	2:F:162:LEU:CD2	2.26	0.65
1:I:49:ILE:HD13	1:K:51[B]:ILE:HG22	1.78	0.65
1:G:31:LEU:HD21	3:G:7003:AG2:HA2	1.78	0.64
1:K:31:LEU:HD21	3:K:7002:AG2:HA2	1.80	0.63
1:G:18[B]:VAL:HG12	2:H:162:LEU:CD2	2.30	0.61
2:D:134:ARG:HE	1:E:45:ASN:ND2	1.91	0.61
2:H:93:ILE:HG22	2:H:144:ILE:HG22	1.82	0.61
2:L:107:ILE:O	2:L:108:MSE:HE2	2.01	0.61
1:G:18[B]:VAL:HG12	2:H:162:LEU:HD22	1.83	0.60
1:E:18[B]:VAL:HG12	2:F:162:LEU:HD23	1.83	0.60
2:J:61:ILE:HD12	2:J:142:GLU:HG3	1.83	0.60
1:A:48:LEU:HB3	2:B:75[B]:THR:HG21	1.83	0.59
2:F:94:SER:HB3	2:F:123:VAL:HG13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:96:ALA:HB2	2:L:127:ALA:HB1	1.83	0.59
2:H:108:MSE:HE3	2:H:126:MSE:HE3	1.83	0.59
2:D:106[B]:LEU:HG	2:D:131:PHE:HE1	1.68	0.59
2:J:163:TRP:CG	2:J:164:TYR:H	2.20	0.59
1:G:18[A]:VAL:HB	2:H:61[A]:ILE:HD13	1.85	0.58
2:H:134:ARG:HE	1:K:45:ASN:ND2	1.96	0.58
2:F:75[B]:THR:HG22	2:F:161:ALA:HA	1.85	0.58
2:F:163:TRP:CG	2:F:164:TYR:H	2.22	0.58
1:C:18:VAL:HG22	2:D:162:LEU:HD22	1.85	0.57
1:I:31:LEU:HB3	2:L:126:MSE:HE2	1.86	0.57
2:D:61:ILE:CD1	2:D:97:ILE:HD11	2.35	0.56
2:D:163:TRP:CG	2:D:164:TYR:H	2.23	0.55
2:L:163:TRP:CG	2:L:164:TYR:H	2.24	0.55
1:E:17:THR:HG22	4:F:197:HOH:O	2.06	0.55
2:H:93:ILE:CG2	2:H:144:ILE:HG22	2.37	0.54
1:I:18:VAL:HG13	2:J:61:ILE:HG12	1.89	0.54
2:B:163:TRP:CG	2:B:164:TYR:H	2.25	0.54
2:D:61:ILE:HD12	2:D:97:ILE:HD11	1.89	0.53
1:A:49:ILE:CD1	1:E:51:ILE:HG22	2.38	0.53
1:G:18[A]:VAL:HG21	2:H:55:MSE:HG3	1.91	0.52
2:H:118:GLU:O	2:H:121[B]:LYS:HG3	2.09	0.52
2:H:106[B]:LEU:CD2	2:H:130:GLY:HA3	2.41	0.51
1:K:51[A]:ILE:HG22	1:K:52:SER:N	2.26	0.51
1:A:48:LEU:HD22	2:B:75[B]:THR:HG21	1.93	0.51
1:G:51[B]:ILE:HG22	1:K:49:ILE:HD13	1.93	0.50
1:I:5:ILE:CD1	1:I:13:LYS:HE3	2.42	0.50
2:J:96:ALA:HB2	2:J:127:ALA:HB1	1.94	0.50
2:D:106[B]:LEU:HG	2:D:131:PHE:CE1	2.47	0.49
1:I:31:LEU:HB3	2:L:126:MSE:CE	2.41	0.49
1:I:39:LEU:HD23	1:I:44:GLY:HA3	1.94	0.49
2:B:106:LEU:HD11	2:B:108:MSE:HE3	1.93	0.49
1:A:48:LEU:HB3	2:B:75[B]:THR:CG2	2.42	0.49
1:I:5:ILE:HD12	1:I:13:LYS:HE3	1.94	0.48
2:D:94:SER:HB3	2:D:123:VAL:HG13	1.95	0.48
2:F:96:ALA:HB2	2:F:127:ALA:HB1	1.95	0.48
1:I:49:ILE:CD1	1:K:51[B]:ILE:HG22	2.42	0.48
2:F:55:MSE:HE2	2:F:105:GLY:HA3	1.94	0.48
2:H:108:MSE:HB3	2:H:126:MSE:HE2	1.95	0.48
2:H:163:TRP:CG	2:H:164:TYR:H	2.32	0.48
2:D:106[B]:LEU:HD11	2:D:134:ARG:HD2	1.96	0.48
1:G:49:ILE:HD13	1:I:51[B]:ILE:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106[A]:LEU:CD2	2:D:130:GLY:HA3	2.44	0.47
1:A:38:LEU:HD12	3:A:7005:AG2:CZ	2.45	0.47
2:D:99:LYS:HE2	2:D:139:ASP:HA	1.97	0.47
1:G:51[A]:ILE:HG21	1:K:47:ASN:OD1	2.15	0.47
1:G:51[B]:ILE:HG22	1:K:49:ILE:CD1	2.44	0.47
1:E:43[B]:ILE:HD11	2:F:157:PHE:CE2	2.49	0.47
1:K:43:ILE:HD12	1:K:48:LEU:HD21	1.97	0.47
2:L:94:SER:HB3	2:L:123:VAL:HG13	1.97	0.47
1:G:51[A]:ILE:HG22	1:G:52:SER:N	2.29	0.46
1:I:16:ASN:HD21	2:J:165:LYS:N	2.06	0.46
1:E:48:LEU:HD22	2:F:75[B]:THR:HG21	1.97	0.46
2:B:94:SER:HB3	2:B:123:VAL:HG13	1.97	0.46
1:A:51[B]:ILE:HG22	1:C:49:ILE:HD13	1.96	0.46
1:G:18[B]:VAL:CG2	2:H:61[B]:ILE:HG12	2.45	0.46
2:H:93:ILE:HG22	2:H:144:ILE:CG2	2.45	0.46
2:J:61:ILE:CD1	2:J:142:GLU:HG3	2.45	0.46
2:D:163:TRP:CD1	2:D:164:TYR:H	2.34	0.46
1:K:24:SER:HB2	2:L:148:HIS:HB2	1.97	0.46
2:B:106:LEU:CD2	2:B:130:GLY:HA3	2.46	0.46
1:E:51:ILE:HG13	2:F:53:PYR:CB	2.46	0.46
1:I:43[B]:ILE:HD11	2:J:157:PHE:CE2	2.51	0.45
2:F:106[B]:LEU:HG	2:F:131:PHE:CE1	2.51	0.45
2:F:64:LEU:HA	2:F:65:PRO:HD3	1.82	0.45
2:H:126:MSE:CE	1:K:31:LEU:HD23	2.47	0.45
3:G:7003:AG2:HB2	2:J:53:PYR:O3	2.17	0.45
2:H:121[B]:LYS:HD2	2:H:121[B]:LYS:C	2.43	0.44
1:E:18[B]:VAL:HG23	2:F:61:ILE:HD13	1.99	0.44
1:G:29:THR:OG1	1:G:32:ASN:ND2	2.50	0.44
1:K:20:LEU:HD21	2:L:95:VAL:CG2	2.46	0.44
1:K:18[B]:VAL:HG21	2:L:55:MSE:HG3	1.99	0.44
2:L:106[A]:LEU:CD2	2:L:130:GLY:HA3	2.47	0.44
1:E:49:ILE:HD11	2:F:72:LEU:HB3	2.00	0.44
1:K:31:LEU:HD11	3:K:7002:AG2:HA2	1.99	0.44
2:B:126:MSE:HE2	1:C:31:LEU:HB3	1.99	0.43
2:L:78:GLY:CA	2:L:109:GLU:HG3	2.48	0.43
2:L:93:ILE:HG22	2:L:144:ILE:HG22	2.00	0.43
1:G:31:LEU:HB3	2:J:126:MSE:HE3	2.00	0.43
1:K:18[A]:VAL:HG13	2:L:61:ILE:HG12	1.99	0.43
2:B:106:LEU:CD1	2:B:108:MSE:HE3	2.49	0.43
1:I:8:LEU:HD21	1:K:49:ILE:HG21	2.00	0.43
1:I:6:ASN:OD1	1:I:8:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:78:GLY:HA3	2:L:109:GLU:HG3	2.00	0.43
1:K:51[A]:ILE:HD11	2:L:74:PRO:HB3	2.01	0.42
1:G:18[B]:VAL:HG23	2:H:61[B]:ILE:HA	2.01	0.42
2:J:94:SER:HB3	2:J:123:VAL:HG13	2.00	0.42
2:D:57:PRO:HD3	2:D:104[B]:CYS:SG	2.60	0.42
1:A:21:VAL:HG11	2:B:64:LEU:HD22	2.02	0.42
1:G:18[B]:VAL:HG11	2:H:55:MSE:HG3	2.02	0.42
2:H:121[A]:LYS:O	2:H:125[A]:GLU:HG3	2.19	0.42
2:L:93:ILE:HG22	2:L:144:ILE:CG2	2.50	0.42
2:B:64:LEU:HA	2:B:65:PRO:HD3	1.82	0.42
2:F:106[B]:LEU:HG	2:F:131:PHE:HE1	1.84	0.42
2:L:77:TYR:HB3	2:L:159:ALA:HB2	2.02	0.42
2:H:99:LYS:C	2:H:99:LYS:HD3	2.44	0.42
1:K:17:THR:CG2	2:L:165:LYS:HG3	2.49	0.42
2:B:106:LEU:HG	2:B:108:MSE:HE3	2.01	0.41
1:K:14:LEU:HA	1:K:15:PRO:HD3	1.94	0.41
3:B:7001:AG2:HA1	1:C:31:LEU:HD11	2.02	0.41
2:D:64:LEU:HA	2:D:65:PRO:HD3	1.85	0.41
2:F:129:ILE:O	2:F:133:MSE:HG3	2.19	0.41
2:F:73[B]:VAL:HA	2:F:74:PRO:HD3	1.87	0.41
2:L:93:ILE:CG2	2:L:144:ILE:HG22	2.50	0.41
2:D:106[B]:LEU:HD12	2:D:131:PHE:HD1	1.85	0.41
2:B:96:ALA:HB2	2:B:127:ALA:HB1	2.03	0.41
1:E:26[B]:GLU:HG2	1:E:27:GLY:N	2.35	0.41
2:H:94:SER:HB3	2:H:123:VAL:HG13	2.02	0.41
2:H:108:MSE:HE3	2:H:126:MSE:CE	2.47	0.41
2:L:106[A]:LEU:HD11	2:L:108:MSE:HE3	2.03	0.41
1:G:18[B]:VAL:HG23	2:H:61[B]:ILE:HG12	2.02	0.41
2:H:61[B]:ILE:CD1	2:H:97:ILE:HD11	2.51	0.41
1:I:51[B]:ILE:HG12	2:J:75:THR:C	2.46	0.41
2:J:163:TRP:CD1	2:J:164:TYR:H	2.39	0.41
1:G:47:ASN:HB2	2:H:72:LEU:HD23	2.03	0.41
2:D:106[A]:LEU:HD21	2:D:130:GLY:HA3	2.02	0.40
1:E:29:THR:OG1	1:E:32:ASN:ND2	2.54	0.40
2:J:55:MSE:O	2:J:104:CYS:HB2	2.21	0.40
2:B:106:LEU:CG	2:B:108:MSE:HE3	2.51	0.40
1:E:20:LEU:HD22	2:F:93:ILE:CG2	2.51	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	47/52 (90%)	45 (96%)	2 (4%)	0	100	100
1	C	47/52 (90%)	45 (96%)	2 (4%)	0	100	100
1	E	52/52 (100%)	50 (96%)	2 (4%)	0	100	100
1	G	41/52 (79%)	40 (98%)	1 (2%)	0	100	100
1	I	49/52 (94%)	47 (96%)	2 (4%)	0	100	100
1	K	45/52 (86%)	43 (96%)	2 (4%)	0	100	100
2	B	113/113 (100%)	112 (99%)	1 (1%)	0	100	100
2	D	118/113 (104%)	116 (98%)	2 (2%)	0	100	100
2	F	115/113 (102%)	113 (98%)	2 (2%)	0	100	100
2	H	116/113 (103%)	114 (98%)	2 (2%)	0	100	100
2	J	114/113 (101%)	112 (98%)	2 (2%)	0	100	100
2	L	112/113 (99%)	111 (99%)	1 (1%)	0	100	100
All	All	969/990 (98%)	948 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	39/40 (98%)	39 (100%)	0	100	100
1	C	39/40 (98%)	38 (97%)	1 (3%)	40	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	43/40 (108%)	42 (98%)	1 (2%)	44	59
1	G	34/40 (85%)	34 (100%)	0	100	100
1	I	41/40 (102%)	40 (98%)	1 (2%)	43	58
1	K	37/40 (92%)	36 (97%)	1 (3%)	39	53
2	B	92/85 (108%)	92 (100%)	0	100	100
2	D	97/85 (114%)	96 (99%)	1 (1%)	68	81
2	F	94/85 (111%)	90 (96%)	4 (4%)	26	35
2	H	95/85 (112%)	94 (99%)	1 (1%)	65	79
2	J	93/85 (109%)	92 (99%)	1 (1%)	65	79
2	L	91/85 (107%)	89 (98%)	2 (2%)	45	61
All	All	795/750 (106%)	782 (98%)	13 (2%)	53	71

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	14	LEU
2	D	109	GLU
1	E	17	THR
2	F	61	ILE
2	F	93	ILE
2	F	123	VAL
2	F	153	LEU
2	H	113	LYS
1	I	16	ASN
2	J	109	GLU
1	K	14	LEU
2	L	93	ILE
2	L	109	GLU

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

Mol	Chain	Res	Type
1	E	32	ASN
1	E	45	ASN
1	G	32	ASN
1	I	16	ASN
1	I	32	ASN

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Mol	Chain	Res	Type
1	K	45	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	AG2	B	7001	-	8,8,8	0.28	0	7,8,8	0.28	0
3	AG2	K	7002	-	8,8,8	0.27	0	7,8,8	0.31	0
3	AG2	A	7005	-	8,8,8	0.28	0	7,8,8	0.34	0
3	AG2	G	7003	-	8,8,8	0.28	0	7,8,8	0.30	0
3	AG2	C	7004	-	8,8,8	0.32	0	7,8,8	0.28	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AG2	B	7001	-	-	0/6/6/6	-
3	AG2	K	7002	-	-	0/6/6/6	-
3	AG2	A	7005	-	-	1/6/6/6	-
3	AG2	G	7003	-	-	0/6/6/6	-
3	AG2	C	7004	-	-	0/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	7005	AG2	CG-CD-NE-CZ

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	7001	AG2	1	0
3	K	7002	AG2	2	0
3	A	7005	AG2	1	0
3	G	7003	AG2	2	0

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, 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	46/52 (88%)	-0.05	2 (4%) 40 36	7, 13, 27, 51	3 (6%)
1	C	48/52 (92%)	-0.13	1 (2%) 63 60	7, 12, 32, 48	1 (2%)
1	E	50/52 (96%)	-0.12	0 100 100	4, 13, 24, 38	4 (8%)
1	G	41/52 (78%)	-0.10	2 (4%) 35 31	5, 13, 27, 44	2 (4%)
1	I	49/52 (94%)	0.31	0 100 100	9, 17, 40, 53	2 (4%)
1	K	45/52 (86%)	0.31	5 (11%) 10 8	5, 14, 55, 71	2 (4%)
2	B	107/113 (94%)	-0.08	0 100 100	4, 16, 30, 36	2 (1%)
2	D	107/113 (94%)	-0.15	0 100 100	5, 15, 30, 36	7 (6%)
2	F	107/113 (94%)	-0.14	1 (0%) 81 79	4, 14, 28, 41	4 (3%)
2	H	107/113 (94%)	-0.02	1 (0%) 81 79	5, 16, 33, 37	5 (4%)
2	J	107/113 (94%)	0.04	1 (0%) 81 79	6, 19, 37, 41	3 (2%)
2	L	107/113 (94%)	-0.00	1 (0%) 81 79	7, 18, 32, 37	1 (0%)
All	All	921/990 (93%)	-0.03	14 (1%) 72 69	4, 16, 34, 71	36 (3%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	8	LEU	5.7
1	K	10	ALA	3.8
1	K	11	TYR	3.7
1	K	9	HIS	3.6
1	K	12	PHE	3.3
1	G	52	SER	2.9
1	C	5	ILE	2.6
1	G	12	PHE	2.6
1	A	52	SER	2.4
1	A	7	PRO	2.4
2	F	58	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	J	165	LYS	2.2
2	L	58	GLU	2.2
2	H	152	LYS	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AG2	C	7004	9/9	0.55	0.28	32,39,41,41	9
3	AG2	G	7003	9/9	0.69	0.20	30,35,40,40	9
3	AG2	K	7002	9/9	0.75	0.20	25,32,37,37	9
3	AG2	A	7005	9/9	0.77	0.17	28,32,40,41	9
3	AG2	B	7001	9/9	0.78	0.18	28,32,38,41	9

6.5 Other polymers [i](#)

There are no such residues in this entry.