



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:43 AM UTC

PDB ID : 7YTO / pdb_00007yto
Title : The Crystal Structure Analysis of Creatine Amidinohydrolase from *Alcaligenes* sp. KS-85
Authors : Chen, R.S.
Deposited on : 2022-08-15
Resolution : 2.31 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

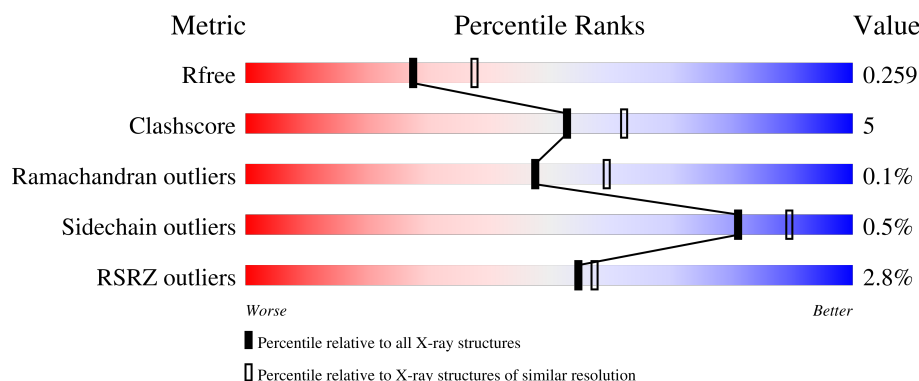
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	404	88% 11% .
1	B	404	2% 84% 14% .
1	C	404	87% 12% .
1	D	404	2% 89% 10% .
1	E	404	4% 85% 14% .

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Mol	Chain	Length	Quality of chain
1	F	404	6% 85% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19352 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 Creatine amidinohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	401	Total	C	N	O	S	0	0	0
			3191	2018	560	591	22			
1	E	401	Total	C	N	O	S	0	0	0
			3193	2021	560	589	23			
1	F	400	Total	C	N	O	S	0	0	0
			3174	2008	555	588	23			
1	A	401	Total	C	N	O	S	0	0	0
			3202	2025	563	591	23			
1	B	400	Total	C	N	O	S	0	0	0
			3194	2021	562	588	23			
1	C	401	Total	C	N	O	S	0	0	0
			3202	2025	563	591	23			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	304	LEU	ILE	conflict	UNP Q9RHU9
D	395	VAL	PHE	conflict	UNP Q9RHU9
E	304	LEU	ILE	conflict	UNP Q9RHU9
E	395	VAL	PHE	conflict	UNP Q9RHU9
F	304	LEU	ILE	conflict	UNP Q9RHU9
F	395	VAL	PHE	conflict	UNP Q9RHU9
A	304	LEU	ILE	conflict	UNP Q9RHU9
A	395	VAL	PHE	conflict	UNP Q9RHU9
B	304	LEU	ILE	conflict	UNP Q9RHU9
B	395	VAL	PHE	conflict	UNP Q9RHU9
C	304	LEU	ILE	conflict	UNP Q9RHU9
C	395	VAL	PHE	conflict	UNP Q9RHU9

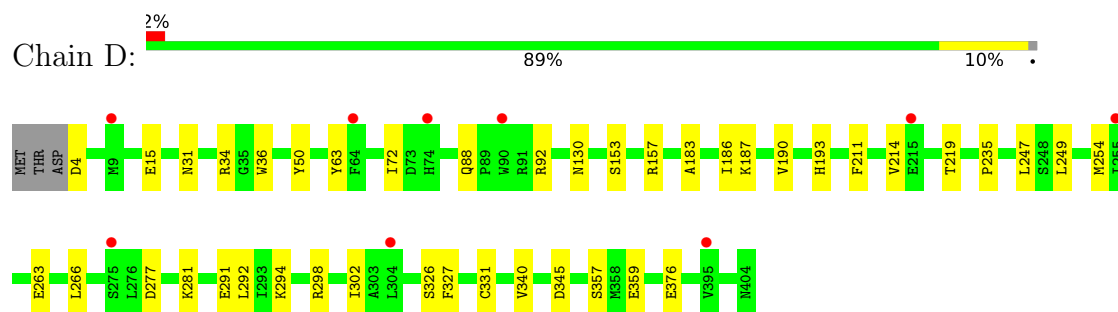
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	31	Total 31	O 31	0	0
2	E	37	Total 37	O 37	0	0
2	F	27	Total 27	O 27	0	0
2	A	38	Total 38	O 38	0	0
2	B	37	Total 37	O 37	0	0
2	C	26	Total 26	O 26	0	0

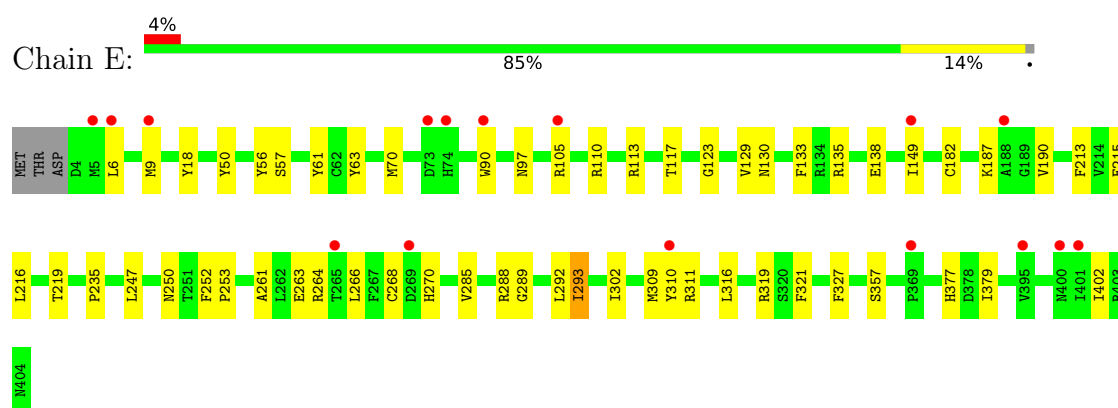
3 Residue-property plots [i](#)

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.

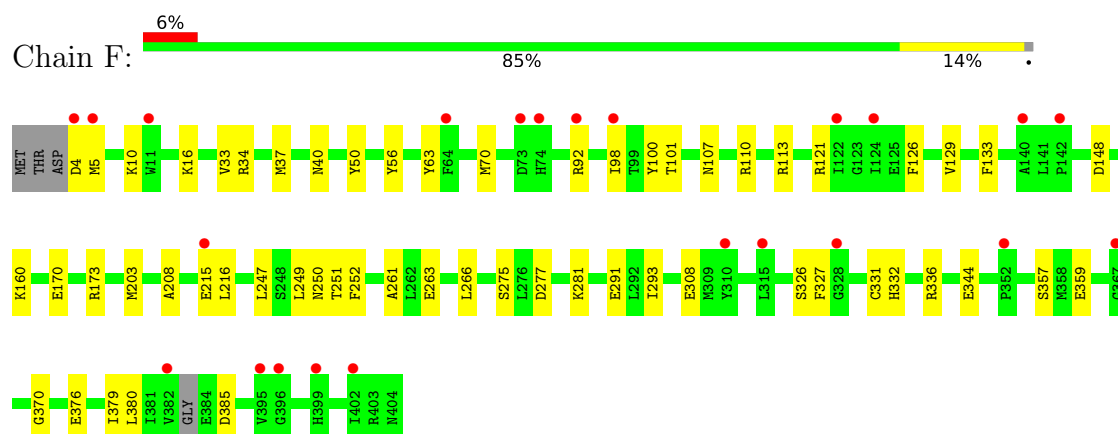
- Molecule 1: Creatine amidinohydrolase



- Molecule 1: Creatine amidinohydrolase

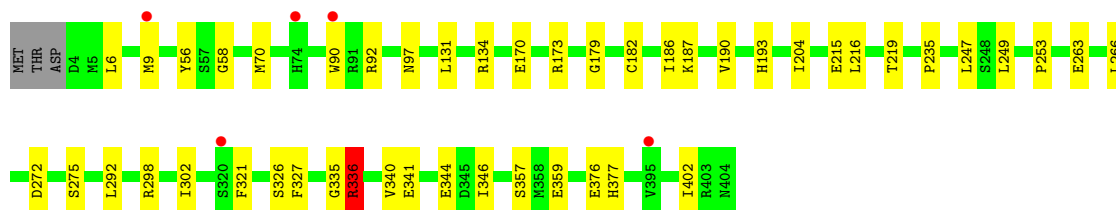


- Molecule 1: Creatine amidinohydrolase



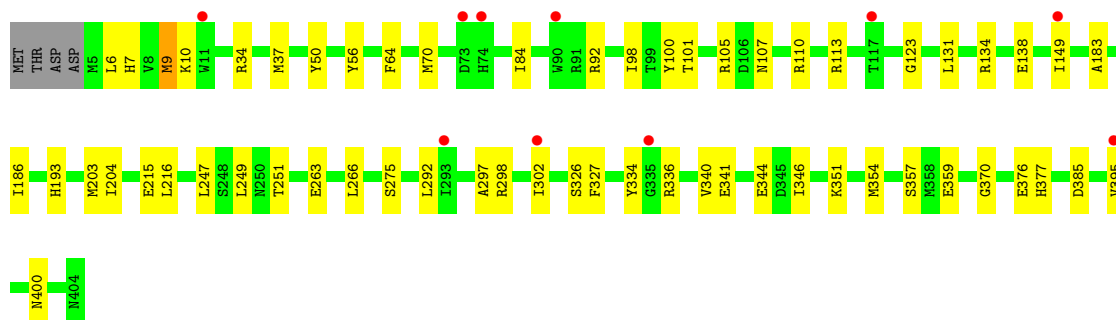
- Molecule 1: Creatine amidinohydrolase

Chain A:  88% 11%



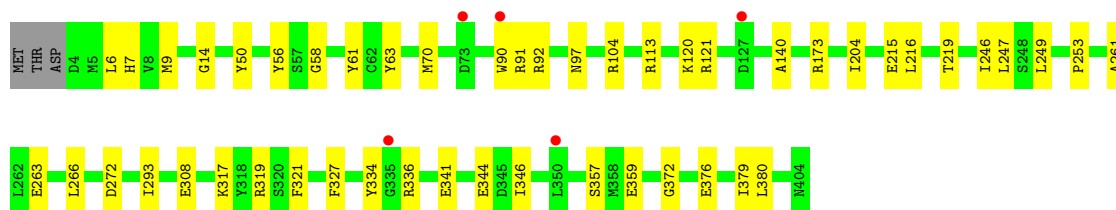
- Molecule 1: Creatine amidinohydrolase

Chain B:  84% 14%



- Molecule 1: Creatine amidinohydrolase

Chain C:  87% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	194.95Å 113.76Å 111.48Å 90.00° 94.90° 90.00°	Depositor
Resolution (Å)	40.00 – 2.31 40.00 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.31) 94.5 (40.00-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.215 , 0.257 0.216 , 0.259	Depositor DCC
R_{free} test set	2006 reflections (1.90%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19352	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.11	0/3283	0.32	0/4446
1	B	0.11	0/3275	0.31	0/4435
1	C	0.11	0/3283	0.31	0/4446
1	D	0.11	0/3272	0.30	0/4433
1	E	0.11	0/3274	0.30	0/4435
1	F	0.10	0/3252	0.28	0/4404
All	All	0.11	0/19639	0.30	0/26599

There are no bond length outliers.

There are no bond angle outliers.

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	3202	0	3072	33	0
1	B	3194	0	3068	38	0
1	C	3202	0	3072	31	0
1	D	3191	0	3047	29	0
1	E	3193	0	3059	37	0
1	F	3174	0	3036	36	0
2	A	38	0	0	0	0
2	B	37	0	0	1	0
2	C	26	0	0	2	0
2	D	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	37	0	0	2	0
2	F	27	0	0	2	0
All	All	19352	0	18354	186	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 5.

All (186) 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:D:331:CYS:SG	2:D:502:HOH:O	2.27	0.92
1:D:219:THR:HG22	1:D:254:MET:H	1.42	0.85
1:D:292:LEU:HB3	1:D:302:ILE:HD12	1.69	0.74
1:B:9:MET:HE1	1:B:101:THR:HG23	1.71	0.73
1:A:336:ARG:HD2	1:A:341:GLU:OE2	1.89	0.73
1:A:292:LEU:HB3	1:A:302:ILE:HD12	1.72	0.72
1:C:341:GLU:HB2	1:C:346:ILE:HD12	1.72	0.71
1:A:247:LEU:HB2	1:A:266:LEU:HB2	1.73	0.70
1:C:56:TYR:HB2	1:C:70:MET:HE1	1.73	0.70
1:E:56:TYR:HB2	1:E:70:MET:HE1	1.74	0.69
1:B:292:LEU:HB3	1:B:302:ILE:HD12	1.73	0.69
1:F:92:ARG:HH12	1:F:215:GLU:HB2	1.60	0.67
1:E:182:CYS:SG	2:E:503:HOH:O	2.53	0.67
1:A:56:TYR:HB2	1:A:70:MET:HE1	1.78	0.66
1:F:16:LYS:NZ	2:F:501:HOH:O	2.29	0.66
1:D:36:TRP:NE1	1:F:385:ASP:OD2	2.29	0.65
1:F:293:ILE:HD12	1:F:380:LEU:HD13	1.79	0.65
1:B:56:TYR:HB2	1:B:70:MET:HE1	1.80	0.64
1:F:129:VAL:HG13	1:F:133:PHE:HB3	1.81	0.63
1:B:327:PHE:HE1	1:B:357:SER:HB3	1.64	0.63
1:A:193:HIS:HB3	1:B:216:LEU:HD13	1.80	0.63
1:C:336:ARG:HD2	1:C:341:GLU:OE2	1.99	0.63
1:E:6:LEU:HD13	1:E:9:MET:HG3	1.79	0.62
1:E:110:ARG:NH2	1:F:308:GLU:OE2	2.29	0.62
1:E:264:ARG:NH1	2:E:502:HOH:O	2.31	0.62
1:A:327:PHE:HE1	1:A:357:SER:HB3	1.65	0.61
1:F:56:TYR:HB2	1:F:70:MET:HE1	1.82	0.61
1:E:288:ARG:NE	1:E:309:MET:SD	2.73	0.60
1:F:247:LEU:HB2	1:F:266:LEU:HB2	1.83	0.60
1:E:90:TRP:HD1	1:E:97:ASN:HB3	1.66	0.60
1:F:277:ASP:OD1	1:F:281:LYS:NZ	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:LEU:HB2	1:D:266:LEU:HB2	1.82	0.60
1:A:344:GLU:N	1:A:344:GLU:OE2	2.35	0.59
1:F:208:ALA:HB2	1:F:216:LEU:HD21	1.84	0.59
1:D:4:ASP:OD2	1:E:311:ARG:NH2	2.33	0.58
1:F:40:ASN:O	1:F:121:ARG:NH1	2.36	0.57
1:B:344:GLU:N	1:B:344:GLU:OE2	2.36	0.56
1:C:173:ARG:NH2	2:C:501:HOH:O	2.39	0.56
1:C:58:GLY:O	1:C:92:ARG:NH1	2.40	0.55
1:D:277:ASP:OD1	1:D:281:LYS:NZ	2.40	0.55
1:E:327:PHE:HE1	1:E:357:SER:HB3	1.71	0.55
1:D:327:PHE:HE1	1:D:357:SER:HB3	1.71	0.55
1:F:101:THR:OG1	1:F:107:ASN:ND2	2.40	0.55
1:B:336:ARG:HD2	1:B:341:GLU:OE2	2.07	0.54
1:D:15:GLU:HG3	1:C:317:LYS:HD2	1.88	0.54
1:A:216:LEU:HD13	1:B:193:HIS:HB3	1.90	0.54
1:E:263:GLU:HB2	1:E:377:HIS:HB3	1.89	0.54
1:D:193:HIS:HB3	1:E:216:LEU:HD13	1.90	0.54
1:A:327:PHE:CE1	1:A:357:SER:HB3	2.44	0.53
1:C:219:THR:HG23	1:C:253:PRO:HA	1.91	0.53
1:A:92:ARG:HE	1:A:215:GLU:CD	2.16	0.53
1:B:247:LEU:HB2	1:B:266:LEU:HB2	1.89	0.53
1:D:187:LYS:O	1:D:190:VAL:HG12	2.09	0.52
1:B:134:ARG:NH1	1:B:138:GLU:OE1	2.42	0.52
1:C:327:PHE:HE1	1:C:357:SER:HB3	1.73	0.52
1:E:57:SER:HB3	1:E:70:MET:SD	2.50	0.52
1:F:327:PHE:CE1	1:F:357:SER:HB3	2.45	0.52
1:B:263:GLU:HB2	1:B:377:HIS:HB3	1.92	0.52
1:E:261:ALA:H	1:E:379:ILE:HD11	1.73	0.52
1:B:10:LYS:HE2	1:B:98:ILE:HG22	1.91	0.52
1:B:327:PHE:CE1	1:B:357:SER:HB3	2.45	0.52
1:D:327:PHE:CE1	1:D:357:SER:HB3	2.44	0.52
1:A:341:GLU:HB2	1:A:346:ILE:HD12	1.92	0.51
1:C:359:GLU:HA	1:C:376:GLU:O	2.10	0.51
1:E:135:ARG:HD2	1:F:291:GLU:OE2	2.11	0.51
1:F:10:LYS:HG2	1:F:98:ILE:HG22	1.93	0.51
1:C:327:PHE:CE1	1:C:357:SER:HB3	2.45	0.51
1:C:121:ARG:NH1	2:C:504:HOH:O	2.44	0.50
1:D:130:ASN:HA	1:E:130:ASN:HA	1.93	0.50
1:B:341:GLU:HB2	1:B:346:ILE:HD12	1.94	0.50
1:B:297:ALA:HB1	1:B:302:ILE:HD11	1.93	0.50
1:F:261:ALA:H	1:F:379:ILE:HD11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:HD11	1:B:134:ARG:HG3	1.94	0.49
1:C:247:LEU:HB2	1:C:266:LEU:HB2	1.93	0.49
1:F:34:ARG:NH2	2:F:502:HOH:O	2.44	0.49
1:B:92:ARG:HE	1:B:215:GLU:CD	2.21	0.49
1:D:326:SER:HB2	1:D:340:VAL:HB	1.95	0.49
1:C:204:ILE:HG23	1:C:216:LEU:HD22	1.95	0.48
1:D:211:PHE:HB2	1:D:214:VAL:HB	1.95	0.48
1:B:183:ALA:HA	1:B:186:ILE:HD12	1.94	0.48
1:C:344:GLU:N	1:C:344:GLU:OE2	2.46	0.48
1:A:58:GLY:O	1:A:92:ARG:NH1	2.47	0.48
1:F:100:TYR:HB2	1:F:107:ASN:HB3	1.95	0.48
1:B:359:GLU:HA	1:B:376:GLU:O	2.13	0.48
1:E:266:LEU:HD13	1:E:402:ILE:HD11	1.96	0.48
1:E:292:LEU:HB3	1:E:302:ILE:HD12	1.96	0.48
1:A:272:ASP:OD1	1:A:275:SER:OG	2.24	0.48
1:E:319:ARG:NH2	1:E:321:PHE:O	2.46	0.47
1:B:249:LEU:HB2	1:B:266:LEU:HD11	1.97	0.47
1:A:90:TRP:HD1	1:A:97:ASN:HB3	1.79	0.47
1:E:90:TRP:CD1	1:E:97:ASN:HB3	2.48	0.47
1:C:92:ARG:HE	1:C:215:GLU:CD	2.22	0.47
1:E:268:CYS:O	1:E:270:HIS:N	2.46	0.47
1:B:105:ARG:NH1	2:B:503:HOH:O	2.39	0.47
1:A:6:LEU:HD13	1:A:9:MET:HG3	1.95	0.47
1:A:335:GLY:O	1:A:336:ARG:HB3	2.15	0.47
1:D:31:ASN:OD1	1:D:34:ARG:NH1	2.48	0.47
1:C:6:LEU:HD13	1:C:9:MET:HG3	1.97	0.47
1:F:92:ARG:NH1	1:F:215:GLU:HB2	2.29	0.46
1:F:359:GLU:HA	1:F:376:GLU:O	2.16	0.46
1:F:126:PHE:CD2	1:F:148:ASP:HB2	2.51	0.46
1:C:14:GLY:HA3	1:C:91:ARG:HD3	1.97	0.46
1:C:50:TYR:CD2	1:C:334:TYR:HB3	2.51	0.46
1:D:36:TRP:CD1	1:F:385:ASP:OD2	2.69	0.46
1:E:18:TYR:HB3	1:E:213:PHE:HB3	1.97	0.46
1:C:246:ILE:HG21	1:C:372:GLY:HA3	1.97	0.46
1:B:50:TYR:CD2	1:B:334:TYR:HB3	2.51	0.46
1:A:263:GLU:HB2	1:A:377:HIS:HB3	1.98	0.45
1:B:249:LEU:O	1:B:263:GLU:HA	2.15	0.45
1:E:327:PHE:CE1	1:E:357:SER:HB3	2.51	0.45
1:E:129:VAL:HG13	1:E:133:PHE:HB3	1.98	0.45
1:D:298:ARG:O	1:D:302:ILE:HG12	2.17	0.45
1:A:170:GLU:OE2	1:A:173:ARG:NH2	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:GLY:HA3	1:B:149:ILE:HG13	1.99	0.45
1:C:249:LEU:O	1:C:263:GLU:HA	2.17	0.44
1:F:33:VAL:HG12	1:F:37:MET:HE2	1.99	0.44
1:A:134:ARG:HG3	1:B:131:LEU:HD11	2.00	0.44
1:B:100:TYR:HB2	1:B:107:ASN:HB3	1.99	0.44
1:F:249:LEU:O	1:F:263:GLU:HA	2.18	0.43
1:F:344:GLU:OE1	1:F:344:GLU:N	2.49	0.43
1:B:395:VAL:O	1:B:400:ASN:ND2	2.51	0.43
1:E:187:LYS:O	1:E:190:VAL:HG12	2.18	0.43
1:F:50:TYR:OH	1:F:63:TYR:HB3	2.19	0.43
1:F:203:MET:SD	1:F:251:THR:HB	2.59	0.43
1:B:110:ARG:HG2	1:B:113:ARG:HH21	1.83	0.43
1:C:261:ALA:H	1:C:379:ILE:HD11	1.84	0.43
1:D:50:TYR:OH	1:D:63:TYR:HB3	2.19	0.43
1:C:50:TYR:OH	1:C:63:TYR:HB3	2.18	0.43
1:D:88:GLN:HE21	1:D:92:ARG:NH1	2.17	0.43
1:B:34:ARG:HA	1:B:37:MET:HE2	2.00	0.43
1:E:61:TYR:HE1	1:E:63:TYR:HB2	1.84	0.43
1:E:247:LEU:HB2	1:E:266:LEU:HB2	1.99	0.43
1:A:249:LEU:HB2	1:A:266:LEU:HD11	2.01	0.43
1:C:272:ASP:OD1	1:C:272:ASP:N	2.51	0.43
1:B:203:MET:SD	1:B:251:THR:HB	2.59	0.43
1:D:249:LEU:O	1:D:263:GLU:HA	2.19	0.42
1:A:204:ILE:HG23	1:A:216:LEU:HD22	2.00	0.42
1:E:50:TYR:OH	1:E:63:TYR:HB3	2.18	0.42
1:A:359:GLU:HA	1:A:376:GLU:O	2.19	0.42
1:F:331:CYS:SG	1:F:332:HIS:N	2.93	0.42
1:B:351:LYS:HB2	1:B:354:MET:HE3	2.02	0.42
1:A:326:SER:HB2	1:A:340:VAL:HB	2.00	0.42
1:B:326:SER:HB2	1:B:340:VAL:HB	2.01	0.42
1:F:126:PHE:HB2	1:F:148:ASP:OD1	2.19	0.42
1:C:90:TRP:HD1	1:C:97:ASN:HB3	1.84	0.42
1:D:183:ALA:HA	1:D:186:ILE:HD12	2.01	0.42
1:E:250:ASN:HB3	1:E:252:PHE:CE2	2.55	0.42
1:C:113:ARG:NH1	1:C:140:ALA:O	2.53	0.42
1:E:123:GLY:HA3	1:E:149:ILE:HD11	2.02	0.41
1:E:311:ARG:HG3	1:E:316:LEU:HD12	2.01	0.41
1:F:250:ASN:HB3	1:F:252:PHE:CZ	2.55	0.41
1:A:182:CYS:O	1:A:186:ILE:HG13	2.20	0.41
1:A:235:PRO:HB2	1:B:215:GLU:HB3	2.01	0.41
1:A:249:LEU:O	1:A:263:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:GLU:HA	1:D:376:GLU:O	2.20	0.41
1:C:319:ARG:NH2	1:C:321:PHE:O	2.50	0.41
1:F:110:ARG:HG2	1:F:113:ARG:NH2	2.35	0.41
1:F:170:GLU:OE2	1:F:173:ARG:NH2	2.32	0.41
1:E:285:VAL:HG21	1:E:310:TYR:CE1	2.56	0.41
1:B:110:ARG:HH21	1:C:308:GLU:HG3	1.86	0.41
1:A:186:ILE:HB	1:A:402:ILE:HG21	2.03	0.41
1:B:275:SER:HB3	1:B:370:GLY:HA2	2.02	0.41
1:C:293:ILE:HD12	1:C:380:LEU:HD22	2.01	0.41
1:D:291:GLU:O	1:D:294:LYS:HE2	2.20	0.41
1:C:61:TYR:HE1	1:C:63:TYR:HB2	1.85	0.41
1:C:120:LYS:HD3	1:C:120:LYS:HA	1.87	0.41
1:A:187:LYS:O	1:A:190:VAL:HG12	2.21	0.41
1:D:153:SER:O	1:D:157:ARG:HG3	2.20	0.41
1:D:235:PRO:HB2	1:E:215:GLU:HB3	2.02	0.41
1:D:345:ASP:OD2	1:E:105:ARG:HG3	2.21	0.41
1:F:92:ARG:HE	1:F:92:ARG:HB2	1.69	0.41
1:F:4:ASP:HB3	1:F:5:MET:H	1.67	0.41
1:F:160:LYS:NZ	1:F:326:SER:OG	2.53	0.41
1:E:113:ARG:O	1:E:117:THR:HG23	2.21	0.40
1:E:219:THR:HG23	1:E:253:PRO:HA	2.02	0.40
1:A:298:ARG:O	1:A:302:ILE:HG12	2.22	0.40
1:C:7:HIS:CE1	1:C:104:ARG:HD3	2.56	0.40
1:E:289:GLY:O	1:E:293:ILE:HD12	2.22	0.40
1:F:275:SER:HB3	1:F:370:GLY:HA2	2.04	0.40
1:A:219:THR:HG23	1:A:253:PRO:HA	2.03	0.40
1:A:321:PHE:HB3	1:B:84:ILE:HB	2.02	0.40
1:B:298:ARG:O	1:B:302:ILE:HG12	2.21	0.40
1:D:92:ARG:HH12	1:E:235:PRO:HD2	1.87	0.40
1:D:219:THR:HG22	1:D:254:MET:N	2.22	0.40
1:A:179:GLY:HA2	1:A:249:LEU:HD11	2.03	0.40
1:B:204:ILE:HG23	1:B:216:LEU:HD22	2.03	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	399/404 (99%)	385 (96%)	13 (3%)	1 (0%)	36	45
1	B	398/404 (98%)	384 (96%)	14 (4%)	0	100	100
1	C	399/404 (99%)	387 (97%)	12 (3%)	0	100	100
1	D	399/404 (99%)	384 (96%)	15 (4%)	0	100	100
1	E	399/404 (99%)	388 (97%)	11 (3%)	0	100	100
1	F	396/404 (98%)	381 (96%)	14 (4%)	1 (0%)	36	45
All	All	2390/2424 (99%)	2309 (97%)	79 (3%)	2 (0%)	48	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	336	ARG
1	A	336	ARG

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	334/339 (98%)	333 (100%)	1 (0%)	86	92
1	B	333/339 (98%)	328 (98%)	5 (2%)	57	73
1	C	334/339 (98%)	334 (100%)	0	100	100
1	D	331/339 (98%)	330 (100%)	1 (0%)	86	92
1	E	332/339 (98%)	330 (99%)	2 (1%)	78	88
1	F	330/339 (97%)	330 (100%)	0	100	100
All	All	1994/2034 (98%)	1985 (100%)	9 (0%)	81	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	72	ILE
1	E	138	GLU
1	E	293	ILE
1	A	336	ARG
1	B	6	LEU
1	B	7	HIS
1	B	9	MET
1	B	64	PHE
1	B	385	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	74	HIS
1	D	75	ASN
1	D	88	GLN
1	D	97	ASN
1	D	201	ASN
1	D	286	HIS
1	D	377	HIS
1	E	97	ASN
1	E	130	ASN
1	E	201	ASN
1	E	282	ASN
1	F	136	GLN
1	F	286	HIS
1	F	399	HIS
1	A	97	ASN
1	B	76	ASN
1	B	286	HIS
1	C	74	HIS
1	C	75	ASN
1	C	97	ASN
1	C	136	GLN
1	C	151	GLN
1	C	270	HIS

5.3.3 RNA ⓘ

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 [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	401/404 (99%)	0.07	5 (1%) 76 78	35, 53, 84, 103	0
1	B	400/404 (99%)	0.26	10 (2%) 58 61	40, 59, 85, 122	0
1	C	401/404 (99%)	0.17	5 (1%) 76 78	35, 58, 85, 127	0
1	D	401/404 (99%)	0.33	9 (2%) 62 65	39, 64, 91, 122	0
1	E	401/404 (99%)	0.37	16 (3%) 42 45	37, 63, 100, 147	0
1	F	400/404 (99%)	0.74	23 (5%) 29 31	54, 79, 114, 145	0
All	All	2404/2424 (99%)	0.32	68 (2%) 55 57	35, 63, 98, 147	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	GLY	5.2
1	C	335	GLY	4.6
1	B	73	ASP	4.1
1	F	11	TRP	3.9
1	D	9	MET	3.7
1	B	74	HIS	3.6
1	B	395	VAL	3.5
1	E	9	MET	3.4
1	E	395	VAL	3.4
1	F	92	ARG	3.4
1	A	74	HIS	3.3
1	E	74	HIS	3.1
1	F	396	GLY	3.1
1	C	127	ASP	3.1
1	F	215	GLU	3.0
1	F	395	VAL	3.0
1	C	350	LEU	2.9
1	E	6	LEU	2.9
1	D	395	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	124	ILE	2.9
1	E	149	ILE	2.8
1	F	98	ILE	2.7
1	B	11	TRP	2.7
1	C	90	TRP	2.7
1	D	215	GLU	2.6
1	D	304	LEU	2.6
1	E	73	ASP	2.6
1	F	122	ILE	2.5
1	D	90	TRP	2.5
1	E	5	MET	2.4
1	B	90	TRP	2.4
1	F	399	HIS	2.4
1	E	265	THR	2.4
1	A	90	TRP	2.4
1	B	117	THR	2.4
1	D	255	ILE	2.4
1	D	275	SER	2.3
1	B	302	ILE	2.3
1	F	315	LEU	2.2
1	E	269	ASP	2.2
1	F	5	MET	2.2
1	F	367	GLY	2.2
1	F	310	TYR	2.2
1	E	401	ILE	2.2
1	B	149	ILE	2.2
1	F	4	ASP	2.2
1	E	369	PRO	2.2
1	F	140	ALA	2.2
1	F	64	PHE	2.2
1	F	73	ASP	2.2
1	A	9	MET	2.2
1	E	310	TYR	2.1
1	F	402	ILE	2.1
1	F	352	PRO	2.1
1	D	74	HIS	2.1
1	F	328	GLY	2.1
1	E	90	TRP	2.1
1	A	395	VAL	2.1
1	D	64	PHE	2.1
1	E	188	ALA	2.1
1	A	320	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	400	ASN	2.1
1	C	73	ASP	2.1
1	F	74	HIS	2.1
1	F	382	VAL	2.0
1	E	105	ARG	2.0
1	F	142	PRO	2.0
1	B	293	ILE	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.