



Full wwPDB X-ray Structure Validation Report i

Aug 15, 2023 – 04:11 PM JST

PDB ID : 7YTO
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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

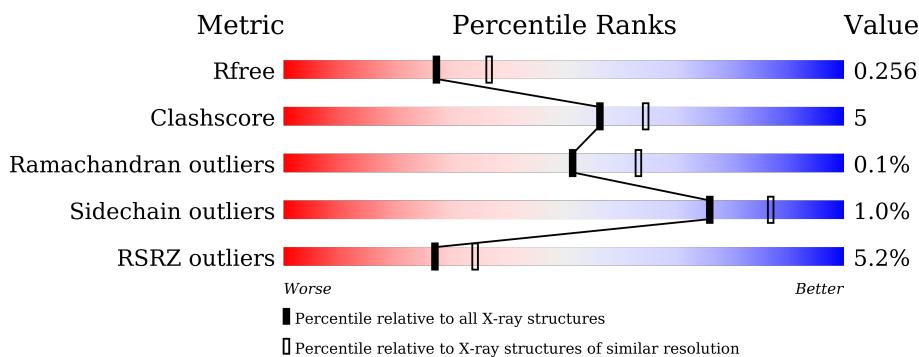
1 Overall quality at a glance

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}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (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 <=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.



2 Entry composition [\(i\)](#)

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 3191	N 2018	O 560	S 591	22	0	0
1	E	401	Total	C 3193	N 2021	O 560	S 589	23	0	0
1	F	400	Total	C 3174	N 2008	O 555	S 588	23	0	0
1	A	401	Total	C 3202	N 2025	O 563	S 591	23	0	0
1	B	400	Total	C 3194	N 2021	O 562	S 588	23	0	0
1	C	401	Total	C 3202	N 2025	O 563	S 591	23	0	0

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

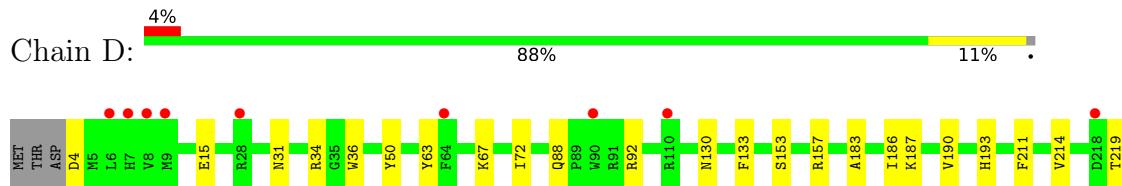
- Molecule 2 is water.

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

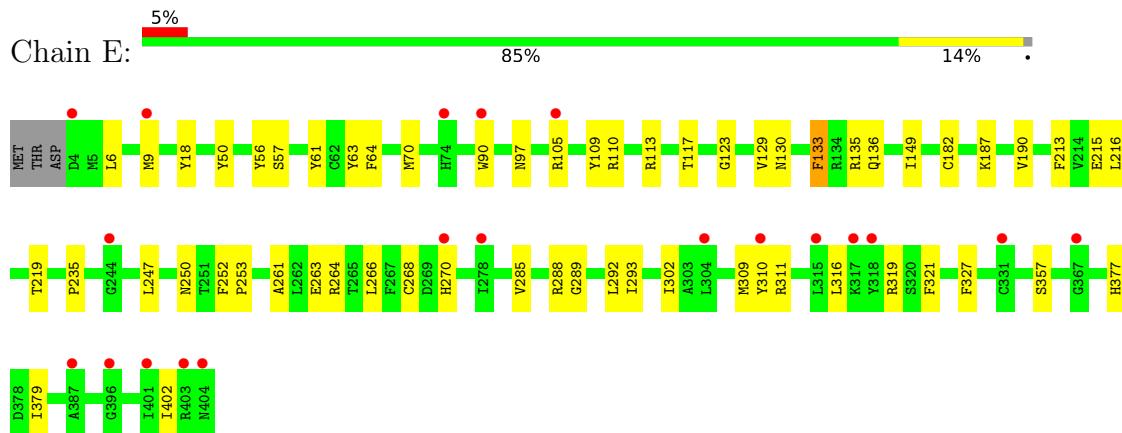
3 Residue-property plots

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.

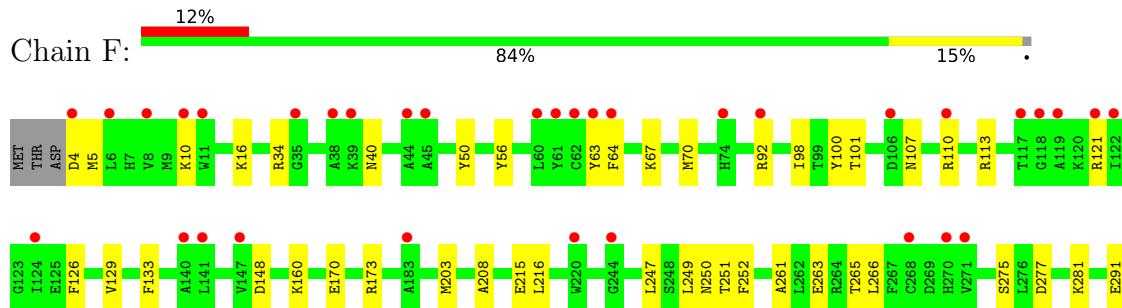
- Molecule 1: Creatine amidinohydrolase



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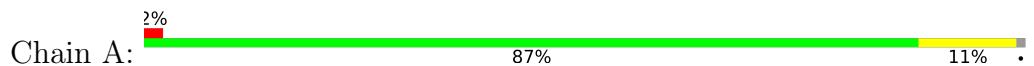


- Molecule 1: Creatine amidinohydrolase

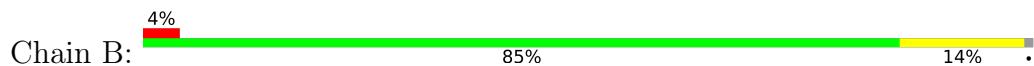




- Molecule 1: Creatine amidinohydrolase



- Molecule 1: Creatine amidinohydrolase



- Molecule 1: Creatine amidinohydrolase



4 Data and refinement statistics (i)

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 38.21 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.31) 94.6 (38.21-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ ¹	1.69 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R , R_{free}	0.215 , 0.257 0.215 , 0.256	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 , 33.9	EDS
L-test for twinning ²	$< L > = 0.49$, $< L^2 > = 0.32$	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 $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality 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	0.25	0/3283	0.43	0/4446
1	B	0.25	0/3275	0.43	0/4435
1	C	0.24	0/3283	0.43	0/4446
1	D	0.24	0/3272	0.42	0/4433
1	E	0.25	0/3274	0.43	0/4435
1	F	0.24	0/3252	0.41	0/4404
All	All	0.25	0/19639	0.43	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	36	0
1	C	3202	0	3072	31	0
1	D	3191	0	3047	29	0
1	E	3193	0	3059	39	0
1	F	3174	0	3036	37	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	187	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 (187) 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	1.70	0.74
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: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: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:C:56:TYR:HB2	1:C:70:MET:HE1	1.77	0.65
1:F:293:ILE:HD12	1:F:380:LEU:HD13	1.79	0.65
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:A:56:TYR:HB2	1:A:70:MET:HE1	1.81	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:56:TYR:HB2	1:E:70:MET:HE1	1.88	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:B:56:TYR:HB2	1:B:70:MET:HE1	1.91	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:ARG:NH2	2:F:502:HOH:O	2.44	0.49
1:F:265:THR:HG1	1:F:375:ARG:H	1.59	0.49
1:D:326:SER:HB2	1:D:340:VAL:HB	1.95	0.49
1:E:109:TYR:OH	1:E:136:GLN:OE1	2.30	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:A:92:ARG:HE	1:A:215:GLU:CD	2.16	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: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:F:56:TYR:HB2	1:F:70:MET:HE1	1.97	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:B:92:ARG:HE	1:B:215:GLU:CD	2.21	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:E:70:MET:HE2	1:E:70:MET:HB3	1.83	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:C:92:ARG:HE	1:C:215:GLU:CD	2.22	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: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:F:70:MET:HE2	1:F:70:MET:HB3	1.82	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:160:LYS:NZ	1:F:326:SER:OG	2.53	0.41
1:F:4:ASP:HB3	1:F:5:MET:H	1.67	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 [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	399/404 (99%)	385 (96%)	13 (3%)	1 (0%)	41 50
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%)	41 50
All	All	2390/2424 (99%)	2309 (97%)	79 (3%)	2 (0%)	51 63

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [\(i\)](#)

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%)	331 (99%)	3 (1%)	78 89
1	B	333/339 (98%)	327 (98%)	6 (2%)	59 74
1	C	334/339 (98%)	330 (99%)	4 (1%)	71 83
1	D	331/339 (98%)	328 (99%)	3 (1%)	78 89
1	E	332/339 (98%)	330 (99%)	2 (1%)	86 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	330/339 (97%)	328 (99%)	2 (1%)	86 93
All	All	1994/2034 (98%)	1974 (99%)	20 (1%)	76 87

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	67	LYS
1	D	72	ILE
1	D	133	PHE
1	E	64	PHE
1	E	133	PHE
1	F	64	PHE
1	F	67	LYS
1	A	64	PHE
1	A	134	ARG
1	A	336	ARG
1	B	6	LEU
1	B	7	HIS
1	B	9	MET
1	B	64	PHE
1	B	133	PHE
1	B	385	ASP
1	C	9	MET
1	C	28	ARG
1	C	64	PHE
1	C	134	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	74	HIS
1	D	88	GLN

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.08	7 (1%) 70 76	35, 53, 84, 103	0
1	B	400/404 (99%)	0.22	15 (3%) 40 47	40, 59, 85, 122	0
1	C	401/404 (99%)	0.18	17 (4%) 36 43	35, 58, 85, 127	0
1	D	401/404 (99%)	0.29	15 (3%) 41 48	39, 64, 91, 122	0
1	E	401/404 (99%)	0.35	20 (4%) 28 36	37, 63, 100, 147	0
1	F	400/404 (99%)	0.78	50 (12%) 3 5	54, 79, 114, 145	0
All	All	2404/2424 (99%)	0.32	124 (5%) 27 34	35, 63, 98, 147	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	401	ILE	4.8
1	B	335	GLY	4.7
1	B	74	HIS	4.6
1	F	122	ILE	4.4
1	F	44	ALA	4.4
1	F	118	GLY	4.4
1	E	9	MET	4.4
1	E	74	HIS	4.3
1	E	396	GLY	4.1
1	F	141	LEU	3.9
1	E	310	TYR	3.8
1	B	383	GLY	3.8
1	F	64	PHE	3.7
1	A	243	SER	3.7
1	F	271	VAL	3.7
1	D	6	LEU	3.6
1	F	314	ASP	3.6
1	A	74	HIS	3.5
1	F	403	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	335	GLY	3.4
1	E	367	GLY	3.4
1	F	124	ILE	3.4
1	A	9	MET	3.3
1	F	6	LEU	3.3
1	D	28	ARG	3.3
1	E	318	TYR	3.3
1	D	308	GLU	3.1
1	C	404	ASN	3.0
1	F	38	ALA	2.9
1	F	183	ALA	2.9
1	E	4	ASP	2.9
1	D	399	HIS	2.9
1	C	268	CYS	2.9
1	E	315	LEU	2.9
1	F	140	ALA	2.8
1	C	312	GLU	2.8
1	D	9	MET	2.8
1	B	331	CYS	2.7
1	F	352	PRO	2.7
1	F	331	CYS	2.7
1	C	403	ARG	2.7
1	F	106	ASP	2.7
1	F	404	ASN	2.7
1	E	403	ARG	2.7
1	E	401	ILE	2.7
1	F	370	GLY	2.7
1	C	401	ILE	2.6
1	A	188	ALA	2.6
1	F	45	ALA	2.6
1	E	270	HIS	2.6
1	F	270	HIS	2.6
1	F	60	LEU	2.5
1	B	268	CYS	2.5
1	E	304	LEU	2.5
1	E	331	CYS	2.5
1	F	268	CYS	2.5
1	E	387	ALA	2.4
1	D	7	HIS	2.4
1	C	402	ILE	2.4
1	F	4	ASP	2.4
1	F	121	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	8	VAL	2.4
1	E	278	ILE	2.4
1	F	332	HIS	2.4
1	E	317	LYS	2.4
1	F	63	TYR	2.4
1	D	64	PHE	2.4
1	B	11	TRP	2.4
1	D	110	ARG	2.4
1	F	61	TYR	2.4
1	D	304	LEU	2.4
1	B	121	ARG	2.3
1	C	90	TRP	2.3
1	E	244	GLY	2.3
1	D	90	TRP	2.3
1	D	218	ASP	2.3
1	B	90	TRP	2.3
1	D	403	ARG	2.3
1	B	117	THR	2.3
1	F	399	HIS	2.3
1	B	384	GLU	2.3
1	F	402	ILE	2.3
1	C	240	ILE	2.3
1	E	105	ARG	2.2
1	F	92	ARG	2.2
1	E	404	ASN	2.2
1	A	187	LYS	2.2
1	F	10	LYS	2.2
1	F	297	ALA	2.2
1	F	220	TRP	2.2
1	D	255	ILE	2.2
1	B	50	TYR	2.2
1	B	39	LYS	2.2
1	F	147	VAL	2.2
1	A	220	TRP	2.2
1	F	110	ARG	2.1
1	F	62	CYS	2.1
1	F	39	LYS	2.1
1	D	8	VAL	2.1
1	C	398	GLU	2.1
1	E	90	TRP	2.1
1	F	308	GLU	2.1
1	C	333	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	347	ASP	2.1
1	C	242	GLN	2.1
1	F	244	GLY	2.1
1	C	350	LEU	2.1
1	F	11	TRP	2.1
1	B	347	ASP	2.1
1	C	241	VAL	2.1
1	C	334	TYR	2.1
1	F	293	ILE	2.1
1	F	292	LEU	2.1
1	B	330	LEU	2.1
1	A	273	ASP	2.1
1	F	335	GLY	2.1
1	C	271	VAL	2.1
1	F	74	HIS	2.0
1	D	404	ASN	2.0
1	F	117	THR	2.0
1	F	119	ALA	2.0
1	C	243	SER	2.0
1	B	15	GLU	2.0
1	F	35	GLY	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 monosaccharides 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.