



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:33 PM UTC

PDB ID : 8Y75 / pdb_00008y75
Title : Crystal structure of the CARF-HTH domain of Csx1-Crn2 from *Marinitoga* sp.
Authors : Zhang, D.; Yuan, C.; Lin, Z.
Deposited on : 2024-02-03
Resolution : 2.40 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

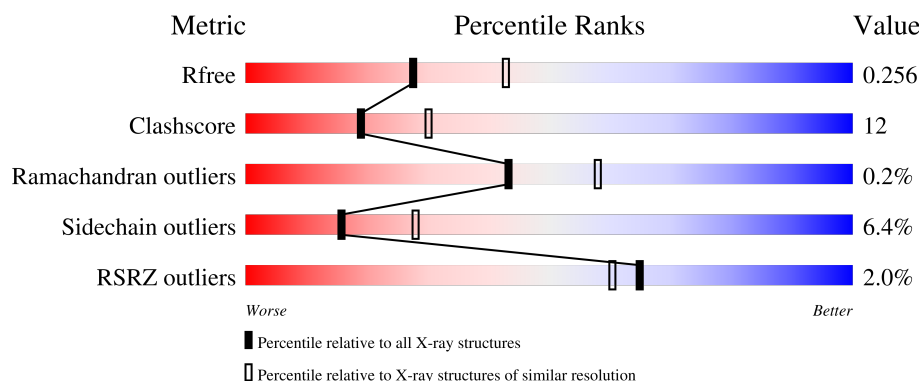
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	444	3% 48%19%31%
1	B	444	3% 47%18%32%
1	C	444	53%14%31%
1	D	444	3% 47%17%32%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10214 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 CRISPR-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2509	1637	399	465	8			
1	B	304	Total	C	N	O	S	0	0	0
			2500	1633	399	460	8			
1	C	305	Total	C	N	O	S	0	0	0
			2516	1643	401	463	9			
1	D	303	Total	C	N	O	S	0	0	0
			2459	1606	390	454	9			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	71	Total	O	0	0
			71	71		
2	B	56	Total	O	0	0
			56	56		
2	C	65	Total	O	0	0
			65	65		
2	D	38	Total	O	0	0
			38	38		

[illegible]

Chain D:

Category	Percentage
Green	47%
Yellow	17%
Orange	3%
Grey	32%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.88Å 193.13Å 61.21Å 90.00° 92.97° 90.00°	Depositor
Resolution (Å)	38.60 – 2.40 38.60 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (38.60-2.40) 98.1 (38.60-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.196 , 0.257 0.200 , 0.256	Depositor DCC
R_{free} test set	1998 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10214	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/2551	0.81	5/3427 (0.1%)
1	B	0.66	1/2542 (0.0%)	1.06	23/3414 (0.7%)
1	C	0.52	1/2558 (0.0%)	0.97	16/3433 (0.5%)
1	D	0.65	2/2500 (0.1%)	1.14	18/3362 (0.5%)
All	All	0.59	4/10151 (0.0%)	1.00	62/13636 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	216	LYS	CE-NZ	6.61	1.69	1.49
1	C	14	ARG	CG-CD	6.02	1.70	1.52
1	B	172	LYS	CD-CE	5.50	1.69	1.52
1	D	146	LYS	CB-CG	5.33	1.68	1.52

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	71	GLU	CG-CD-OE1	21.23	167.23	118.40
1	D	71	GLU	CG-CD-OE2	-19.15	74.36	118.40
1	B	172	LYS	CG-CD-CE	-12.43	82.72	111.30
1	C	82	GLU	CA-CB-CG	12.36	138.81	114.10
1	C	14	ARG	CB-CG-CD	-11.78	84.20	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	14	ARG	CG-CD-NE	11.59	137.50	112.00
1	C	81	ASN	CA-C-N	-11.56	104.16	122.65
1	C	81	ASN	C-N-CA	-11.56	104.16	122.65
1	D	216	LYS	CG-CD-CE	10.16	134.67	111.30
1	D	71	GLU	OE1-CD-OE2	-9.73	99.54	122.90
1	C	82	GLU	N-CA-CB	9.10	123.85	110.56
1	B	212	LYS	CB-CG-CD	9.02	132.05	111.30
1	B	74	LYS	CG-CD-CE	-8.89	90.86	111.30
1	A	301	GLU	CB-CG-CD	8.88	127.69	112.60
1	A	3	LYS	N-CA-CB	8.46	124.48	110.52
1	B	240	LEU	N-CA-CB	8.33	122.48	110.16
1	C	216	LYS	CA-CB-CG	-8.30	97.50	114.10
1	D	286	LYS	CB-CG-CD	-7.87	93.20	111.30
1	B	196	GLU	CB-CA-C	-7.43	99.11	110.92
1	D	297	LYS	CD-CE-NZ	-7.41	88.20	111.90
1	C	13	GLY	CA-C-N	-7.33	108.04	121.52
1	C	13	GLY	C-N-CA	-7.33	108.04	121.52
1	B	74	LYS	CA-CB-CG	7.29	128.68	114.10
1	B	71	GLU	CB-CA-C	7.17	124.44	110.67
1	D	297	LYS	N-CA-CB	-7.04	99.80	110.01
1	C	236	ARG	CB-CG-CD	-6.98	95.24	111.30
1	B	267	SER	CB-CA-C	6.72	122.62	109.72
1	B	240	LEU	CB-CA-C	-6.71	99.44	110.85
1	D	146	LYS	CB-CG-CD	6.50	126.26	111.30
1	B	71	GLU	N-CA-CB	-6.46	100.26	110.28
1	C	82	GLU	CA-C-N	-6.36	110.42	120.47
1	C	82	GLU	C-N-CA	-6.36	110.42	120.47
1	A	3	LYS	CB-CA-C	-6.34	98.82	109.48
1	D	70	ASN	CA-C-N	6.17	128.55	120.28
1	D	70	ASN	C-N-CA	6.17	128.55	120.28
1	D	297	LYS	CA-CB-CG	6.03	126.17	114.10
1	B	290	LYS	CA-CB-CG	-5.98	102.14	114.10
1	B	63	GLU	CA-CB-CG	5.94	125.98	114.10
1	C	236	ARG	CG-CD-NE	-5.90	99.03	112.00
1	D	150	GLU	CA-CB-CG	5.88	125.85	114.10
1	B	68	GLU	CA-CB-CG	5.79	125.68	114.10
1	D	274	LEU	N-CA-C	-5.76	104.90	111.07
1	C	168	GLU	N-CA-C	5.73	118.64	110.10
1	D	286	LYS	CA-CB-CG	5.72	125.55	114.10
1	D	146	LYS	CA-CB-CG	5.50	125.11	114.10
1	C	239	LYS	CA-CB-CG	-5.49	103.12	114.10
1	B	239	LYS	CA-C-N	-5.45	112.55	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	239	LYS	C-N-CA	-5.45	112.55	120.29
1	A	248	PRO	N-CA-C	-5.40	102.65	110.80
1	B	260	LYS	N-CA-CB	-5.33	102.13	109.91
1	B	260	LYS	CD-CE-NZ	-5.32	94.87	111.90
1	D	228	GLU	N-CA-C	-5.29	106.87	113.38
1	B	71	GLU	CG-CD-OE2	-5.24	106.35	118.40
1	B	260	LYS	CA-CB-CG	5.20	124.49	114.10
1	A	305	LEU	CD1-CG-CD2	5.19	122.22	110.80
1	C	14	ARG	N-CA-C	-5.12	106.20	112.90
1	D	296	GLN	CA-C-N	5.09	127.06	120.44
1	D	296	GLN	C-N-CA	5.09	127.06	120.44
1	B	70	ASN	CA-C-N	5.05	127.99	120.31
1	B	70	ASN	C-N-CA	5.05	127.99	120.31
1	B	266	GLU	CA-C-N	-5.02	112.73	122.06
1	B	266	GLU	C-N-CA	-5.02	112.73	122.06

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	236	ARG	Sidechain
1	B	71	GLU	Sidechain
1	C	14	ARG	Sidechain
1	C	236	ARG	Sidechain
1	D	14	ARG	Sidechain
1	D	200	ARG	Sidechain

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	2509	0	2595	80	0
1	B	2500	0	2593	54	1
1	C	2516	0	2620	51	0
1	D	2459	0	2515	70	1
2	A	71	0	0	6	0
2	B	56	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	65	0	0	6	0
2	D	38	0	0	3	0
All	All	10214	0	10323	240	1

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 12.

All (240) 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:216:LYS:CE	1:D:216:LYS:NZ	1.69	1.55
1:D:271:GLU:O	1:D:275:CYS:HB2	1.53	1.04
1:B:168:GLU:HG3	1:B:176:LYS:HE2	1.53	0.90
1:A:147:ASN:HB3	1:C:192:THR:HG21	1.54	0.88
1:D:272:PHE:HA	1:D:275:CYS:CB	2.06	0.86
1:A:146:LYS:HG2	1:A:150:GLU:HG3	1.56	0.85
1:A:122:LYS:HE3	1:A:158:LYS:HD3	1.59	0.83
1:B:168:GLU:O	1:B:175:LYS:HA	1.81	0.80
1:D:212:LYS:HD3	1:D:216:LYS:NZ	1.97	0.80
1:D:216:LYS:NZ	1:D:216:LYS:CD	2.47	0.78
1:A:201:TYR:HB2	1:A:203:ILE:HG13	1.67	0.77
1:A:298:ILE:O	1:A:301:GLU:HG3	1.85	0.77
1:B:39:ASN:HD21	1:B:179:ILE:HG21	1.53	0.73
1:B:21:TYR:HB3	1:B:29:MET:HG3	1.68	0.73
1:D:147:ASN:O	1:D:150:GLU:HB2	1.89	0.72
1:B:204:THR:HB	1:B:238:LEU:HG	1.71	0.71
1:C:10:LEU:HB3	1:C:56:VAL:HG12	1.73	0.69
1:D:272:PHE:HA	1:D:275:CYS:HB2	1.74	0.69
1:A:227:ASN:ND2	2:A:502:HOH:O	2.26	0.68
1:A:305:LEU:CD2	1:D:216:LYS:HE3	2.23	0.68
1:A:122:LYS:HE3	1:A:158:LYS:CD	2.24	0.67
1:A:182:ILE:O	1:A:185:THR:HG22	1.95	0.67
1:A:225:ASN:ND2	1:A:228:GLU:HG2	2.10	0.66
1:B:68:GLU:CD	1:B:68:GLU:H	2.04	0.66
1:A:24:GLU:HA	1:A:282:LEU:HD13	1.76	0.65
1:B:185:THR:HA	1:B:188:LEU:CD1	2.26	0.65
1:D:272:PHE:HA	1:D:275:CYS:HB3	1.79	0.65
1:B:73:ALA:O	1:B:76:ILE:HG22	1.97	0.64
1:D:108:MET:HE3	1:D:141:THR:OG1	1.98	0.64
1:D:212:LYS:HD3	1:D:216:LYS:HZ3	1.62	0.64
1:A:205:GLU:OE2	1:C:200:ARG:NH2	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:HE2	1:A:174:LEU:HD21	1.62	0.63
1:D:142:VAL:HG11	1:D:159:ILE:HD11	1.81	0.63
1:D:272:PHE:CA	1:D:275:CYS:HB2	2.29	0.62
1:A:297:LYS:HE3	2:A:501:HOH:O	1.98	0.62
1:A:185:THR:OG1	1:C:141:THR:HG22	2.00	0.62
1:B:146:LYS:HG2	1:B:157:MET:HB2	1.81	0.61
1:D:50:VAL:HB	1:D:88:ILE:HD12	1.83	0.61
1:A:166:ILE:HD13	1:C:99:LYS:HA	1.83	0.60
1:B:184:GLN:O	1:B:188:LEU:HG	2.01	0.60
1:C:149:MET:HE3	1:C:153:ASN:HB2	1.82	0.60
1:C:116:LEU:HD23	1:C:149:MET:HE1	1.82	0.60
1:A:172:LYS:O	1:A:174:LEU:N	2.34	0.60
1:A:305:LEU:HD21	1:D:216:LYS:HE3	1.84	0.60
1:D:271:GLU:C	1:D:275:CYS:HB2	2.26	0.59
1:B:197:GLU:HB3	1:B:203:ILE:HB	1.83	0.59
1:A:134:MET:HA	1:A:134:MET:HE2	1.85	0.59
1:C:14:ARG:HD3	1:C:16:TYR:CZ	2.37	0.59
1:B:12:LYS:HG3	1:B:60:VAL:HG22	1.83	0.59
1:D:138:THR:O	1:D:141:THR:HG22	2.02	0.59
1:A:189:SER:O	1:A:193:ILE:HG12	2.03	0.58
1:C:158:LYS:O	1:C:159:ILE:HD13	2.02	0.58
1:D:237:GLU:OE1	1:D:260:LYS:CE	2.51	0.58
1:D:272:PHE:CA	1:D:275:CYS:CB	2.81	0.58
1:B:150:GLU:HG3	1:B:155:LEU:O	2.04	0.58
1:C:19:PHE:CD2	1:C:174:LEU:HD11	2.39	0.58
1:C:44:LYS:NZ	1:C:86:TYR:O	2.34	0.58
1:B:254:ILE:HG13	1:B:255:ALA:N	2.19	0.57
1:A:222:LYS:H	1:A:222:LYS:HD2	1.70	0.57
1:A:32:LYS:HD2	1:A:37:LEU:HD23	1.86	0.56
1:A:142:VAL:HG21	1:A:159:ILE:HD11	1.88	0.56
1:A:25:HIS:HB3	1:A:27:GLU:OE2	2.06	0.56
1:D:212:LYS:HD3	1:D:216:LYS:HZ2	1.69	0.55
1:B:168:GLU:CB	1:B:176:LYS:HB3	2.37	0.55
1:C:242:GLU:HA	1:C:245:LEU:HD12	1.88	0.55
1:B:222:LYS:H	1:B:222:LYS:HE2	1.71	0.54
1:A:297:LYS:CE	2:A:501:HOH:O	2.55	0.54
1:D:158:LYS:O	1:D:159:ILE:HD13	2.07	0.54
1:B:222:LYS:H	1:B:222:LYS:CE	2.20	0.54
1:B:207:MET:O	1:B:211:LEU:HG	2.08	0.54
1:A:115:LEU:HB3	1:A:149:MET:HE2	1.90	0.53
1:A:204:THR:HG22	2:A:523:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ASN:ND2	1:B:179:ILE:HD13	2.23	0.53
1:B:154:LYS:NZ	2:B:507:HOH:O	2.41	0.53
1:A:262:ASN:O	1:A:266:GLU:HG2	2.08	0.53
1:D:32:LYS:HD2	1:D:37:LEU:HD12	1.91	0.53
1:D:237:GLU:CD	1:D:260:LYS:HE2	2.34	0.53
1:C:241:PHE:CE2	1:C:245:LEU:HD11	2.43	0.53
1:B:207:MET:HB3	1:B:238:LEU:HD21	1.91	0.53
1:D:80:LEU:O	1:D:83:ILE:HG22	2.09	0.52
1:D:37:LEU:HD21	1:D:83:ILE:HB	1.90	0.52
1:C:44:LYS:NZ	2:C:503:HOH:O	2.35	0.52
1:B:258:ILE:HG21	1:B:303:LEU:HG	1.91	0.52
1:A:186:LEU:HD22	1:C:140:SER:HB2	1.91	0.52
1:D:148:LEU:C	1:D:150:GLU:H	2.17	0.52
1:B:272:PHE:HA	1:B:275:CYS:HB2	1.92	0.52
1:A:293:VAL:HG13	1:A:297:LYS:HE3	1.92	0.52
1:A:192:THR:HG21	1:C:147:ASN:OD1	2.10	0.51
1:C:37:LEU:HD13	1:C:79:GLU:HG2	1.90	0.51
1:D:23:ILE:HG12	1:D:281:ASN:HB3	1.92	0.51
1:D:169:GLU:O	1:D:170:ILE:C	2.53	0.51
1:B:74:LYS:HA	1:B:77:LEU:HB2	1.92	0.51
1:A:229:LEU:O	1:A:268:SER:OG	2.22	0.51
1:B:27:GLU:HG2	1:B:28:LYS:N	2.25	0.51
1:B:138:THR:O	1:B:142:VAL:HG23	2.11	0.51
1:B:168:GLU:HB2	1:B:176:LYS:HB3	1.93	0.51
1:C:19:PHE:HD2	1:C:174:LEU:HD11	1.76	0.51
1:C:28:LYS:HE3	1:C:42:LEU:HD22	1.93	0.50
1:D:12:LYS:HD3	2:D:507:HOH:O	2.11	0.50
1:A:4:ILE:HA	1:A:122:LYS:O	2.11	0.50
1:C:28:LYS:HB3	2:C:501:HOH:O	2.11	0.50
1:A:305:LEU:HD22	1:D:216:LYS:HE3	1.93	0.50
1:A:293:VAL:O	1:A:297:LYS:HG2	2.12	0.50
1:C:153:ASN:HB3	1:C:155:LEU:HB2	1.94	0.50
1:D:237:GLU:OE1	1:D:260:LYS:HE2	2.12	0.50
1:C:273:LYS:HE3	2:C:534:HOH:O	2.12	0.49
1:B:168:GLU:HB2	1:B:176:LYS:O	2.12	0.49
1:D:289:GLN:O	1:D:293:VAL:HG13	2.12	0.49
1:A:186:LEU:CD2	1:C:140:SER:HB2	2.41	0.49
1:C:123:VAL:HG13	1:C:157:MET:HG2	1.93	0.49
1:A:105:GLU:HG3	2:C:560:HOH:O	2.12	0.49
1:C:14:ARG:HD3	1:C:16:TYR:CE2	2.47	0.49
1:B:213:ASN:HB2	2:B:552:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:GLU:HB3	1:C:271:GLU:HG2	1.94	0.49
1:D:240:LEU:O	1:D:240:LEU:HD22	2.13	0.48
1:A:16:TYR:CZ	1:A:173:ASN:ND2	2.81	0.48
1:B:78:ASN:O	1:B:82:GLU:HG2	2.13	0.48
1:B:86:TYR:HB2	1:B:88:ILE:HD12	1.95	0.48
1:B:172:LYS:NZ	2:B:509:HOH:O	2.45	0.48
1:C:82:GLU:HB2	1:C:85:ASN:ND2	2.28	0.48
1:A:298:ILE:HA	1:A:301:GLU:CG	2.44	0.48
1:B:257:SER:HB3	2:B:539:HOH:O	2.14	0.48
1:D:250:PRO:O	1:D:252:GLU:N	2.46	0.48
1:B:241:PHE:CD1	1:B:241:PHE:C	2.91	0.48
1:C:84:LYS:HE3	1:C:90:VAL:HB	1.96	0.48
1:D:237:GLU:OE1	1:D:260:LYS:HE3	2.14	0.48
1:D:258:ILE:HG21	1:D:303:LEU:HG	1.96	0.48
1:A:261:ILE:HG21	1:A:299:VAL:HG21	1.95	0.47
1:C:276:SER:O	1:C:279:SER:OG	2.29	0.47
1:D:65:LEU:HG	1:D:77:LEU:HD11	1.95	0.47
1:B:53:ILE:HD13	1:B:114:LEU:HD22	1.95	0.47
1:B:102:GLU:O	1:B:106:ILE:HG13	2.15	0.47
1:A:286:LYS:HE3	2:C:509:HOH:O	2.14	0.47
1:D:216:LYS:O	1:D:219:ALA:HB3	2.14	0.47
1:D:243:GLU:OE1	1:D:246:LYS:HE3	2.13	0.47
1:A:116:LEU:HD23	1:A:149:MET:HE1	1.96	0.47
1:B:185:THR:HA	1:B:188:LEU:HG	1.97	0.47
1:B:237:GLU:OE2	1:B:237:GLU:HA	2.13	0.47
1:D:145:PHE:O	1:D:149:MET:HB2	2.15	0.47
1:B:21:TYR:CE1	1:B:176:LYS:HG2	2.50	0.47
1:D:294:ASP:HA	1:D:297:LYS:HD3	1.95	0.47
1:B:62:ASN:HA	1:B:66:TYR:CD2	2.51	0.46
1:A:149:MET:O	1:A:153:ASN:N	2.42	0.46
1:D:170:ILE:HD12	1:D:174:LEU:HG	1.96	0.46
1:A:196:GLU:HG3	1:C:151:LYS:CE	2.45	0.46
1:A:185:THR:HA	1:A:188:LEU:HG	1.96	0.46
1:A:305:LEU:HA	1:A:305:LEU:HD23	1.56	0.46
1:A:150:GLU:HG2	1:A:155:LEU:O	2.16	0.46
1:D:243:GLU:OE1	1:D:246:LYS:CE	2.64	0.46
1:A:260:LYS:HA	1:A:260:LYS:HD3	1.83	0.46
1:C:123:VAL:HG12	1:C:155:LEU:CD2	2.46	0.46
1:D:40:ALA:HB2	1:D:52:ILE:HD11	1.97	0.45
1:A:239:LYS:O	1:A:243:GLU:HG3	2.16	0.45
1:B:15:TYR:HB3	1:B:76:ILE:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ILE:O	1:C:273:LYS:HB2	2.16	0.45
1:A:172:LYS:O	1:A:173:ASN:C	2.59	0.45
1:D:70:ASN:HB3	1:D:73:ALA:HB3	1.99	0.45
1:A:24:GLU:HB2	1:A:25:HIS:CE1	2.51	0.45
1:C:122:LYS:NZ	2:C:512:HOH:O	2.50	0.45
1:D:15:TYR:HB3	1:D:76:ILE:HD11	2.00	0.44
1:D:33:ARG:N	1:D:79:GLU:OE2	2.34	0.44
1:D:195:LEU:HD12	1:D:195:LEU:HA	1.88	0.44
1:D:37:LEU:CD1	1:D:83:ILE:HD13	2.48	0.44
1:D:44:LYS:HG3	1:D:88:ILE:HD11	1.99	0.44
1:A:19:PHE:CE2	1:A:174:LEU:HD21	2.49	0.44
1:C:174:LEU:C	1:C:174:LEU:HD13	2.42	0.44
1:D:37:LEU:HD13	1:D:83:ILE:HD13	2.00	0.44
1:A:267:SER:HB2	2:A:537:HOH:O	2.17	0.44
1:B:2:LYS:HD3	1:B:121:ASN:OD1	2.17	0.44
1:C:142:VAL:HG12	1:C:186:LEU:HG	2.00	0.44
1:A:76:ILE:HD13	1:A:76:ILE:HA	1.56	0.43
1:A:79:GLU:HA	1:A:82:GLU:HG2	2.00	0.43
1:A:296:GLN:HB3	2:A:501:HOH:O	2.18	0.43
1:A:131:LEU:HB3	1:C:165:GLU:OE1	2.18	0.43
1:A:4:ILE:HD11	1:A:48:ASN:HD22	1.84	0.43
1:D:175:LYS:HB3	1:D:175:LYS:HE3	1.48	0.43
1:D:208:ILE:HG13	1:D:235:SER:HB3	2.01	0.43
1:D:244:LEU:O	1:D:249:SER:HB2	2.18	0.43
1:A:32:LYS:HD2	1:A:37:LEU:CD2	2.49	0.43
1:A:53:ILE:HG21	1:A:114:LEU:HD11	2.00	0.43
1:D:154:LYS:O	2:D:501:HOH:O	2.21	0.43
1:B:257:SER:O	1:B:260:LYS:HB3	2.18	0.43
1:D:10:LEU:HA	1:D:10:LEU:HD12	1.78	0.43
1:D:265:LEU:HD12	1:D:265:LEU:HA	1.83	0.43
1:B:146:LYS:HB3	1:B:146:LYS:HE3	1.75	0.43
1:A:55:PHE:CD1	1:A:93:ARG:HB2	2.54	0.43
1:B:144:TYR:CZ	1:B:148:LEU:HD22	2.54	0.43
1:B:168:GLU:HG3	1:B:176:LYS:CE	2.36	0.43
1:D:160:VAL:HA	1:D:180:LEU:O	2.19	0.43
1:A:298:ILE:HA	1:A:301:GLU:HG3	2.01	0.42
1:D:29:MET:HE1	1:D:176:LYS:HD2	2.01	0.42
1:A:172:LYS:C	1:A:174:LEU:N	2.77	0.42
1:B:279:SER:HA	1:B:282:LEU:HD12	2.01	0.42
1:A:201:TYR:CZ	1:C:203:ILE:HD13	2.55	0.42
1:A:298:ILE:C	1:A:301:GLU:HG3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:SER:C	1:D:24:GLU:N	2.77	0.42
1:A:149:MET:HE3	1:A:149:MET:HB3	1.88	0.42
1:C:53:ILE:HG21	1:C:114:LEU:HD21	2.01	0.42
1:A:201:TYR:CE2	1:C:203:ILE:HD13	2.55	0.42
1:C:119:LYS:HD2	1:C:119:LYS:HA	1.69	0.42
1:D:159:ILE:HG13	1:D:186:LEU:HD23	2.00	0.42
1:D:293:VAL:O	1:D:297:LYS:HB2	2.20	0.42
1:B:172:LYS:O	1:B:174:LEU:N	2.52	0.42
1:A:165:GLU:HB3	1:C:131:LEU:HD13	2.01	0.42
1:A:295:PHE:CD1	1:A:295:PHE:C	2.94	0.42
1:C:37:LEU:HD22	1:C:83:ILE:HD13	2.01	0.42
1:A:33:ARG:NE	1:A:75:ASN:HB3	2.35	0.41
1:A:172:LYS:C	1:A:174:LEU:H	2.28	0.41
1:A:164:TYR:HA	1:A:177:VAL:HG22	2.02	0.41
1:D:12:LYS:HG2	1:D:64:PHE:HB2	2.03	0.41
1:A:207:MET:HB3	1:A:207:MET:HE3	1.76	0.41
1:B:19:PHE:HE2	1:B:174:LEU:HD21	1.86	0.41
1:C:286:LYS:HB3	1:C:286:LYS:HE3	1.77	0.41
1:A:4:ILE:CD1	1:A:122:LYS:HD3	2.51	0.41
1:C:168:GLU:OE1	1:C:168:GLU:HA	2.21	0.41
1:B:2:LYS:HB3	1:B:121:ASN:OD1	2.21	0.41
1:D:250:PRO:C	1:D:252:GLU:H	2.29	0.41
1:A:64:PHE:CD2	1:A:65:LEU:HD12	2.56	0.41
1:A:199:GLU:OE1	1:A:298:ILE:HG12	2.21	0.41
1:A:293:VAL:CG1	1:A:297:LYS:HE3	2.51	0.41
1:B:203:ILE:HG22	2:B:529:HOH:O	2.20	0.41
1:B:247:ILE:O	1:B:248:PRO:C	2.63	0.41
1:C:3:LYS:HG3	1:C:49:ASP:HB3	2.02	0.41
1:C:286:LYS:HE3	1:C:287:PRO:HD3	2.02	0.41
1:A:12:LYS:HG3	1:A:60:VAL:HG22	2.03	0.41
1:A:241:PHE:HE1	1:A:254:ILE:HG23	1.86	0.40
1:C:186:LEU:HD13	1:C:186:LEU:HA	1.90	0.40
1:D:32:LYS:HE3	2:D:536:HOH:O	2.21	0.40
1:D:301:GLU:O	1:D:301:GLU:HG3	2.20	0.40
1:B:52:ILE:O	1:B:90:VAL:HA	2.21	0.40
1:C:147:ASN:OD1	1:C:147:ASN:C	2.64	0.40
1:B:113:LYS:HE2	2:B:540:HOH:O	2.21	0.40
1:C:250:PRO:HB2	1:C:253:LYS:HG3	2.03	0.40
1:D:158:LYS:C	1:D:159:ILE:HD13	2.45	0.40
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.83	0.40
1:C:65:LEU:HA	1:C:65:LEU:HD12	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:VAL:HG11	1:D:159:ILE:CD1	2.50	0.40
1:D:198:PHE:HZ	1:D:299:VAL:HG23	1.86	0.40
1:C:5:LEU:HD11	1:C:53:ILE:HD12	2.04	0.40
1:D:240:LEU:O	1:D:244:LEU:HG	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLU:OE1	1:D:286:LYS:NZ[1_556]	2.10	0.10

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	303/444 (68%)	299 (99%)	4 (1%)	0	100	100
1	B	302/444 (68%)	296 (98%)	6 (2%)	0	100	100
1	C	303/444 (68%)	300 (99%)	3 (1%)	0	100	100
1	D	299/444 (67%)	287 (96%)	10 (3%)	2 (1%)	18	28
All	All	1207/1776 (68%)	1182 (98%)	23 (2%)	2 (0%)	43	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	170	ILE
1	D	251	PRO

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	282/416 (68%)	267 (95%)	15 (5%)	20	36
1	B	281/416 (68%)	258 (92%)	23 (8%)	10	18
1	C	284/416 (68%)	276 (97%)	8 (3%)	38	60
1	D	272/416 (65%)	246 (90%)	26 (10%)	8	12
All	All	1119/1664 (67%)	1047 (94%)	72 (6%)	16	28

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	76	ILE
1	A	154	LYS
1	A	158	LYS
1	A	159	ILE
1	A	172	LYS
1	A	204	THR
1	A	210	VAL
1	A	232	SER
1	A	233	SER
1	A	246	LYS
1	A	249	SER
1	A	254	ILE
1	A	268	SER
1	A	277	LYS
1	B	10	LEU
1	B	26	SER
1	B	56	VAL
1	B	68	GLU
1	B	74	LYS
1	B	81	ASN
1	B	141	THR
1	B	185	THR
1	B	186	LEU

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Mol	Chain	Res	Type
1	B	189	SER
1	B	192	THR
1	B	203	ILE
1	B	210	VAL
1	B	222	LYS
1	B	233	SER
1	B	237	GLU
1	B	239	LYS
1	B	249	SER
1	B	254	ILE
1	B	269	ILE
1	B	274	LEU
1	B	275	CYS
1	B	290	LYS
1	C	26	SER
1	C	61	LYS
1	C	142	VAL
1	C	150	GLU
1	C	186	LEU
1	C	222	LYS
1	C	253	LYS
1	C	305	LEU
1	D	65	LEU
1	D	71	GLU
1	D	91	SER
1	D	147	ASN
1	D	148	LEU
1	D	153	ASN
1	D	166	ILE
1	D	169	GLU
1	D	170	ILE
1	D	175	LYS
1	D	185	THR
1	D	186	LEU
1	D	195	LEU
1	D	199	GLU
1	D	213	ASN
1	D	222	LYS
1	D	239	LYS
1	D	240	LEU
1	D	245	LEU
1	D	254	ILE

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Mol	Chain	Res	Type
1	D	258	ILE
1	D	260	LYS
1	D	263	ASP
1	D	265	LEU
1	D	275	CYS
1	D	297	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	147	ASN
1	A	289	GLN
1	B	39	ASN
1	B	70	ASN
1	B	281	ASN
1	C	85	ASN
1	C	153	ASN
1	C	281	ASN
1	D	70	ASN
1	D	227	ASN
1	D	281	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	305/444 (68%)	-0.10	5 (1%) 70 66	29, 47, 80, 118	0
1	B	304/444 (68%)	0.16	6 (1%) 65 60	31, 56, 93, 128	0
1	C	305/444 (68%)	-0.05	1 (0%) 90 88	29, 49, 84, 121	0
1	D	303/444 (68%)	0.38	12 (3%) 42 38	33, 63, 107, 136	0
All	All	1217/1776 (68%)	0.10	24 (1%) 65 60	29, 53, 97, 136	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	170	ILE	4.0
1	D	252	GLU	3.6
1	D	168	GLU	3.5
1	B	24	GLU	3.2
1	D	152	ALA	3.2
1	A	152	ALA	3.0
1	D	274	LEU	2.9
1	D	254	ILE	2.9
1	A	301	GLU	2.8
1	D	229	LEU	2.7
1	B	59	GLU	2.7
1	D	275	CYS	2.6
1	A	186	LEU	2.5
1	B	240	LEU	2.5
1	D	251	PRO	2.4
1	D	304	PRO	2.2
1	A	173	ASN	2.2
1	A	172	LYS	2.2
1	B	267	SER	2.1
1	B	196	GLU	2.1
1	D	66	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	14	ARG	2.0
1	B	250	PRO	2.0
1	D	259	TYR	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.