



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:39 AM UTC

PDB ID : 6Z3U / pdb_00006z3u
Title : Structure of the CAK complex form Chaetomium thermophilum
Authors : Peissert, S.; Kuper, J.; Kisker, C.
Deposited on : 2020-05-22
Resolution : 2.60 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

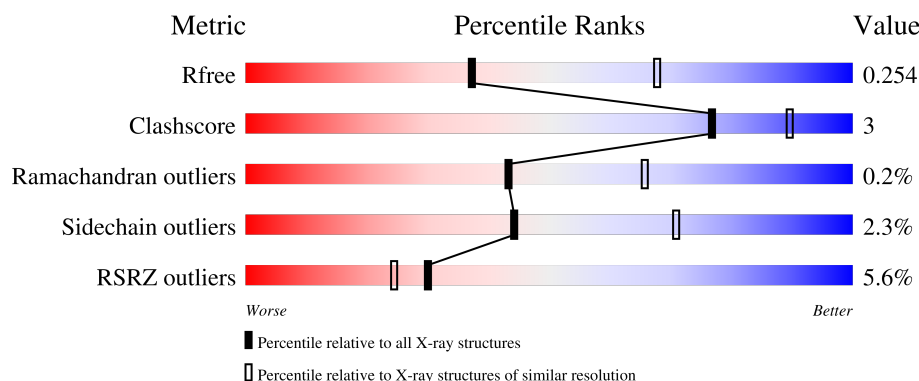
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	425	6% 67% 6% 27%
1	D	425	4% 67% 7% 26%
2	B	437	4% 67% 7% 26%
2	E	437	4% 66% 7% 26%
3	C	69	% 87% 7% ...

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Mol	Chain	Length	Quality of chain
3	F	69	% 88% 9%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22711 atoms, of which 11313 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 CYCLIN domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	312	Total	C	H	N	O	S	0	0	0
			5039	1599	2517	449	463	11			
1	D	314	Total	C	H	N	O	S	0	0	0
			5061	1605	2528	451	466	11			

- Molecule 2 is a protein called Protein kinase domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	322	Total	C	H	N	O	S	0	0	0
			5237	1678	2624	462	460	13			
2	E	323	Total	C	H	N	O	S	0	0	0
			5250	1682	2630	463	462	13			

- Molecule 3 is a protein called RING-type domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	66	Total	C	H	N	O	S	0	0	0
			1041	344	503	90	102	2			
3	F	67	Total	C	H	N	O	S	0	0	0
			1061	353	511	91	104	2			

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total	0	0
			1 Cl		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total	0	0
			4 O		

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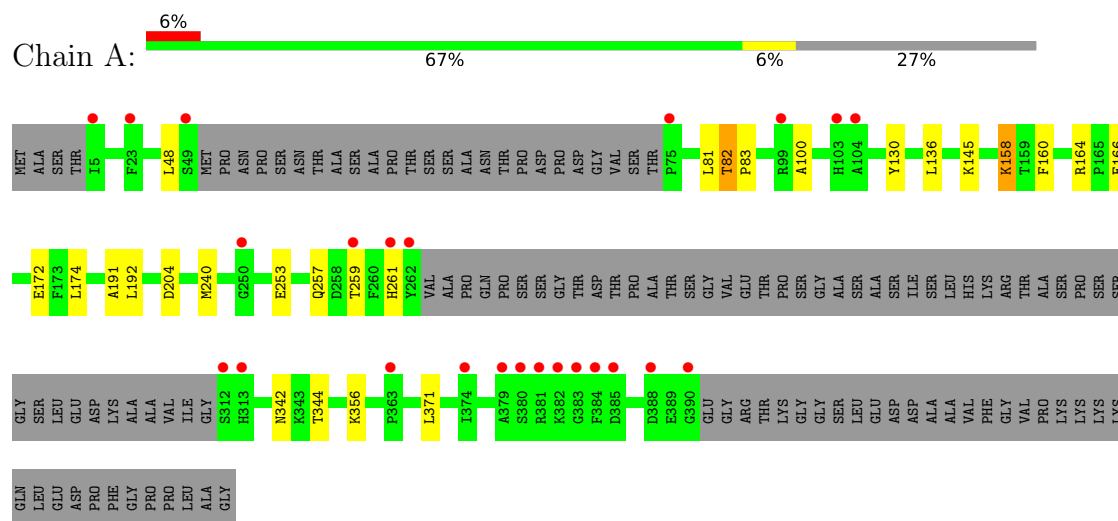
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	6	Total 6	O 6	0	0
5	D	4	Total 4	O 4	0	0
5	E	7	Total 7	O 7	0	0

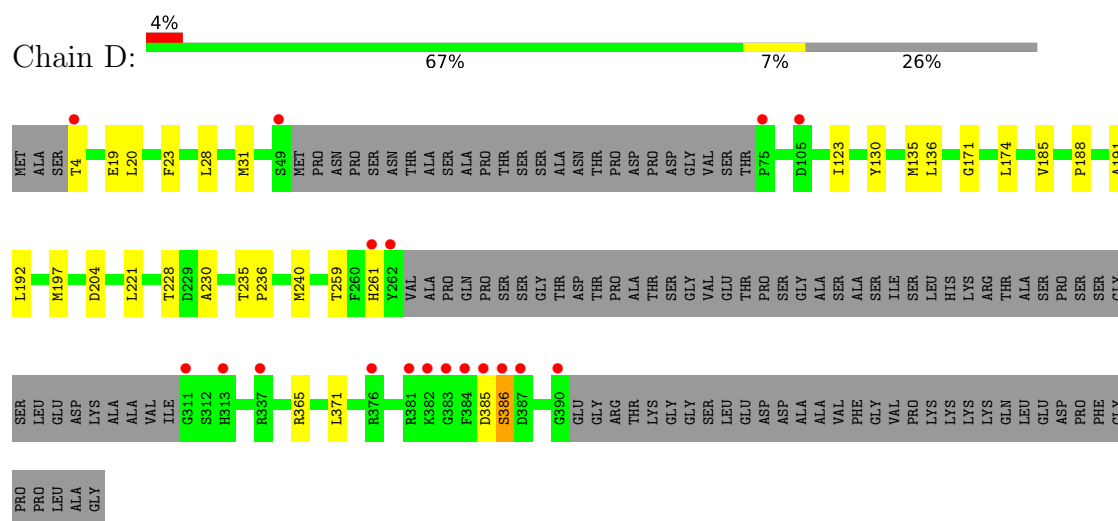
3 Residue-property plots [i](#)

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: CYCLIN domain-containing protein



• Molecule 1: CYCLIN domain-containing protein



• Molecule 2: Protein kinase domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.44Å 85.24Å 160.40Å 90.00° 96.93° 90.00°	Depositor
Resolution (Å)	75.87 – 2.60 75.87 – 2.60	Depositor EDS
% Data completeness (in resolution range)	50.4 (75.87-2.60) 50.4 (75.87-2.60)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.62Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.18rc4_3812	Depositor
R, R_{free}	0.203 , 0.249 0.215 , 0.254	Depositor DCC
R_{free} test set	1653 reflections (2.46%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.5	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	0.91	EDS
Total number of atoms	22711	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.52% 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](#)

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

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	0.13	0/2574	0.31	0/3471
1	D	0.13	0/2585	0.30	0/3486
2	B	0.13	0/2684	0.30	0/3635
2	E	0.13	0/2691	0.31	0/3646
3	C	0.11	0/552	0.28	0/742
3	F	0.12	0/565	0.28	0/760
All	All	0.13	0/11651	0.30	0/15740

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	2522	2517	2517	14	0
1	D	2533	2528	2527	19	0
2	B	2613	2624	2624	14	0
2	E	2620	2630	2630	17	0
3	C	538	503	502	4	0
3	F	550	511	511	5	0
4	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	0	0	0
5	B	6	0	0	0	0
5	D	4	0	0	0	0
5	E	7	0	0	0	0
All	All	11398	11313	11311	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (66) 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:B:253:THR:HG22	2:B:255:ASN:H	1.44	0.83
2:E:253:THR:HG22	2:E:255:ASN:H	1.48	0.79
2:B:359:LEU:HD11	2:B:377:MET:HG3	1.75	0.68
2:B:274:GLY:O	2:B:277:VAL:HG22	2.00	0.61
2:B:218:HIS:NE2	2:B:238:ASP:O	2.35	0.59
1:D:259:THR:HG21	3:F:324:PHE:HE1	1.69	0.58
1:A:100:ALA:HB1	1:A:160:PHE:HE1	1.66	0.57
1:D:197:MET:HE1	3:F:316:ILE:HG12	1.86	0.57
1:D:130:TYR:OH	1:D:365:ARG:NH2	2.37	0.57
2:B:363:THR:HG22	2:B:377:MET:HE2	1.85	0.56
2:E:218:HIS:NE2	2:E:238:ASP:O	2.39	0.56
2:B:256:VAL:O	2:B:262:ARG:NH1	2.40	0.55
1:A:204:ASP:OD1	1:A:204:ASP:N	2.40	0.54
2:B:296:LEU:HD11	2:B:312:ILE:CD1	2.38	0.54
2:E:359:LEU:HD11	2:E:377:MET:HG2	1.89	0.54
2:E:204:LEU:HD13	2:E:226:LEU:HD21	1.89	0.54
2:E:274:GLY:O	2:E:277:VAL:HG22	2.08	0.53
1:A:145:LYS:NZ	1:A:172:GLU:OE1	2.42	0.53
2:B:246:ALA:HB2	2:B:252:MET:HE3	1.92	0.52
1:D:192:LEU:HD12	1:D:240:MET:HE3	1.92	0.52
1:A:82:THR:HG22	1:A:83:PRO:HD2	1.92	0.51
2:B:198:LYS:NZ	2:B:385:THR:O	2.44	0.51
1:D:259:THR:HG21	3:F:324:PHE:CE1	2.46	0.51
1:D:19:GLU:HG3	1:D:20:LEU:HD13	1.93	0.51
1:D:191:ALA:HB1	3:F:323:ALA:HA	1.93	0.50
1:D:204:ASP:OD1	1:D:204:ASP:N	2.39	0.50
1:D:188:PRO:HG2	1:D:221:LEU:HD22	1.94	0.49
2:E:124:ILE:HD12	2:E:124:ILE:N	2.27	0.49
3:C:313:LEU:H	3:C:313:LEU:HD22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:198:LYS:NZ	2:E:385:THR:O	2.46	0.48
2:E:124:ILE:HD12	2:E:124:ILE:H	1.78	0.48
2:E:296:LEU:HD11	2:E:312:ILE:CD1	2.45	0.47
1:A:81:LEU:HD23	1:A:356:LYS:HD2	1.97	0.47
2:B:95:GLY:N	2:B:108:LEU:O	2.44	0.47
1:A:253:GLU:O	1:A:257:GLN:HG2	2.15	0.46
1:D:23:PHE:CE2	1:D:31:MET:HE1	2.50	0.46
1:D:31:MET:HE3	1:D:123:ILE:HD11	1.97	0.46
2:E:177:LEU:HD12	2:E:229:ALA:O	2.15	0.46
3:C:313:LEU:HD13	3:C:313:LEU:N	2.30	0.45
1:A:158:LYS:NZ	1:A:158:LYS:HB3	2.31	0.45
1:D:130:TYR:CE1	1:D:174:LEU:HD21	2.52	0.44
2:B:109:GLY:O	2:B:119:VAL:N	2.48	0.44
2:E:246:ALA:HB2	2:E:252:MET:HE3	1.99	0.44
1:D:228:THR:HG23	1:D:230:ALA:H	1.83	0.44
1:A:136:LEU:C	1:A:136:LEU:HD23	2.43	0.43
1:A:191:ALA:HB1	3:C:323:ALA:HA	2.00	0.43
1:D:130:TYR:CD1	1:D:174:LEU:HD21	2.53	0.43
1:A:192:LEU:HD12	1:A:240:MET:HE3	2.00	0.43
1:D:385:ASP:OD1	1:D:386:SER:N	2.52	0.42
1:A:130:TYR:CD1	1:A:174:LEU:HD21	2.55	0.42
1:D:136:LEU:C	1:D:136:LEU:HD23	2.44	0.42
2:B:279:ILE:HG13	2:B:377:MET:HE1	2.01	0.42
2:E:95:GLY:N	2:E:108:LEU:O	2.48	0.42
2:B:358:ASP:OD2	2:B:380:HIS:NE2	2.45	0.42
2:E:109:GLY:O	2:E:119:VAL:N	2.52	0.42
1:A:164:ARG:NE	1:A:166:GLU:OE1	2.51	0.41
1:A:342:ASN:OD1	1:A:344:THR:N	2.47	0.41
1:D:235:THR:HG21	3:F:326:GLY:HA3	2.02	0.41
1:A:259:THR:HG21	3:C:324:PHE:HE2	1.85	0.41
2:B:296:LEU:HD11	2:B:312:ILE:HD11	2.02	0.41
1:D:235:THR:HG23	1:D:236:PRO:HD2	2.02	0.41
2:E:282:VAL:HG11	2:E:377:MET:HE1	2.03	0.41
2:E:77:THR:N	2:E:78:PRO:CD	2.84	0.41
2:E:219:ARG:CZ	2:E:256:VAL:HG11	2.51	0.41
1:D:135:MET:HE1	1:D:171:GLY:HA3	2.04	0.40
2:E:77:THR:HB	2:E:78:PRO:HD3	2.04	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	306/425 (72%)	300 (98%)	6 (2%)	0	100	100
1	D	308/425 (72%)	301 (98%)	7 (2%)	0	100	100
2	B	320/437 (73%)	313 (98%)	6 (2%)	1 (0%)	36	58
2	E	321/437 (74%)	314 (98%)	5 (2%)	2 (1%)	21	42
3	C	64/69 (93%)	64 (100%)	0	0	100	100
3	F	65/69 (94%)	65 (100%)	0	0	100	100
All	All	1384/1862 (74%)	1357 (98%)	24 (2%)	3 (0%)	43	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	257	ILE
2	E	257	ILE
2	E	220	ASP

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	267/354 (75%)	262 (98%)	5 (2%)	50	75
1	D	268/354 (76%)	262 (98%)	6 (2%)	45	72
2	B	275/370 (74%)	269 (98%)	6 (2%)	45	72
2	E	276/370 (75%)	272 (99%)	4 (1%)	59	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	55/57 (96%)	51 (93%)	4 (7%)	13	29
3	F	56/57 (98%)	54 (96%)	2 (4%)	31	58
All	All	1197/1562 (77%)	1170 (98%)	27 (2%)	44	71

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	82	THR
1	A	158	LYS
1	A	261	HIS
1	A	371	LEU
2	B	119	VAL
2	B	126	VAL
2	B	149	ARG
2	B	180	LEU
2	B	326	LEU
2	B	360	LEU
3	C	288	ARG
3	C	304	GLN
3	C	313	LEU
3	C	327	LEU
1	D	4	THR
1	D	28	LEU
1	D	185	VAL
1	D	261	HIS
1	D	371	LEU
1	D	386	SER
2	E	119	VAL
2	E	180	LEU
2	E	326	LEU
2	E	360	LEU
3	F	288	ARG
3	F	327	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	257	GLN

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Mol	Chain	Res	Type
1	A	349	GLN
1	A	351	GLN
1	A	358	ASN
2	B	85	ASN
2	B	166	GLN
3	C	303	GLN
1	D	27	GLN
1	D	358	ASN
2	E	365	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	312/425 (73%)	0.65	24 (7%)	19 15	34, 66, 101, 137	0
1	D	314/425 (73%)	0.18	18 (5%)	29 24	21, 44, 77, 161	0
2	B	322/437 (73%)	0.12	16 (4%)	34 28	21, 40, 90, 113	0
2	E	323/437 (73%)	-0.01	19 (5%)	28 23	15, 31, 82, 120	0
3	C	66/69 (95%)	0.35	1 (1%)	72 68	41, 64, 86, 95	0
3	F	67/69 (97%)	0.01	1 (1%)	72 68	23, 41, 69, 84	0
All	All	1404/1862 (75%)	0.23	79 (5%)	30 24	15, 45, 91, 161	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	384	PHE	7.1
1	D	384	PHE	7.0
2	B	78	PRO	7.0
2	E	128	ALA	5.7
2	B	103	TYR	5.4
1	A	5	ILE	5.1
1	A	75	PRO	4.9
1	D	382	LYS	4.8
2	E	126	VAL	4.7
2	E	103	TYR	4.6
1	A	262	TYR	4.5
1	A	382	LYS	4.5
2	B	126	VAL	4.4
1	D	390	GLY	4.3
1	D	381	ARG	4.3
1	A	383	GLY	4.2
1	D	262	TYR	4.1
2	B	102	THR	4.0
1	D	75	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
2	E	130	TYR	3.7
1	D	385	ASP	3.7
1	A	49	SER	3.7
2	B	237	ALA	3.6
1	D	311	GLY	3.6
2	E	102	THR	3.5
1	A	381	ARG	3.5
1	A	103	HIS	3.4
2	E	113	ASP	3.3
2	E	77	THR	3.3
2	B	96	LYS	3.1
1	D	383	GLY	3.0
1	A	379	ALA	3.0
1	D	4	THR	2.9
3	F	338	GLY	2.9
2	E	78	PRO	2.9
2	E	237	ALA	2.7
1	D	386	SER	2.7
3	C	338	GLY	2.7
2	E	112	ARG	2.7
2	B	131	LYS	2.7
1	A	312	SER	2.6
2	B	128	ALA	2.6
1	D	313	HIS	2.6
2	E	125	LYS	2.6
2	E	83	GLN	2.6
2	E	129	GLN	2.5
2	E	127	GLN	2.5
2	E	399	SER	2.4
1	A	259	THR	2.4
1	D	49	SER	2.4
1	A	250	GLY	2.4
2	B	81	VAL	2.4
1	A	380	SER	2.3
1	A	385	ASP	2.3
1	D	387	ASP	2.3
2	E	86	GLU	2.3
1	A	104	ALA	2.3
2	E	96	LYS	2.3
2	B	125	LYS	2.2
2	B	399	SER	2.2
1	A	23	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	261	HIS	2.2
2	E	90	ARG	2.2
2	E	188	GLU	2.2
1	D	337	ARG	2.2
1	D	105	ASP	2.2
1	D	261	HIS	2.1
1	D	376	ARG	2.1
1	A	99	ARG	2.1
1	A	374	ILE	2.1
2	B	111	SER	2.1
2	B	90	ARG	2.1
1	A	313	HIS	2.1
2	B	130	TYR	2.1
1	A	388	ASP	2.0
1	A	363	PRO	2.0
2	B	80	PRO	2.0
2	B	129	GLN	2.0
1	A	390	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 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
4	CL	E	501	1/1	0.99	0.03	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.