Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2020 – 09:05 AM GMT

PDB ID	:	6Z3U
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 following versions of software and data (see references ①) were used in the production of this report:

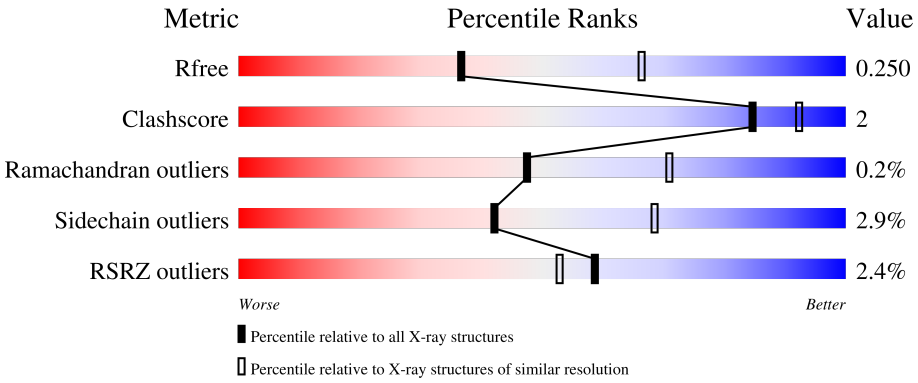
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on 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.

Mol	Chain	Length	Quality of chain
1	A	425	3% 68% 5% 27%
1	D	425	2% 68% 5% 26%
2	B	437	% 68% 6% 26%
2	E	437	2% 67% 7% 26%
3	C	69	6% 87% 7%

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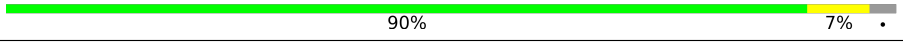
Mol	Chain	Length	Quality of chain
3	F	69	

2 Entry composition

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 (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is water.

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

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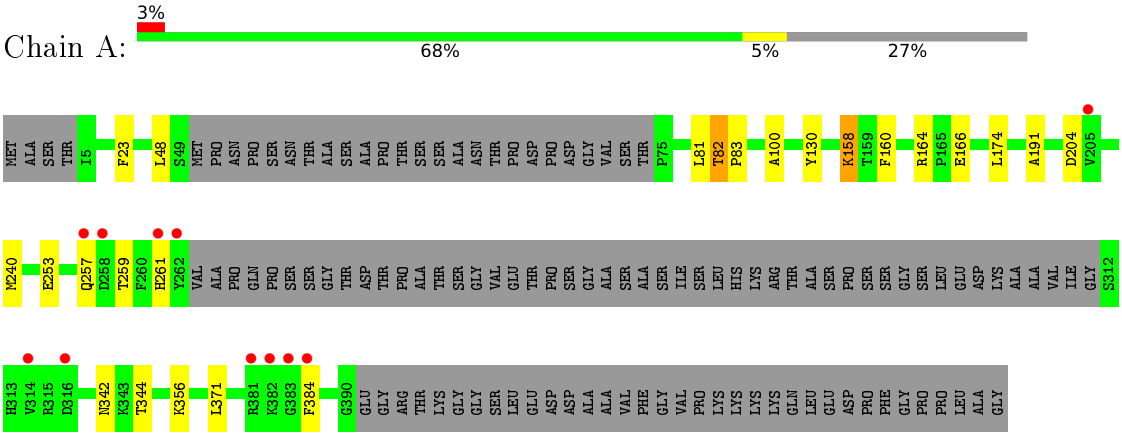
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	6	Total O 6 6	0	0
5	D	4	Total O 4 4	0	0
5	E	7	Total O 7 7	0	0

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.

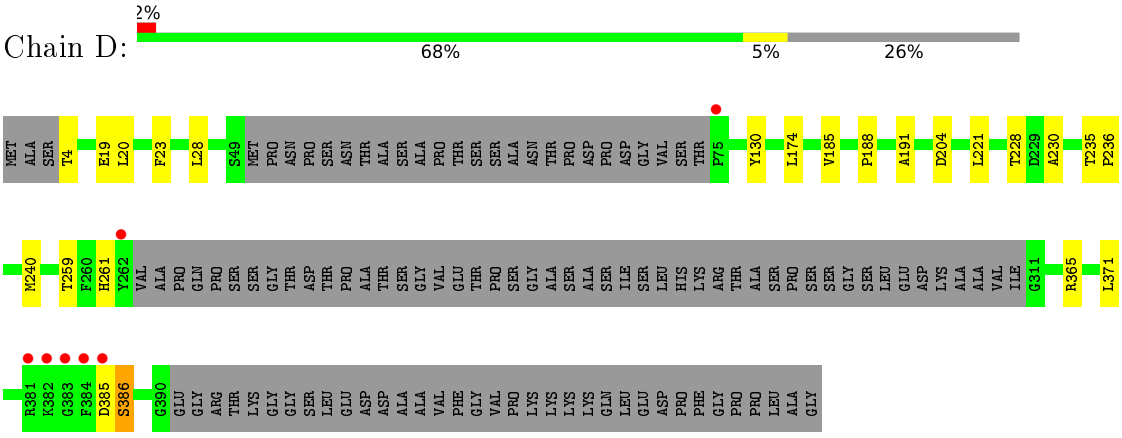
- Molecule 1: CYCLIN domain-containing protein

Chain A:



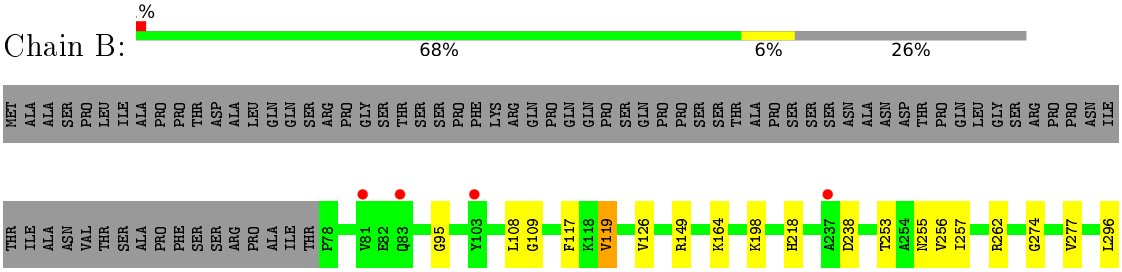
- Molecule 1: CYCLIN domain-containing protein

Chain D:



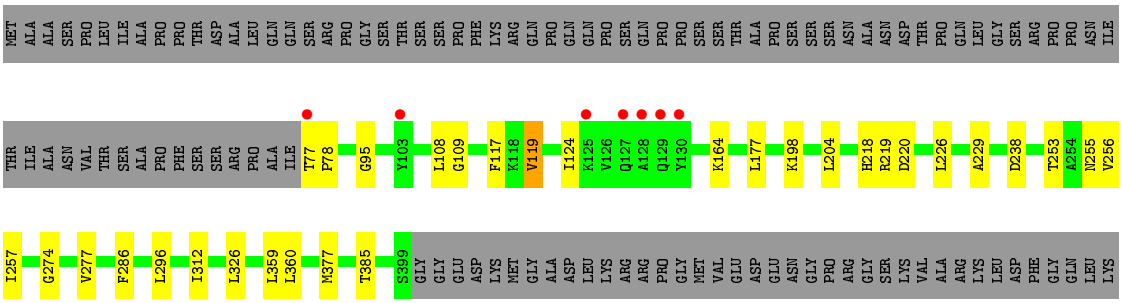
- Molecule 2: Protein kinase domain-containing protein

Chain B:



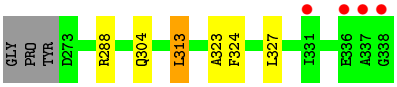
• Molecule 2: Protein kinase domain-containing protein

Chain E:



• Molecule 3: RING-type domain-containing protein

Chain C:



• Molecule 3: RING-type domain-containing protein

Chain F:

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.37 (at 2.62Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.18rc4_3812	Depositor
R, R_{free}	0.203 , 0.249 0.215 , 0.250	Depositor DCC
R_{free} test set	1653 reflections (4.89%)	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 , 39.1	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	0.91	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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

5.1 Standard geometry

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	0.25	0/2574	0.40	0/3471
1	D	0.26	0/2585	0.41	0/3486
2	B	0.25	0/2684	0.43	0/3635
2	E	0.25	0/2691	0.43	0/3646
3	C	0.26	0/552	0.40	0/742
3	F	0.26	0/565	0.40	0/760
All	All	0.25	0/11651	0.42	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

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	11	0
1	D	2533	2528	2527	13	0
2	B	2613	2624	2624	11	0
2	E	2620	2630	2630	15	0
3	C	538	503	502	4	0
3	F	550	511	511	4	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	52	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 2.

All (52) 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:130:TYR:OH	1:D:365:ARG:NH2	2.37	0.57
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: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:N	1:D:204:ASP:OD1	2.39	0.50
1:D:188:PRO:HG2	1:D:221:LEU:HD22	1.94	0.49
2:E:124:ILE:N	2:E:124:ILE:HD12	2.27	0.49
3:C:313:LEU:H	3:C:313:LEU:HD22	1.77	0.48
2:E:198:LYS:NZ	2:E:385:THR:O	2.46	0.48
2:E:124:ILE:H	2:E:124:ILE:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLU:O	1:A:257:GLN:HG2	2.15	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:HB3	1:A:158:LYS:NZ	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
1:D:228:THR:HG23	1:D:230:ALA:H	1.83	0.44
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: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
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:219:ARG:CZ	2:E:256:VAL:HG11	2.51	0.41
2:E:77:THR:N	2:E:78:PRO:CD	2.84	0.41
2:E:77:THR:HB	2:E:78:PRO:HD3	2.04	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	306/425 (72%)	300 (98%)	6 (2%)	0	100	100
1	D	308/425 (72%)	301 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	320/437 (73%)	313 (98%)	6 (2%)	1 (0%)	41 64
2	E	321/437 (74%)	314 (98%)	5 (2%)	2 (1%)	25 47
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%)	47 71

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%)	259 (97%)	8 (3%)	41 67
1	D	268/354 (76%)	260 (97%)	8 (3%)	41 67
2	B	275/370 (74%)	268 (98%)	7 (2%)	47 73
2	E	276/370 (75%)	270 (98%)	6 (2%)	52 76
3	C	55/57 (96%)	51 (93%)	4 (7%)	14 28
3	F	56/57 (98%)	54 (96%)	2 (4%)	35 61
All	All	1197/1562 (77%)	1162 (97%)	35 (3%)	42 68

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	PHE
1	A	48	LEU
1	A	82	THR
1	A	158	LYS

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Mol	Chain	Res	Type
1	A	240	MET
1	A	261	HIS
1	A	371	LEU
1	A	384	PHE
2	B	117	PHE
2	B	119	VAL
2	B	126	VAL
2	B	149	ARG
2	B	164	LYS
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	23	PHE
1	D	28	LEU
1	D	185	VAL
1	D	240	MET
1	D	261	HIS
1	D	371	LEU
1	D	386	SER
2	E	117	PHE
2	E	119	VAL
2	E	164	LYS
2	E	286	PHE
2	E	326	LEU
2	E	360	LEU
3	F	288	ARG
3	F	327	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

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

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, 95^{th} 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%)	0.38	11 (3%) 44 36	33, 60, 93, 124	0
1	D	314/425 (73%)	0.14	7 (2%) 62 56	19, 40, 70, 145	0
2	B	322/437 (73%)	0.08	4 (1%) 79 76	20, 37, 80, 103	0
2	E	323/437 (73%)	0.06	7 (2%) 62 56	14, 28, 73, 109	0
3	C	66/69 (95%)	0.41	4 (6%) 21 16	39, 57, 81, 87	0
3	F	67/69 (97%)	-0.06	0 100 100	22, 38, 61, 78	0
All	All	1404/1862 (75%)	0.16	33 (2%) 59 53	14, 42, 83, 145	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	7.1
1	D	381	ARG	5.8
1	D	384	PHE	5.7
1	D	75	PRO	4.6
2	E	129	GLN	4.4
1	A	384	PHE	4.4
1	A	383	GLY	4.3
1	A	381	ARG	4.0
1	D	262	TYR	4.0
1	D	382	LYS	3.8
1	A	382	LYS	3.6
2	E	103	TYR	3.4
3	C	338	GLY	3.2
2	E	128	ALA	3.1
3	C	336	GLU	2.9
2	E	130	TYR	2.8
1	D	383	GLY	2.8
2	B	103	TYR	2.8
1	D	385	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	81	VAL	2.6
1	A	257	GLN	2.5
2	E	127	GLN	2.5
2	E	77	THR	2.5
1	A	258	ASP	2.4
2	B	237	ALA	2.4
1	A	261	HIS	2.4
1	A	314	VAL	2.3
2	B	83	GLN	2.3
3	C	337	ALA	2.3
3	C	331	ILE	2.2
1	A	316	ASP	2.2
2	E	125	LYS	2.1
1	A	205	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
4	CL	E	501	1/1	0.99	0.09	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.