



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:17 PM GMT

PDB ID : 3AJ2
Title : The structure of AxCeSD octamer (C-terminal HIS-tag) from Acetobacter xylinum
Authors : Hu, S.Q.; Tajima, K.; Zhou, Y.; Tanaka, I.; Yao, M.
Deposited on : 2010-05-20
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

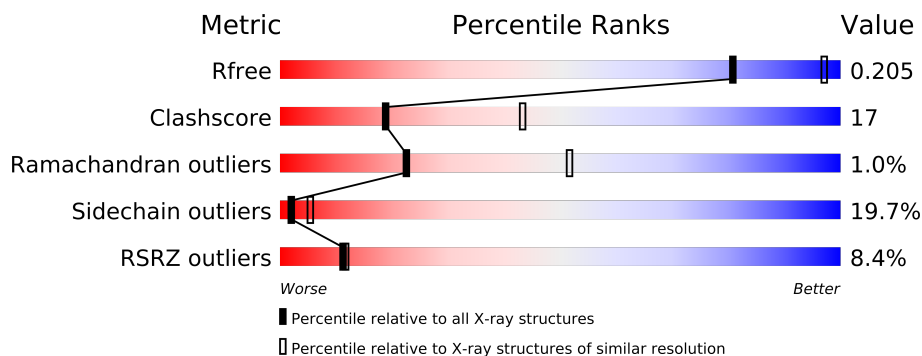
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	162	
1	B	162	
1	C	162	
1	D	162	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5046 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Cellulose synthase operon protein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1155	732	198	220	5			
1	B	158	Total	C	N	O	S	0	0	0
			1247	786	221	235	5			
1	C	145	Total	C	N	O	S	0	0	0
			1137	725	193	214	5			
1	D	158	Total	C	N	O	S	0	0	0
			1246	786	221	234	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	157	HIS	-	EXPRESSION TAG	UNP P37719
A	158	HIS	-	EXPRESSION TAG	UNP P37719
A	159	HIS	-	EXPRESSION TAG	UNP P37719
A	160	HIS	-	EXPRESSION TAG	UNP P37719
A	161	HIS	-	EXPRESSION TAG	UNP P37719
A	162	HIS	-	EXPRESSION TAG	UNP P37719
B	157	HIS	-	EXPRESSION TAG	UNP P37719
B	158	HIS	-	EXPRESSION TAG	UNP P37719
B	159	HIS	-	EXPRESSION TAG	UNP P37719
B	160	HIS	-	EXPRESSION TAG	UNP P37719
B	161	HIS	-	EXPRESSION TAG	UNP P37719
B	162	HIS	-	EXPRESSION TAG	UNP P37719
C	157	HIS	-	EXPRESSION TAG	UNP P37719
C	158	HIS	-	EXPRESSION TAG	UNP P37719
C	159	HIS	-	EXPRESSION TAG	UNP P37719
C	160	HIS	-	EXPRESSION TAG	UNP P37719
C	161	HIS	-	EXPRESSION TAG	UNP P37719
C	162	HIS	-	EXPRESSION TAG	UNP P37719
D	157	HIS	-	EXPRESSION TAG	UNP P37719
D	158	HIS	-	EXPRESSION TAG	UNP P37719
D	159	HIS	-	EXPRESSION TAG	UNP P37719

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Chain	Residue	Modelled	Actual	Comment	Reference
D	160	HIS	-	EXPRESSION TAG	UNP P37719
D	161	HIS	-	EXPRESSION TAG	UNP P37719
D	162	HIS	-	EXPRESSION TAG	UNP P37719

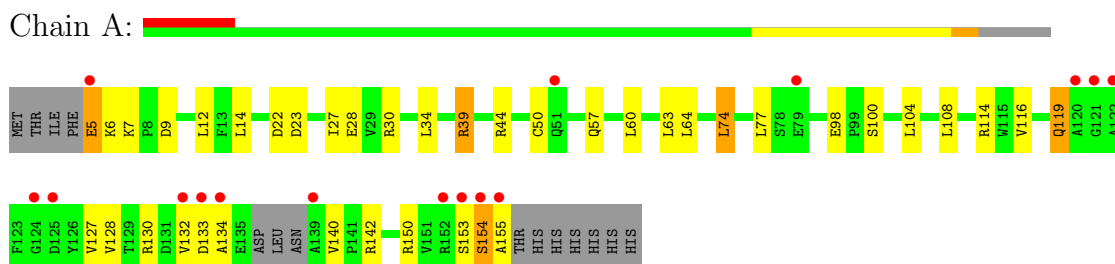
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	65	Total 65	O 65	0	0
2	B	52	Total 52	O 52	0	0
2	C	65	Total 65	O 65	0	0
2	D	79	Total 79	O 79	0	0

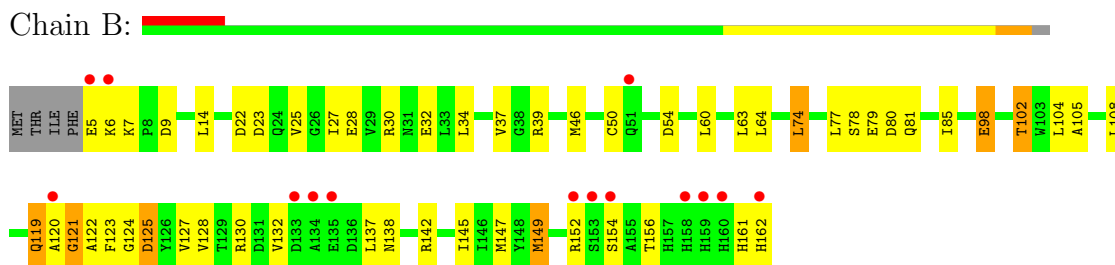
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

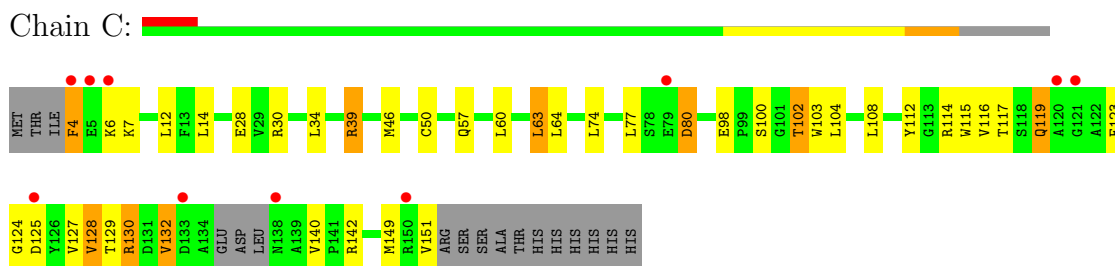
- Molecule 1: Cellulose synthase operon protein D



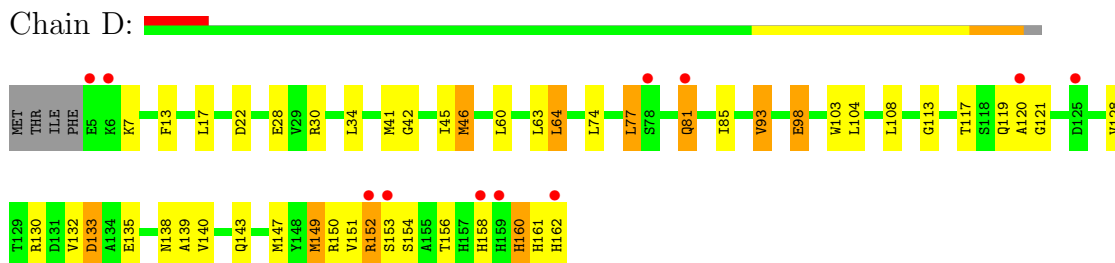
- Molecule 1: Cellulose synthase operon protein D



- Molecule 1: Cellulose synthase operon protein D



- Molecule 1: Cellulose synthase operon protein D



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	133.35Å 133.35Å 217.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.70 19.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.80-2.70) 99.7 (19.80-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.209 , 0.276 0.214 , 0.205	Depositor DCC
R_{free} test set	2715 reflections (11.12%)	DCC
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.40$	Xtriage
Outliers	3 of 27126 reflections (0.011%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5046	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.29 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.6114e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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	0.86	0/1176	0.91	0/1599
1	B	0.79	1/1275 (0.1%)	0.92	4/1735 (0.2%)
1	C	0.80	0/1159	0.87	0/1577
1	D	0.83	0/1274	0.87	3/1735 (0.2%)
All	All	0.82	1/4884 (0.0%)	0.89	7/6646 (0.1%)

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	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	32	GLU	CG-CD	5.13	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	79	GLU	N-CA-C	-5.44	96.30	111.00
1	B	74	LEU	CA-CB-CG	5.43	127.80	115.30
1	D	22	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	D	154	SER	N-CA-C	5.14	124.88	111.00
1	B	142	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	9	ASP	CB-CG-OD2	5.10	122.89	118.30
1	D	64	LEU	CB-CG-CD1	5.03	119.54	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	ALA	Peptide
1	B	78	SER	Peptide
1	D	160	HIS	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1155	0	78	18	0
1	B	1247	0	127	22	0
1	C	1137	0	59	22	0
1	D	1246	0	127	27	0
2	A	65	0	0	4	0
2	B	52	0	0	6	0
2	C	65	0	0	8	0
2	D	79	0	0	9	0
All	All	5046	0	391	86	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (86) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:160:HIS:CD2	1:D:161:HIS:H	1.51	1.29
1:D:160:HIS:HD2	1:D:161:HIS:N	1.59	1.00
1:D:160:HIS:CD2	1:D:161:HIS:N	2.35	0.92
1:A:50:CYS:N	1:A:119:GLN:NE2	2.23	0.87
1:B:50:CYS:N	1:B:119:GLN:NE2	2.32	0.77
1:B:98:GLU:CG	2:B:197:HOH:O	2.33	0.76
1:A:39:ARG:NH2	1:A:114:ARG:NH2	2.34	0.76
1:B:120:ALA:O	1:B:122:ALA:N	2.21	0.73
1:C:112:TYR:CA	2:C:241:HOH:O	2.38	0.71
1:A:127:VAL:CG1	1:A:128:VAL:N	2.54	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:151:VAL:HG12	2:C:205:HOH:O	1.92	0.70
1:B:30:ARG:NH2	1:B:98:GLU:OE2	2.28	0.66
1:A:6:LYS:HA	2:A:172:HOH:O	1.96	0.65
2:C:258:HOH:O	1:D:41:MET:CG	2.44	0.65
1:D:93:VAL:CG1	1:D:93:VAL:O	2.45	0.64
1:D:98:GLU:CG	2:D:171:HOH:O	2.45	0.63
1:D:152:ARG:HD2	2:D:199:HOH:O	1.98	0.63
1:B:39:ARG:NH1	2:B:194:HOH:O	2.34	0.61
1:A:44:ARG:NH1	2:A:196:HOH:O	2.34	0.61
1:D:45:ILE:CD1	2:D:233:HOH:O	2.50	0.60
1:D:152:ARG:CD	2:D:199:HOH:O	2.49	0.59
1:C:30:ARG:NH2	1:C:98:GLU:OE2	2.35	0.59
1:C:4:PHE:N	1:C:4:PHE:CD2	2.71	0.58
1:A:154:SER:O	1:A:155:ALA:HB3	2.03	0.58
1:D:160:HIS:HD2	1:D:161:HIS:H	0.74	0.57
1:A:132:VAL:O	1:A:132:VAL:CG1	2.53	0.57
1:B:123:PHE:O	1:B:125:ASP:N	2.38	0.57
1:C:115:TRP:CE3	2:C:241:HOH:O	2.53	0.56
1:B:105:ALA:CA	2:B:231:HOH:O	2.53	0.56
1:D:133:ASP:OD1	1:D:133:ASP:N	2.38	0.56
1:A:9:ASP:HB2	2:A:209:HOH:O	2.06	0.56
1:B:102:THR:CG2	1:B:102:THR:O	2.53	0.55
1:C:39:ARG:NE	1:C:114:ARG:NH2	2.54	0.55
1:C:4:PHE:HD2	1:C:4:PHE:N	2.05	0.55
1:B:145:ILE:CG1	2:B:231:HOH:O	2.55	0.54
1:D:162:HIS:HB2	2:D:285:HOH:O	2.06	0.54
1:A:30:ARG:NH2	1:A:98:GLU:OE2	2.41	0.54
1:B:80:ASP:OD1	1:B:81:GLN:N	2.40	0.54
1:D:119:GLN:O	1:D:121:GLY:N	2.41	0.53
1:B:5:GLU:OE1	1:C:6:LYS:HD3	2.08	0.53
1:D:162:HIS:HB2	2:D:262:HOH:O	2.09	0.52
1:A:100:SER:O	1:A:142:ARG:NH1	2.42	0.52
1:D:162:HIS:CB	2:D:285:HOH:O	2.57	0.51
1:A:6:LYS:HG3	1:A:6:LYS:O	2.11	0.51
1:A:5:GLU:OE1	1:A:5:GLU:CA	2.58	0.51
1:A:5:GLU:OE1	1:A:5:GLU:HA	2.12	0.49
1:C:127:VAL:CG1	1:C:128:VAL:N	2.76	0.49
1:C:57:GLN:OE1	1:C:74:LEU:N	2.45	0.49
1:D:30:ARG:NH2	1:D:98:GLU:OE1	2.45	0.49
1:B:105:ALA:CB	2:B:231:HOH:O	2.60	0.49
1:C:102:THR:CG2	2:C:191:HOH:O	2.61	0.49
1:A:57:GLN:OE1	1:A:74:LEU:N	2.46	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:22:ASP:OD1	1:A:30:ARG:CD	2.61	0.48
1:B:161:HIS:O	1:B:162:HIS:ND1	2.47	0.48
1:A:154:SER:O	1:A:155:ALA:CB	2.62	0.48
1:C:117:THR:C	1:C:119:GLN:N	2.67	0.48
1:B:85:ILE:N	1:B:147:MET:O	2.46	0.48
1:B:120:ALA:C	1:B:122:ALA:N	2.68	0.47
1:B:128:VAL:CG2	1:B:149:MET:SD	3.02	0.47
1:B:54:ASP:OD2	1:C:142:ARG:NH2	2.47	0.47
1:C:98:GLU:O	1:C:130:ARG:NH1	2.48	0.47
1:C:116:VAL:O	1:C:119:GLN:CB	2.62	0.47
1:D:113:GLY:O	1:D:117:THR:OG1	2.32	0.47
1:C:50:CYS:N	1:C:119:GLN:OE1	2.47	0.46
1:D:160:HIS:O	1:D:161:HIS:CG	2.69	0.46
1:D:139:ALA:N	2:D:290:HOH:O	2.47	0.46
1:B:22:ASP:OD1	1:B:30:ARG:CD	2.64	0.46
1:D:147:MET:CE	2:D:263:HOH:O	2.64	0.46
1:C:102:THR:O	1:C:102:THR:CG2	2.64	0.45
1:D:13:PHE:O	1:D:17:LEU:N	2.50	0.45
1:B:28:GLU:CB	2:B:243:HOH:O	2.66	0.43
1:C:98:GLU:N	2:C:191:HOH:O	2.51	0.43
1:D:85:ILE:N	1:D:147:MET:O	2.51	0.43
1:A:5:GLU:N	1:A:5:GLU:OE1	2.52	0.43
1:C:30:ARG:CD	1:C:103:TRP:NE1	2.82	0.42
1:B:120:ALA:O	1:B:121:GLY:C	2.58	0.42
1:D:42:GLY:O	1:D:46:MET:CE	2.69	0.41
1:D:77:LEU:O	1:D:81:GLN:N	2.54	0.41
1:C:130:ARG:NH2	2:C:173:HOH:O	2.53	0.41
1:C:80:ASP:N	1:C:80:ASP:OD1	2.53	0.41
1:A:116:VAL:O	1:A:119:GLN:CB	2.68	0.41
2:A:209:HOH:O	1:B:7:LYS:CE	2.69	0.41
1:D:30:ARG:CD	1:D:103:TRP:NE1	2.84	0.40
1:B:46:MET:CE	1:D:46:MET:SD	3.09	0.40
1:C:63:LEU:CD1	2:C:202:HOH:O	2.68	0.40
1:D:128:VAL:CG2	1:D:149:MET:SD	3.09	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	144/162 (89%)	135 (94%)	9 (6%)	0	100	100
1	B	156/162 (96%)	148 (95%)	6 (4%)	2 (1%)	18	43
1	C	141/162 (87%)	132 (94%)	7 (5%)	2 (1%)	16	41
1	D	156/162 (96%)	143 (92%)	11 (7%)	2 (1%)	18	43
All	All	597/648 (92%)	558 (94%)	33 (6%)	6 (1%)	22	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	121	GLY
1	D	120	ALA
1	B	124	GLY
1	D	135	GLU
1	C	124	GLY
1	C	132	VAL

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	126/140 (90%)	103 (82%)	23 (18%)	2	6
1	B	136/140 (97%)	109 (80%)	27 (20%)	2	5
1	C	124/140 (89%)	98 (79%)	26 (21%)	1	4
1	D	136/140 (97%)	109 (80%)	27 (20%)	2	5
All	All	522/560 (93%)	419 (80%)	103 (20%)	2	5

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	7	LYS
1	A	12	LEU
1	A	14	LEU
1	A	23	ASP
1	A	27	ILE
1	A	28	GLU
1	A	34	LEU
1	A	39	ARG
1	A	60	LEU
1	A	63	LEU
1	A	64	LEU
1	A	74	LEU
1	A	77	LEU
1	A	104	LEU
1	A	108	LEU
1	A	119	GLN
1	A	130	ARG
1	A	133	ASP
1	A	140	VAL
1	A	150	ARG
1	A	153	SER
1	A	154	SER
1	B	6	LYS
1	B	14	LEU
1	B	23	ASP
1	B	25	VAL
1	B	27	ILE
1	B	34	LEU
1	B	37	VAL
1	B	60	LEU
1	B	63	LEU
1	B	64	LEU
1	B	74	LEU
1	B	77	LEU
1	B	98	GLU
1	B	102	THR
1	B	104	LEU
1	B	108	LEU
1	B	119	GLN
1	B	125	ASP
1	B	127	VAL
1	B	130	ARG

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Mol	Chain	Res	Type
1	B	132	VAL
1	B	137	LEU
1	B	138	ASN
1	B	149	MET
1	B	152	ARG
1	B	154	SER
1	B	156	THR
1	C	4	PHE
1	C	7	LYS
1	C	12	LEU
1	C	14	LEU
1	C	28	GLU
1	C	34	LEU
1	C	39	ARG
1	C	46	MET
1	C	60	LEU
1	C	63	LEU
1	C	64	LEU
1	C	77	LEU
1	C	80	ASP
1	C	100	SER
1	C	102	THR
1	C	104	LEU
1	C	108	LEU
1	C	119	GLN
1	C	123	PHE
1	C	125	ASP
1	C	128	VAL
1	C	129	THR
1	C	130	ARG
1	C	132	VAL
1	C	140	VAL
1	C	149	MET
1	D	7	LYS
1	D	28	GLU
1	D	34	LEU
1	D	46	MET
1	D	60	LEU
1	D	63	LEU
1	D	64	LEU
1	D	74	LEU
1	D	77	LEU

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Mol	Chain	Res	Type
1	D	81	GLN
1	D	93	VAL
1	D	98	GLU
1	D	104	LEU
1	D	108	LEU
1	D	130	ARG
1	D	132	VAL
1	D	133	ASP
1	D	138	ASN
1	D	140	VAL
1	D	143	GLN
1	D	149	MET
1	D	150	ARG
1	D	151	VAL
1	D	152	ARG
1	D	153	SER
1	D	156	THR
1	D	158	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	160	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 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	148/162 (91%)	0.21	16 (10%) 6 6	39, 54, 108, 122	0
1	B	158/162 (97%)	-0.04	14 (8%) 10 10	38, 56, 104, 118	0
1	C	145/162 (89%)	0.14	10 (6%) 17 18	42, 58, 114, 125	0
1	D	158/162 (97%)	0.01	11 (6%) 16 17	41, 55, 96, 115	0
All	All	609/648 (93%)	0.08	51 (8%) 11 12	38, 56, 105, 125	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	SER	8.5
1	D	5	GLU	6.2
1	A	155	ALA	6.1
1	C	138	ASN	5.8
1	C	4	PHE	5.6
1	D	159	HIS	5.6
1	A	153	SER	5.4
1	B	5	GLU	5.2
1	C	150	ARG	4.6
1	A	125	ASP	4.5
1	C	120	ALA	4.3
1	A	121	GLY	4.2
1	C	5	GLU	4.0
1	D	162	HIS	3.7
1	A	133	ASP	3.6
1	C	125	ASP	3.6
1	C	133	ASP	3.5
1	B	159	HIS	3.4
1	D	120	ALA	3.4
1	A	5	GLU	3.2
1	A	120	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	6	LYS	3.2
1	B	160	HIS	3.2
1	B	134	ALA	3.1
1	C	79	GLU	3.0
1	A	124	GLY	3.0
1	B	135	GLU	3.0
1	B	120	ALA	3.0
1	B	162	HIS	2.8
1	D	6	LYS	2.7
1	D	158	HIS	2.7
1	B	152	ARG	2.6
1	A	134	ALA	2.6
1	C	121	GLY	2.6
1	A	152	ARG	2.5
1	D	152	ARG	2.5
1	B	158	HIS	2.4
1	B	133	ASP	2.4
1	A	139	ALA	2.3
1	B	6	LYS	2.3
1	D	125	ASP	2.3
1	A	51	GLN	2.3
1	A	132	VAL	2.2
1	B	153	SER	2.2
1	B	154	SER	2.1
1	D	78	SER	2.1
1	B	51	GLN	2.1
1	A	122	ALA	2.1
1	A	79	GLU	2.1
1	D	81	GLN	2.0
1	D	153	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.