Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:17 AM GMT

PDB ID	:	3A8E
Title	:	The structure of AxCesD octamer complexed with cellopentaose
Authors	:	Hu, S.Q.; Tajima, K.; Zhou, Y.; Yao, M.; Tanaka, I.
Deposited on	:	2009-10-05
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

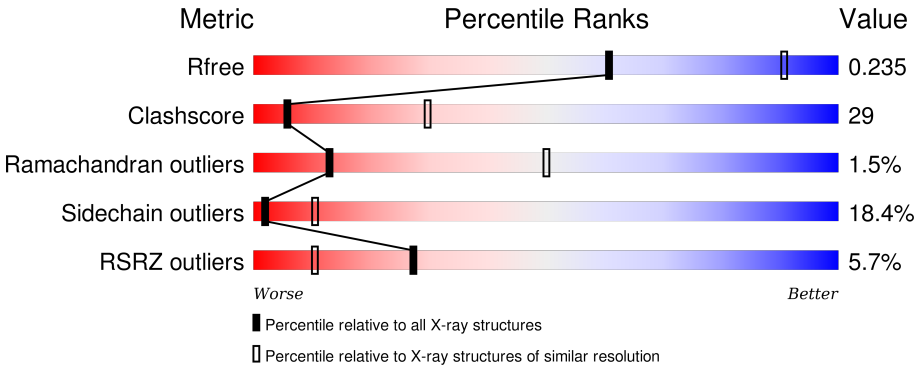
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. 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	162	7% 55% 30% 7% 9%
1	B	162	5% 61% 30% 6%
1	C	162	4% 54% 32% 12%
1	D	162	6% 51% 31% 10% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CE5	A	801	-	-	-	X
2	CE5	A	802[A]	-	-	-	X
2	CE5	A	802[B]	-	-	-	X
2	CE5	C	803	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5230 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 Cellulose synthase operon protein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1162	740	196	221	5			
1	B	158	Total	C	N	O	S	0	0	0
			1247	789	219	234	5			
1	C	159	Total	C	N	O	S	0	0	0
			1257	795	222	235	5			
1	D	148	Total	C	N	O	S	0	0	0
			1162	740	196	221	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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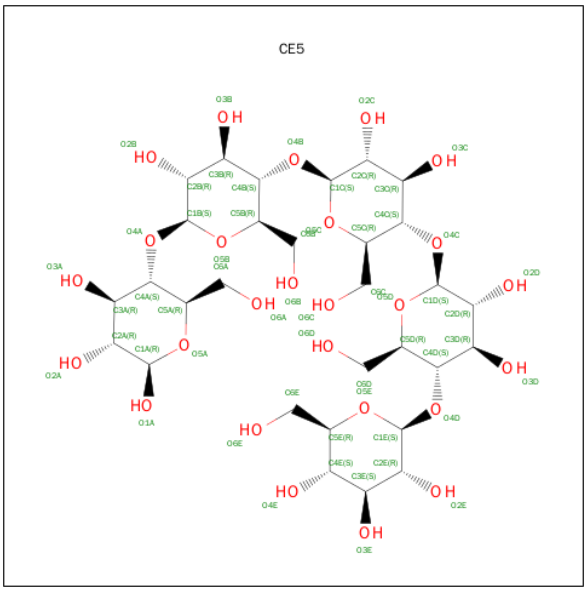
Chain	Residue	Modelled	Actual	Comment	Reference
D	160	HIS	-	EXPRESSION TAG	UNP P37719
D	161	HIS	-	EXPRESSION TAG	UNP P37719
D	162	HIS	-	EXPRESSION TAG	UNP P37719

- Molecule 2 is SUGAR (CELLOPENTAOSE) (three-letter code: CE5) (formula: $C_{30}H_{52}O_{26}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 56 30 26	0	0
2	A	1	Total C O 112 60 52	0	1
2	C	1	Total C O 56 30 26	0	0

- Molecule 3 is water.

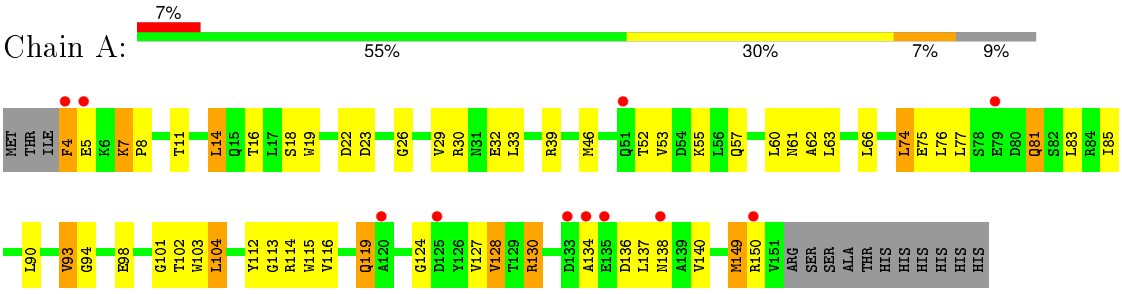
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	45	Total O 45 45	0	0
3	B	42	Total O 42 42	0	0
3	C	46	Total O 46 46	0	0
3	D	45	Total O 45 45	0	0

3 Residue-property plots (i)

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.

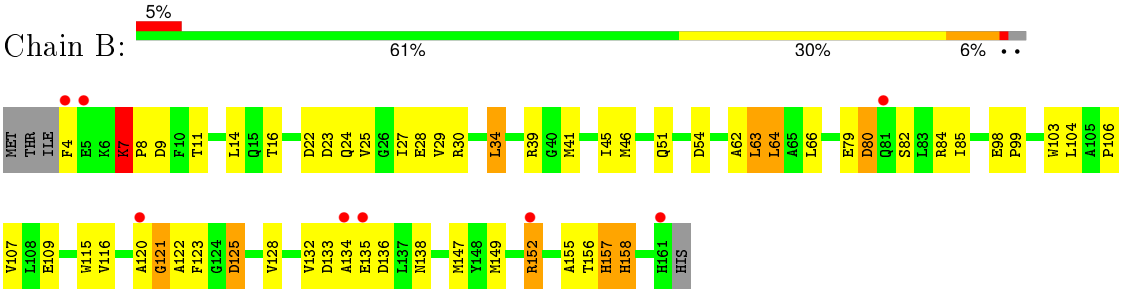
- Molecule 1: Cellulose synthase operon protein D

Chain A:



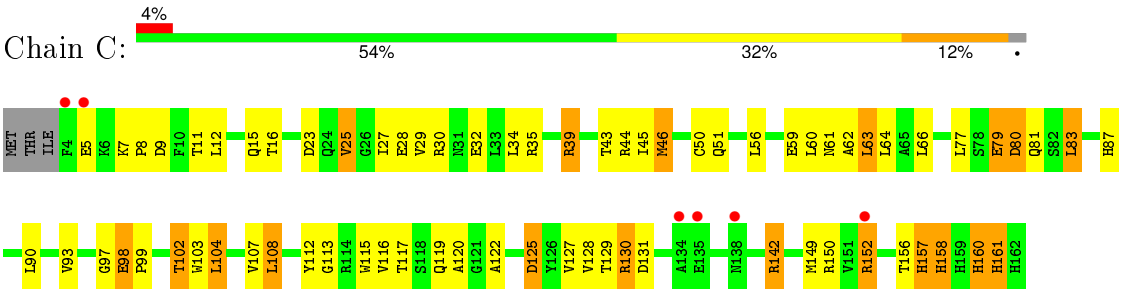
- Molecule 1: Cellulose synthase operon protein D

Chain B:



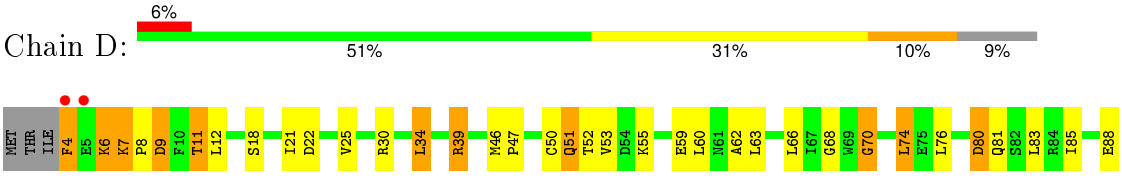
- Molecule 1: Cellulose synthase operon protein D

Chain C:



- Molecule 1: Cellulose synthase operon protein D

Chain D:




V93
E98
W103
P106
V107
L108
E109
G113
R114
W115
V116
T117
A120
G121
A122
F123
G124
D125
Y126
V127
V128
T129
R130
D131
V132
D133
A134
E135
D136
L137
N138
R142
I146
M147
Y148
M149
R150
V151
ARG
SER
SER
ALA
THR
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	132.88Å 132.88Å 216.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 3.00 19.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.94-3.00) 100.0 (19.94-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	0.78 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.242 , 0.293 0.236 , 0.235	Depositor DCC
R_{free} test set	2015 reflections (11.41%)	DCC
Wilson B-factor (Å^2)	65.8	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	Xtriage
Outliers	1 of 19684 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5230	wwPDB-VP
Average B, all atoms (Å^2)	56.0	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 48.53 % 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 8.4891e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CE5

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	0.38	0/1185	0.63	1/1614 (0.1%)
1	B	0.40	0/1275	0.63	0/1736
1	C	0.38	0/1286	0.63	0/1751
1	D	0.40	0/1185	0.67	0/1614
All	All	0.39	0/4931	0.64	1/6715 (0.0%)

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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	7	LYS	Peptide

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	1162	0	1160	48	0
1	B	1247	0	1230	73	0
1	C	1257	0	1237	75	0
1	D	1162	0	1160	64	0
2	A	168	0	156	48	0
2	C	56	0	52	15	0
3	A	45	0	0	3	0
3	B	42	0	0	1	0
3	C	46	0	0	3	0
3	D	45	0	0	3	0
All	All	5230	0	4995	290	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 29.

All (290) 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:7:LYS:HB3	1:D:8:PRO:CD	1.69	1.22
1:A:7:LYS:HB3	1:A:8:PRO:CD	1.69	1.21
1:B:155:ALA:HB1	1:B:158:HIS:CG	1.82	1.13
1:A:7:LYS:HB3	1:A:8:PRO:HD2	1.31	1.09
1:B:7:LYS:HB3	1:B:8:PRO:CD	1.84	1.07
1:B:7:LYS:HB3	1:B:8:PRO:HD3	1.36	1.06
1:D:7:LYS:HB3	1:D:8:PRO:HD3	1.37	1.03
1:A:112:TYR:HA	3:A:214:HOH:O	1.58	1.03
1:B:156:THR:N	1:B:158:HIS:CD2	2.32	0.97
1:B:158:HIS:H	1:B:158:HIS:CD2	1.63	0.96
2:A:802[A]:CE5:H3C	2:A:802[A]:CE5:C2D	1.95	0.96
2:A:802[B]:CE5:H3C	2:A:802[B]:CE5:C2D	1.97	0.95
2:A:802[B]:CE5:H3D	1:B:66:LEU:HD12	1.50	0.94
1:D:39:ARG:HG2	1:D:39:ARG:HH11	1.27	0.93
2:C:803:CE5:H3C	2:C:803:CE5:C2D	2.00	0.92
2:A:801:CE5:H3C	2:A:801:CE5:C2D	1.99	0.92
2:A:802[A]:CE5:H3D	1:C:66:LEU:HD12	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:LYS:HE2	1:C:7:LYS:HA	1.48	0.91
2:A:802[A]:CE5:H2D	2:A:802[A]:CE5:H3C	1.53	0.91
2:A:802[B]:CE5:H6A1	2:A:802[B]:CE5:H1B	1.52	0.90
1:A:30:ARG:HD2	1:A:103:TRP:NE1	1.86	0.90
1:A:81:GLN:HE21	1:A:81:GLN:HA	1.33	0.90
1:C:128:VAL:HG22	1:C:149:MET:SD	2.12	0.90
1:D:30:ARG:HD2	1:D:103:TRP:HE1	1.35	0.89
2:C:803:CE5:H6A1	2:C:803:CE5:H1B	1.55	0.89
2:C:803:CE5:O3A	1:D:62:ALA:HA	1.72	0.89
2:A:802[A]:CE5:H6A1	2:A:802[A]:CE5:H1B	1.56	0.88
1:B:80:ASP:HB2	1:B:82:SER:HB3	1.55	0.87
1:B:155:ALA:HB1	1:B:158:HIS:CB	2.05	0.86
2:C:803:CE5:H2D	2:C:803:CE5:H3C	1.58	0.85
1:B:156:THR:HG23	1:B:157:HIS:HD2	1.38	0.85
1:D:7:LYS:HB3	1:D:8:PRO:HD2	1.56	0.85
2:A:802[B]:CE5:H3C	2:A:802[B]:CE5:H2D	1.57	0.85
1:A:7:LYS:HB3	1:A:8:PRO:HD3	1.58	0.84
2:A:801:CE5:H3C	2:A:801:CE5:H2D	1.59	0.84
1:C:64:LEU:HD12	3:C:270:HOH:O	1.78	0.84
1:C:156:THR:HB	1:C:158:HIS:CD2	2.13	0.84
2:A:802[B]:CE5:H4D	1:D:9:ASP:OD1	1.77	0.83
1:A:62:ALA:HB1	2:A:801:CE5:O3E	1.77	0.83
1:D:30:ARG:HD2	1:D:103:TRP:NE1	1.91	0.83
2:A:801:CE5:H6A1	2:A:801:CE5:H1B	1.58	0.83
1:D:7:LYS:CB	1:D:8:PRO:CD	2.54	0.82
1:C:9:ASP:OD2	2:C:803:CE5:H4D	1.81	0.81
1:A:11:THR:HG21	2:A:802[A]:CE5:H4E	1.61	0.80
1:C:7:LYS:HB3	1:C:8:PRO:CD	2.12	0.79
1:B:134:ALA:O	1:B:135:GLU:HG2	1.82	0.79
1:C:50:CYS:H	1:C:119:GLN:NE2	1.81	0.79
1:A:7:LYS:CB	1:A:8:PRO:CD	2.57	0.78
1:A:81:GLN:HE21	1:A:81:GLN:CA	1.95	0.77
1:B:158:HIS:HD2	1:B:158:HIS:H	1.32	0.77
1:B:158:HIS:N	1:B:158:HIS:CD2	2.47	0.77
1:B:155:ALA:HB1	1:B:158:HIS:HB2	1.66	0.77
1:A:81:GLN:NE2	1:A:81:GLN:HA	1.96	0.77
2:A:802[A]:CE5:O3E	1:C:62:ALA:HB1	1.86	0.76
1:C:7:LYS:HB3	1:C:8:PRO:HD2	1.66	0.76
2:A:802[B]:CE5:O3A	1:C:62:ALA:HA	1.86	0.76
1:D:132:VAL:HG21	1:D:137:LEU:HA	1.68	0.76
2:A:802[B]:CE5:O3E	1:B:62:ALA:HB1	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:802[A]:CE5:H2B	1:B:66:LEU:HD12	1.69	0.74
1:C:160:HIS:ND1	1:C:160:HIS:O	2.19	0.74
1:C:50:CYS:H	1:C:119:GLN:HE22	1.34	0.74
1:A:22:ASP:OD1	1:A:30:ARG:HD3	1.88	0.73
1:A:115:TRP:CE3	3:A:214:HOH:O	2.42	0.73
2:C:803:CE5:H6A1	2:C:803:CE5:C1B	2.18	0.73
2:A:801:CE5:C1B	2:A:801:CE5:H6A1	2.18	0.72
1:B:85:ILE:HD11	1:B:149:MET:HE3	1.69	0.72
1:A:4:PHE:O	1:A:5:GLU:HG2	1.89	0.72
1:B:156:THR:HG23	1:B:157:HIS:CD2	2.25	0.71
1:C:7:LYS:CE	1:C:7:LYS:HA	2.19	0.71
2:A:802[A]:CE5:H3B	1:D:9:ASP:OD1	1.90	0.70
1:C:30:ARG:HD2	1:C:103:TRP:NE1	2.06	0.70
1:D:74:LEU:HD12	1:D:85:ILE:HG12	1.74	0.70
2:A:802[A]:CE5:C1B	2:A:802[A]:CE5:H6A1	2.22	0.70
1:B:41:MET:HE1	1:B:107:VAL:HG11	1.74	0.70
1:B:30:ARG:HD2	1:B:103:TRP:NE1	2.07	0.69
1:D:51:GLN:HG2	1:D:55:LYS:HD3	1.74	0.69
1:A:93:VAL:HG13	1:A:93:VAL:O	1.93	0.69
2:A:802[B]:CE5:H6A1	2:A:802[B]:CE5:C1B	2.21	0.68
1:C:127:VAL:HG13	1:C:152:ARG:HG2	1.74	0.68
1:A:7:LYS:CB	1:A:8:PRO:HD2	2.17	0.68
2:A:802[A]:CE5:O3A	1:B:62:ALA:HA	1.94	0.68
1:C:152:ARG:HH21	1:C:152:ARG:HG3	1.59	0.68
1:D:137:LEU:H	1:D:137:LEU:HD12	1.59	0.67
1:B:128:VAL:HG22	1:B:149:MET:SD	2.35	0.67
1:A:62:ALA:HA	2:A:801:CE5:O4E	1.94	0.67
1:C:97:GLY:C	1:C:98:GLU:OE2	2.33	0.67
1:B:157:HIS:H	1:B:157:HIS:CD2	2.10	0.66
1:B:7:LYS:CB	1:B:8:PRO:CD	2.68	0.66
1:A:14:LEU:HB3	1:A:93:VAL:CG2	2.25	0.66
1:D:125:ASP:O	1:D:126:TYR:HD1	1.78	0.66
1:A:62:ALA:O	2:A:801:CE5:H3E	1.96	0.66
1:D:4:PHE:N	1:D:4:PHE:CD1	2.63	0.65
1:D:130:ARG:HA	1:D:147:MET:HG2	1.76	0.65
1:A:14:LEU:HB3	1:A:93:VAL:HG21	1.79	0.65
1:B:41:MET:CE	1:B:107:VAL:CG1	2.74	0.65
1:A:30:ARG:NH2	1:A:98:GLU:OE2	2.25	0.64
1:D:39:ARG:HG2	1:D:39:ARG:NH1	2.05	0.64
2:A:801:CE5:O2D	2:A:801:CE5:H3C	1.97	0.64
2:A:802[B]:CE5:H3C	2:A:802[B]:CE5:O2D	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:LYS:CB	1:D:8:PRO:HD2	2.25	0.64
1:D:109:GLU:CD	1:D:130:ARG:HB3	2.18	0.64
1:B:157:HIS:N	1:B:158:HIS:CD2	2.66	0.64
1:B:157:HIS:N	1:B:158:HIS:HD2	1.96	0.64
1:C:116:VAL:HG21	1:C:149:MET:SD	2.39	0.63
2:A:802[A]:CE5:O2D	2:A:802[A]:CE5:H3C	1.98	0.63
1:C:152:ARG:HH21	1:C:152:ARG:CG	2.11	0.63
1:D:132:VAL:HG11	1:D:136:ASP:O	2.00	0.62
1:C:98:GLU:OE2	1:C:98:GLU:N	2.33	0.62
1:A:30:ARG:HD2	1:A:103:TRP:HE1	1.65	0.61
1:C:25:VAL:HG13	1:C:29:VAL:HB	1.82	0.61
1:D:34:LEU:HB3	1:D:106:PRO:HB2	1.82	0.61
1:B:135:GLU:HA	1:B:138:ASN:HB2	1.82	0.61
1:C:7:LYS:HE2	1:C:7:LYS:CA	2.26	0.61
1:D:117:THR:HG23	1:D:124:GLY:HA2	1.83	0.60
2:C:803:CE5:O2D	2:C:803:CE5:H3C	2.01	0.60
1:D:22:ASP:OD1	1:D:30:ARG:HD2	2.02	0.60
1:D:107:VAL:HG23	3:D:200:HOH:O	2.01	0.60
1:B:155:ALA:C	1:B:158:HIS:CD2	2.75	0.59
1:B:157:HIS:HD2	1:B:157:HIS:H	1.50	0.59
1:C:113:GLY:HA2	1:C:149:MET:HE1	1.84	0.59
1:C:127:VAL:CG1	1:C:152:ARG:HG2	2.32	0.59
2:A:802[B]:CE5:O5E	1:D:11:THR:HG21	2.03	0.59
1:B:41:MET:HE3	1:B:107:VAL:CG1	2.33	0.58
1:C:9:ASP:CG	2:C:803:CE5:H4D	2.22	0.58
1:C:99:PRO:O	1:C:102:THR:HB	2.04	0.58
1:B:7:LYS:HB3	1:B:8:PRO:HD2	1.84	0.58
1:D:22:ASP:OD1	1:D:30:ARG:CD	2.52	0.58
1:D:113:GLY:HA2	1:D:149:MET:HE1	1.86	0.57
1:B:120:ALA:O	1:B:121:GLY:O	2.22	0.57
1:C:152:ARG:HG3	1:C:152:ARG:NH2	2.20	0.57
1:D:9:ASP:C	1:D:9:ASP:OD2	2.42	0.57
1:B:41:MET:HE1	1:B:107:VAL:CG1	2.34	0.57
1:C:156:THR:CB	1:C:158:HIS:CD2	2.87	0.56
1:B:156:THR:N	1:B:158:HIS:HD2	2.01	0.56
2:A:802[A]:CE5:H2D	2:A:802[A]:CE5:C3C	2.31	0.56
1:A:62:ALA:HB1	2:A:801:CE5:HO3E	1.71	0.56
1:D:132:VAL:CG1	1:D:134:ALA:HB3	2.36	0.56
1:C:11:THR:HG21	2:C:803:CE5:H4E	1.87	0.55
1:B:123:PHE:HD1	1:B:123:PHE:N	2.04	0.55
1:C:39:ARG:O	1:C:43:THR:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:GLY:HA3	1:D:88:GLU:O	2.05	0.55
1:B:34:LEU:HB3	1:B:106:PRO:HB2	1.89	0.55
1:C:90:LEU:HD11	1:C:104:LEU:HB3	1.88	0.55
1:A:93:VAL:CG1	1:A:93:VAL:O	2.54	0.55
1:B:54:ASP:OD1	1:D:142:ARG:NH2	2.39	0.55
1:C:11:THR:HB	2:C:803:CE5:H2E	1.89	0.55
1:D:132:VAL:O	1:D:135:GLU:HA	2.07	0.55
1:B:156:THR:C	1:B:158:HIS:HD2	2.09	0.54
1:D:127:VAL:O	1:D:149:MET:HA	2.07	0.54
2:A:802[B]:CE5:O2E	1:B:66:LEU:HD13	2.07	0.54
1:B:123:PHE:N	1:B:123:PHE:CD1	2.74	0.54
2:A:802[B]:CE5:C3C	2:A:802[B]:CE5:H2D	2.36	0.54
1:B:155:ALA:CB	1:B:158:HIS:HB2	2.35	0.54
2:A:802[A]:CE5:C3D	1:C:66:LEU:HD12	2.32	0.54
1:C:30:ARG:HH22	1:C:98:GLU:CD	2.11	0.54
1:D:60:LEU:HD12	1:D:74:LEU:HD21	1.91	0.53
1:B:41:MET:CE	1:B:107:VAL:HG13	2.38	0.53
1:B:125:ASP:OD1	1:B:152:ARG:HD2	2.08	0.53
1:C:50:CYS:N	1:C:119:GLN:NE2	2.56	0.53
1:D:51:GLN:HG2	1:D:55:LYS:CD	2.38	0.53
2:A:802[B]:CE5:H6D2	1:D:11:THR:HG21	1.90	0.53
1:C:112:TYR:O	1:C:116:VAL:HG22	2.09	0.53
1:A:81:GLN:NE2	1:A:81:GLN:CA	2.66	0.52
1:B:156:THR:H	1:B:158:HIS:CD2	2.22	0.52
1:D:135:GLU:O	1:D:135:GLU:HG2	2.09	0.52
2:A:802[B]:CE5:C4D	1:D:9:ASP:OD1	2.54	0.52
1:D:21:ILE:O	1:D:25:VAL:HG22	2.10	0.52
1:C:90:LEU:HD13	1:C:108:LEU:HD22	1.92	0.52
1:B:30:ARG:HD2	1:B:103:TRP:HE1	1.74	0.51
1:D:39:ARG:CG	1:D:39:ARG:HH11	2.11	0.51
1:B:85:ILE:HD11	1:B:149:MET:CE	2.39	0.51
1:A:11:THR:HG21	2:A:802[A]:CE5:C4E	2.35	0.51
1:C:28:GLU:OE1	1:C:28:GLU:HA	2.10	0.51
2:C:803:CE5:C6D	2:C:803:CE5:O5E	2.58	0.51
1:B:28:GLU:OE2	1:B:28:GLU:HA	2.11	0.51
2:A:801:CE5:H3A	1:B:11:THR:HG21	1.93	0.51
1:A:39:ARG:HD2	1:A:114:ARG:HD3	1.91	0.51
1:C:125:ASP:N	1:C:125:ASP:OD2	2.44	0.51
1:A:90:LEU:HD11	1:A:104:LEU:HB3	1.93	0.50
1:A:116:VAL:O	1:A:119:GLN:HB2	2.11	0.50
1:B:157:HIS:N	1:B:157:HIS:CD2	2.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:THR:OG1	1:D:55:LYS:HG3	2.12	0.50
1:D:132:VAL:CG2	1:D:137:LEU:HA	2.38	0.50
2:A:801:CE5:H2D	2:A:801:CE5:C3C	2.37	0.50
1:D:126:TYR:HA	1:D:150:ARG:O	2.12	0.50
1:C:161:HIS:O	1:C:161:HIS:ND1	2.44	0.50
1:A:60:LEU:HD22	1:A:115:TRP:CE3	2.46	0.49
1:C:8:PRO:HB3	1:D:68:GLY:O	2.12	0.49
1:D:132:VAL:HG12	1:D:135:GLU:N	2.28	0.49
1:C:7:LYS:HD3	1:C:8:PRO:HD3	1.93	0.49
1:B:155:ALA:CB	1:B:158:HIS:CG	2.75	0.48
1:A:113:GLY:HA2	1:A:149:MET:HE1	1.94	0.48
1:C:157:HIS:ND1	1:C:157:HIS:N	2.57	0.48
2:A:802[B]:CE5:C3D	1:B:66:LEU:HD12	2.33	0.48
1:D:132:VAL:HG21	3:D:228:HOH:O	2.13	0.48
1:A:134:ALA:HA	1:A:137:LEU:HB2	1.95	0.48
1:B:25:VAL:HG13	1:B:29:VAL:HB	1.95	0.48
1:B:85:ILE:CD1	1:B:149:MET:CE	2.91	0.48
1:C:50:CYS:SG	1:C:59:GLU:HG3	2.53	0.48
1:A:94:GLY:O	1:A:101:GLY:HA2	2.14	0.48
1:A:52:THR:OG1	1:A:55:LYS:HG3	2.14	0.47
1:B:41:MET:HE3	1:B:107:VAL:HG13	1.96	0.47
1:B:116:VAL:CG1	1:B:123:PHE:HD2	2.26	0.47
1:D:130:ARG:O	1:D:146:ILE:O	2.33	0.47
1:D:116:VAL:HG21	1:D:149:MET:HG2	1.97	0.47
1:C:93:VAL:CG2	1:C:104:LEU:HD22	2.44	0.47
1:B:64:LEU:HD13	1:B:115:TRP:HH2	1.79	0.47
1:D:6:LYS:O	1:D:7:LYS:HG2	2.13	0.47
1:B:85:ILE:CD1	1:B:149:MET:HE3	2.40	0.47
2:C:803:CE5:C3C	2:C:803:CE5:C2D	2.83	0.47
1:C:30:ARG:HD2	1:C:103:TRP:HE1	1.75	0.47
1:A:14:LEU:HB3	1:A:93:VAL:HG22	1.96	0.47
1:A:26:GLY:HA3	3:A:188:HOH:O	2.14	0.47
1:C:79:GLU:HG2	1:C:79:GLU:H	1.52	0.47
1:D:39:ARG:CG	1:D:39:ARG:NH1	2.75	0.46
1:C:60:LEU:HD22	1:C:115:TRP:CE3	2.50	0.46
1:B:98:GLU:HA	1:B:99:PRO:HA	1.69	0.46
1:C:142:ARG:HA	1:C:142:ARG:HD3	1.70	0.46
1:B:103:TRP:O	1:B:106:PRO:HD2	2.15	0.46
1:D:50:CYS:SG	1:D:59:GLU:HG3	2.56	0.46
1:C:130:ARG:HG3	1:C:131:ASP:N	2.30	0.46
2:A:802[A]:CE5:O2E	1:C:66:LEU:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:VAL:HA	1:D:148:TYR:O	2.15	0.46
2:A:802[A]:CE5:C2B	1:B:66:LEU:HD12	2.43	0.46
1:A:137:LEU:HA	1:A:140:VAL:HG22	1.98	0.45
1:C:83:LEU:HB3	1:C:149:MET:HB3	1.99	0.45
1:C:97:GLY:CA	1:C:98:GLU:OE2	2.64	0.45
1:B:122:ALA:HB3	1:B:123:PHE:CE1	2.51	0.45
2:C:803:CE5:C3C	2:C:803:CE5:H2D	2.39	0.45
1:B:41:MET:CE	1:B:107:VAL:HG11	2.40	0.45
1:B:109:GLU:HA	1:B:147:MET:CE	2.46	0.45
1:C:7:LYS:CB	1:C:8:PRO:CD	2.86	0.45
1:D:22:ASP:OD1	1:D:30:ARG:HD3	2.17	0.45
1:D:137:LEU:HD12	1:D:137:LEU:N	2.28	0.45
1:C:102:THR:O	1:C:102:THR:HG23	2.16	0.44
1:D:80:ASP:O	1:D:81:GLN:HB2	2.16	0.44
1:B:45:ILE:HG22	1:C:45:ILE:HG22	1.99	0.44
1:A:22:ASP:OD1	1:A:30:ARG:CD	2.62	0.44
1:C:113:GLY:O	1:C:117:THR:HB	2.18	0.44
1:A:4:PHE:CD2	1:A:4:PHE:N	2.85	0.44
1:B:122:ALA:HB3	1:B:123:PHE:CD1	2.52	0.44
1:A:130:ARG:O	1:A:130:ARG:HG3	2.17	0.44
1:B:79:GLU:HG2	1:B:80:ASP:OD1	2.18	0.44
1:A:83:LEU:HB3	1:A:149:MET:HB3	2.00	0.44
1:C:27:ILE:HG12	1:C:98:GLU:OE1	2.18	0.43
2:A:802[A]:CE5:C2D	2:A:802[A]:CE5:C3C	2.78	0.43
2:C:803:CE5:H6D2	2:C:803:CE5:O6E	2.19	0.43
1:D:93:VAL:HG23	1:D:93:VAL:O	2.18	0.43
1:D:18:SER:HA	1:D:103:TRP:CZ2	2.53	0.43
1:B:79:GLU:H	1:B:79:GLU:CD	2.21	0.43
1:B:80:ASP:N	1:B:80:ASP:OD1	2.52	0.43
1:C:104:LEU:HD12	1:C:107:VAL:HG21	2.01	0.43
1:A:127:VAL:HG12	1:A:128:VAL:H	1.83	0.43
2:A:802[A]:CE5:O5E	2:A:802[A]:CE5:H6D2	2.19	0.43
1:A:127:VAL:O	1:A:149:MET:HA	2.19	0.43
1:B:155:ALA:HB1	1:B:158:HIS:ND1	2.28	0.43
1:A:18:SER:HA	1:A:103:TRP:CZ2	2.54	0.43
1:C:87:HIS:CD2	1:C:87:HIS:C	2.92	0.43
1:A:76:LEU:HD11	1:A:81:GLN:HE22	1.84	0.43
1:C:50:CYS:SG	1:C:56:LEU:HA	2.59	0.42
1:C:12:LEU:O	1:C:16:THR:HG23	2.19	0.42
1:C:5:GLU:O	1:C:7:LYS:CE	2.68	0.42
1:D:127:VAL:HG12	1:D:128:VAL:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:GLN:NE2	2:C:803:CE5:O3E	2.53	0.42
1:C:32:GLU:OE1	1:C:35:ARG:NH1	2.51	0.42
1:B:22:ASP:OD1	1:B:30:ARG:HD3	2.19	0.42
1:A:57:GLN:HG2	1:A:61:ASN:ND2	2.34	0.42
1:D:134:ALA:O	1:D:135:GLU:HB3	2.19	0.42
1:C:63:LEU:HD12	1:C:63:LEU:HA	1.91	0.42
1:D:60:LEU:HD22	1:D:115:TRP:CE3	2.55	0.42
1:D:46:MET:HB2	1:D:47:PRO:HD2	2.02	0.42
1:B:156:THR:CA	1:B:158:HIS:HD2	2.33	0.41
1:C:93:VAL:HG22	1:C:104:LEU:HD22	2.02	0.41
1:C:80:ASP:OD1	1:C:80:ASP:C	2.58	0.41
1:C:46:MET:HB3	3:C:185:HOH:O	2.19	0.41
1:D:106:PRO:HD2	3:D:200:HOH:O	2.19	0.41
1:C:102:THR:O	1:C:102:THR:CG2	2.68	0.41
3:B:166:HOH:O	1:C:44:ARG:HD2	2.20	0.41
1:A:74:LEU:HD12	1:A:85:ILE:HG12	2.01	0.41
2:A:802[B]:CE5:H1E	2:A:802[B]:CE5:H5D	1.96	0.41
1:D:132:VAL:O	1:D:135:GLU:CA	2.68	0.41
1:B:156:THR:CA	1:B:158:HIS:CD2	3.04	0.41
2:A:802[B]:CE5:C1B	2:A:802[B]:CE5:C6A	2.95	0.41
2:A:802[B]:CE5:O5E	2:A:802[B]:CE5:H6D2	2.21	0.41
2:A:801:CE5:C6A	2:A:801:CE5:H1B	2.38	0.41
1:C:5:GLU:O	1:C:7:LYS:HE3	2.21	0.41
1:B:63:LEU:HD12	1:B:63:LEU:HA	1.97	0.40
1:C:80:ASP:O	1:C:81:GLN:HB2	2.21	0.40
1:C:61:ASN:HA	3:C:270:HOH:O	2.20	0.40
1:A:57:GLN:HG2	1:A:61:ASN:HD21	1.85	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	146/162 (90%)	130 (89%)	14 (10%)	2 (1%)	14 51
1	B	156/162 (96%)	147 (94%)	7 (4%)	2 (1%)	15 53
1	C	157/162 (97%)	143 (91%)	12 (8%)	2 (1%)	15 53
1	D	146/162 (90%)	138 (94%)	5 (3%)	3 (2%)	9 40
All	All	605/648 (93%)	558 (92%)	38 (6%)	9 (2%)	13 50

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	121	GLY
1	C	122	ALA
1	D	7	LYS
1	D	70	GLY
1	C	120	ALA
1	D	120	ALA
1	B	7	LYS
1	A	7	LYS
1	A	124	GLY

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	127/140 (91%)	102 (80%)	25 (20%)	1 9
1	B	136/140 (97%)	113 (83%)	23 (17%)	2 13
1	C	137/140 (98%)	112 (82%)	25 (18%)	2 11
1	D	127/140 (91%)	103 (81%)	24 (19%)	2 10
All	All	527/560 (94%)	430 (82%)	97 (18%)	2 10

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	14	LEU

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Mol	Chain	Res	Type
1	A	16	THR
1	A	19	TRP
1	A	23	ASP
1	A	29	VAL
1	A	32	GLU
1	A	33	LEU
1	A	46	MET
1	A	53	VAL
1	A	63	LEU
1	A	74	LEU
1	A	75	GLU
1	A	77	LEU
1	A	81	GLN
1	A	93	VAL
1	A	102	THR
1	A	104	LEU
1	A	119	GLN
1	A	128	VAL
1	A	130	ARG
1	A	136	ASP
1	A	138	ASN
1	A	149	MET
1	A	150	ARG
1	B	4	PHE
1	B	9	ASP
1	B	14	LEU
1	B	16	THR
1	B	23	ASP
1	B	24	GLN
1	B	27	ILE
1	B	34	LEU
1	B	39	ARG
1	B	46	MET
1	B	51	GLN
1	B	63	LEU
1	B	64	LEU
1	B	80	ASP
1	B	84	ARG
1	B	104	LEU
1	B	125	ASP
1	B	132	VAL
1	B	133	ASP

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Mol	Chain	Res	Type
1	B	136	ASP
1	B	152	ARG
1	B	157	HIS
1	B	158	HIS
1	C	23	ASP
1	C	25	VAL
1	C	34	LEU
1	C	39	ARG
1	C	46	MET
1	C	51	GLN
1	C	63	LEU
1	C	77	LEU
1	C	79	GLU
1	C	80	ASP
1	C	83	LEU
1	C	98	GLU
1	C	102	THR
1	C	104	LEU
1	C	108	LEU
1	C	125	ASP
1	C	129	THR
1	C	130	ARG
1	C	142	ARG
1	C	150	ARG
1	C	152	ARG
1	C	157	HIS
1	C	158	HIS
1	C	160	HIS
1	C	161	HIS
1	D	4	PHE
1	D	6	LYS
1	D	9	ASP
1	D	11	THR
1	D	12	LEU
1	D	34	LEU
1	D	39	ARG
1	D	51	GLN
1	D	53	VAL
1	D	63	LEU
1	D	66	LEU
1	D	74	LEU
1	D	76	LEU

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Mol	Chain	Res	Type
1	D	80	ASP
1	D	83	LEU
1	D	98	GLU
1	D	114	ARG
1	D	123	PHE
1	D	130	ARG
1	D	136	ASP
1	D	137	LEU
1	D	138	ASN
1	D	142	ARG
1	D	149	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	81	GLN
1	A	138	ASN
1	B	51	GLN
1	B	157	HIS
1	B	158	HIS
1	C	15	GLN
1	C	119	GLN
1	C	158	HIS
1	D	57	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CE5	A	801	-	60,60,60	0.50	0	89,89,89	1.29	9 (10%)
2	CE5	A	802[A]	-	60,60,60	0.50	0	89,89,89	1.34	10 (11%)
2	CE5	A	802[B]	-	60,60,60	0.50	0	89,89,89	1.35	12 (13%)
2	CE5	C	803	-	60,60,60	0.57	0	89,89,89	1.32	10 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CE5	A	801	-	-	0/26/126/126	0/5/5/5
2	CE5	A	802[A]	-	-	0/26/126/126	0/5/5/5
2	CE5	A	802[B]	-	-	0/26/126/126	0/5/5/5
2	CE5	C	803	-	-	0/26/126/126	0/5/5/5

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	802[A]	CE5	O4C-C1D-O5D	-3.73	101.23	110.68
2	A	802[B]	CE5	O4C-C1D-O5D	-3.69	101.33	110.68
2	C	803	CE5	O4C-C1D-O5D	-3.30	102.33	110.68
2	A	801	CE5	O4C-C1D-O5D	-3.09	102.87	110.68
2	A	802[B]	CE5	O5D-C1D-C2D	-2.29	105.59	110.28
2	A	801	CE5	O3E-C3E-C2E	-2.19	105.41	110.34
2	A	802[A]	CE5	O5D-C1D-C2D	-2.19	105.79	110.28
2	A	802[B]	CE5	O5E-C1E-C2E	-2.14	105.89	110.28
2	C	803	CE5	O2D-C2D-C3D	-2.10	105.60	110.34
2	A	802[B]	CE5	O2D-C2D-C3D	-2.02	105.79	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	803	CE5	O4D-C4D-C5D	2.04	114.68	109.32
2	A	802[B]	CE5	C2A-C3A-C4A	2.04	114.09	109.60
2	A	801	CE5	C2D-C3D-C4D	2.12	114.26	109.60
2	A	801	CE5	C2A-C3A-C4A	2.14	114.30	109.60
2	A	801	CE5	C3E-C4E-C5E	2.19	114.01	110.20
2	C	803	CE5	C2D-C3D-C4D	2.21	114.44	109.60
2	C	803	CE5	O5E-C5E-C6E	2.21	111.93	106.36
2	A	802[A]	CE5	C2A-C3A-C4A	2.23	114.50	109.60
2	C	803	CE5	C2A-C3A-C4A	2.29	114.63	109.60
2	A	802[B]	CE5	C4E-C3E-C2E	2.30	115.08	110.79
2	A	802[A]	CE5	O4D-C4D-C5D	2.33	115.44	109.32
2	A	802[A]	CE5	C3E-C4E-C5E	2.35	114.30	110.20
2	A	802[B]	CE5	C2D-C3D-C4D	2.38	114.84	109.60
2	A	802[B]	CE5	C1D-O4C-C4C	2.41	124.31	118.01
2	A	802[A]	CE5	O4A-C4A-C5A	2.42	115.68	109.32
2	A	802[B]	CE5	O4A-C4A-C5A	2.42	115.69	109.32
2	A	802[B]	CE5	O4D-C4D-C5D	2.43	115.71	109.32
2	A	802[B]	CE5	C3E-C4E-C5E	2.44	114.45	110.20
2	A	801	CE5	O4A-C4A-C5A	2.46	115.80	109.32
2	C	803	CE5	C1D-O4C-C4C	2.54	124.64	118.01
2	A	801	CE5	C1D-O4C-C4C	2.60	124.81	118.01
2	A	802[A]	CE5	C1D-O4C-C4C	2.64	124.92	118.01
2	C	803	CE5	O4A-C4A-C5A	2.67	116.33	109.32
2	A	802[A]	CE5	C4E-C3E-C2E	2.68	115.79	110.79
2	A	802[A]	CE5	C2D-C3D-C4D	2.84	115.84	109.60
2	C	803	CE5	C4E-C3E-C2E	3.40	117.14	110.79
2	A	801	CE5	C4E-C3E-C2E	3.50	117.32	110.79
2	A	801	CE5	O4C-C1D-C2D	5.01	120.29	108.10
2	A	802[A]	CE5	O4C-C1D-C2D	5.29	120.98	108.10
2	C	803	CE5	O4C-C1D-C2D	5.30	121.00	108.10
2	A	802[B]	CE5	O4C-C1D-C2D	5.41	121.26	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	CE5	12	0
2	A	802[A]	CE5	18	0
2	A	802[B]	CE5	18	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	803	CE5	15	0

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	148/162 (91%)	-0.15	11 (7%) 17 6	30, 49, 108, 156	0
1	B	158/162 (97%)	-0.15	8 (5%) 32 12	32, 47, 92, 146	0
1	C	159/162 (98%)	-0.17	6 (3%) 44 18	28, 47, 94, 139	0
1	D	148/162 (91%)	-0.07	10 (6%) 20 7	29, 45, 107, 157	0
All	All	613/648 (94%)	-0.14	35 (5%) 27 10	28, 47, 102, 157	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	GLU	6.4
1	D	120	ALA	5.8
1	B	4	PHE	5.6
1	C	4	PHE	4.8
1	D	134	ALA	4.6
1	D	135	GLU	4.4
1	C	138	ASN	4.4
1	D	133	ASP	4.4
1	C	5	GLU	4.3
1	A	134	ALA	4.2
1	D	136	ASP	4.1
1	B	134	ALA	4.0
1	A	135	GLU	4.0
1	A	4	PHE	3.6
1	C	135	GLU	3.5
1	B	135	GLU	3.5
1	A	138	ASN	3.5
1	A	79	GLU	3.2
1	A	125	ASP	3.1
1	D	122	ALA	3.0
1	D	4	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	161	HIS	2.9
1	D	5	GLU	2.9
1	B	81	GLN	2.8
1	D	121	GLY	2.8
1	C	134	ALA	2.8
1	A	5	GLU	2.8
1	A	133	ASP	2.7
1	D	138	ASN	2.6
1	B	120	ALA	2.6
1	C	152	ARG	2.5
1	A	51	GLN	2.2
1	B	152	ARG	2.1
1	A	150	ARG	2.0
1	A	120	ALA	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	CE5	A	801	56/56	0.57	0.55	4.43	54,55,55,55	56
2	CE5	A	802[A]	56/56	0.62	0.54	3.37	53,54,55,55	56
2	CE5	A	802[B]	56/56	0.62	0.54	3.33	53,54,55,56	56
2	CE5	C	803	56/56	0.62	0.50	3.31	53,54,56,56	56

6.5 Other polymers (i)

There are no such residues in this entry.