Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:40 AM UTC

PDB ID	:	3AJ1 / pdb_00003aj1
Title	:	The structure of AxCeSD octamer (N-terminal HIS-tag) from Acetobacter xylinum
Authors	:	Hu, S.Q.; Tajima, K.; Zhou, Y.; Tanaka, I.; Yao, M.
Deposited on	:	2010-05-20
Resolution	:	2.50 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:

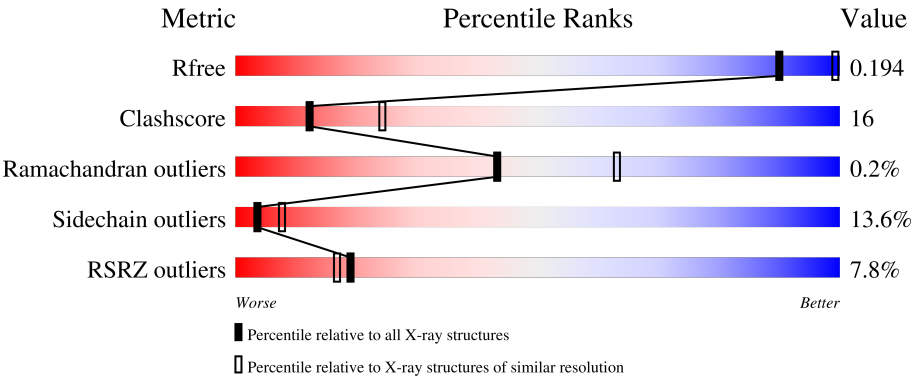
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 <=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	167	8% 65% 20% • • 10%
1	B	167	8% 68% 20% 6% 7%
1	C	167	8% 65% 22% • 10%
1	D	167	5% 60% 26% • 10%
1	E	167	8% 57% 27% 8% • 7%

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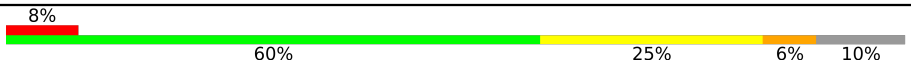
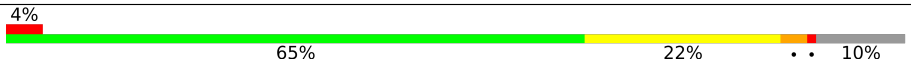
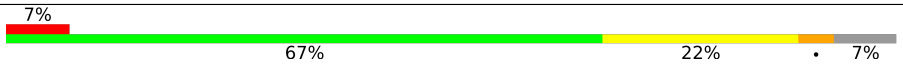
Mol	Chain	Length	Quality of chain
1	F	167	
1	G	167	
1	H	167	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9931 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	151	Total	C	N	O	S	Se	0	0	0
			1177	745	202	225	1	4			
1	B	156	Total	C	N	O	S	Se	0	0	0
			1220	774	207	233	1	5			
1	C	151	Total	C	N	O	S	Se	0	0	0
			1178	745	202	226	1	4			
1	D	151	Total	C	N	O	S	Se	0	0	0
			1177	745	202	225	1	4			
1	E	155	Total	C	N	O	S	Se	0	0	0
			1212	769	206	232	1	4			
1	F	151	Total	C	N	O	S	Se	0	0	0
			1177	745	202	225	1	4			
1	G	151	Total	C	N	O	S	Se	0	0	0
			1177	745	202	225	1	4			
1	H	156	Total	C	N	O	S	Se	0	0	0
			1221	774	207	234	1	5			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MSE	-	expression tag	UNP P37719
A	-9	ARG	-	expression tag	UNP P37719
A	-8	GLY	-	expression tag	UNP P37719
A	-7	SER	-	expression tag	UNP P37719
A	-6	HIS	-	expression tag	UNP P37719
A	-5	HIS	-	expression tag	UNP P37719
A	-4	HIS	-	expression tag	UNP P37719
A	-3	HIS	-	expression tag	UNP P37719
A	-2	HIS	-	expression tag	UNP P37719
A	-1	HIS	-	expression tag	UNP P37719
A	0	GLY	-	expression tag	UNP P37719
B	-10	MSE	-	expression tag	UNP P37719
B	-9	ARG	-	expression tag	UNP P37719

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP P37719
B	-7	SER	-	expression tag	UNP P37719
B	-6	HIS	-	expression tag	UNP P37719
B	-5	HIS	-	expression tag	UNP P37719
B	-4	HIS	-	expression tag	UNP P37719
B	-3	HIS	-	expression tag	UNP P37719
B	-2	HIS	-	expression tag	UNP P37719
B	-1	HIS	-	expression tag	UNP P37719
B	0	GLY	-	expression tag	UNP P37719
C	-10	MSE	-	expression tag	UNP P37719
C	-9	ARG	-	expression tag	UNP P37719
C	-8	GLY	-	expression tag	UNP P37719
C	-7	SER	-	expression tag	UNP P37719
C	-6	HIS	-	expression tag	UNP P37719
C	-5	HIS	-	expression tag	UNP P37719
C	-4	HIS	-	expression tag	UNP P37719
C	-3	HIS	-	expression tag	UNP P37719
C	-2	HIS	-	expression tag	UNP P37719
C	-1	HIS	-	expression tag	UNP P37719
C	0	GLY	-	expression tag	UNP P37719
D	-10	MSE	-	expression tag	UNP P37719
D	-9	ARG	-	expression tag	UNP P37719
D	-8	GLY	-	expression tag	UNP P37719
D	-7	SER	-	expression tag	UNP P37719
D	-6	HIS	-	expression tag	UNP P37719
D	-5	HIS	-	expression tag	UNP P37719
D	-4	HIS	-	expression tag	UNP P37719
D	-3	HIS	-	expression tag	UNP P37719
D	-2	HIS	-	expression tag	UNP P37719
D	-1	HIS	-	expression tag	UNP P37719
D	0	GLY	-	expression tag	UNP P37719
E	-10	MSE	-	expression tag	UNP P37719
E	-9	ARG	-	expression tag	UNP P37719
E	-8	GLY	-	expression tag	UNP P37719
E	-7	SER	-	expression tag	UNP P37719
E	-6	HIS	-	expression tag	UNP P37719
E	-5	HIS	-	expression tag	UNP P37719
E	-4	HIS	-	expression tag	UNP P37719
E	-3	HIS	-	expression tag	UNP P37719
E	-2	HIS	-	expression tag	UNP P37719
E	-1	HIS	-	expression tag	UNP P37719
E	0	GLY	-	expression tag	UNP P37719

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-10	MSE	-	expression tag	UNP P37719
F	-9	ARG	-	expression tag	UNP P37719
F	-8	GLY	-	expression tag	UNP P37719
F	-7	SER	-	expression tag	UNP P37719
F	-6	HIS	-	expression tag	UNP P37719
F	-5	HIS	-	expression tag	UNP P37719
F	-4	HIS	-	expression tag	UNP P37719
F	-3	HIS	-	expression tag	UNP P37719
F	-2	HIS	-	expression tag	UNP P37719
F	-1	HIS	-	expression tag	UNP P37719
F	0	GLY	-	expression tag	UNP P37719
G	-10	MSE	-	expression tag	UNP P37719
G	-9	ARG	-	expression tag	UNP P37719
G	-8	GLY	-	expression tag	UNP P37719
G	-7	SER	-	expression tag	UNP P37719
G	-6	HIS	-	expression tag	UNP P37719
G	-5	HIS	-	expression tag	UNP P37719
G	-4	HIS	-	expression tag	UNP P37719
G	-3	HIS	-	expression tag	UNP P37719
G	-2	HIS	-	expression tag	UNP P37719
G	-1	HIS	-	expression tag	UNP P37719
G	0	GLY	-	expression tag	UNP P37719
H	-10	MSE	-	expression tag	UNP P37719
H	-9	ARG	-	expression tag	UNP P37719
H	-8	GLY	-	expression tag	UNP P37719
H	-7	SER	-	expression tag	UNP P37719
H	-6	HIS	-	expression tag	UNP P37719
H	-5	HIS	-	expression tag	UNP P37719
H	-4	HIS	-	expression tag	UNP P37719
H	-3	HIS	-	expression tag	UNP P37719
H	-2	HIS	-	expression tag	UNP P37719
H	-1	HIS	-	expression tag	UNP P37719
H	0	GLY	-	expression tag	UNP P37719

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	52	Total O 52 52	0	0
2	B	47	Total O 47 47	0	0
2	C	45	Total O 45 45	0	0

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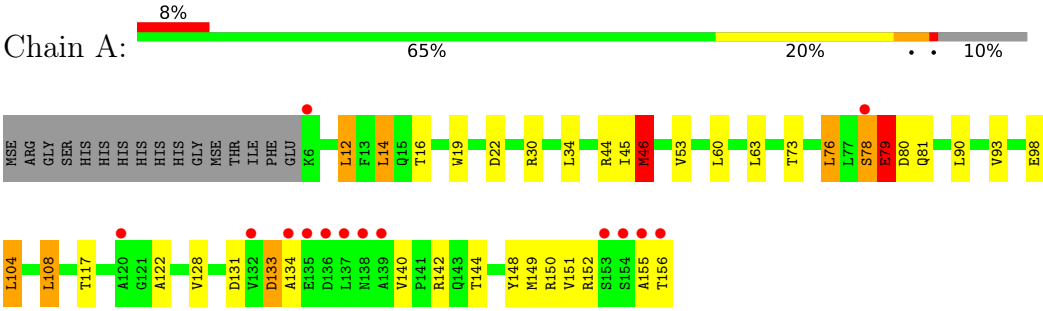
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	54	Total O 54 54	0	0
2	E	48	Total O 48 48	0	0
2	F	52	Total O 52 52	0	0
2	G	42	Total O 42 42	0	0
2	H	52	Total O 52 52	0	0

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.

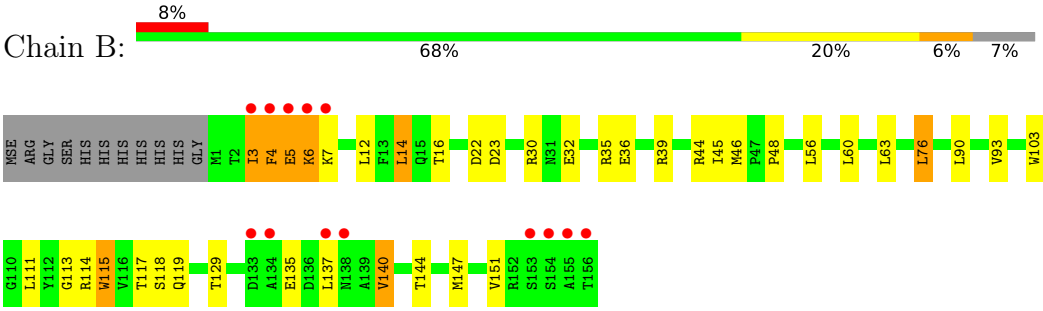
• Molecule 1: Cellulose synthase operon protein D

Chain A:



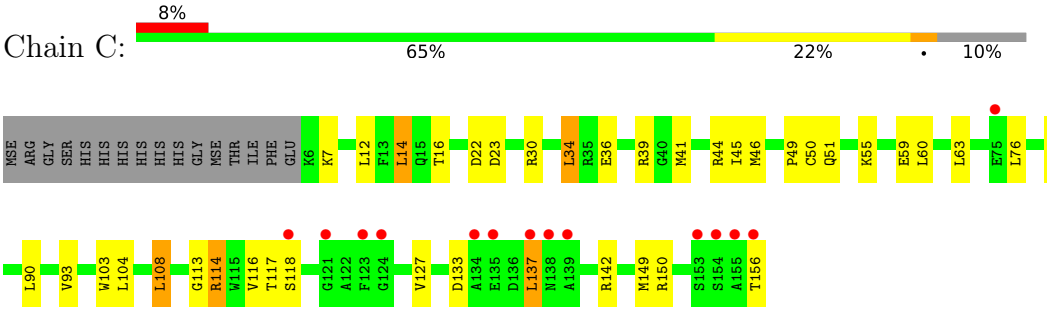
• Molecule 1: Cellulose synthase operon protein D

Chain B:



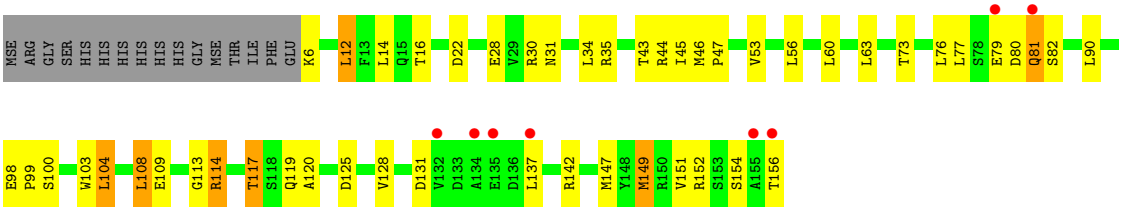
• Molecule 1: Cellulose synthase operon protein D

Chain C:



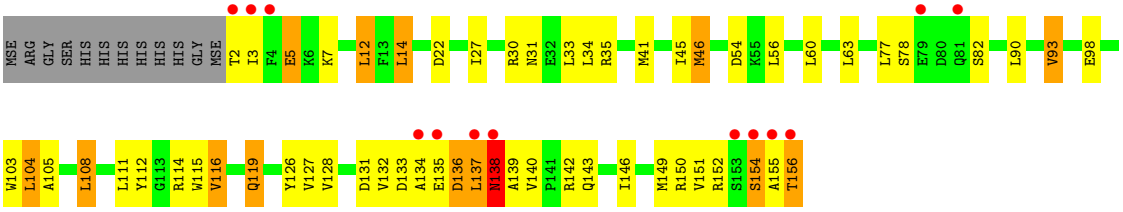
• Molecule 1: Cellulose synthase operon protein D

Chain D:



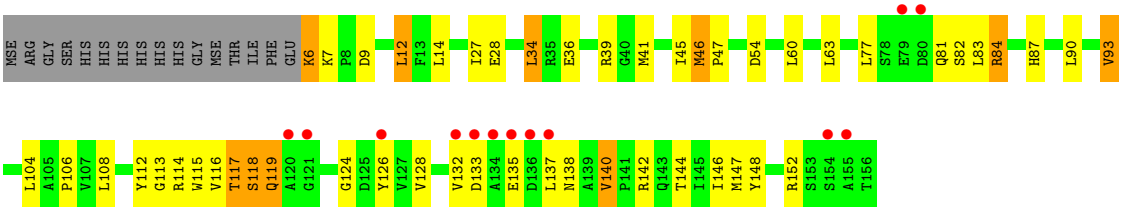
• Molecule 1: Cellulose synthase operon protein D

Chain E:



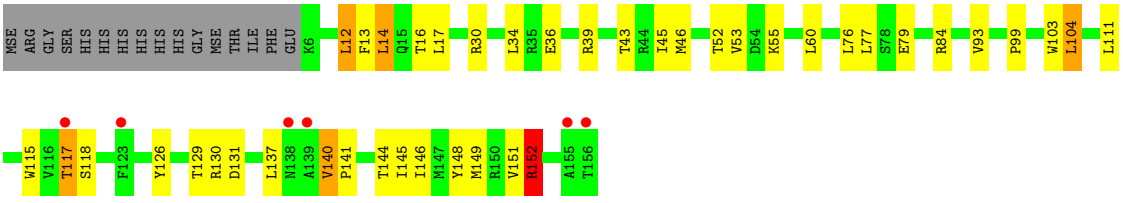
• Molecule 1: Cellulose synthase operon protein D

Chain F:



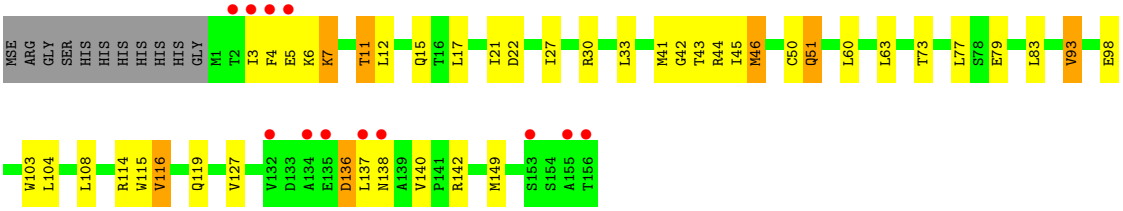
• Molecule 1: Cellulose synthase operon protein D

Chain G:



• Molecule 1: Cellulose synthase operon protein D

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	77.70Å 77.70Å 213.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.87 – 2.50 19.87 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.87-2.50) 99.2 (19.87-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.203 , 0.257 0.206 , 0.194	Depositor DCC
R_{free} test set	4986 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å^2)	43.9	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l 0.074 for h,-h-k,-l 0.031 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9931	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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

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	0.68	0/1195	0.93	3/1621 (0.2%)
1	B	0.69	0/1239	0.95	1/1680 (0.1%)
1	C	0.68	0/1196	0.95	1/1621 (0.1%)
1	D	0.75	0/1195	0.97	2/1621 (0.1%)
1	E	0.65	0/1231	1.00	7/1670 (0.4%)
1	F	0.68	1/1195 (0.1%)	0.95	1/1621 (0.1%)
1	G	0.61	0/1195	0.90	2/1621 (0.1%)
1	H	0.73	0/1240	0.99	2/1680 (0.1%)
All	All	0.69	1/9686 (0.0%)	0.96	19/13135 (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	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	118	SER	C-N	5.54	1.39	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	152	ARG	N-CA-C	7.88	120.63	111.02
1	H	46	MSE	N-CA-C	7.09	116.48	108.25
1	A	46	MSE	N-CA-C	7.00	116.37	108.25
1	E	138	ASN	N-CA-C	6.71	118.44	107.23
1	E	139	ALA	N-CA-C	6.53	120.55	112.58
1	E	154	SER	N-CA-C	6.29	118.22	111.36
1	C	82	SER	N-CA-C	6.28	117.71	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	80	ASP	N-CA-C	-6.23	104.96	113.30
1	E	82	SER	N-CA-C	6.05	118.26	109.07
1	H	6	LYS	N-CA-C	5.50	117.69	108.23
1	A	79	GLU	N-CA-C	5.46	116.84	107.28
1	G	117	THR	N-CA-C	5.20	117.35	111.11
1	B	115	TRP	N-CA-C	5.19	118.77	112.23
1	E	140	VAL	CA-C-N	5.11	125.10	119.89
1	E	140	VAL	C-N-CA	5.11	125.10	119.89
1	F	27	ILE	N-CA-C	5.11	115.33	110.42
1	D	47	PRO	CA-C-N	-5.10	115.12	120.38
1	D	47	PRO	C-N-CA	-5.10	115.12	120.38
1	E	46	MSE	N-CA-C	5.04	116.40	108.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	138	ASN	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	1177	0	1180	34	0
1	B	1220	0	1225	36	0
1	C	1178	0	1180	36	0
1	D	1177	0	1180	47	0
1	E	1212	0	1213	47	0
1	F	1177	0	1180	40	0
1	G	1177	0	1180	37	0
1	H	1221	0	1225	42	0
2	A	52	0	0	5	0
2	B	47	0	0	1	0
2	C	45	0	0	2	0
2	D	54	0	0	4	0
2	E	48	0	0	4	0
2	F	52	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	42	0	0	2	0
2	H	52	0	0	2	0
All	All	9931	0	9563	296	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 16.

All (296) 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:E:116:VAL:CG1	1:E:149:MSE:HE3	1.38	1.52
1:E:116:VAL:HG13	1:E:149:MSE:CE	1.53	1.37
1:H:50:CYS:H	1:H:119:GLN:NE2	1.45	1.15
1:F:46:MSE:HE2	1:F:47:PRO:HD2	1.19	1.14
1:D:81:GLN:HE21	1:D:81:GLN:HA	0.98	1.10
1:F:46:MSE:HE3	1:F:115:TRP:HD1	1.15	1.07
1:B:56:LEU:HD13	1:B:119:GLN:HG2	1.34	1.05
1:C:46:MSE:HE1	1:C:118:SER:HB2	1.36	1.04
1:F:46:MSE:HE3	1:F:115:TRP:CD1	1.93	1.04
1:F:46:MSE:CE	1:F:115:TRP:HD1	1.70	1.02
1:B:109:GLU:CG	1:B:147:MSE:HE2	1.90	1.02
1:H:138:ASN:HB3	1:H:140:VAL:HG13	1.41	1.00
1:E:131:ASP:OD1	1:E:134:ALA:HB3	1.66	0.95
1:D:81:GLN:HA	1:D:81:GLN:NE2	1.80	0.94
1:B:109:GLU:HG3	1:B:147:MSE:HE2	1.49	0.91
1:F:46:MSE:HE2	1:F:47:PRO:CD	2.02	0.90
1:D:81:GLN:HE21	1:D:81:GLN:CA	1.85	0.89
1:H:30:ARG:HD2	1:H:103:TRP:NE1	1.86	0.89
1:F:46:MSE:CE	1:F:115:TRP:CD1	2.53	0.88
1:E:134:ALA:HA	1:E:137:LEU:HB2	1.53	0.88
1:F:6:LYS:HB3	2:F:375:HOH:O	1.74	0.86
1:F:113:GLY:O	1:F:117:THR:HB	1.77	0.84
1:H:50:CYS:H	1:H:119:GLN:HE22	1.25	0.84
1:B:30:ARG:HD2	1:B:103:TRP:NE1	1.92	0.83
1:B:109:GLU:HG3	1:B:147:MSE:CE	2.09	0.83
1:F:46:MSE:HE1	1:F:115:TRP:HA	1.61	0.82
1:A:53:VAL:HG21	1:A:76:LEU:HD22	1.59	0.82
1:B:109:GLU:HG2	1:B:147:MSE:HE2	1.59	0.81
1:E:116:VAL:HG11	1:E:149:MSE:HE3	1.58	0.81
1:H:50:CYS:N	1:H:119:GLN:NE2	2.27	0.80
1:H:30:ARG:HD2	1:H:103:TRP:HE1	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:ARG:HH12	1:D:117:THR:HG21	1.47	0.78
1:D:81:GLN:HG3	1:D:151:VAL:HG23	1.67	0.77
1:B:56:LEU:CD1	1:B:119:GLN:HG2	2.12	0.76
1:C:22:ASP:OD1	1:C:30:ARG:HD3	1.85	0.76
1:H:138:ASN:CB	1:H:140:VAL:HG13	2.16	0.76
2:F:406:HOH:O	1:G:46:MSE:HE3	1.84	0.76
1:C:93:VAL:HG12	1:C:93:VAL:O	1.85	0.75
1:E:127:VAL:HG12	1:E:154:SER:HA	1.68	0.75
1:B:46:MSE:HG2	2:B:158:HOH:O	1.86	0.74
1:C:30:ARG:HD2	1:C:103:TRP:NE1	2.02	0.74
1:G:140:VAL:HG13	1:G:144:THR:HB	1.70	0.74
1:E:126:TYR:CD2	1:E:149:MSE:HE2	2.22	0.74
1:F:128:VAL:HG11	1:F:147:MSE:CE	2.18	0.74
1:F:84:ARG:HG3	1:F:148:TYR:CE1	2.24	0.73
1:B:56:LEU:HD13	1:B:119:GLN:CG	2.14	0.72
1:E:127:VAL:HG13	1:E:152:ARG:O	1.89	0.72
1:G:30:ARG:HD2	1:G:103:TRP:HE1	1.53	0.72
1:F:128:VAL:HG11	1:F:147:MSE:HE3	1.72	0.72
1:F:112:TYR:HB2	1:F:147:MSE:HE1	1.71	0.72
1:H:43:THR:HG22	1:H:114:ARG:HE	1.54	0.71
1:B:14:LEU:HB3	1:B:93:VAL:HG11	1.72	0.71
1:E:93:VAL:O	1:E:93:VAL:HG13	1.90	0.71
1:G:30:ARG:HD2	1:G:103:TRP:NE1	2.06	0.70
1:E:116:VAL:CG1	1:E:149:MSE:CE	2.35	0.70
1:F:128:VAL:CG1	1:F:147:MSE:HE3	2.22	0.70
1:A:90:LEU:HD13	1:A:108:LEU:HD22	1.73	0.69
1:H:93:VAL:HG12	1:H:93:VAL:O	1.91	0.68
1:C:142:ARG:NH1	1:E:54:ASP:OD2	2.26	0.68
1:A:14:LEU:HB3	1:A:93:VAL:CG1	2.22	0.68
1:E:116:VAL:HG13	1:E:149:MSE:HE3	0.70	0.68
1:H:46:MSE:SE	2:H:345:HOH:O	2.62	0.68
1:D:43:THR:O	1:D:46:MSE:HE2	1.94	0.68
1:E:14:LEU:HB3	1:E:93:VAL:CG2	2.25	0.67
1:F:93:VAL:O	1:F:93:VAL:CG1	2.41	0.67
1:B:113:GLY:O	1:B:117:THR:HG23	1.95	0.67
1:H:50:CYS:N	1:H:119:GLN:HE22	1.91	0.67
1:H:22:ASP:OD1	1:H:30:ARG:HD3	1.95	0.67
1:B:22:ASP:OD1	1:B:30:ARG:HD3	1.95	0.66
1:A:79:GLU:OE1	1:A:79:GLU:HA	1.94	0.66
1:D:43:THR:O	1:D:46:MSE:CE	2.44	0.66
1:D:100:SER:O	1:D:142:ARG:HD2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:VAL:HG12	1:G:93:VAL:O	1.96	0.66
1:E:126:TYR:CG	1:E:149:MSE:HE2	2.31	0.65
1:A:73:THR:HG23	2:A:256:HOH:O	1.97	0.65
1:F:114:ARG:HD3	2:F:202:HOH:O	1.95	0.64
1:E:155:ALA:O	1:E:156:THR:HB	1.98	0.64
1:C:14:LEU:HB3	1:C:93:VAL:CG1	2.28	0.64
1:G:12:LEU:HD13	1:H:41:MSE:HG2	1.81	0.63
1:B:93:VAL:HG12	1:B:93:VAL:O	1.98	0.63
1:H:50:CYS:H	1:H:119:GLN:HE21	1.42	0.62
1:D:43:THR:C	1:D:46:MSE:HE2	2.23	0.62
1:G:36:GLU:OE2	1:G:39:ARG:NH1	2.32	0.62
1:D:30:ARG:HD2	1:D:103:TRP:NE1	2.15	0.62
1:G:12:LEU:CD1	1:H:41:MSE:HG2	2.30	0.62
1:F:93:VAL:O	1:F:93:VAL:HG12	1.99	0.62
1:B:45:ILE:HG22	1:C:45:ILE:HG22	1.81	0.62
1:G:117:THR:HA	1:G:149:MSE:HE1	1.81	0.62
1:A:93:VAL:CG2	1:A:104:LEU:HD22	2.30	0.61
1:D:81:GLN:O	1:D:151:VAL:HG22	1.99	0.61
1:E:151:VAL:C	2:E:398:HOH:O	2.44	0.60
1:G:52:THR:CG2	1:G:55:LYS:HG3	2.30	0.60
1:C:114:ARG:O	1:C:118:SER:HB3	2.02	0.60
1:E:30:ARG:HD2	1:E:103:TRP:NE1	2.17	0.60
1:A:30:ARG:HD2	1:A:103:TRP:HE1	1.66	0.60
1:D:6:LYS:HB3	2:D:269:HOH:O	2.02	0.60
1:B:30:ARG:HD2	1:B:103:TRP:HE1	1.66	0.60
1:H:93:VAL:O	1:H:93:VAL:CG1	2.49	0.60
1:A:14:LEU:HB3	1:A:93:VAL:HG13	1.84	0.59
1:B:14:LEU:HB3	1:B:93:VAL:CG1	2.32	0.59
1:C:14:LEU:HB3	1:C:93:VAL:HG11	1.83	0.59
1:H:60:LEU:HD22	1:H:115:TRP:CE3	2.36	0.59
1:E:112:TYR:O	1:E:116:VAL:HB	2.02	0.59
1:D:128:VAL:HG22	1:D:149:MSE:HG3	1.84	0.59
1:E:14:LEU:HB3	1:E:93:VAL:HG22	1.85	0.58
1:E:127:VAL:CG1	1:E:154:SER:HA	2.33	0.58
1:H:3:ILE:HD12	1:H:3:ILE:H	1.67	0.58
1:D:22:ASP:OD1	1:D:30:ARG:HD3	2.03	0.58
1:D:109:GLU:CG	1:D:147:MSE:HE2	2.34	0.58
1:G:117:THR:HA	1:G:149:MSE:CE	2.33	0.57
1:F:90:LEU:HD13	1:F:108:LEU:HD22	1.85	0.57
1:B:6:LYS:HG3	1:B:6:LYS:O	2.06	0.56
1:E:30:ARG:HD2	1:E:103:TRP:HE1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:116:VAL:CG1	1:H:149:MSE:SE	3.03	0.56
1:A:30:ARG:HD2	1:A:103:TRP:NE1	2.21	0.56
1:D:43:THR:HA	1:D:46:MSE:HE2	1.88	0.56
1:G:144:THR:C	1:G:145:ILE:HD12	2.30	0.56
1:D:30:ARG:HH22	1:D:98:GLU:CD	2.14	0.56
1:H:138:ASN:HB3	1:H:140:VAL:CG1	2.27	0.56
1:G:14:LEU:HB3	1:G:93:VAL:CG1	2.35	0.56
1:D:46:MSE:HG2	2:D:158:HOH:O	2.04	0.55
1:D:80:ASP:O	1:D:81:GLN:C	2.49	0.55
1:E:14:LEU:HD23	1:E:93:VAL:HG21	1.88	0.55
1:G:84:ARG:HD2	2:G:352:HOH:O	2.05	0.55
1:H:30:ARG:NH2	1:H:98:GLU:OE1	2.34	0.55
1:A:93:VAL:HG21	1:A:104:LEU:HD22	1.87	0.55
1:C:93:VAL:O	1:C:93:VAL:CG1	2.54	0.55
1:A:140:VAL:CG1	1:A:144:THR:HB	2.36	0.55
1:D:30:ARG:NH2	1:D:98:GLU:OE1	2.38	0.55
1:E:93:VAL:O	1:E:93:VAL:CG1	2.55	0.55
1:A:117:THR:HA	1:A:122:ALA:HB3	1.89	0.55
1:G:111:LEU:HD11	1:G:115:TRP:CZ2	2.42	0.55
1:C:41:MSE:HG2	1:D:12:LEU:HD13	1.87	0.55
1:H:83:LEU:HB3	1:H:149:MSE:HB3	1.89	0.55
1:C:16:THR:HG22	1:D:44:ARG:NE	2.22	0.55
1:H:7:LYS:HB3	1:H:7:LYS:HZ2	1.72	0.54
1:B:48:PRO:O	1:B:119:GLN:NE2	2.41	0.54
1:B:32:GLU:OE2	1:B:35:ARG:NH1	2.41	0.54
1:E:142:ARG:HG2	1:E:143:GLN:OE1	2.08	0.54
1:F:142:ARG:HD2	2:F:383:HOH:O	2.08	0.54
1:C:133:ASP:O	1:C:137:LEU:HB2	2.08	0.53
1:F:124:GLY:HA3	1:F:126:TYR:CE1	2.43	0.53
1:E:14:LEU:HB3	1:E:93:VAL:HG21	1.88	0.53
1:F:36:GLU:OE2	1:F:39:ARG:NH1	2.41	0.53
1:A:100:SER:O	1:A:142:ARG:HD2	2.09	0.53
1:B:36:GLU:OE1	1:B:39:ARG:NH1	2.42	0.53
1:D:90:LEU:HD13	1:D:108:LEU:HD22	1.91	0.53
1:D:109:GLU:HG2	1:D:147:MSE:HE2	1.91	0.53
1:A:30:ARG:NH2	1:A:98:GLU:OE1	2.40	0.52
1:C:46:MSE:CE	1:C:118:SER:HB2	2.26	0.52
1:E:60:LEU:HD22	1:E:115:TRP:CE3	2.44	0.52
1:H:116:VAL:HG13	1:H:149:MSE:SE	2.59	0.52
1:F:45:ILE:HG22	1:G:45:ILE:HG22	1.91	0.52
1:C:36:GLU:OE2	1:C:39:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:ASP:O	1:F:137:LEU:HD12	2.10	0.52
1:G:17:LEU:HD21	1:H:17:LEU:HD21	1.92	0.52
1:B:4:PHE:CG	1:B:4:PHE:O	2.63	0.51
1:E:12:LEU:HD13	1:F:41:MSE:HG2	1.92	0.51
1:F:135:GLU:O	1:F:140:VAL:HG13	2.10	0.51
1:D:46:MSE:HE1	1:E:46:MSE:SE	2.60	0.51
1:H:42:GLY:O	1:H:46:MSE:HG3	2.10	0.51
1:F:84:ARG:HG3	1:F:148:TYR:CZ	2.45	0.51
1:F:140:VAL:HG11	1:F:146:ILE:HD11	1.92	0.51
1:G:14:LEU:HB3	1:G:93:VAL:HG11	1.92	0.51
1:B:22:ASP:OD2	1:B:30:ARG:NH1	2.44	0.50
1:C:116:VAL:CG1	1:C:149:MSE:SE	3.08	0.50
1:B:109:GLU:N	1:B:147:MSE:HE1	2.26	0.50
1:A:53:VAL:CG2	1:A:76:LEU:HD22	2.36	0.50
1:E:46:MSE:HB3	2:E:333:HOH:O	2.11	0.50
1:F:54:ASP:OD1	1:H:142:ARG:NH2	2.45	0.50
1:A:44:ARG:NE	1:B:16:THR:HG22	2.26	0.50
1:G:126:TYR:HB2	1:G:149:MSE:HE2	1.93	0.50
1:A:19:TRP:HH2	1:C:49:PRO:O	1.95	0.50
1:F:34:LEU:HB3	1:F:106:PRO:HB2	1.93	0.50
1:D:81:GLN:CG	1:D:152:ARG:O	2.60	0.50
1:G:52:THR:HG23	1:G:55:LYS:HG3	1.94	0.50
1:C:116:VAL:HG12	1:C:149:MSE:SE	2.63	0.49
1:G:111:LEU:HD21	1:G:115:TRP:CH2	2.47	0.49
1:C:44:ARG:NH2	2:C:160:HOH:O	2.29	0.49
1:A:22:ASP:OD1	1:A:30:ARG:HD3	2.12	0.49
1:D:45:ILE:HG22	1:E:45:ILE:HG22	1.93	0.49
1:D:43:THR:CA	1:D:46:MSE:HE2	2.43	0.49
1:G:152:ARG:HH11	1:G:152:ARG:CG	2.26	0.49
1:D:114:ARG:NH1	1:D:117:THR:HG21	2.22	0.48
1:D:119:GLN:O	1:D:120:ALA:HB3	2.12	0.48
1:B:90:LEU:HD13	1:B:108:LEU:HD22	1.95	0.48
1:A:134:ALA:CB	2:A:359:HOH:O	2.60	0.48
1:D:46:MSE:CE	1:E:46:MSE:SE	3.11	0.48
1:E:31:ASN:O	1:E:35:ARG:HG3	2.13	0.48
1:E:126:TYR:CB	1:E:149:MSE:HE2	2.43	0.48
1:H:116:VAL:HG11	1:H:149:MSE:SE	2.63	0.48
1:D:120:ALA:HA	2:D:167:HOH:O	2.13	0.48
1:F:46:MSE:CE	1:F:47:PRO:HD2	2.14	0.48
1:F:128:VAL:CG1	1:F:147:MSE:CE	2.86	0.48
1:D:109:GLU:HG3	1:D:147:MSE:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:O	1:A:16:THR:HG23	2.14	0.47
1:H:11:THR:O	1:H:15:GLN:HG3	2.14	0.47
1:E:5:GLU:HB3	2:E:349:HOH:O	2.14	0.47
1:H:42:GLY:HA3	1:H:114:ARG:HG2	1.95	0.47
1:A:45:ILE:HG22	1:H:45:ILE:HG22	1.96	0.47
1:F:114:ARG:O	1:F:118:SER:HB3	2.15	0.47
1:D:73:THR:HG23	2:D:174:HOH:O	2.13	0.47
1:C:14:LEU:HB3	1:C:93:VAL:HG13	1.97	0.47
1:G:129:THR:HG22	2:G:409:HOH:O	2.15	0.47
1:H:3:ILE:HD13	2:H:405:HOH:O	2.14	0.47
1:B:135:GLU:HG2	1:B:140:VAL:HG11	1.97	0.46
1:A:76:LEU:HD21	1:A:155:ALA:H	1.79	0.46
1:D:31:ASN:O	1:D:35:ARG:HG3	2.14	0.46
1:E:22:ASP:OD1	1:E:30:ARG:HD3	2.15	0.46
1:G:152:ARG:HH11	1:G:152:ARG:HG2	1.80	0.46
1:E:151:VAL:O	2:E:398:HOH:O	2.21	0.46
1:G:36:GLU:HA	1:G:39:ARG:HD2	1.96	0.46
1:H:3:ILE:HD12	1:H:3:ILE:N	2.30	0.46
1:D:56:LEU:HD22	1:D:119:GLN:HG3	1.98	0.46
1:G:103:TRP:CE3	1:G:104:LEU:HD13	2.51	0.46
1:F:87:HIS:O	1:F:144:THR:HA	2.15	0.46
1:H:51:GLN:H	1:H:51:GLN:CD	2.24	0.46
1:A:134:ALA:HB1	2:A:359:HOH:O	2.15	0.46
1:C:51:GLN:N	1:C:51:GLN:CD	2.74	0.45
1:E:131:ASP:O	1:E:135:GLU:HG3	2.15	0.45
1:C:127:VAL:O	1:C:149:MSE:HA	2.16	0.45
1:A:22:ASP:OD1	1:A:30:ARG:CD	2.64	0.45
1:E:56:LEU:HD13	1:E:119:GLN:HG2	1.98	0.45
1:G:52:THR:HG23	1:G:55:LYS:H	1.82	0.45
1:A:30:ARG:HH22	1:A:98:GLU:CD	2.24	0.45
1:C:30:ARG:HG2	1:C:34:LEU:HD22	1.99	0.45
1:D:53:VAL:HG21	1:D:76:LEU:HD13	1.99	0.44
1:B:60:LEU:HD22	1:B:115:TRP:CE3	2.51	0.44
1:F:46:MSE:CE	1:F:115:TRP:HA	2.40	0.44
1:C:16:THR:CG2	1:D:44:ARG:NE	2.81	0.44
1:C:116:VAL:HG11	1:C:149:MSE:SE	2.67	0.44
1:H:3:ILE:HG22	1:H:5:GLU:H	1.83	0.44
1:A:46:MSE:HB3	2:A:157:HOH:O	2.16	0.44
1:A:149:MSE:HE2	1:A:149:MSE:HB3	1.96	0.44
1:E:90:LEU:HD13	1:E:108:LEU:HD22	2.00	0.44
1:B:22:ASP:CG	1:B:30:ARG:HH11	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:GLU:O	1:H:5:GLU:HG3	2.18	0.43
1:C:30:ARG:HD2	1:C:103:TRP:HE1	1.80	0.43
1:B:3:ILE:HD11	1:H:5:GLU:HA	2.00	0.43
1:B:44:ARG:O	1:C:45:ILE:HA	2.18	0.43
1:B:140:VAL:HG22	1:B:144:THR:HG21	2.00	0.43
1:C:7:LYS:HE2	2:C:316:HOH:O	2.17	0.43
1:E:108:LEU:HG	1:E:112:TYR:HE2	1.83	0.43
1:B:93:VAL:HG23	1:B:104:LEU:HD22	2.01	0.43
1:C:50:CYS:SG	1:C:59:GLU:HG3	2.58	0.43
1:G:13:PHE:HD2	1:G:14:LEU:HD13	1.83	0.43
1:D:76:LEU:HD21	1:D:154:SER:O	2.17	0.43
1:E:105:ALA:O	1:E:108:LEU:HB2	2.19	0.43
1:H:50:CYS:HB2	1:H:119:GLN:HE21	1.84	0.43
1:B:5:GLU:C	1:B:7:LYS:H	2.27	0.43
1:C:41:MSE:HG2	1:D:12:LEU:CD1	2.49	0.43
1:D:114:ARG:HH11	1:D:125:ASP:HB3	1.84	0.43
1:F:119:GLN:HE21	1:F:119:GLN:HB2	1.58	0.43
1:D:114:ARG:HH12	1:D:117:THR:CG2	2.26	0.42
1:A:131:ASP:OD2	1:A:133:ASP:OD2	2.37	0.42
1:A:140:VAL:HG13	1:A:144:THR:HB	2.01	0.42
1:E:103:TRP:HE3	1:E:104:LEU:HD13	1.83	0.42
2:A:177:HOH:O	1:C:55:LYS:HD3	2.19	0.42
1:H:51:GLN:OE1	1:H:51:GLN:N	2.50	0.42
1:G:43:THR:O	1:G:46:MSE:HE2	2.19	0.42
1:A:78:SER:O	1:A:79:GLU:HG2	2.19	0.42
1:B:111:LEU:HD11	1:B:115:TRP:CZ2	2.54	0.42
1:H:136:ASP:OD2	1:H:137:LEU:N	2.53	0.42
1:A:103:TRP:HE3	1:A:104:LEU:HD13	1.84	0.41
1:E:30:ARG:HH22	1:E:98:GLU:CD	2.28	0.41
1:G:99:PRO:HD2	1:G:130:ARG:HH22	1.84	0.41
1:A:14:LEU:HB3	1:A:93:VAL:HG11	2.01	0.41
1:F:83:LEU:HD12	1:F:116:VAL:HG11	2.02	0.41
1:D:90:LEU:HD13	1:D:108:LEU:CD2	2.50	0.41
1:F:128:VAL:HG12	1:F:147:MSE:HE3	1.97	0.41
1:C:49:PRO:O	1:C:51:GLN:NE2	2.54	0.41
1:E:135:GLU:HG2	1:E:146:ILE:HG12	2.02	0.41
1:G:14:LEU:HB3	1:G:93:VAL:HG13	2.00	0.41
1:G:93:VAL:O	1:G:93:VAL:CG1	2.66	0.41
1:G:16:THR:HG22	1:H:44:ARG:NE	2.36	0.41
1:G:103:TRP:HE3	1:G:104:LEU:HD13	1.86	0.41
1:E:133:ASP:HA	1:E:136:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:LEU:HG	1:H:21:ILE:HD12	2.01	0.41
1:B:48:PRO:HD3	1:C:44:ARG:NH1	2.35	0.41
1:G:131:ASP:HB2	1:G:148:TYR:HD1	1.85	0.41
1:A:131:ASP:OD1	1:A:148:TYR:CE2	2.74	0.41
1:A:128:VAL:HG22	1:A:149:MSE:HG2	2.02	0.40
1:D:114:ARG:NH1	1:D:117:THR:CG2	2.83	0.40
1:E:22:ASP:OD1	1:E:30:ARG:CD	2.69	0.40
1:G:140:VAL:HG21	1:G:146:ILE:HD11	2.03	0.40
1:C:113:GLY:O	1:C:117:THR:HG23	2.21	0.40
1:F:6:LYS:HD3	1:F:6:LYS:N	2.35	0.40
1:G:140:VAL:HA	1:G:141:PRO:HD2	1.94	0.40
1:C:90:LEU:HD13	1:C:108:LEU:HD22	2.03	0.40
1:D:103:TRP:CE3	1:D:104:LEU:HD13	2.56	0.40
1:D:98:GLU:HA	1:D:99:PRO:HA	1.94	0.40
1:D:113:GLY:O	1:D:117:THR:HB	2.20	0.40
1:E:41:MSE:HG2	1:F:12:LEU:HD13	2.03	0.40
1:B:76:LEU:HD12	1:B:76:LEU:HA	1.97	0.40
1:C:81:GLN:HB2	1:C:150:ARG:HH11	1.86	0.40
1:F:113:GLY:O	1:F:117:THR:CB	2.59	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	149/167 (89%)	142 (95%)	6 (4%)	1 (1%)	18	34
1	B	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	21	38
1	C	149/167 (89%)	142 (95%)	7 (5%)	0	100	100
1	D	149/167 (89%)	143 (96%)	6 (4%)	0	100	100
1	E	153/167 (92%)	144 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	149/167 (89%)	145 (97%)	3 (2%)	1 (1%)	18 34
1	G	149/167 (89%)	144 (97%)	5 (3%)	0	100 100
1	H	154/167 (92%)	147 (96%)	7 (4%)	0	100 100
All	All	1206/1336 (90%)	1153 (96%)	50 (4%)	3 (0%)	43 63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	5	GLU
1	F	152	ARG
1	A	152	ARG

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	129/137 (94%)	113 (88%)	16 (12%)	4 9
1	B	134/137 (98%)	118 (88%)	16 (12%)	5 11
1	C	129/137 (94%)	116 (90%)	13 (10%)	7 15
1	D	129/137 (94%)	110 (85%)	19 (15%)	3 6
1	E	133/137 (97%)	107 (80%)	26 (20%)	1 2
1	F	129/137 (94%)	108 (84%)	21 (16%)	2 4
1	G	129/137 (94%)	115 (89%)	14 (11%)	6 13
1	H	134/137 (98%)	117 (87%)	17 (13%)	4 9
All	All	1046/1096 (95%)	904 (86%)	142 (14%)	3 8

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	14	LEU
1	A	34	LEU

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Mol	Chain	Res	Type
1	A	46	MSE
1	A	60	LEU
1	A	63	LEU
1	A	76	LEU
1	A	78	SER
1	A	79	GLU
1	A	81	GLN
1	A	104	LEU
1	A	108	LEU
1	A	133	ASP
1	A	150	ARG
1	A	151	VAL
1	A	156	THR
1	B	3	ILE
1	B	4	PHE
1	B	6	LYS
1	B	12	LEU
1	B	14	LEU
1	B	23	ASP
1	B	63	LEU
1	B	76	LEU
1	B	104	LEU
1	B	108	LEU
1	B	114	ARG
1	B	118	SER
1	B	129	THR
1	B	137	LEU
1	B	140	VAL
1	B	151	VAL
1	C	12	LEU
1	C	14	LEU
1	C	23	ASP
1	C	34	LEU
1	C	60	LEU
1	C	63	LEU
1	C	76	LEU
1	C	79	GLU
1	C	104	LEU
1	C	108	LEU
1	C	114	ARG
1	C	137	LEU
1	C	156	THR

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Mol	Chain	Res	Type
1	D	12	LEU
1	D	14	LEU
1	D	16	THR
1	D	28	GLU
1	D	34	LEU
1	D	60	LEU
1	D	63	LEU
1	D	77	LEU
1	D	79	GLU
1	D	81	GLN
1	D	82	SER
1	D	104	LEU
1	D	108	LEU
1	D	114	ARG
1	D	117	THR
1	D	131	ASP
1	D	137	LEU
1	D	149	MSE
1	D	156	THR
1	E	2	THR
1	E	3	ILE
1	E	5	GLU
1	E	7	LYS
1	E	12	LEU
1	E	14	LEU
1	E	27	ILE
1	E	33	LEU
1	E	34	LEU
1	E	63	LEU
1	E	77	LEU
1	E	78	SER
1	E	93	VAL
1	E	104	LEU
1	E	108	LEU
1	E	111	LEU
1	E	114	ARG
1	E	116	VAL
1	E	119	GLN
1	E	128	VAL
1	E	132	VAL
1	E	136	ASP
1	E	137	LEU

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Mol	Chain	Res	Type
1	E	138	ASN
1	E	150	ARG
1	E	156	THR
1	F	6	LYS
1	F	7	LYS
1	F	9	ASP
1	F	12	LEU
1	F	14	LEU
1	F	28	GLU
1	F	34	LEU
1	F	46	MSE
1	F	60	LEU
1	F	63	LEU
1	F	77	LEU
1	F	81	GLN
1	F	82	SER
1	F	84	ARG
1	F	93	VAL
1	F	104	LEU
1	F	117	THR
1	F	119	GLN
1	F	132	VAL
1	F	138	ASN
1	F	140	VAL
1	G	12	LEU
1	G	14	LEU
1	G	34	LEU
1	G	53	VAL
1	G	60	LEU
1	G	76	LEU
1	G	77	LEU
1	G	79	GLU
1	G	104	LEU
1	G	118	SER
1	G	137	LEU
1	G	140	VAL
1	G	151	VAL
1	G	152	ARG
1	H	4	PHE
1	H	7	LYS
1	H	11	THR
1	H	12	LEU

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Mol	Chain	Res	Type
1	H	27	ILE
1	H	33	LEU
1	H	51	GLN
1	H	63	LEU
1	H	73	THR
1	H	77	LEU
1	H	79	GLU
1	H	93	VAL
1	H	104	LEU
1	H	108	LEU
1	H	116	VAL
1	H	127	VAL
1	H	136	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	B	51	GLN
1	B	138	ASN
1	B	143	GLN
1	C	15	GLN
1	D	81	GLN
1	D	138	ASN
1	E	138	ASN
1	F	81	GLN
1	F	119	GLN
1	F	138	ASN
1	H	15	GLN
1	H	119	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 (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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, 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	147/167 (88%)	0.28	14 (9%)	14	12	38, 53, 86, 92	0
1	B	151/167 (90%)	0.33	13 (8%)	16	14	41, 52, 87, 102	0
1	C	147/167 (88%)	0.35	14 (9%)	14	12	43, 54, 90, 97	0
1	D	147/167 (88%)	0.21	8 (5%)	31	27	43, 53, 85, 90	0
1	E	151/167 (90%)	0.35	13 (8%)	16	14	46, 58, 89, 101	0
1	F	147/167 (88%)	0.49	13 (8%)	15	14	47, 62, 92, 101	0
1	G	147/167 (88%)	0.38	6 (4%)	41	37	50, 60, 90, 98	0
1	H	151/167 (90%)	0.34	12 (7%)	18	16	43, 55, 90, 104	0
All	All	1188/1336 (88%)	0.34	93 (7%)	19	17	38, 57, 89, 104	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	THR	6.9
1	B	156	THR	6.5
1	B	155	ALA	6.0
1	D	156	THR	4.7
1	H	4	PHE	4.6
1	A	135	GLU	4.5
1	H	156	THR	4.4
1	H	3	ILE	4.4
1	H	155	ALA	4.4
1	A	137	LEU	4.4
1	H	134	ALA	4.3
1	E	155	ALA	4.2
1	F	80	ASP	3.9
1	G	117	THR	3.9
1	F	155	ALA	3.9
1	E	135	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	2	THR	3.9
1	C	138	ASN	3.8
1	D	81	GLN	3.8
1	A	134	ALA	3.8
1	E	4	PHE	3.8
1	C	155	ALA	3.7
1	A	155	ALA	3.7
1	E	156	THR	3.6
1	B	3	ILE	3.6
1	B	4	PHE	3.5
1	C	118	SER	3.5
1	E	3	ILE	3.5
1	H	138	ASN	3.5
1	B	137	LEU	3.4
1	F	79	GLU	3.4
1	D	134	ALA	3.4
1	F	134	ALA	3.4
1	G	155	ALA	3.3
1	G	139	ALA	3.3
1	A	154	SER	3.3
1	C	137	LEU	3.3
1	B	6	LYS	3.3
1	B	133	ASP	3.2
1	B	138	ASN	3.2
1	C	135	GLU	3.2
1	A	132	VAL	3.2
1	H	135	GLU	3.1
1	E	2	THR	3.1
1	F	154	SER	3.0
1	H	132	VAL	3.0
1	H	137	LEU	3.0
1	B	134	ALA	3.0
1	G	138	ASN	3.0
1	D	137	LEU	2.9
1	C	134	ALA	2.9
1	F	120	ALA	2.9
1	A	120	ALA	2.9
1	D	135	GLU	2.8
1	B	154	SER	2.8
1	E	81	GLN	2.8
1	G	156	THR	2.8
1	C	123	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	156	THR	2.6
1	C	121	GLY	2.6
1	G	123	PHE	2.6
1	F	137	LEU	2.6
1	F	135	GLU	2.5
1	C	139	ALA	2.5
1	A	139	ALA	2.5
1	D	155	ALA	2.5
1	C	154	SER	2.5
1	B	5	GLU	2.5
1	E	138	ASN	2.5
1	A	138	ASN	2.4
1	F	132	VAL	2.4
1	H	5	GLU	2.4
1	H	153	SER	2.3
1	A	6	LYS	2.3
1	A	153	SER	2.2
1	F	133	ASP	2.2
1	D	132	VAL	2.2
1	F	126	TYR	2.2
1	E	154	SER	2.2
1	B	7	LYS	2.2
1	E	137	LEU	2.2
1	F	121	GLY	2.1
1	B	153	SER	2.1
1	F	136	ASP	2.1
1	E	79	GLU	2.1
1	C	75	GLU	2.1
1	D	79	GLU	2.1
1	A	78	SER	2.1
1	A	136	ASP	2.1
1	C	124	GLY	2.1
1	E	134	ALA	2.0
1	E	153	SER	2.0
1	C	153	SER	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.