



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 06:35 PM BST

PDB ID : 1NB5
Title : Crystal structure of stefin A in complex with cathepsin H
Authors : Jenko, S.; Dolenc, I.; Guncar, G.; Dobersek, A.; Podobnik, M.; Turk, D.
Deposited on : 2002-12-02
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

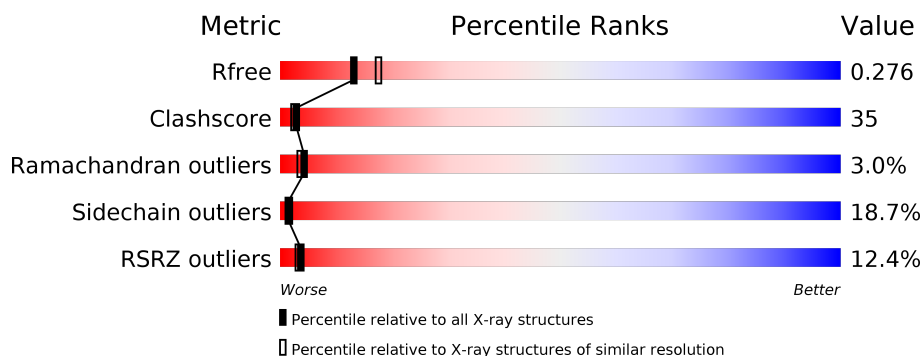
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	220	<div> <div>8%</div> <div>45%</div> <div>43%</div> <div>12%</div> </div>
1	B	220	<div> <div>9%</div> <div>43%</div> <div>46%</div> <div>10%</div> </div>
1	C	220	<div> <div>10%</div> <div>46%</div> <div>44%</div> <div>10%</div> </div>
1	D	220	<div> <div>7%</div> <div>47%</div> <div>44%</div> <div>9%</div> </div>
2	P	8	<div> <div>75%</div> <div>50%</div> <div>25%</div> <div>25%</div> </div>
2	R	8	<div> <div>50%</div> <div>38%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	S	8	
2	T	8	
3	I	98	
3	J	98	
3	K	98	
3	L	98	
4	E	3	
4	F	3	
4	G	3	
4	H	3	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10312 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 Cathepsin H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	60	0	0
			1706	1085	283	322	16			
1	B	220	Total	C	N	O	S	70	0	0
			1706	1085	283	322	16			
1	C	220	Total	C	N	O	S	71	0	0
			1706	1085	283	322	16			
1	D	220	Total	C	N	O	S	63	0	0
			1706	1085	283	322	16			

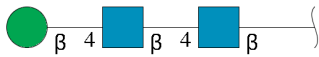
- Molecule 2 is a protein called Cathepsin H MINI CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	8	Total	C	N	O	S	8	0	0
			58	32	10	15	1			
2	R	8	Total	C	N	O	S	15	0	0
			58	32	10	15	1			
2	S	8	Total	C	N	O	S	13	0	0
			58	32	10	15	1			
2	T	8	Total	C	N	O	S	17	0	0
			58	32	10	15	1			

- Molecule 3 is a protein called STEFIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	98	Total	C	N	O	S	41	0	0
			775	492	126	155	2			
3	J	98	Total	C	N	O	S	39	0	0
			775	492	126	155	2			
3	K	98	Total	C	N	O	S	64	0	0
			775	492	126	155	2			
3	L	98	Total	C	N	O	S	62	0	0
			775	492	126	155	2			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

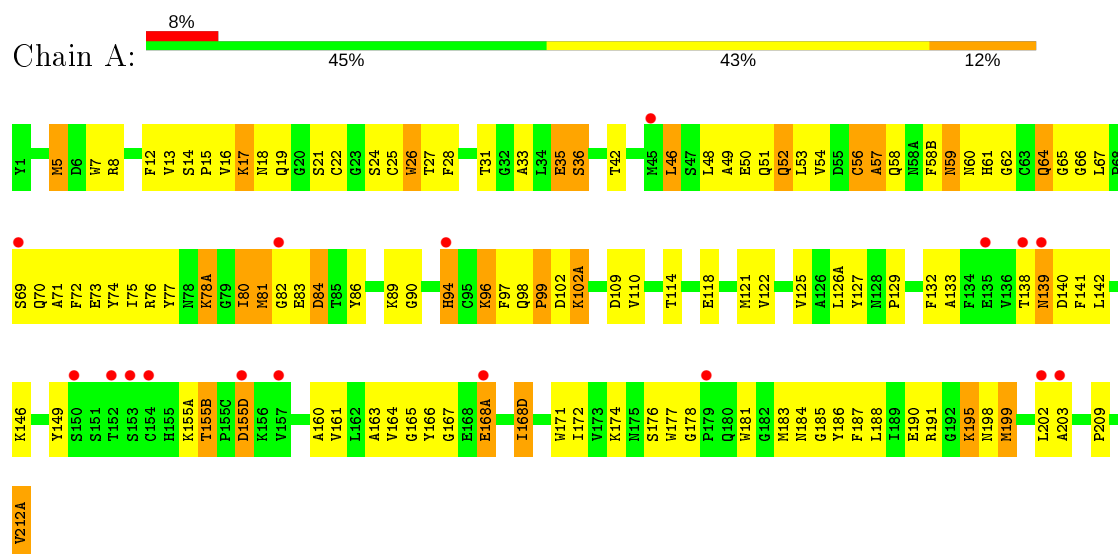


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

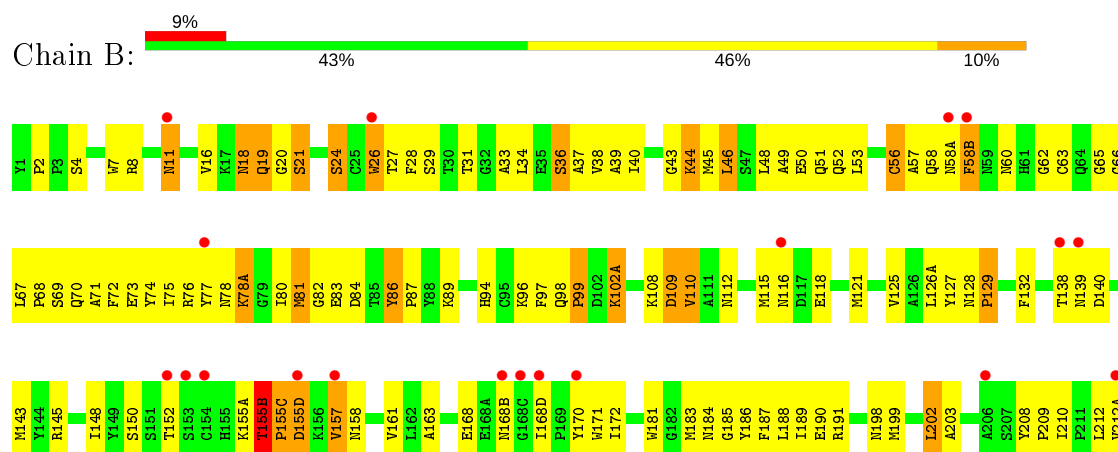
3 Residue-property plots

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: Cathepsin H

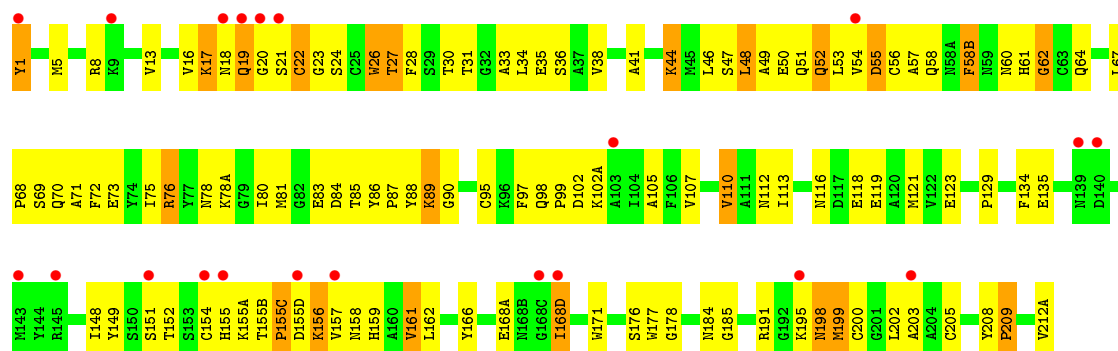


• Molecule 1: Cathepsin H

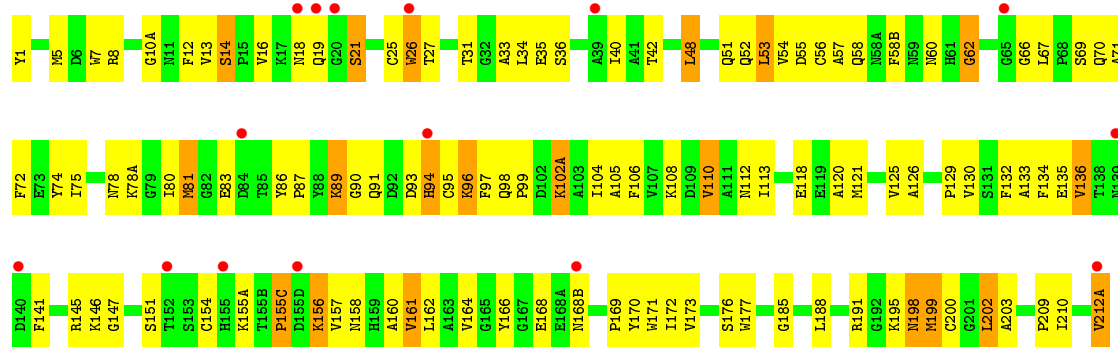


• Molecule 1: Cathepsin H

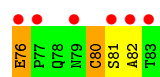
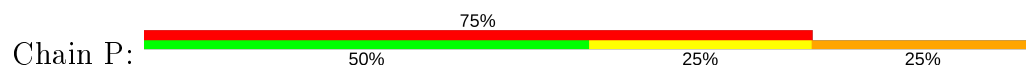




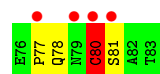
• Molecule 1: Cathepsin H



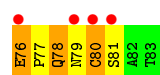
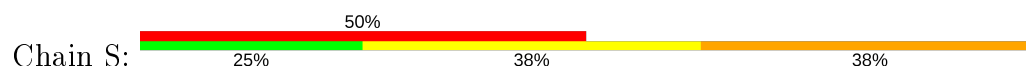
• Molecule 2: Cathepsin H MINI CHAIN



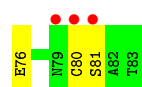
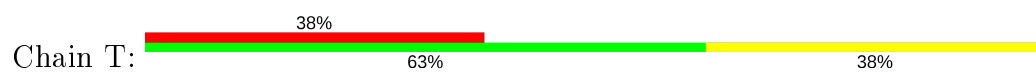
• Molecule 2: Cathepsin H MINI CHAIN



• Molecule 2: Cathepsin H MINI CHAIN



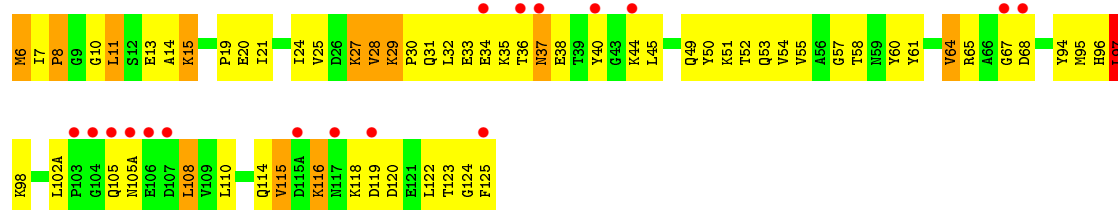
• Molecule 2: Cathepsin H MINI CHAIN



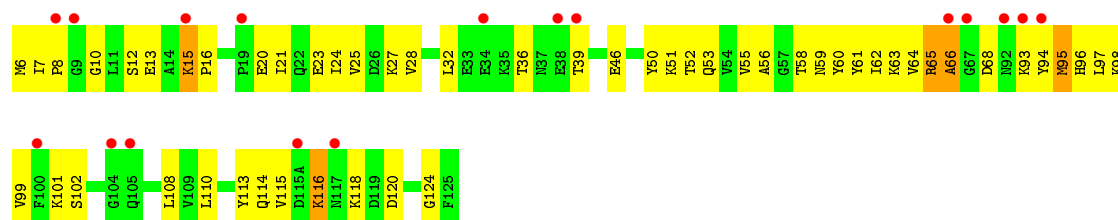
• Molecule 3: STEFIN A



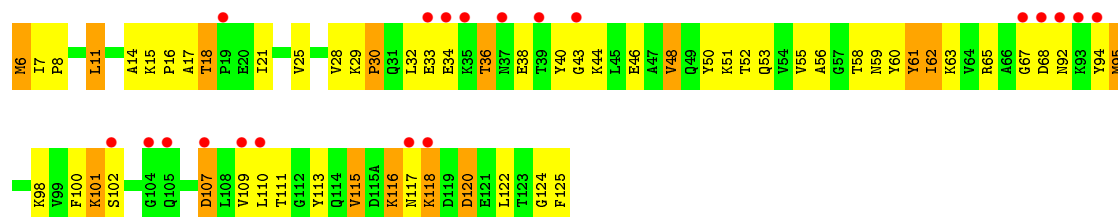
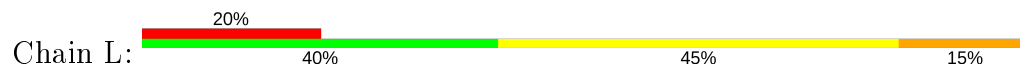
• Molecule 3: STEFIN A



• Molecule 3: STEFIN A



• Molecule 3: STEFIN A



- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

UAG1
UAG2
BMA3

- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  33% 67%

UAG1
UAG2
BMA3

- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  33% 33% 33%

UAG1
UAG2
BMA3

- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33% 33% 33%

UAG1
UAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.63Å 97.58Å 162.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40 10.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.40) 87.9 (10.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	MAIN	Depositor
R, R_{free}	0.235 , 0.274 0.268 , 0.276	Depositor DCC
R_{free} test set	2844 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.936	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 80.3	EDS
L-test for twinning ¹	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10312	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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 56.69 % 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 2.6402e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.50	0/1753	0.75	1/2377 (0.0%)
1	B	0.51	0/1753	0.83	5/2377 (0.2%)
1	C	0.50	0/1753	0.72	0/2377
1	D	0.51	2/1753 (0.1%)	0.74	0/2377
2	P	0.40	0/58	0.88	0/77
2	R	0.34	0/58	0.77	0/77
2	S	0.56	0/58	0.82	0/77
2	T	0.46	0/58	0.74	0/77
3	I	0.52	0/788	0.81	1/1062 (0.1%)
3	J	0.61	0/788	0.88	3/1062 (0.3%)
3	K	0.50	0/788	0.77	0/1062
3	L	0.48	0/788	0.77	0/1062
All	All	0.51	2/10396 (0.0%)	0.78	10/14064 (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
3	K	0	1
3	L	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	212(A)	VAL	C-OXT	5.82	1.34	1.23
1	D	25	CYS	CB-SG	-5.68	1.72	1.81

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155(C)	PRO	N-CA-C	9.65	137.19	112.10
1	B	58(A)	ASN	N-CA-C	8.54	134.05	111.00
3	J	36	THR	N-CA-C	6.97	129.83	111.00
3	J	11	LEU	CA-CB-CG	6.44	130.11	115.30
3	J	97	LEU	CA-CB-CG	5.69	128.39	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	113	TYR	Sidechain
3	L	113	TYR	Sidechain

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	1706	0	1622	130	1
1	B	1706	0	1622	125	2
1	C	1706	0	1622	99	2
1	D	1706	0	1622	107	0
2	P	58	0	47	24	0
2	R	58	0	47	10	0
2	S	58	0	47	6	0
2	T	58	0	47	6	0
3	I	775	0	777	76	0
3	J	775	0	777	64	7
3	K	775	0	777	44	1
3	L	775	0	777	41	7
4	E	39	0	34	9	0
4	F	39	0	34	11	0
4	G	39	0	34	2	0
4	H	39	0	34	3	0
All	All	10312	0	9920	667	10

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 35.

The worst 5 of 667 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)
3:I:45:LEU:HD22	3:I:64:VAL:CG1	1.23	1.64
3:I:45:LEU:CD2	3:I:66:ALA:HB2	1.32	1.56
3:I:45:LEU:CD2	3:I:64:VAL:CG1	1.86	1.50
1:B:8:ARG:NH2	1:B:172:ILE:HG21	1.62	1.11
2:S:81:SER:HA	3:K:7:ILE:HG12	1.26	1.11

The worst 5 of 10 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:119:ASP:OD2	3:L:107:ASP:CG[4_465]	1.37	0.83
3:J:119:ASP:OD1	3:L:107:ASP:OD2[4_465]	1.42	0.78
3:J:119:ASP:OD2	3:L:107:ASP:OD2[4_465]	1.47	0.73
3:J:119:ASP:CG	3:L:107:ASP:OD2[4_465]	1.54	0.66
1:A:84:ASP:O	3:L:115:VAL:CG2[4_455]	1.55	0.65

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	218/220 (99%)	191 (88%)	22 (10%)	5 (2%)	6	7
1	B	218/220 (99%)	184 (84%)	26 (12%)	8 (4%)	3	2
1	C	218/220 (99%)	182 (84%)	29 (13%)	7 (3%)	4	3
1	D	218/220 (99%)	190 (87%)	24 (11%)	4 (2%)	8	10
2	P	6/8 (75%)	4 (67%)	1 (17%)	1 (17%)	0	0
2	R	6/8 (75%)	5 (83%)	0	1 (17%)	0	0
2	S	6/8 (75%)	4 (67%)	1 (17%)	1 (17%)	0	0
2	T	6/8 (75%)	5 (83%)	1 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	96/98 (98%)	79 (82%)	14 (15%)	3 (3%)	4	3
3	J	96/98 (98%)	83 (86%)	10 (10%)	3 (3%)	4	3
3	K	96/98 (98%)	82 (85%)	12 (12%)	2 (2%)	7	8
3	L	96/98 (98%)	82 (85%)	11 (12%)	3 (3%)	4	3
All	All	1280/1304 (98%)	1091 (85%)	151 (12%)	38 (3%)	4	3

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	155(B)	THR
1	B	155(C)	PRO
1	D	155(C)	PRO
1	D	156	LYS
3	L	67	GLY

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	181/181 (100%)	146 (81%)	35 (19%)	1	1
1	B	181/181 (100%)	148 (82%)	33 (18%)	1	2
1	C	181/181 (100%)	152 (84%)	29 (16%)	2	3
1	D	181/181 (100%)	156 (86%)	25 (14%)	3	4
2	P	7/7 (100%)	5 (71%)	2 (29%)	0	0
2	R	7/7 (100%)	6 (86%)	1 (14%)	3	4
2	S	7/7 (100%)	4 (57%)	3 (43%)	0	0
2	T	7/7 (100%)	6 (86%)	1 (14%)	3	4
3	I	85/85 (100%)	72 (85%)	13 (15%)	2	3
3	J	85/85 (100%)	65 (76%)	20 (24%)	1	1
3	K	85/85 (100%)	71 (84%)	14 (16%)	2	2
3	L	85/85 (100%)	57 (67%)	28 (33%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1092/1092 (100%)	888 (81%)	204 (19%)	1 2

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	44	LYS
1	C	52	GLN
3	L	58	THR
3	J	54	VAL
3	J	116	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	70	GLN
3	J	49	GLN
1	D	98	GLN
1	B	116	ASN
1	B	198	ASN

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 ⓘ

12 monosaccharides 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
4	NAG	E	1	1,4	14,14,15	0.86	1 (7%)	17,19,21	1.17	2 (11%)
4	NAG	E	2	4	14,14,15	0.44	0	17,19,21	0.87	1 (5%)
4	BMA	E	3	4	11,11,12	0.81	0	15,15,17	1.48	3 (20%)
4	NAG	F	1	1,4	14,14,15	0.47	0	17,19,21	1.72	3 (17%)
4	NAG	F	2	4	14,14,15	0.58	0	17,19,21	1.14	1 (5%)
4	BMA	F	3	4	11,11,12	0.36	0	15,15,17	0.51	0
4	NAG	G	1	1,4	14,14,15	1.02	2 (14%)	17,19,21	1.04	2 (11%)
4	NAG	G	2	4	14,14,15	0.55	0	17,19,21	0.88	0
4	BMA	G	3	4	11,11,12	0.68	0	15,15,17	0.73	0
4	NAG	H	1	1,4	14,14,15	0.70	0	17,19,21	1.21	2 (11%)
4	NAG	H	2	4	14,14,15	0.58	0	17,19,21	0.96	1 (5%)
4	BMA	H	3	4	11,11,12	0.52	0	15,15,17	0.73	0

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
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	NAG	C4-C5	2.17	1.57	1.53
4	G	1	NAG	C4-C3	2.17	1.57	1.52
4	E	1	NAG	C4-C5	2.11	1.57	1.53

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	F	1	NAG	C1-O5-C5	3.63	117.11	112.19
4	F	1	NAG	C3-C4-C5	3.60	116.66	110.24
4	F	1	NAG	O5-C1-C2	3.48	116.78	111.29
4	E	3	BMA	C2-C3-C4	3.43	116.83	110.89
4	E	3	BMA	C3-C4-C5	3.18	115.92	110.24

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	4	0
4	G	1	NAG	1	0
4	E	2	NAG	4	0
4	G	2	NAG	1	0
4	H	2	NAG	3	0
4	F	2	NAG	2	0
4	E	1	NAG	4	0
4	F	3	BMA	5	0
4	E	3	BMA	1	0

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 ⓘ

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(Å²)	Q<0.9
1	A	216/220 (98%)	0.65	17 (7%)	12	11	14, 36, 59, 79	13 (6%)
1	B	216/220 (98%)	0.65	19 (8%)	10	9	15, 35, 57, 67	15 (6%)
1	C	217/220 (98%)	0.81	21 (9%)	7	7	19, 36, 60, 78	16 (7%)
1	D	216/220 (98%)	0.77	15 (6%)	16	15	15, 37, 58, 75	14 (6%)
2	P	8/8 (100%)	3.32	6 (75%)	0	0	34, 52, 61, 65	2 (25%)
2	R	6/8 (75%)	2.38	4 (66%)	0	0	31, 53, 67, 69	1 (16%)
2	S	6/8 (75%)	2.55	4 (66%)	0	0	49, 64, 67, 68	0
2	T	6/8 (75%)	3.02	3 (50%)	0	0	42, 60, 69, 72	1 (16%)
3	I	98/98 (100%)	1.03	16 (16%)	1	1	16, 39, 59, 78	11 (11%)
3	J	98/98 (100%)	1.03	17 (17%)	1	1	17, 39, 64, 77	12 (12%)
3	K	96/98 (97%)	1.07	17 (17%)	1	1	18, 51, 67, 78	13 (13%)
3	L	96/98 (97%)	1.25	20 (20%)	1	0	21, 49, 68, 79	11 (11%)
All	All	1279/1304 (98%)	0.88	159 (12%)	4	3	14, 39, 64, 79	109 (8%)

The worst 5 of 159 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	66	ALA	11.3
3	I	105(A)	ASN	10.0
3	J	105(A)	ASN	9.7
1	B	155(D)	ASP	9.3
2	P	82	ALA	9.2

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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	E	3	11/12	0.53	0.34	43,61,65,68	0
4	BMA	H	3	11/12	0.65	0.21	42,54,65,69	0
4	BMA	G	3	11/12	0.72	0.26	36,49,63,67	0
4	NAG	E	1	14/15	0.81	0.27	43,50,69,70	0
4	NAG	F	1	14/15	0.82	0.22	30,49,57,58	0
4	BMA	F	3	11/12	0.83	0.22	40,52,61,70	0
4	NAG	G	2	14/15	0.83	0.21	21,39,47,49	0
4	NAG	H	1	14/15	0.85	0.21	21,32,53,54	0
4	NAG	F	2	14/15	0.86	0.17	5,53,57,58	0
4	NAG	G	1	14/15	0.89	0.17	13,32,53,57	0
4	NAG	H	2	14/15	0.91	0.14	28,41,49,54	0
4	NAG	E	2	14/15	0.93	0.17	22,50,65,68	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.