



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 10:40 pm GMT

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

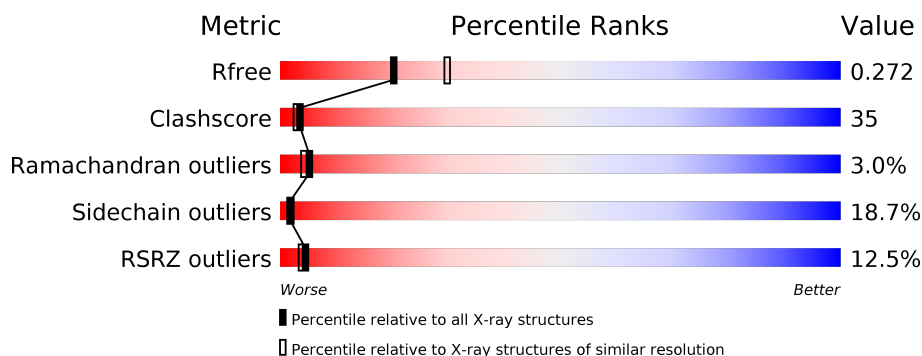
# 1 Overall quality at a glance

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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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  $\geq 3$ , 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  $\leq 5\%$ . 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% 43% 12%</div> </div>
1	B	220	<div> <div>9%</div> <div>43% 46% 10%</div> </div>
1	C	220	<div> <div>10%</div> <div>46% 44% 10%</div> </div>
1	D	220	<div> <div>7%</div> <div>47% 44% 9%</div> </div>
2	P	8	<div> <div>75%</div> <div>50% 25% 25%</div> </div>
2	R	8	<div> <div>50%</div> <div>50% 38% 13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	S	8	<div><div></div><div>50%</div><div>25%</div><div>38%</div><div>38%</div></div>
2	T	8	<div><div></div><div>38%</div><div>63%</div><div>38%</div></div>
3	I	98	<div><div></div><div>16%</div><div>51%</div><div>41%</div><div>8%</div></div>
3	J	98	<div><div></div><div>18%</div><div>36%</div><div>51%</div><div>12%</div></div>
3	K	98	<div><div></div><div>15%</div><div>46%</div><div>49%</div><div>5%</div></div>
3	L	98	<div><div></div><div>20%</div><div>40%</div><div>45%</div><div>15%</div></div>

## 2 Entry composition

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			

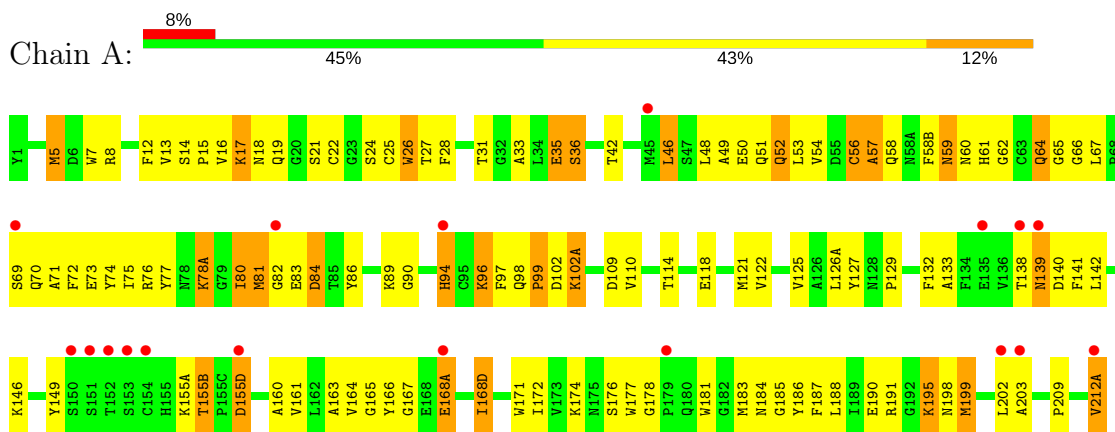
- Molecule 4 is a polymer of unknown type called SUGAR (NAG-NAG-BMA).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	B	3	Total	C	N	O	0	0
			39	22	2	15		
4	C	3	Total	C	N	O	0	0
			39	22	2	15		
4	D	3	Total	C	N	O	0	0
			39	22	2	15		

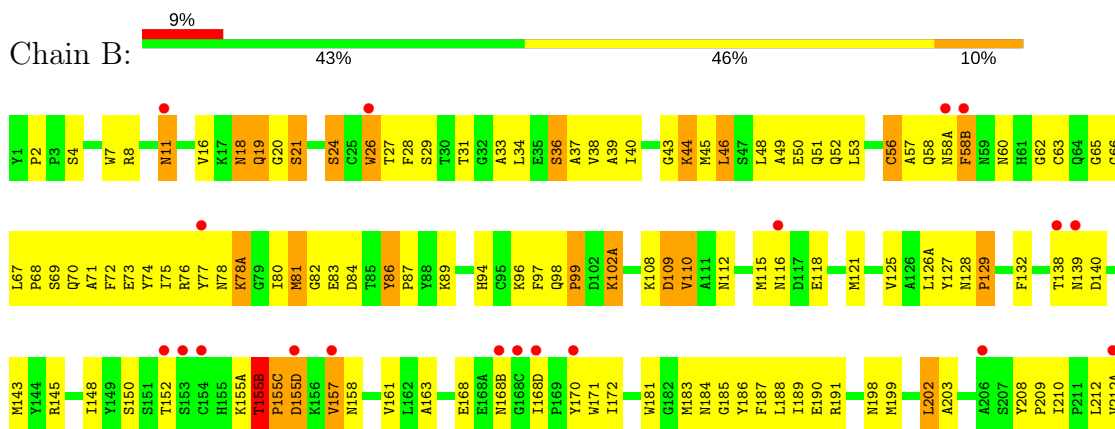
### 3 Residue-property plots [i](#)

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

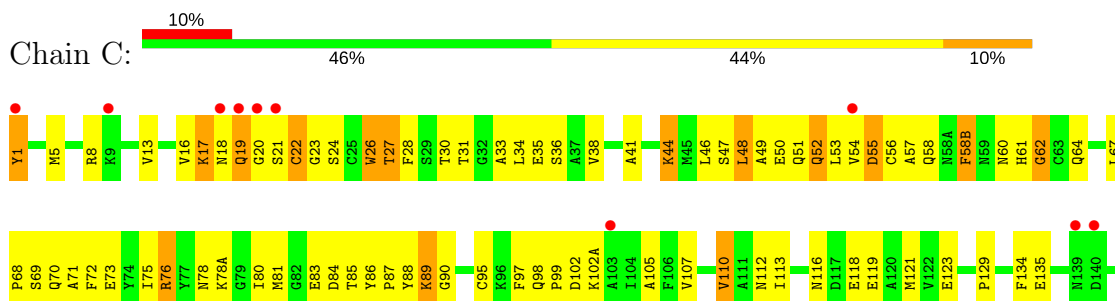
#### • Molecule 1: Cathepsin H

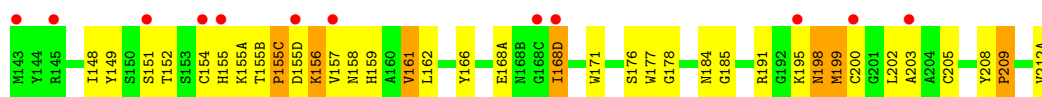


#### • Molecule 1: Cathepsin H

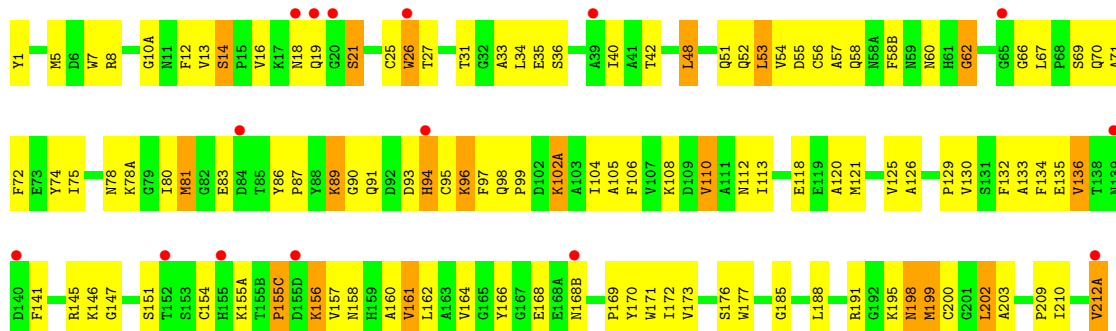


#### • Molecule 1: Cathepsin H

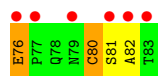
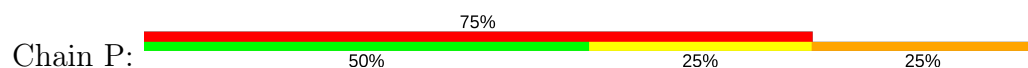




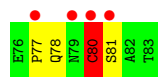
● Molecule 1: Cathepsin H



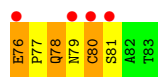
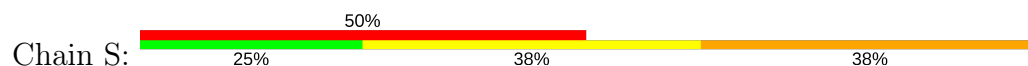
● Molecule 2: Cathepsin H MINI CHAIN



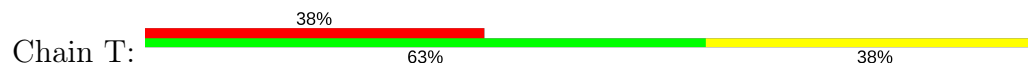
● Molecule 2: Cathepsin H MINI CHAIN



● Molecule 2: Cathepsin H MINI CHAIN

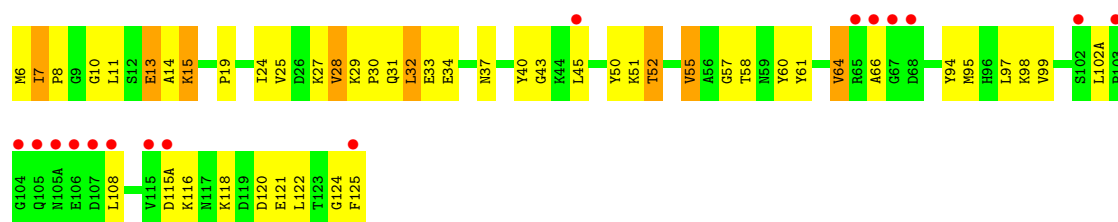


● Molecule 2: Cathepsin H MINI CHAIN

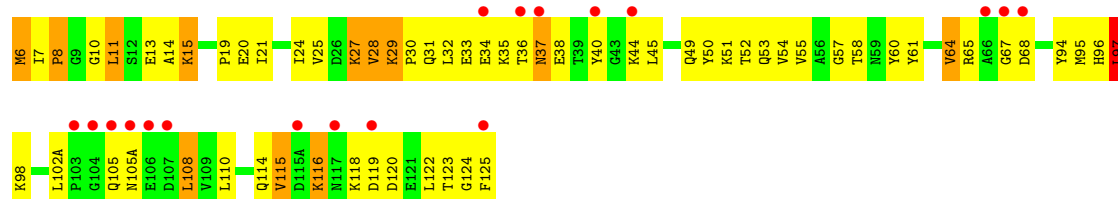


● Molecule 3: STEFIN A

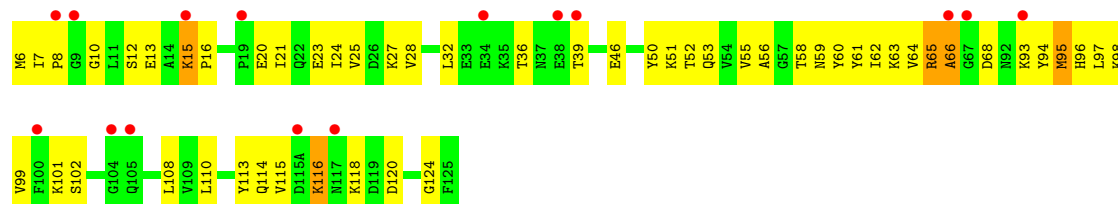




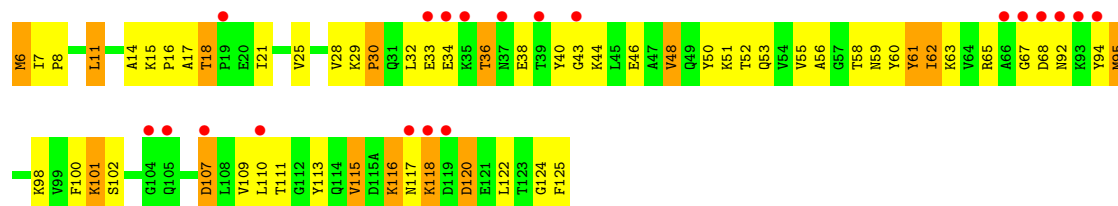
● Molecule 3: STEFIN A



● Molecule 3: STEFIN A



● Molecule 3: STEFIN A





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 0.263 , 0.272	Depositor DCC
$R_{free}$ test set	2529 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.936	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 80.3	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Theoretical 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	A	39	0	34	9	0
4	B	39	0	34	11	0
4	C	39	0	34	2	0
4	D	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%)	7	8
1	B	218/220 (99%)	184 (84%)	26 (12%)	8 (4%)	4	3
1	C	218/220 (99%)	182 (84%)	29 (13%)	7 (3%)	5	4
1	D	218/220 (99%)	190 (87%)	24 (11%)	4 (2%)	10	12
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%)	5	4
3	J	96/98 (98%)	83 (86%)	10 (10%)	3 (3%)	5	4
3	K	96/98 (98%)	82 (85%)	12 (12%)	2 (2%)	8	9
3	L	96/98 (98%)	82 (85%)	11 (12%)	3 (3%)	5	4
All	All	1280/1304 (98%)	1091 (85%)	151 (12%)	38 (3%)	5	4

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

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 carbohydrates 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	A	213	1,4	14,14,15	0.85	1 (7%)	15,19,21	1.29	2 (13%)
4	NAG	A	214	4	14,14,15	0.44	0	15,19,21	0.92	1 (6%)
4	BMA	A	215	4	11,11,12	0.81	0	13,15,17	1.58	2 (15%)
4	NAG	B	213	1,4	14,14,15	0.46	0	15,19,21	1.77	3 (20%)
4	NAG	B	214	4	14,14,15	0.57	0	15,19,21	1.22	2 (13%)
4	BMA	B	215	4	11,11,12	0.35	0	13,15,17	0.53	0
4	NAG	C	213	1,4	14,14,15	1.02	2 (14%)	15,19,21	1.15	2 (13%)
4	NAG	C	214	4	14,14,15	0.56	0	15,19,21	0.93	0
4	BMA	C	215	4	11,11,12	0.70	0	13,15,17	0.76	0
4	NAG	D	213	1,4	14,14,15	0.69	0	15,19,21	1.24	1 (6%)
4	NAG	D	214	4	14,14,15	0.57	0	15,19,21	1.06	2 (13%)
4	BMA	D	215	4	11,11,12	0.51	0	13,15,17	0.77	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	A	213	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	214	4	-	0/6/23/26	0/1/1/1
4	BMA	A	215	4	-	0/2/19/22	0/1/1/1
4	NAG	B	213	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	214	4	-	0/6/23/26	0/1/1/1
4	BMA	B	215	4	-	0/2/19/22	0/1/1/1
4	NAG	C	213	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	214	4	-	0/6/23/26	0/1/1/1
4	BMA	C	215	4	-	0/2/19/22	0/1/1/1
4	NAG	D	213	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	214	4	-	0/6/23/26	0/1/1/1
4	BMA	D	215	4	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	213	NAG	C4-C5	2.09	1.57	1.53
4	C	213	NAG	C4-C5	2.15	1.57	1.53
4	C	213	NAG	C4-C3	2.16	1.57	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	213	NAG	O5-C1-C2	-3.66	106.39	111.47
4	C	213	NAG	O5-C1-C2	-2.97	107.34	111.47
4	D	214	NAG	C2-N2-C7	-2.89	118.72	122.94
4	A	214	NAG	C2-N2-C7	-2.85	118.78	122.94
4	B	214	NAG	C2-N2-C7	-2.82	118.83	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	213	NAG	4	0
4	A	214	NAG	4	0
4	A	215	BMA	1	0
4	B	213	NAG	4	0
4	B	214	NAG	2	0
4	B	215	BMA	5	0
4	C	213	NAG	1	0
4	C	214	NAG	1	0
4	D	214	NAG	3	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 [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	216/220 (98%)	0.66	18 (8%)	12 11	14, 36, 59, 79	13 (6%)
1	B	216/220 (98%)	0.66	19 (8%)	11 9	15, 35, 57, 67	15 (6%)
1	C	217/220 (98%)	0.81	22 (10%)	8 7	19, 36, 60, 78	16 (7%)
1	D	216/220 (98%)	0.77	15 (6%)	18 16	15, 37, 58, 75	14 (6%)
2	P	8/8 (100%)	3.34	6 (75%)	0 0	34, 52, 61, 65	2 (25%)
2	R	6/8 (75%)	2.37	4 (66%)	0 0	31, 53, 67, 69	1 (16%)
2	S	6/8 (75%)	2.58	4 (66%)	0 0	49, 64, 67, 68	0
2	T	6/8 (75%)	3.10	3 (50%)	0 0	42, 60, 69, 72	1 (16%)
3	I	98/98 (100%)	1.03	16 (16%)	2 2	16, 39, 59, 78	11 (11%)
3	J	98/98 (100%)	1.02	18 (18%)	1 1	17, 39, 64, 77	12 (12%)
3	K	96/98 (97%)	1.07	15 (15%)	2 2	18, 51, 67, 78	13 (13%)
3	L	96/98 (97%)	1.27	20 (20%)	1 1	21, 49, 68, 79	11 (11%)
All	All	1279/1304 (98%)	0.88	160 (12%)	4 4	14, 39, 64, 79	109 (8%)

The worst 5 of 160 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	66	ALA	11.2
3	I	105(A)	ASN	10.0
3	J	105(A)	ASN	9.5
2	P	82	ALA	9.4
1	B	155(D)	ASP	9.3

### 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](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	C	214	14/15	0.84	0.20	0.58	21,39,47,49	0
4	NAG	A	213	14/15	0.81	0.27	0.18	43,50,69,70	0
4	NAG	B	213	14/15	0.82	0.22	-0.27	30,49,57,58	0
4	NAG	D	213	14/15	0.86	0.21	-0.39	21,32,53,54	0
4	NAG	C	213	14/15	0.89	0.17	-0.60	13,32,53,57	0
4	NAG	D	214	14/15	0.91	0.15	-0.91	28,41,49,54	0
4	NAG	B	214	14/15	0.86	0.16	-1.28	5,53,57,58	0
4	NAG	A	214	14/15	0.93	0.17	-1.29	22,50,65,68	0
4	BMA	B	215	11/12	0.83	0.22	-	40,52,61,70	0
4	BMA	D	215	11/12	0.66	0.21	-	42,54,65,69	0
4	BMA	C	215	11/12	0.70	0.26	-	36,49,63,67	0
4	BMA	A	215	11/12	0.53	0.34	-	43,61,65,68	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.