wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:45 PM GMT

PDB ID	:	1LQ8
Title	:	Crystal structure of cleaved protein C inhibitor
Authors	:	Huntington, J.A.; Kjellberg, M.; Stenflo, J.
Deposited on	:	2002-05-09
Resolution	:	2.40 Å(reported)

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

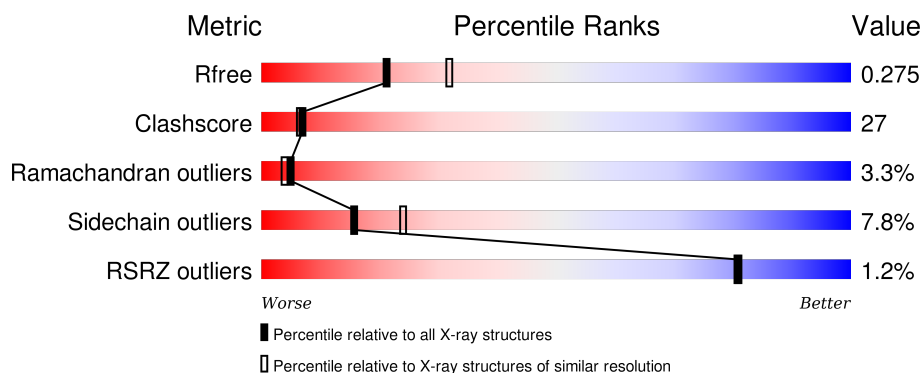|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.275
Clashscore		27
Ramachandran outliers		3.3%
Sidechain outliers		7.8%
RSRZ outliers		1.2%

Worse ← → *Better*

▌ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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. 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	346	57% · 31% · 7% · 5%
1	C	346	% · 48% · 39% · 7% · 5%
1	E	346	2% · 49% · 40% · 5% · 5%
1	G	346	% · 56% · 34% · · · 5%
2	B	31	3% · 48% · 39% · 6% · 6%

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Mol	Chain	Length	Quality of chain
2	D	31	52% 26% 13% · 6%
2	F	31	3% 32% 58% 10%
2	H	31	48% 39% 6% 6%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MAN	G	6	-	-	-	X
8	IPA	A	901	-	-	-	X
8	IPA	C	902	-	-	-	X
8	IPA	G	903	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 11658 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 plasma serine protease inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	23	0	0
			2598	1653	442	491	12			
1	C	328	Total	C	N	O	S	17	0	0
			2587	1647	438	490	12			
1	E	329	Total	C	N	O	S	34	0	0
			2598	1653	442	491	12			
1	G	330	Total	C	N	O	S	18	0	0
			2604	1656	443	493	12			

- Molecule 2 is a protein called plasma serine protease inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	29	Total	C	N	O	S	0	0	0
			245	160	45	39	1			
2	D	29	Total	C	N	O	S	0	0	0
			245	160	45	39	1			
2	F	28	Total	C	N	O	S	0	0	0
			237	156	43	37	1			
2	H	29	Total	C	N	O	S	0	0	0
			245	160	45	39	1			

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).
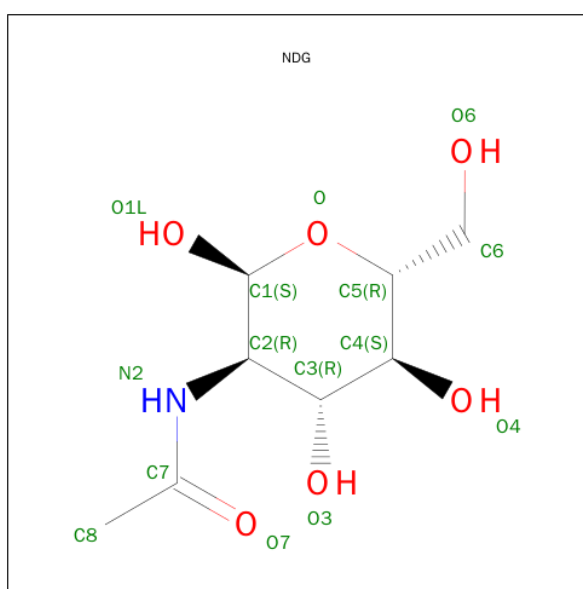
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	3	Total	C	O	0	0
			34	18	16		

- Molecule 8 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).

IPA

C3

C2

C1

O H

O2
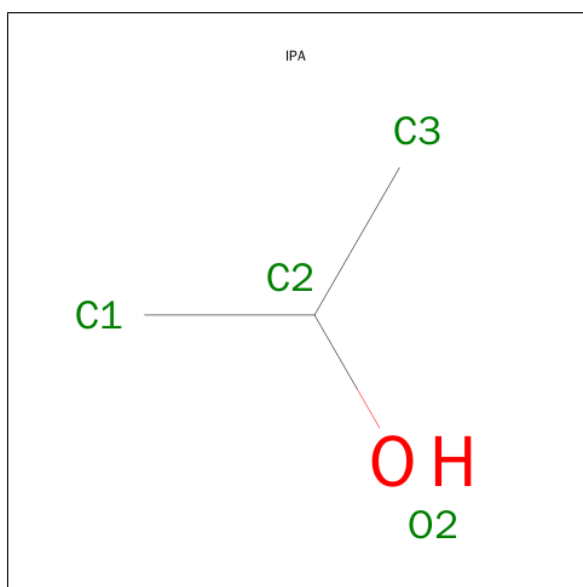
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 4	C 3	O 1	0	0
8	C	1	Total 4	C 3	O 1	0	0
8	G	1	Total 4	C 3	O 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	28	Total 28	O 28	0	0
9	B	4	Total 4	O 4	0	0
9	C	18	Total 18	O 18	0	0
9	D	10	Total 10	O 10	0	0
9	E	15	Total 15	O 15	0	0
9	F	1	Total 1	O 1	0	0
9	G	21	Total 21	O 21	0	0
9	H	2	Total 2	O 2	0	0

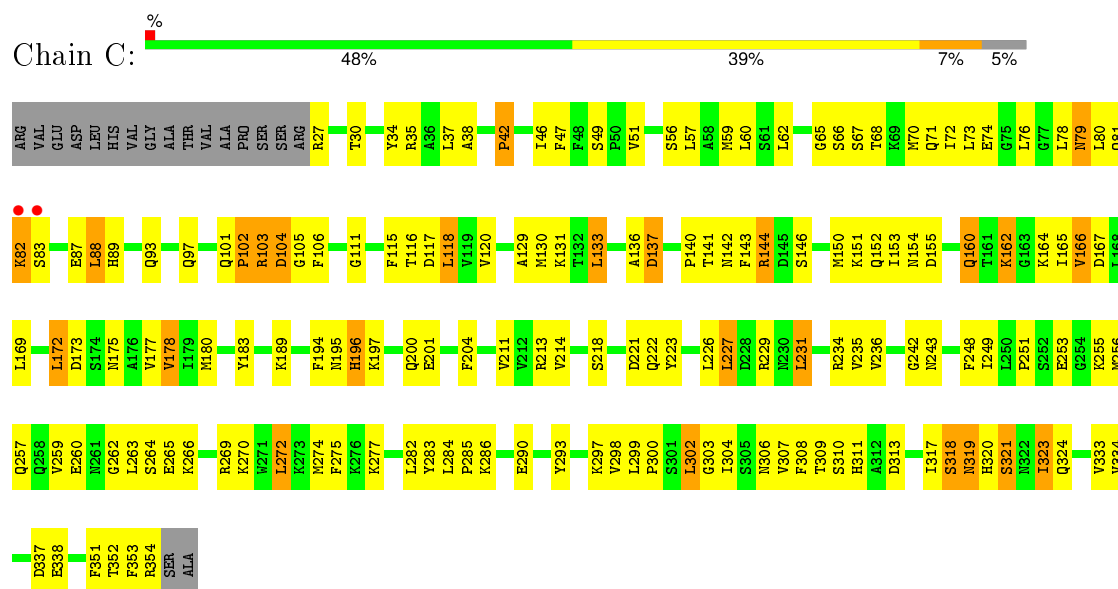W O R L D W I D E
PDB
PROTEIN DATA BANK

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: plasma serine protease inhibitor
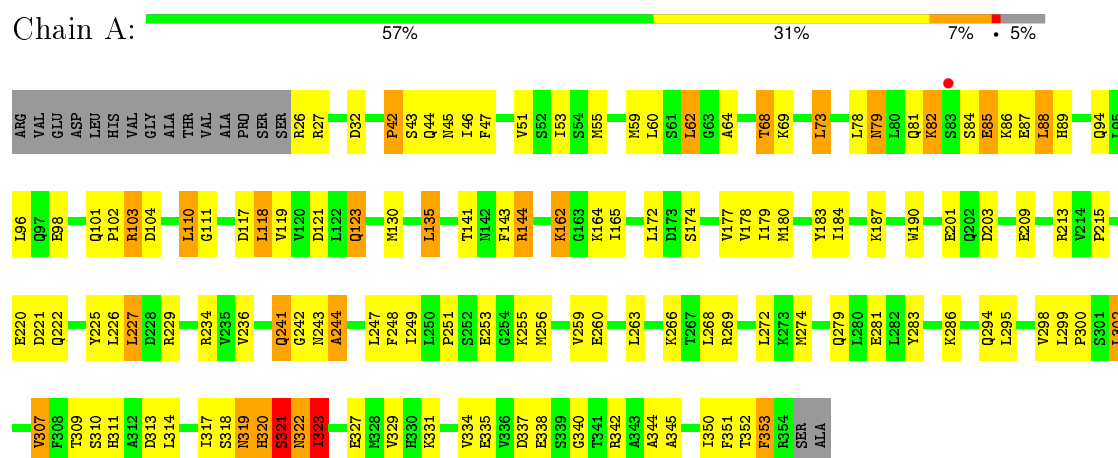
Chain A:

57%   31%   7% · 5%

- Molecule 1: plasma serine protease inhibitor

Chain C:

48%   39%   7% 5%

- Molecule 1: plasma serine protease inhibitor

Chain E:

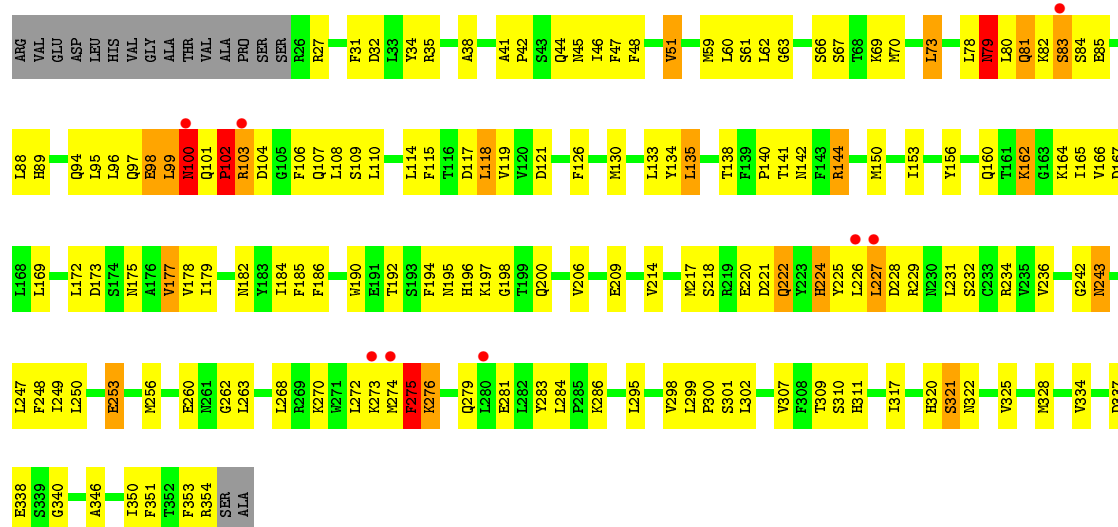2%   49%   40%   5% · 5%

• Molecule 1: plasma serine protease inhibitor

Chain G:

• Molecule 2: plasma serine protease inhibitor

Chain B:

• Molecule 2: plasma serine protease inhibitor

Chain D:

• Molecule 2: plasma serine protease inhibitor

Chain F:

ARG LEU ASN S360 Q361 R362 L363 V364 F365 N366 R367 P368 F369 L370 M371 F372 D375 N376 N377 I378 L379 F380 L381 G382 K383 V384 N385 R386 P387

• Molecule 2: plasma serine protease inhibitor

Chain H:

48%   39%   6%   6%

ARG LEU N359 S360 Q361 R362 L363 F372 I373 V374 D375 N376 N377 I378 L379 F380 V384 N385 R386 P387
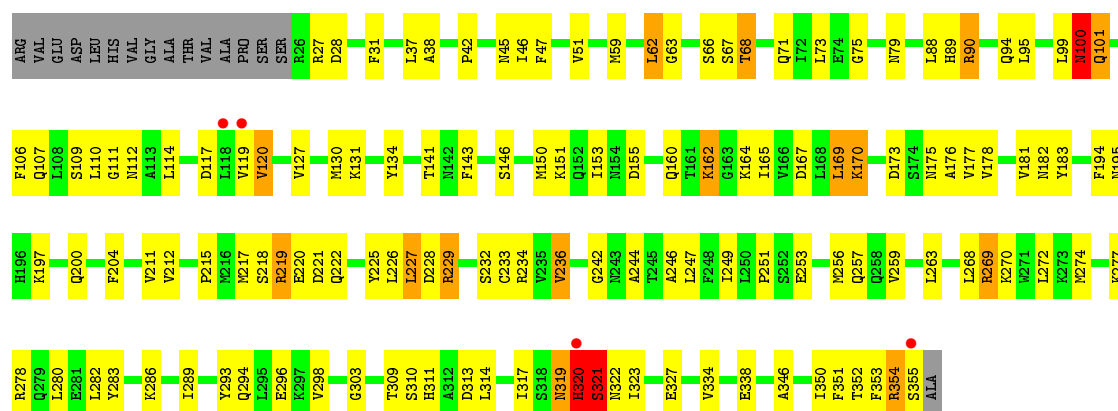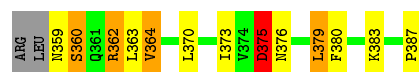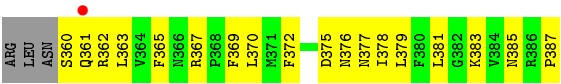
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.20Å 244.03Å 66.40Å 90.00° 91.98° 90.00°	Depositor
Resolution (Å)	45.66 – 2.40 44.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	80.6 (45.66-2.40) 80.7 (44.91-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.222 , 0.279 0.222 , 0.275	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	53.9	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 36.4	EDS
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	1 of 55033 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11658	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.43	0/2646	0.69	1/3570 (0.0%)
1	C	0.42	0/2635	0.68	0/3556
1	E	0.39	0/2646	0.67	1/3570 (0.0%)
1	G	0.39	0/2652	0.68	1/3578 (0.0%)
2	B	0.46	0/250	0.83	0/335
2	D	0.45	0/250	0.83	1/335 (0.3%)
2	F	0.37	0/242	0.77	0/324
2	H	0.46	0/250	0.90	1/335 (0.3%)
All	All	0.41	0/11571	0.69	5/15603 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	321	SER	N-CA-C	-5.50	96.14	111.00
2	D	375	ASP	N-CA-C	-5.24	96.85	111.00
2	H	375	ASP	N-CA-C	-5.11	97.19	111.00
1	A	82	LYS	N-CA-C	-5.05	97.37	111.00
1	E	79	ASN	N-CA-C	5.04	124.62	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2598	0	2603	125	0
1	C	2587	0	2588	168	0
1	E	2598	0	2607	160	0
1	G	2604	0	2610	128	0
2	B	245	0	253	16	0
2	D	245	0	253	16	0
2	F	237	0	247	29	0
2	H	245	0	253	18	0
3	A	28	0	25	2	0
3	G	28	0	25	5	0
4	A	28	0	25	6	0
5	C	28	0	25	7	0
6	C	28	0	26	3	0
6	G	14	0	13	1	0
7	G	34	0	30	2	0
8	A	4	0	8	2	0
8	C	4	0	8	0	0
8	G	4	0	8	0	0
9	A	28	0	0	2	0
9	B	4	0	0	0	0
9	C	18	0	0	1	0
9	D	10	0	0	0	0
9	E	15	0	0	4	0
9	F	1	0	0	0	0
9	G	21	0	0	1	0
9	H	2	0	0	0	0
All	All	11658	0	11607	610	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 27.

The worst 5 of 610 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:C:164:LYS:HA	1:C:164:LYS:HE2	1.33	1.06
4:A:3:NAG:O3	4:A:7:NAG:H2	1.60	1.02
1:G:309:THR:HG22	1:G:311:HIS:H	1.21	1.00
1:G:120:VAL:HG21	1:G:177:VAL:HB	1.44	0.99
1:A:266:LYS:HG3	1:A:269:ARG:HH22	1.25	0.99

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	327/346 (94%)	296 (90%)	20 (6%)	11 (3%)	5	4
1	C	326/346 (94%)	297 (91%)	19 (6%)	10 (3%)	5	4
1	E	327/346 (94%)	282 (86%)	30 (9%)	15 (5%)	3	2
1	G	328/346 (95%)	295 (90%)	24 (7%)	9 (3%)	6	6
2	B	27/31 (87%)	23 (85%)	4 (15%)	0	100	100
2	D	27/31 (87%)	25 (93%)	1 (4%)	1 (4%)	4	3
2	F	26/31 (84%)	23 (88%)	3 (12%)	0	100	100
2	H	27/31 (87%)	24 (89%)	2 (7%)	1 (4%)	4	3
All	All	1415/1508 (94%)	1265 (89%)	103 (7%)	47 (3%)	5	4

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	GLU
1	A	321	SER
1	A	322	ASN
1	A	323	ILE
1	C	42	PRO

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	288/301 (96%)	263 (91%)	25 (9%)	13	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	287/301 (95%)	262 (91%)	25 (9%)	13	19
1	E	288/301 (96%)	268 (93%)	20 (7%)	19	30
1	G	289/301 (96%)	268 (93%)	21 (7%)	17	27
2	B	28/30 (93%)	26 (93%)	2 (7%)	18	28
2	D	28/30 (93%)	23 (82%)	5 (18%)	2	2
2	F	27/30 (90%)	27 (100%)	0	100	100
2	H	28/30 (93%)	27 (96%)	1 (4%)	42	63
All	All	1263/1324 (95%)	1164 (92%)	99 (8%)	16	24

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	227	LEU
2	D	375	ASP
1	G	236	VAL
1	C	231	LEU
1	C	302	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	97	GLN
1	E	222	GLN
1	G	261	ASN
1	E	107	GLN
1	E	243	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

11 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	#$|Z| > 2$
3	NDG	A	1	1,3	14,14,15	0.67	0	15,19,21	0.89	1 (6%)
3	NDG	A	2	3	14,14,15	1.27	1 (7%)	15,19,21	0.96	2 (13%)
4	NAG	A	3	1,4	14,14,15	0.95	0	15,19,21	0.77	0
4	NAG	A	7	4	14,14,15	0.92	1 (7%)	15,19,21	0.80	0
5	NDG	C	8	1,5	14,14,15	0.66	0	15,19,21	0.77	1 (6%)
5	NAG	C	9	5	14,14,15	0.75	1 (7%)	15,19,21	0.70	0
3	NDG	G	357	1,3	14,14,15	0.92	0	15,19,21	0.72	0
3	NDG	G	358	3	14,14,15	0.84	0	15,19,21	0.70	0
7	MAN	G	4	7	12,12,12	0.75	0	17,17,17	1.18	1 (5%)
7	MAN	G	5	7	11,11,12	0.64	0	14,15,17	0.92	1 (7%)
7	MAN	G	6	7	11,11,12	0.58	0	14,15,17	0.92	1 (7%)

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
3	NDG	A	1	1,3	-	0/6/23/26	0/1/1/1
3	NDG	A	2	3	-	0/6/23/26	0/1/1/1
4	NAG	A	3	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	7	4	-	1/6/23/26	0/1/1/1
5	NDG	C	8	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	9	5	-	1/6/23/26	0/1/1/1
3	NDG	G	357	1,3	-	0/6/23/26	0/1/1/1
3	NDG	G	358	3	-	0/6/23/26	0/1/1/1
7	MAN	G	4	7	-	0/2/22/22	0/1/1/1
7	MAN	G	5	7	-	0/2/19/22	1/1/1/1
7	MAN	G	6	7	-	0/2/19/22	1/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	9	NAG	C1-C2	2.23	1.55	1.52
4	A	7	NAG	C1-C2	2.85	1.56	1.52
3	A	2	NDG	C1-C2	3.63	1.57	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	4	MAN	C3-C4-C5	-3.49	104.12	110.20
5	C	8	NDG	C2-N2-C7	-2.23	120.17	123.04
3	A	2	NDG	C4-C3-C2	-2.11	107.94	111.23
3	A	1	NDG	C3-C4-C5	-2.05	106.62	110.20
3	A	2	NDG	C1-O-C5	2.25	115.11	112.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	9	NAG	O7-C7-N2-C2
4	A	7	NAG	O7-C7-N2-C2

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	5	MAN	C1-C2-C3-C4-C5-O5
7	G	6	MAN	C1-C2-C3-C4-C5-O5

10 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	NDG	2	0
3	A	2	NDG	2	0
4	A	3	NAG	6	0
4	A	7	NAG	4	0
5	C	8	NDG	6	0
5	C	9	NAG	4	0
3	G	357	NDG	1	0
3	G	358	NDG	5	0
7	G	4	MAN	1	0
7	G	6	MAN	2	0

5.6 Ligand geometry (i)

6 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
8	IPA	A	901	-	3,3,3	0.37	0	3,3,3	0.40	0
6	NDG	C	10	1	14,14,15	0.76	0	15,19,21	0.60	0
6	NDG	C	357	1	14,14,15	0.85	1 (7%)	15,19,21	0.77	1 (6%)
8	IPA	C	902	-	3,3,3	0.32	0	3,3,3	0.39	0
6	NDG	G	359	1	14,14,15	0.76	0	15,19,21	0.87	1 (6%)
8	IPA	G	903	-	3,3,3	0.31	0	3,3,3	0.37	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
8	IPA	A	901	-	-	0/0/0/0	0/0/0/0
6	NDG	C	10	1	-	0/6/23/26	0/1/1/1
6	NDG	C	357	1	-	0/6/23/26	0/1/1/1
8	IPA	C	902	-	-	0/0/0/0	0/0/0/0
6	NDG	G	359	1	-	1/6/23/26	0/1/1/1
8	IPA	G	903	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	357	NDG	C1-C2	2.21	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	359	NDG	C2-N2-C7	-2.47	119.86	123.04
6	C	357	NDG	C2-N2-C7	-2.29	120.10	123.04

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	359	NDG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	901	IPA	2	0
6	C	10	NDG	3	0
6	G	359	NDG	1	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	329/346 (95%)	-0.19	1 (0%)	94	94	43, 57, 87, 105	6 (1%)
1	C	328/346 (94%)	-0.14	2 (0%)	90	90	42, 61, 86, 104	4 (1%)
1	E	329/346 (95%)	0.02	8 (2%)	62	61	42, 66, 99, 118	9 (2%)
1	G	330/346 (95%)	-0.15	4 (1%)	81	81	40, 61, 85, 106	6 (1%)
2	B	29/31 (93%)	-0.10	1 (3%)	49	49	41, 50, 81, 92	0
2	D	29/31 (93%)	-0.32	0	100	100	41, 49, 70, 89	0
2	F	28/31 (90%)	0.16	1 (3%)	46	47	55, 65, 105, 107	0
2	H	29/31 (93%)	-0.09	0	100	100	44, 52, 74, 83	0
All	All	1431/1508 (94%)	-0.11	17 (1%)	81	81	40, 61, 92, 118	25 (1%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	320	HIS	3.5
1	E	103	ARG	3.3
1	E	274	MET	3.1
1	E	226	LEU	3.1
1	C	82	LYS	2.9

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, 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	LLDF	B-factors($Å^2$)	Q<0.9
7	MAN	G	6	11/12	0.70	0.21	3.73	144,146,147,148	0
3	NDG	A	1	14/15	0.83	0.19	0.57	92,95,98,104	0
5	NDG	C	8	14/15	0.87	0.17	0.42	100,105,108,114	0
3	NDG	G	357	14/15	0.81	0.17	-0.38	87,92,95,100	0
3	NDG	A	2	14/15	0.73	0.33	-	109,111,113,113	0
7	MAN	G	5	11/12	0.61	0.43	-	152,153,153,153	0
4	NAG	A	3	14/15	0.54	0.26	-	109,114,117,122	0
4	NAG	A	7	14/15	0.48	0.48	-	125,128,129,129	0
7	MAN	G	4	12/12	0.61	0.29	-	151,154,155,155	0
3	NDG	G	358	14/15	0.82	0.44	-	104,107,107,108	0
5	NAG	C	9	14/15	0.81	0.23	-	117,119,120,120	0

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, 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	LLDF	B-factors($Å^2$)	Q<0.9
8	IPA	C	902	4/4	0.87	0.33	8.56	98,99,99,99	0
8	IPA	A	901	4/4	0.97	0.18	4.62	63,64,64,65	0
8	IPA	G	903	4/4	0.96	0.20	4.46	79,79,79,80	0
6	NDG	C	10	14/15	0.74	0.25	1.49	114,116,117,117	0
6	NDG	C	357	14/15	0.66	0.29	-	100,105,107,107	0
6	NDG	G	359	14/15	0.78	0.48	-	100,103,108,108	0

6.5 Other polymers (i)

There are no such residues in this entry.