



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:34 PM GMT

PDB ID : 1G5G
Title : FRAGMENT OF FUSION PROTEIN FROM NEWCASTLE DISEASE VIRUS
Authors : Lawrence, M.C.; Smith, B.J.
Deposited on : 2000-11-01
Resolution : 3.30 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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

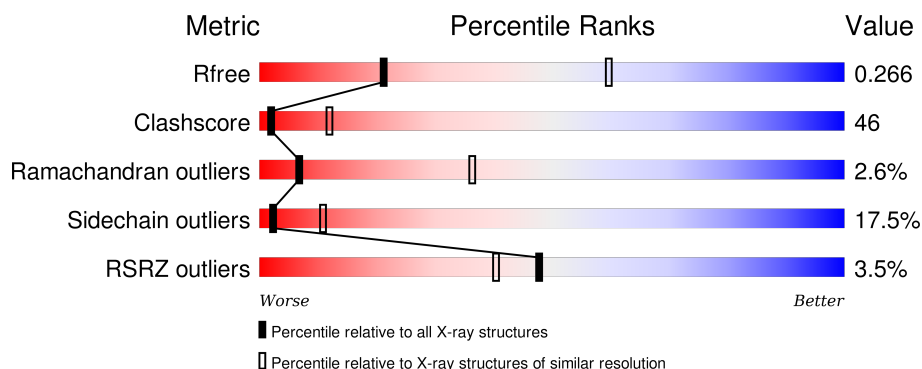
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 $\leq 5\%$. 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	481	 3% 27% 38% 9% 26%
1	B	481	 3% 29% 35% 10% 26%
1	C	481	 3% 30% 36% 9% 26%
1	D	481	 3% 27% 38% 9% 26%
1	E	481	 2% 30% 35% 9% 26%

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Mol	Chain	Length	Quality of chain
1	F	481	

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
2	NAG	A	851	-	-	-	X
4	NAG	C	4471	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16341 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 FUSION PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2675	1679	440	538	18			
1	B	357	Total	C	N	O	S	0	0	0
			2675	1679	440	538	18			
1	C	357	Total	C	N	O	S	0	0	0
			2675	1679	440	538	18			
1	D	357	Total	C	N	O	S	0	0	0
			2675	1679	440	538	18			
1	E	357	Total	C	N	O	S	0	0	0
			2675	1679	440	538	18			
1	F	357	Total	C	N	O	S	0	0	0
			2675	1679	440	538	18			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	ASN	ASP	CONFLICT	UNP P35936
A	265	SER	GLY	CONFLICT	UNP P35936
A	500	SER	ALA	CONFLICT	UNP P35936
A	501	ARG	LEU	CONFLICT	UNP P35936
A	502	GLU	-	PURIFICATION TAG	UNP P35936
A	503	GLN	-	PURIFICATION TAG	UNP P35936
A	504	LYS	-	PURIFICATION TAG	UNP P35936
A	506	ILE	-	PURIFICATION TAG	UNP P35936
A	507	SER	-	PURIFICATION TAG	UNP P35936
A	508	GLU	-	PURIFICATION TAG	UNP P35936
A	509	GLU	-	PURIFICATION TAG	UNP P35936
A	510	ASP	-	PURIFICATION TAG	UNP P35936
A	511	LEU	-	PURIFICATION TAG	UNP P35936
A	512	ASN	-	PURIFICATION TAG	UNP P35936
B	170	ASN	ASP	CONFLICT	UNP P35936
B	265	SER	GLY	CONFLICT	UNP P35936
B	500	SER	ALA	CONFLICT	UNP P35936

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Chain	Residue	Modelled	Actual	Comment	Reference
B	501	ARG	LEU	CONFLICT	UNP P35936
B	502	GLU	-	PURIFICATION TAG	UNP P35936
B	503	GLN	-	PURIFICATION TAG	UNP P35936
B	504	LYS	-	PURIFICATION TAG	UNP P35936
B	506	ILE	-	PURIFICATION TAG	UNP P35936
B	507	SER	-	PURIFICATION TAG	UNP P35936
B	508	GLU	-	PURIFICATION TAG	UNP P35936
B	509	GLU	-	PURIFICATION TAG	UNP P35936
B	510	ASP	-	PURIFICATION TAG	UNP P35936
B	511	LEU	-	PURIFICATION TAG	UNP P35936
B	512	ASN	-	PURIFICATION TAG	UNP P35936
C	170	ASN	ASP	CONFLICT	UNP P35936
C	265	SER	GLY	CONFLICT	UNP P35936
C	500	SER	ALA	CONFLICT	UNP P35936
C	501	ARG	LEU	CONFLICT	UNP P35936
C	502	GLU	-	PURIFICATION TAG	UNP P35936
C	503	GLN	-	PURIFICATION TAG	UNP P35936
C	504	LYS	-	PURIFICATION TAG	UNP P35936
C	506	ILE	-	PURIFICATION TAG	UNP P35936
C	507	SER	-	PURIFICATION TAG	UNP P35936
C	508	GLU	-	PURIFICATION TAG	UNP P35936
C	509	GLU	-	PURIFICATION TAG	UNP P35936
C	510	ASP	-	PURIFICATION TAG	UNP P35936
C	511	LEU	-	PURIFICATION TAG	UNP P35936
C	512	ASN	-	PURIFICATION TAG	UNP P35936
D	170	ASN	ASP	CONFLICT	UNP P35936
D	265	SER	GLY	CONFLICT	UNP P35936
D	500	SER	ALA	CONFLICT	UNP P35936
D	501	ARG	LEU	CONFLICT	UNP P35936
D	502	GLU	-	PURIFICATION TAG	UNP P35936
D	503	GLN	-	PURIFICATION TAG	UNP P35936
D	504	LYS	-	PURIFICATION TAG	UNP P35936
D	506	ILE	-	PURIFICATION TAG	UNP P35936
D	507	SER	-	PURIFICATION TAG	UNP P35936
D	508	GLU	-	PURIFICATION TAG	UNP P35936
D	509	GLU	-	PURIFICATION TAG	UNP P35936
D	510	ASP	-	PURIFICATION TAG	UNP P35936
D	511	LEU	-	PURIFICATION TAG	UNP P35936
D	512	ASN	-	PURIFICATION TAG	UNP P35936
E	170	ASN	ASP	CONFLICT	UNP P35936
E	265	SER	GLY	CONFLICT	UNP P35936
E	500	SER	ALA	CONFLICT	UNP P35936

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Chain	Residue	Modelled	Actual	Comment	Reference
E	501	ARG	LEU	CONFLICT	UNP P35936
E	502	GLU	-	PURIFICATION TAG	UNP P35936
E	503	GLN	-	PURIFICATION TAG	UNP P35936
E	504	LYS	-	PURIFICATION TAG	UNP P35936
E	506	ILE	-	PURIFICATION TAG	UNP P35936
E	507	SER	-	PURIFICATION TAG	UNP P35936
E	508	GLU	-	PURIFICATION TAG	UNP P35936
E	509	GLU	-	PURIFICATION TAG	UNP P35936
E	510	ASP	-	PURIFICATION TAG	UNP P35936
E	511	LEU	-	PURIFICATION TAG	UNP P35936
E	512	ASN	-	PURIFICATION TAG	UNP P35936
F	170	ASN	ASP	CONFLICT	UNP P35936
F	265	SER	GLY	CONFLICT	UNP P35936
F	500	SER	ALA	CONFLICT	UNP P35936
F	501	ARG	LEU	CONFLICT	UNP P35936
F	502	GLU	-	PURIFICATION TAG	UNP P35936
F	503	GLN	-	PURIFICATION TAG	UNP P35936
F	504	LYS	-	PURIFICATION TAG	UNP P35936
F	506	ILE	-	PURIFICATION TAG	UNP P35936
F	507	SER	-	PURIFICATION TAG	UNP P35936
F	508	GLU	-	PURIFICATION TAG	UNP P35936
F	509	GLU	-	PURIFICATION TAG	UNP P35936
F	510	ASP	-	PURIFICATION TAG	UNP P35936
F	511	LEU	-	PURIFICATION TAG	UNP P35936
F	512	ASN	-	PURIFICATION TAG	UNP P35936

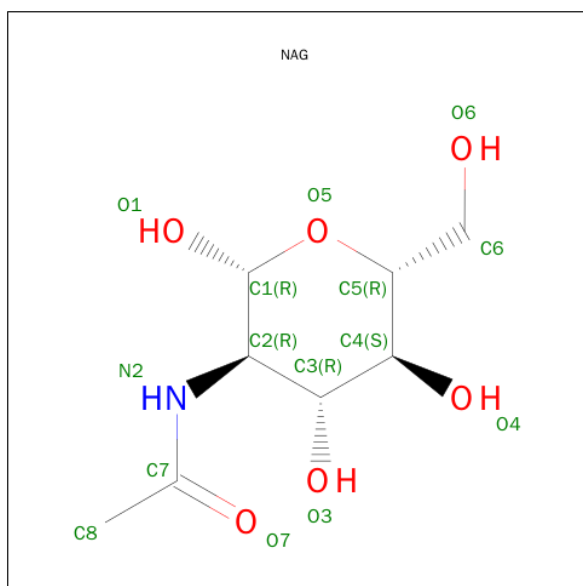
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		

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

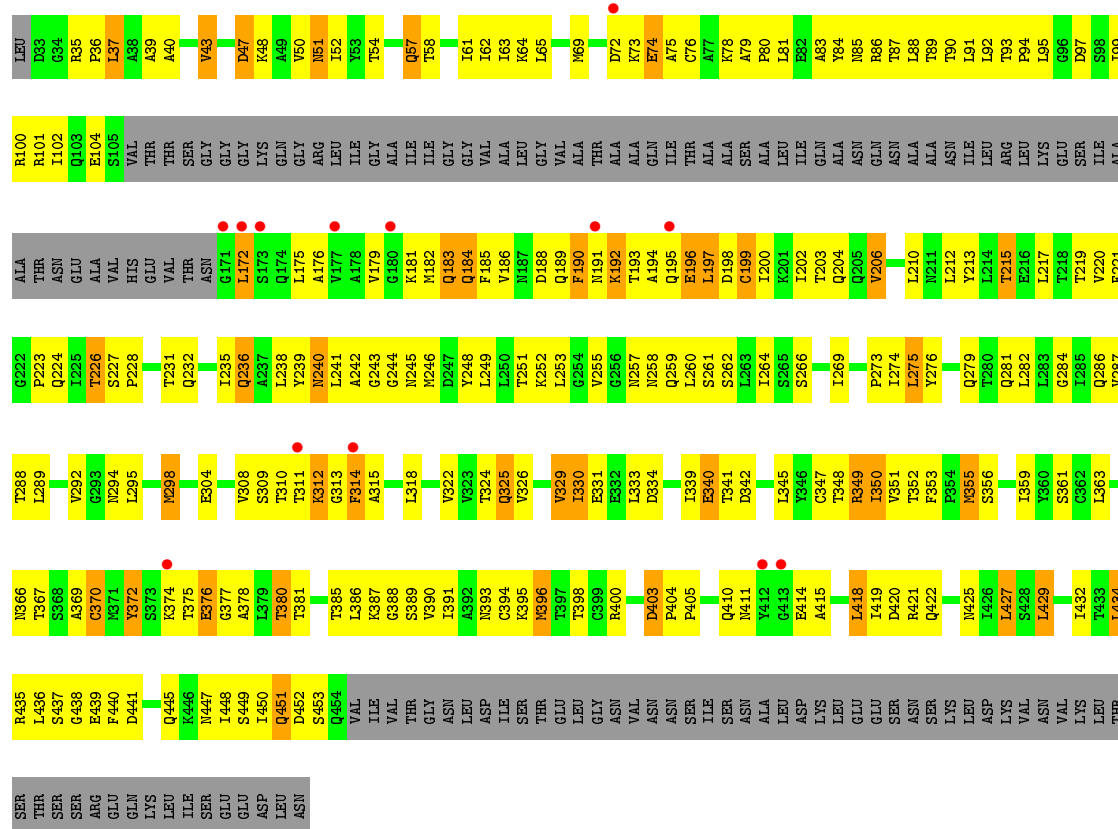
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

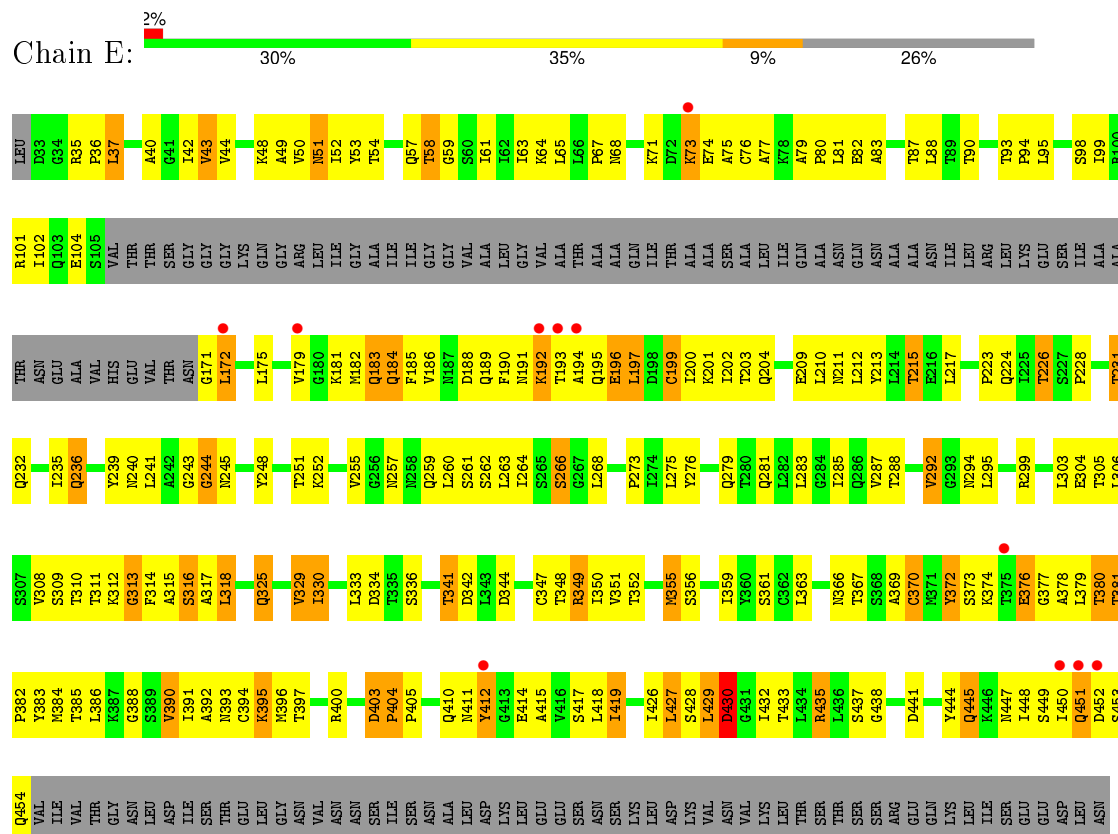


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

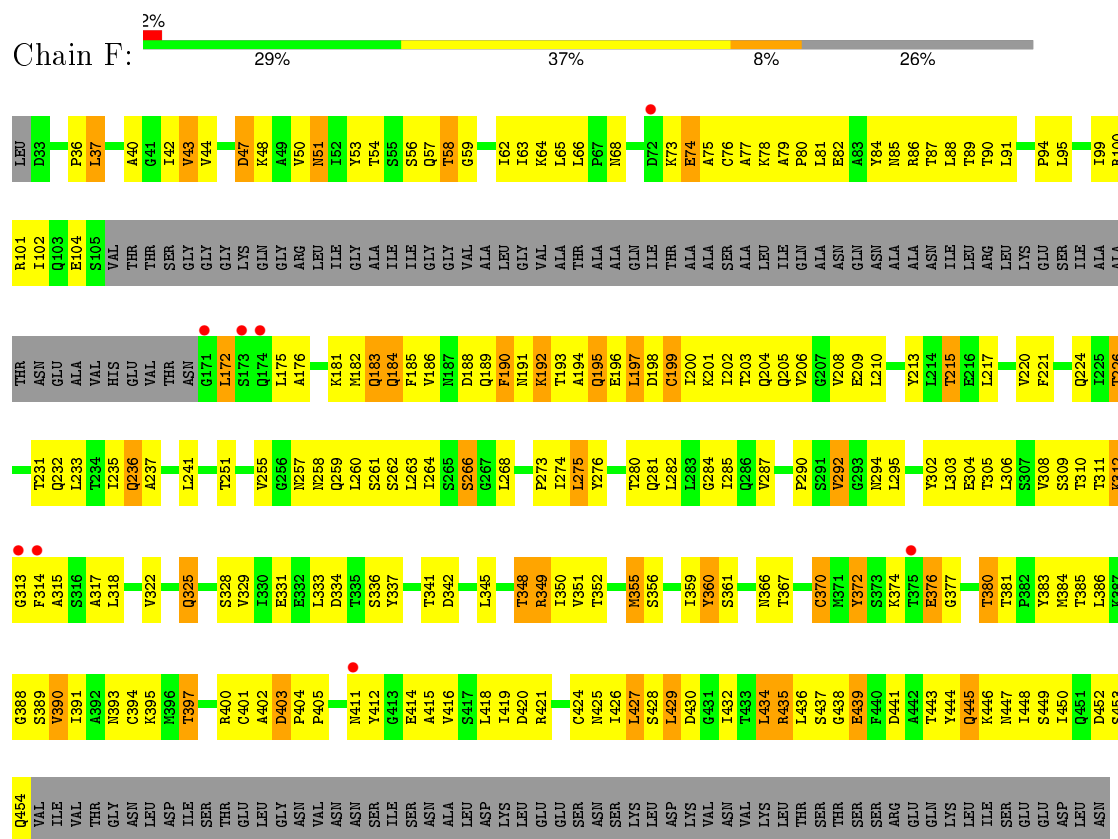




• Molecule 1: FUSION PROTEIN



● Molecule 1: FUSION PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	134.39Å 308.33Å 243.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30 24.84 – 3.29	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.30) 95.8 (24.84-3.29)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.30Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.224 , 0.273 0.225 , 0.266	Depositor DCC
R_{free} test set	3465 reflections (5.13%)	DCC
Wilson B-factor (Å ²)	72.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	10 of 73052 reflections (0.014%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16341	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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 34.87 % 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 6.3763e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	0.43	0/2708	0.73	1/3683 (0.0%)
1	B	0.42	0/2708	0.73	0/3683
1	C	0.42	0/2708	0.74	1/3683 (0.0%)
1	D	0.44	0/2708	0.73	1/3683 (0.0%)
1	E	0.42	0/2708	0.74	0/3683
1	F	0.43	0/2708	0.73	0/3683
All	All	0.43	0/16248	0.73	3/22098 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	ILE	N-CA-C	-5.41	96.39	111.00
1	C	339	ILE	N-CA-C	-5.35	96.56	111.00
1	D	339	ILE	N-CA-C	-5.10	97.22	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	2675	0	2716	311	0
1	B	2675	0	2717	313	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2675	0	2716	329	0
1	D	2675	0	2717	297	0
1	E	2675	0	2716	310	0
1	F	2675	0	2717	318	0
2	A	28	0	25	6	0
2	B	56	0	50	5	0
2	C	28	0	25	1	0
2	D	28	0	25	1	0
2	E	28	0	25	1	0
2	F	28	0	25	2	0
3	A	39	0	34	5	0
4	C	14	0	13	7	0
4	D	14	0	13	0	0
4	E	14	0	13	5	0
4	F	14	0	13	0	0
All	All	16341	0	16560	1521	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 46.

The worst 5 of 1521 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:A:255:VAL:HG13	1:A:292:VAL:HG11	1.23	1.19
1:D:255:VAL:HG13	1:D:292:VAL:HG11	1.27	1.10
1:E:314:PHE:HB3	1:E:374:LYS:HD3	1.32	1.10
1:C:405:PRO:CG	1:F:64:LYS:HD2	1.81	1.10
1:A:314:PHE:HB3	1:A:374:LYS:HD3	1.31	1.09

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	353/481 (73%)	304 (86%)	40 (11%)	9 (2%)	7	37
1	B	353/481 (73%)	299 (85%)	40 (11%)	14 (4%)	4	24
1	C	353/481 (73%)	290 (82%)	56 (16%)	7 (2%)	9	43
1	D	353/481 (73%)	299 (85%)	48 (14%)	6 (2%)	11	47
1	E	353/481 (73%)	302 (86%)	40 (11%)	11 (3%)	5	32
1	F	353/481 (73%)	289 (82%)	56 (16%)	8 (2%)	8	39
All	All	2118/2886 (73%)	1783 (84%)	280 (13%)	55 (3%)	7	36

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	72	ASP
1	B	403	ASP
1	B	412	TYR
1	C	403	ASP
1	D	310	THR

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	307/406 (76%)	254 (83%)	53 (17%)	2	11
1	B	307/406 (76%)	256 (83%)	51 (17%)	3	13
1	C	307/406 (76%)	250 (81%)	57 (19%)	2	9
1	D	307/406 (76%)	249 (81%)	58 (19%)	2	8
1	E	307/406 (76%)	260 (85%)	47 (15%)	3	16
1	F	307/406 (76%)	251 (82%)	56 (18%)	2	9
All	All	1842/2436 (76%)	1520 (82%)	322 (18%)	2	11

5 of 322 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	396	MET

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Mol	Chain	Res	Type
1	D	206	VAL
1	F	329	VAL
1	C	420	ASP
1	D	47	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	325	GLN
1	D	224	GLN
1	F	257	ASN
1	C	422	GLN
1	D	103	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 ⓘ

17 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	NAG	A	4471	1,3	14,14,15	0.67	0	15,19,21	0.77	1 (6%)
3	NAG	A	4472	3	14,14,15	1.07	1 (7%)	15,19,21	1.14	1 (6%)
3	BMA	A	4473	3	11,11,12	0.58	0	14,15,17	0.65	0
2	NAG	A	851	1,2	14,14,15	0.55	0	15,19,21	0.84	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	852	2	14,14,15	0.47	0	15,19,21	0.66	0
2	NAG	B	1911	1,2	14,14,15	0.81	0	15,19,21	1.32	3 (20%)
2	NAG	B	1912	2	14,14,15	0.80	1 (7%)	15,19,21	0.76	1 (6%)
2	NAG	B	851	1,2	14,14,15	0.49	0	15,19,21	0.85	1 (6%)
2	NAG	B	852	2	14,14,15	0.47	0	15,19,21	0.96	1 (6%)
2	NAG	C	851	1,2	14,14,15	0.53	0	15,19,21	0.78	0
2	NAG	C	852	2	14,14,15	0.45	0	15,19,21	0.87	1 (6%)
2	NAG	D	851	1,2	14,14,15	0.57	0	15,19,21	0.79	1 (6%)
2	NAG	D	852	2	14,14,15	0.66	0	15,19,21	0.75	1 (6%)
2	NAG	E	851	1,2	14,14,15	0.66	0	15,19,21	0.68	0
2	NAG	E	852	2	14,14,15	0.55	0	15,19,21	0.84	1 (6%)
2	NAG	F	851	1,2	14,14,15	0.54	0	15,19,21	0.77	1 (6%)
2	NAG	F	852	2	14,14,15	0.51	0	15,19,21	0.71	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
3	NAG	A	4471	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	4472	3	-	0/6/23/26	0/1/1/1
3	BMA	A	4473	3	-	0/2/19/22	0/1/1/1
2	NAG	A	851	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	852	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1911	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1912	2	-	0/6/23/26	0/1/1/1
2	NAG	B	851	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	852	2	-	0/6/23/26	0/1/1/1
2	NAG	C	851	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	852	2	-	0/6/23/26	0/1/1/1
2	NAG	D	851	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	852	2	-	0/6/23/26	0/1/1/1
2	NAG	E	851	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	852	2	-	0/6/23/26	0/1/1/1
2	NAG	F	851	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	852	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1912	NAG	C1-C2	2.04	1.55	1.52
3	A	4472	NAG	C1-C2	3.13	1.56	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	852	NAG	C2-N2-C7	-2.87	119.35	123.04
2	B	851	NAG	C2-N2-C7	-2.71	119.55	123.04
2	E	852	NAG	C2-N2-C7	-2.54	119.78	123.04
2	B	1911	NAG	C2-N2-C7	-2.54	119.78	123.04
2	B	852	NAG	C2-N2-C7	-2.44	119.91	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4471	NAG	2	0
3	A	4472	NAG	2	0
3	A	4473	BMA	3	0
2	A	851	NAG	2	0
2	A	852	NAG	5	0
2	B	1911	NAG	3	0
2	B	1912	NAG	3	0
2	B	851	NAG	1	0
2	B	852	NAG	1	0
2	C	852	NAG	1	0
2	D	852	NAG	1	0
2	E	852	NAG	1	0
2	F	851	NAG	2	0

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is

the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	4471	1	14,14,15	0.52	0	15,19,21	0.75	1 (6%)
4	NAG	D	1911	1	14,14,15	0.53	0	15,19,21	0.69	0
4	NAG	E	4471	1	14,14,15	0.77	1 (7%)	15,19,21	0.80	0
4	NAG	F	1911	1	14,14,15	0.77	1 (7%)	15,19,21	0.63	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	C	4471	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1911	1	-	0/6/23/26	0/1/1/1
4	NAG	E	4471	1	-	0/6/23/26	0/1/1/1
4	NAG	F	1911	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1911	NAG	C1-C2	2.06	1.55	1.52
4	E	4471	NAG	C1-C2	2.09	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	4471	NAG	C2-N2-C7	-2.35	120.02	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	4471	NAG	7	0
4	E	4471	NAG	5	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	357/481 (74%)	-0.22	14 (3%) 43 36	7, 34, 87, 100	0
1	B	357/481 (74%)	-0.18	15 (4%) 40 33	3, 35, 89, 100	0
1	C	357/481 (74%)	-0.19	15 (4%) 40 33	7, 33, 90, 100	0
1	D	357/481 (74%)	-0.22	13 (3%) 46 39	6, 33, 88, 100	0
1	E	357/481 (74%)	-0.17	11 (3%) 52 46	7, 34, 86, 100	0
1	F	357/481 (74%)	-0.22	8 (2%) 65 59	5, 33, 87, 99	0
All	All	2142/2886 (74%)	-0.20	76 (3%) 48 40	3, 34, 88, 100	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	173	SER	11.3
1	B	173	SER	4.8
1	F	174	GLN	4.3
1	E	172	LEU	4.2
1	E	412	TYR	4.2

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(\AA^2)	Q<0.9
2	NAG	A	851	14/15	0.90	0.40	3.99	49,55,64,65	0
2	NAG	D	851	14/15	0.89	0.23	0.97	48,59,71,73	0
2	NAG	C	851	14/15	0.92	0.26	0.74	34,40,49,52	0
2	NAG	F	851	14/15	0.94	0.18	-0.33	38,45,53,56	0
2	NAG	B	851	14/15	0.94	0.13	-1.08	46,53,56,59	0
2	NAG	E	851	14/15	0.90	0.16	-1.52	49,55,64,64	0
2	NAG	A	852	14/15	0.88	0.44	-	61,66,75,77	0
2	NAG	B	1911	14/15	0.76	0.66	-	84,90,95,96	0
3	NAG	A	4471	14/15	0.40	0.76	-	90,95,98,98	0
2	NAG	B	852	14/15	0.87	0.32	-	55,60,63,68	0
2	NAG	E	852	14/15	0.89	0.28	-	66,70,75,79	0
2	NAG	C	852	14/15	0.90	0.43	-	40,43,48,53	0
2	NAG	F	852	14/15	0.86	0.33	-	48,49,54,57	0
3	NAG	A	4472	14/15	0.53	0.98	-	97,100,100,100	0
2	NAG	D	852	14/15	0.85	0.29	-	66,72,73,75	0
2	NAG	B	1912	14/15	0.46	0.89	-	93,100,100,100	0
3	BMA	A	4473	11/12	0.72	0.81	-	98,100,100,100	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(\AA^2)	Q<0.9
4	NAG	F	1911	14/15	0.81	0.46	-	91,95,100,100	0
4	NAG	E	4471	14/15	0.72	0.56	-	84,90,100,100	0
4	NAG	D	1911	14/15	0.69	0.66	-	99,100,100,100	0
4	NAG	C	4471	14/15	0.78	0.47	-	79,86,91,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.