



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:31 PM GMT

PDB ID : 1FZD
Title : STRUCTURE OF RECOMBINANT ALPHAEC DOMAIN FROM HUMAN FIBRINOGEN-420
Authors : Spraggon, G.; Applegate, D.; Everse, S.J.; Zhang, J.-Z.; Veerapandian, L.; Redman, C.; Doolittle, R.F.; Grieninger, G.
Deposited on : 1998-06-22
Resolution : 2.10 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

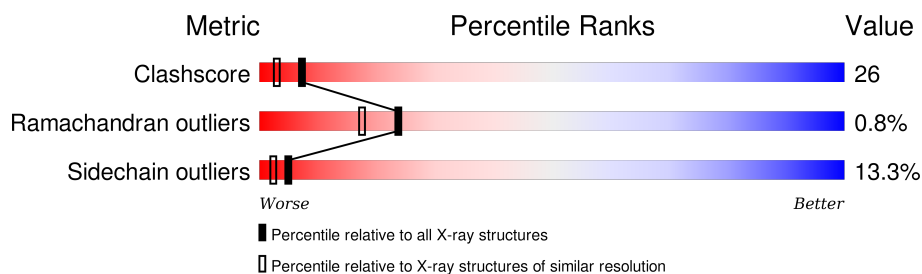
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	201	 69% 19% 7% ..
1	B	201	 73% 15% 7% ..
1	C	201	 71% 20% . . .
1	D	201	 71% 20% . . .
1	E	201	 61% 28% 7% ..
1	F	201	 63% 26% 8% ..
1	G	201	 60% 30% 6% ..

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Mol	Chain	Length	Quality of chain
1	H	201	

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	MAN	A	13	-	-	X	-
2	MAN	A	14	X	-	X	-
2	MAN	A	15	-	-	X	-
2	NAG	C	12	-	-	X	-
2	MAN	C	13	-	-	X	-
2	MAN	C	14	X	-	X	-
2	MAN	C	15	X	-	-	-
2	NAG	D	10	-	X	-	-
2	NAG	D	12	-	-	X	-
2	MAN	D	13	-	-	X	-
2	MAN	D	15	X	-	-	-
3	NAG	E	10	-	X	X	-
3	NAG	G	10	-	-	X	-
3	NAG	G	11	-	-	X	-
3	NAG	H	10	-	-	X	-
3	NAG	H	11	-	-	X	-
4	NAG	B	12	-	-	X	-
4	MAN	B	13	-	-	X	-
4	MAN	B	14	X	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13595 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 FIBRINOGEN-420.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	B	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	C	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	D	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	E	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	F	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	G	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	H	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			

- Molecule 2 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	6	Total	C	N	O	0	0
			75	42	3	30		
2	C	6	Total	C	N	O	0	0
			75	42	3	30		
2	D	6	Total	C	N	O	0	0
			75	42	3	30		

- Molecule 3 is SUGAR (6-MER) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	5	Total	C	N	O	0	0
			60	34	2	24		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	2	Total	C	N	O	1	0
			28	16	2	10		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total Ca 1 1	0	0
6	D	1	Total Ca 1 1	0	0
6	E	1	Total Ca 1 1	0	0
6	H	1	Total Ca 1 1	0	0
6	B	1	Total Ca 1 1	0	0
6	C	1	Total Ca 1 1	0	0
6	A	1	Total Ca 1 1	0	0
6	F	1	Total Ca 1 1	0	0

- Molecule 7 is water.

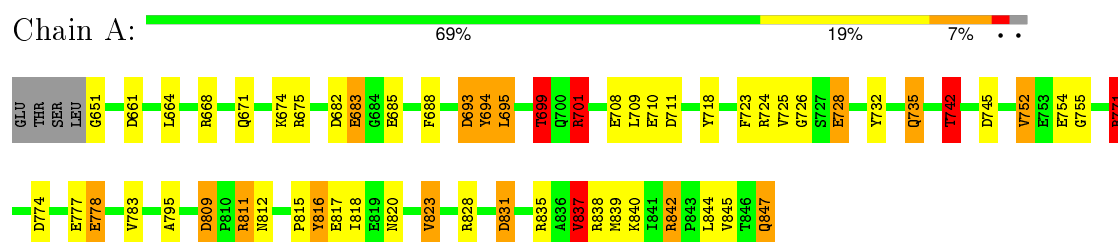
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	70	Total O 70 70	0	0
7	B	76	Total O 76 76	0	0
7	C	71	Total O 71 71	0	0
7	D	74	Total O 74 74	0	0
7	E	52	Total O 52 52	0	0
7	F	63	Total O 63 63	0	0
7	G	56	Total O 56 56	0	0
7	H	34	Total O 34 34	0	0

3 Residue-property plots [i](#)

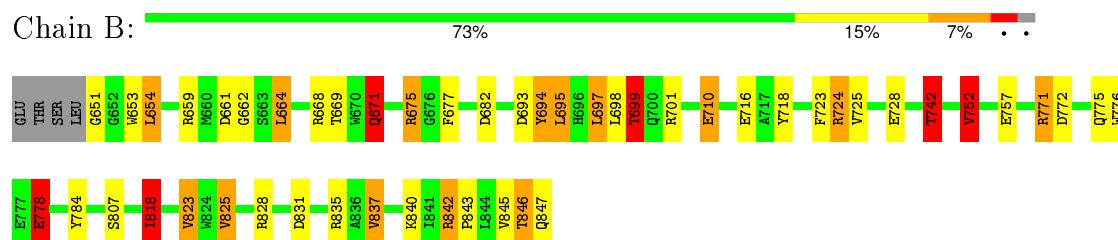
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

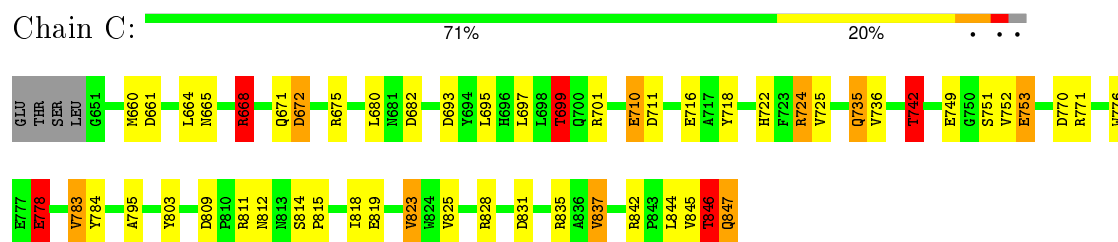
• Molecule 1: FIBRINOGEN-420



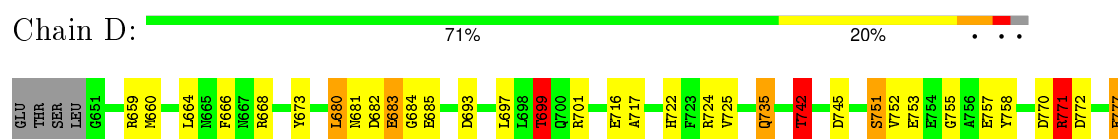
• Molecule 1: FIBRINOGEN-420



• Molecule 1: FIBRINOGEN-420



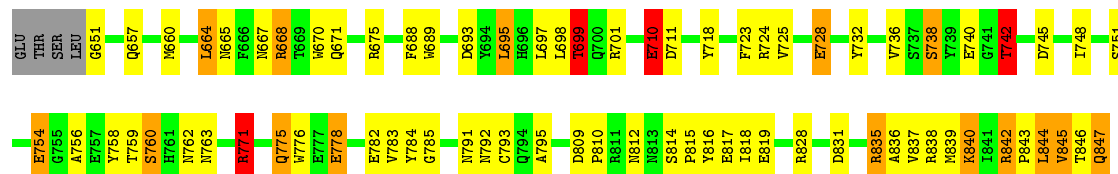
• Molecule 1: FIBRINOGEN-420





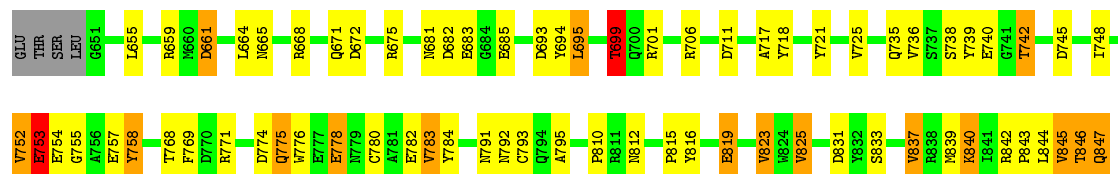
• Molecule 1: FIBRINOGEN-420

Chain E:



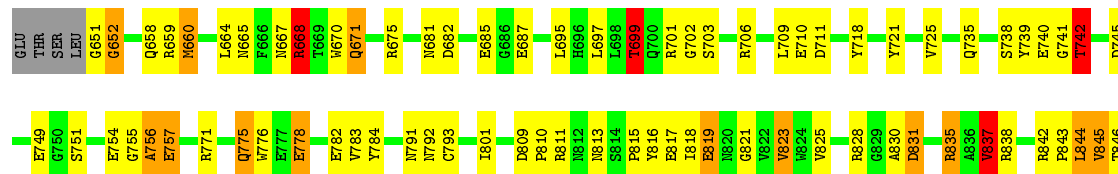
• Molecule 1: FIBRINOGEN-420

Chain F:



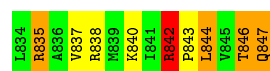
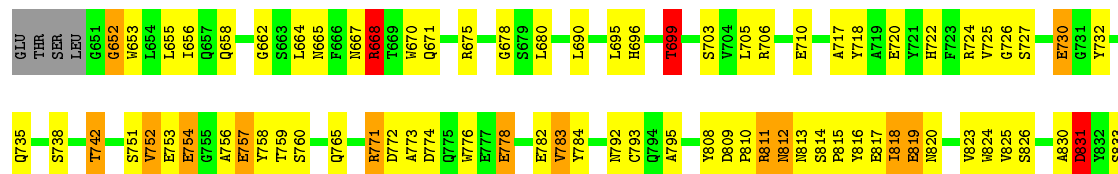
• Molecule 1: FIBRINOGEN-420

Chain G:



• Molecule 1: FIBRINOGEN-420

Chain H:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.25Å 105.18Å 71.14Å 104.60° 108.95° 71.47°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	91.2 (20.00-2.10)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC, X-PLOR	Depositor
R, R_{free}	0.195 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13595	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.85	0/1628	1.96	46/2208 (2.1%)
1	B	0.82	0/1628	1.81	37/2208 (1.7%)
1	C	0.77	0/1628	1.66	28/2208 (1.3%)
1	D	0.79	0/1628	1.75	29/2208 (1.3%)
1	E	0.60	0/1628	1.41	26/2208 (1.2%)
1	F	0.58	0/1628	1.35	14/2208 (0.6%)
1	G	0.56	0/1628	1.34	12/2208 (0.5%)
1	H	0.52	0/1628	1.41	16/2208 (0.7%)
All	All	0.70	0/13024	1.60	208/17664 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	2
1	G	0	1
2	A	1	0
2	C	2	0
2	D	1	0
4	B	1	0
All	All	5	8

There are no bond length outliers.

The worst 5 of 208 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	771	ARG	CD-NE-CZ	37.32	175.85	123.60
1	B	771	ARG	CD-NE-CZ	28.31	163.23	123.60
1	D	668	ARG	NE-CZ-NH2	-17.90	111.35	120.30
1	D	659	ARG	NE-CZ-NH1	16.59	128.60	120.30
1	B	840	LYS	CA-CB-CG	13.12	142.26	113.40

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	14	MAN	C1
4	B	14	MAN	C1
2	C	14	MAN	C1
2	C	15	MAN	C1
2	D	15	MAN	C1

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	795	ALA	Mainchain
1	B	723	PHE	Mainchain
1	C	846	THR	Mainchain
1	D	666	PHE	Mainchain
1	D	803	TYR	Mainchain

5.2 Too-close contacts

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	1585	0	1421	29	0
1	B	1585	0	1418	42	0
1	C	1585	0	1420	31	5
1	D	1585	0	1421	33	1
1	E	1585	0	1422	58	0
1	F	1585	0	1421	108	0
1	G	1585	0	1422	107	0
1	H	1585	0	1422	114	6
2	A	75	0	64	19	0
2	C	75	0	64	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	75	0	64	12	0
3	B	14	0	10	5	0
3	E	28	0	26	17	0
3	G	28	0	26	13	0
3	H	28	0	26	17	0
4	B	60	0	49	25	0
5	F	28	0	25	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	70	0	0	4	0
7	B	76	0	0	8	0
7	C	71	0	0	0	0
7	D	74	0	0	7	0
7	E	52	0	0	5	0
7	F	63	0	0	3	0
7	G	56	0	0	7	0
7	H	34	0	0	6	0
All	All	13595	0	11721	641	6

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 26.

The worst 5 of 641 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:F:758:TYR:CD1	1:F:792:ASN:HB3	1.25	1.63
3:B:10:NAG:C2	3:B:10:NAG:C3	1.76	1.61
1:F:842:ARG:CZ	1:F:847:GLN:HB2	1.25	1.61
1:E:667:ASN:HD21	3:E:10:NAG:C1	0.99	1.61
1:F:842:ARG:CZ	1:F:847:GLN:CB	1.83	1.56

The worst 5 of 6 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)
1:C:847:GLN:OXT	1:H:678:GLY:O[1_445]	0.94	1.26
1:D:847:GLN:O	1:H:722:HIS:ND1[1_545]	1.73	0.47
1:C:847:GLN:C	1:H:678:GLY:O[1_445]	1.88	0.32
1:C:847:GLN:NE2	1:H:680:LEU:O[1_445]	2.03	0.17
1:C:847:GLN:OXT	1:H:678:GLY:C[1_445]	2.13	0.07

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	195/201 (97%)	184 (94%)	11 (6%)	0	100	100
1	B	195/201 (97%)	188 (96%)	7 (4%)	0	100	100
1	C	195/201 (97%)	184 (94%)	10 (5%)	1 (0%)	34	30
1	D	195/201 (97%)	183 (94%)	11 (6%)	1 (0%)	34	30
1	E	195/201 (97%)	187 (96%)	7 (4%)	1 (0%)	34	30
1	F	195/201 (97%)	181 (93%)	10 (5%)	4 (2%)	9	3
1	G	195/201 (97%)	176 (90%)	16 (8%)	3 (2%)	13	7
1	H	195/201 (97%)	175 (90%)	17 (9%)	3 (2%)	13	7
All	All	1560/1608 (97%)	1458 (94%)	89 (6%)	13 (1%)	24	17

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	846	THR
1	G	756	ALA
1	C	846	THR
1	F	754	GLU
1	H	652	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	159/163 (98%)	138 (87%)	21 (13%)	5	2
1	B	159/163 (98%)	140 (88%)	19 (12%)	6	3
1	C	159/163 (98%)	143 (90%)	16 (10%)	9	5
1	D	159/163 (98%)	141 (89%)	18 (11%)	7	4
1	E	159/163 (98%)	137 (86%)	22 (14%)	4	2
1	F	159/163 (98%)	131 (82%)	28 (18%)	2	1
1	G	159/163 (98%)	137 (86%)	22 (14%)	4	2
1	H	159/163 (98%)	136 (86%)	23 (14%)	4	2
All	All	1272/1304 (98%)	1103 (87%)	169 (13%)	5	2

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	675	ARG
1	E	844	LEU
1	H	778	GLU
1	E	695	LEU
1	E	751	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	813	ASN
1	G	658	GLN
1	G	792	ASN
1	E	667	ASN
1	F	763	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 ⓘ

25 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$
2	NAG	A	10	1,2	14,14,15	0.86	1 (7%)	15,19,21	0.78	0
2	NAG	A	11	2	14,14,15	0.54	0	15,19,21	1.18	3 (20%)
2	NAG	A	12	2	14,14,15	0.61	0	15,19,21	1.32	1 (6%)
2	MAN	A	13	2	11,11,12	0.78	0	14,15,17	0.75	0
2	MAN	A	14	2	11,11,12	0.89	1 (9%)	14,15,17	1.82	3 (21%)
2	MAN	A	15	2	11,11,12	0.95	0	14,15,17	1.86	2 (14%)
4	NDG	B	11	3,4	14,14,15	0.83	0	15,19,21	0.79	1 (6%)
4	NAG	B	12	4	14,14,15	0.86	0	15,19,21	1.49	2 (13%)
4	MAN	B	13	4	11,11,12	1.46	2 (18%)	14,15,17	1.71	3 (21%)
4	MAN	B	14	4	11,11,12	0.85	0	14,15,17	2.22	3 (21%)
4	MAN	B	15	4	10,10,12	0.69	0	14,14,17	1.20	2 (14%)
2	NAG	C	10	1,2	14,14,15	0.46	0	15,19,21	0.69	0
2	NAG	C	11	2	14,14,15	0.67	0	15,19,21	1.34	2 (13%)
2	NAG	C	12	2	14,14,15	0.89	0	15,19,21	0.79	0
2	MAN	C	13	2	11,11,12	0.66	0	14,15,17	1.09	1 (7%)
2	MAN	C	14	2	11,11,12	0.59	0	14,15,17	1.12	1 (7%)
2	MAN	C	15	2	11,11,12	0.93	1 (9%)	14,15,17	1.13	2 (14%)
2	NAG	D	10	1,2	14,14,15	6.07	11 (78%)	15,19,21	5.69	13 (86%)
2	NAG	D	11	2	14,14,15	0.79	1 (7%)	15,19,21	0.95	1 (6%)
2	NAG	D	12	2	14,14,15	0.91	1 (7%)	15,19,21	2.13	4 (26%)
2	MAN	D	13	2	11,11,12	0.81	0	14,15,17	1.26	1 (7%)
2	MAN	D	14	2	11,11,12	1.02	1 (9%)	14,15,17	1.75	4 (28%)
2	MAN	D	15	2	11,11,12	0.69	0	14,15,17	1.34	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	F	10	1,5	14,14,15	0.64	0	15,19,21	1.08	1 (6%)
5	NAG	F	11	5	14,14,15	0.77	0	15,19,21	1.48	3 (20%)

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
2	NAG	A	10	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	11	2	-	0/6/23/26	0/1/1/1
2	NAG	A	12	2	-	0/6/23/26	0/1/1/1
2	MAN	A	13	2	-	0/2/19/22	0/1/1/1
2	MAN	A	14	2	1/1/4/5	0/2/19/22	1/1/1/1
2	MAN	A	15	2	-	0/2/19/22	0/1/1/1
4	NDG	B	11	3,4	-	0/6/23/26	0/1/1/1
4	NAG	B	12	4	-	0/6/23/26	0/1/1/1
4	MAN	B	13	4	-	0/2/19/22	0/1/1/1
4	MAN	B	14	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	B	15	4	-	0/0/17/22	0/1/1/1
2	NAG	C	10	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	11	2	-	0/6/23/26	0/1/1/1
2	NAG	C	12	2	-	0/6/23/26	0/1/1/1
2	MAN	C	13	2	-	0/2/19/22	0/1/1/1
2	MAN	C	14	2	1/1/4/5	0/2/19/22	0/1/1/1
2	MAN	C	15	2	1/1/4/5	0/2/19/22	1/1/1/1
2	NAG	D	10	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	11	2	-	0/6/23/26	0/1/1/1
2	NAG	D	12	2	-	0/6/23/26	0/1/1/1
2	MAN	D	13	2	-	0/2/19/22	0/1/1/1
2	MAN	D	14	2	-	0/2/19/22	0/1/1/1
2	MAN	D	15	2	1/1/4/5	0/2/19/22	0/1/1/1
5	NAG	F	10	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	11	5	-	0/6/23/26	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	10	NAG	O7-C7	-9.67	1.00	1.23
2	D	10	NAG	C8-C7	-7.89	1.34	1.50
2	D	10	NAG	C4-C5	-3.00	1.46	1.53
2	D	14	MAN	C2-C3	-2.41	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	12	NAG	C8-C7	2.00	1.54	1.50

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	10	NAG	O7-C7-N2	-9.43	102.65	121.86
2	D	10	NAG	O4-C4-C3	-8.15	91.99	110.34
2	D	10	NAG	O6-C6-C5	-6.77	88.96	111.33
2	D	10	NAG	C3-C4-C5	-6.42	99.01	110.20
2	D	12	NAG	C2-N2-C7	-6.18	115.09	123.04

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	14	MAN	C1
2	D	15	MAN	C1
2	A	14	MAN	C1
4	B	14	MAN	C1
2	C	15	MAN	C1

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	15	MAN	C1-C2-C3-C4-C5-O5
2	A	14	MAN	C1-C2-C3-C4-C5-O5

19 monomers are involved in 84 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	11	NAG	4	0
2	A	12	NAG	3	0
2	A	13	MAN	6	0
2	A	14	MAN	13	0
2	A	15	MAN	9	0
4	B	11	NDG	1	0
4	B	12	NAG	9	0
4	B	13	MAN	17	0
4	B	14	MAN	15	0
4	B	15	MAN	5	0
2	C	11	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	12	NAG	12	0
2	C	13	MAN	22	0
2	C	14	MAN	13	0
2	C	15	MAN	3	0
2	D	12	NAG	8	0
2	D	13	MAN	12	0
2	D	14	MAN	4	0
5	F	10	NAG	1	0

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 for Mogul analysis.

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	B	10	1,4	14,14,15	6.72	12 (85%)	15,19,21	3.83	9 (60%)
3	NAG	E	10	1,3	14,14,15	8.21	11 (78%)	15,19,21	6.05	12 (80%)
3	NAG	E	11	3	14,14,15	0.58	0	15,19,21	0.81	1 (6%)
3	NAG	G	10	1	14,14,15	0.55	0	15,19,21	1.40	2 (13%)
3	NAG	G	11	-	14,14,15	0.52	0	15,19,21	1.21	2 (13%)
3	NAG	H	10	1	14,14,15	0.50	0	15,19,21	1.12	2 (13%)
3	NAG	H	11	-	14,14,15	0.71	0	15,19,21	0.92	1 (6%)

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	B	10	1,4	-	0/6/23/26	0/1/1/1
3	NAG	E	10	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	11	3	-	0/6/23/26	0/1/1/1
3	NAG	G	10	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	11	-	-	0/6/23/26	0/1/1/1
3	NAG	H	10	1	-	0/6/23/26	0/1/1/1
3	NAG	H	11	-	-	0/6/23/26	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	10	NAG	C1-C2	-15.90	1.30	1.52
3	B	10	NAG	O3-C3	-13.78	1.10	1.43
3	B	10	NAG	C1-C2	-6.37	1.43	1.52
3	E	10	NAG	C2-N2	-4.76	1.37	1.46
3	B	10	NAG	O4-C4	-4.71	1.31	1.43

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	10	NAG	C2-N2-C7	-11.91	107.74	123.04
3	E	10	NAG	O5-C5-C6	-11.72	81.97	107.35
3	B	10	NAG	O7-C7-N2	-9.00	103.52	121.86
3	E	10	NAG	O6-C6-C5	-7.33	87.10	111.33
3	B	10	NAG	C3-C2-N2	-5.20	98.11	110.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	10	NAG	5	0
3	E	10	NAG	17	0
3	E	11	NAG	2	0
3	G	10	NAG	13	0
3	G	11	NAG	9	0
3	H	10	NAG	15	0
3	H	11	NAG	10	0

5.7 Other polymers ⓘ

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 ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.