



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:04 AM GMT

PDB ID : 2FFD
Title : Fibrinogen Fragment D with "A" knob peptide mimic GPRVVE
Authors : Betts, L.
Deposited on : 2005-12-19
Resolution : 2.89 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

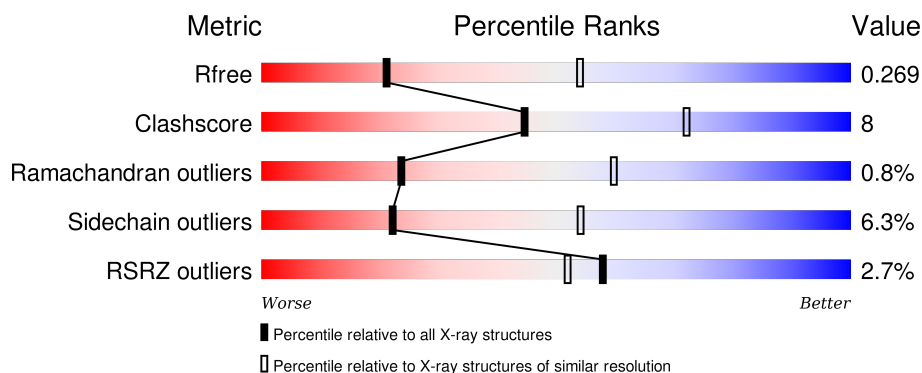
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	66	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>• •</div> </div> </div>
1	D	66	<div> <div>11%</div> <div> <div></div> <div>71%</div> <div>14%</div> <div>• 14%</div> </div> </div>
2	B	313	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>
2	E	313	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>• 6%</div> </div> </div>
3	C	311	<div> <div>•</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	311	<p>4% 73% 16% 8%</p>
4	G	6	<p>33% 33% 33%</p>
4	H	6	<p>50% 17% 33%</p>
4	I	6	<p>33% 17% 17% 33%</p>
4	J	6	<p>50% 17% 33%</p>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10894 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 alpha/alpha-E Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	65	Total	C	N	O	S	0	0	0
			530	327	100	100	3			
1	D	57	Total	C	N	O	S	0	0	0
			466	286	88	89	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2428	1515	429	462	22			
2	E	295	Total	C	N	O	S	0	0	0
			2369	1480	418	449	22			

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	298	Total	C	N	O	S	0	0	0
			2391	1517	402	461	11			
3	F	285	Total	C	N	O	S	0	0	0
			2283	1450	384	438	11			

- Molecule 4 is a protein called GLY-PRO-ARG-VAL-VAL-GLU peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			29	18	7	4			
4	H	4	Total	C	N	O	0	0	0
			29	18	7	4			
4	I	4	Total	C	N	O	0	0	0
			29	18	7	4			
4	J	4	Total	C	N	O	0	0	0
			29	18	7	4			

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	3	Total	C	N	O	0	0
			38	22	2	14		
5	E	3	Total	C	N	O	0	0
			38	22	2	14		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		
6	F	1	Total	Ca	0	0
			1	1		
6	E	1	Total	Ca	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	10	Total	O	0	0
			10	10		
7	B	57	Total	O	0	0
			57	57		
7	C	26	Total	O	0	0
			26	26		
7	D	6	Total	O	0	0
			6	6		
7	E	76	Total	O	0	0
			76	76		
7	F	52	Total	O	0	0
			52	52		
7	H	1	Total	O	0	0
			1	1		
7	I	2	Total	O	0	0
			2	2		
7	J	1	Total	O	0	0
			1	1		

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.

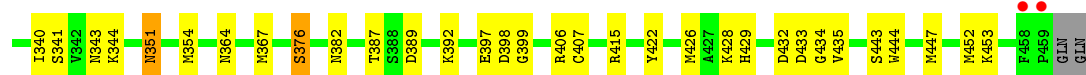
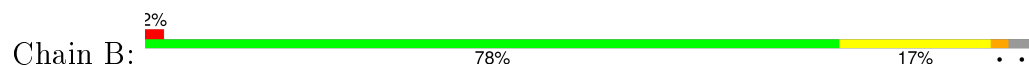
- Molecule 1: Fibrinogen alpha/alpha-E Chain



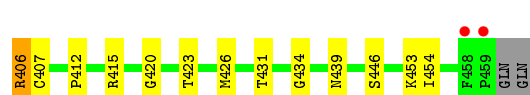
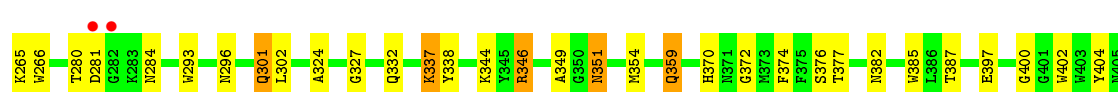
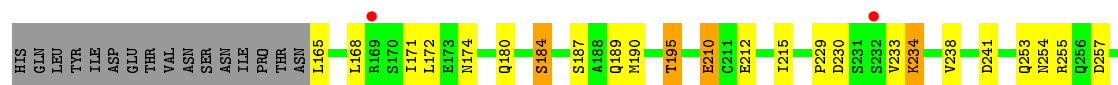
- Molecule 1: Fibrinogen alpha/alpha-E Chain



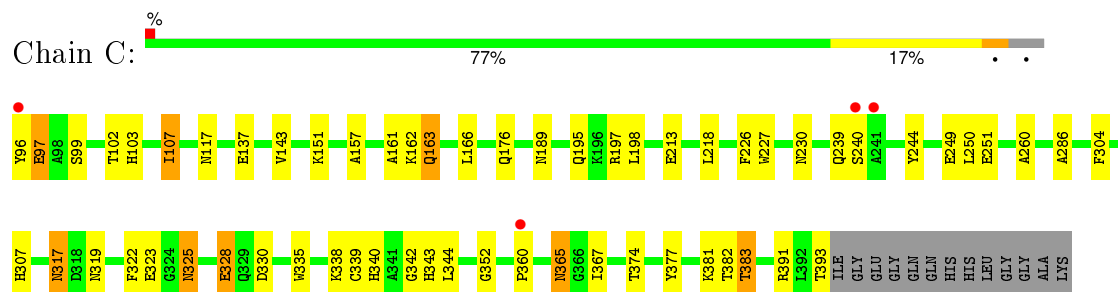
- Molecule 2: Fibrinogen beta chain



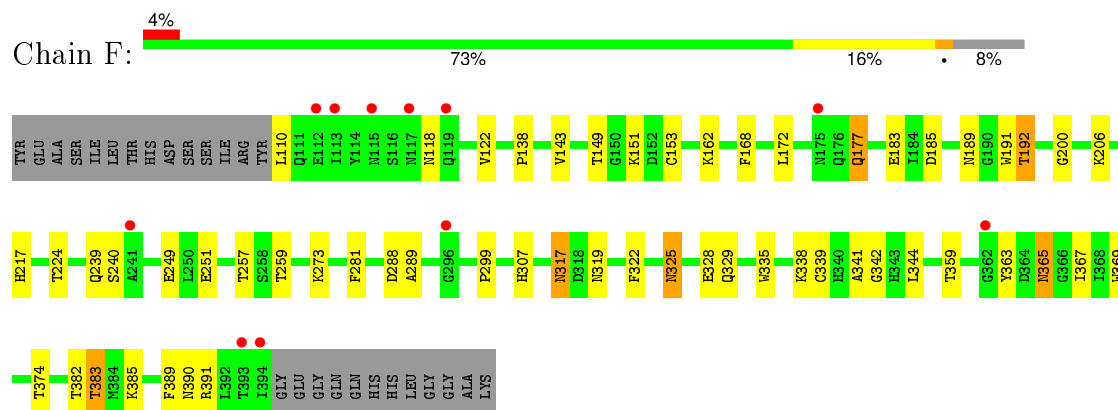
- Molecule 2: Fibrinogen beta chain



- Molecule 3: Fibrinogen gamma chain



- Molecule 3: Fibrinogen gamma chain



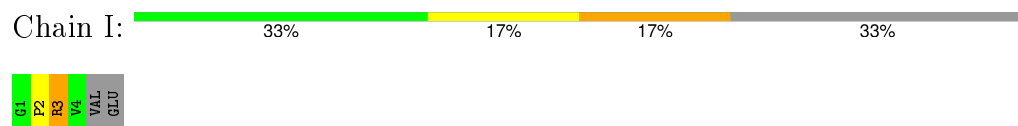
- Molecule 4: GLY-PRO-ARG-VAL-VAL-GLU peptide



- Molecule 4: GLY-PRO-ARG-VAL-VAL-GLU peptide



- Molecule 4: GLY-PRO-ARG-VAL-VAL-GLU peptide



- Molecule 4: GLY-PRO-ARG-VAL-VAL-GLU peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.52Å 94.65Å 227.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.89 17.86 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.7 (20.00-2.89) 98.2 (17.86-2.89)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.87Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.211 , 0.268 0.215 , 0.269	Depositor DCC
R_{free} test set	2160 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 42903 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10894	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	0.39	0/531	0.54	0/709
1	D	0.38	0/466	0.59	0/621
2	B	0.42	0/2490	0.56	0/3364
2	E	0.44	0/2430	0.60	0/3280
3	C	0.40	0/2457	0.51	0/3324
3	F	0.44	0/2346	0.55	0/3173
4	G	0.65	0/29	0.53	0/38
4	H	0.66	0/29	0.61	0/38
4	I	0.73	0/29	0.69	0/38
4	J	0.52	0/29	0.46	0/38
All	All	0.42	0/10836	0.56	0/14623

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	530	0	556	12	0
1	D	466	0	488	7	0
2	B	2428	0	2295	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2369	0	2238	46	0
3	C	2391	0	2235	35	0
3	F	2283	0	2138	41	0
4	G	29	0	34	0	0
4	H	29	0	34	5	0
4	I	29	0	34	2	0
4	J	29	0	34	2	0
5	B	38	0	34	2	0
5	E	38	0	34	4	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	A	10	0	0	0	0
7	B	57	0	0	0	0
7	C	26	0	0	0	0
7	D	6	0	0	0	0
7	E	76	0	0	2	0
7	F	52	0	0	4	0
7	H	1	0	0	0	0
7	I	2	0	0	0	0
7	J	1	0	0	1	0
All	All	10894	0	10154	164	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 8.

The worst 5 of 164 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)
2:B:343:ASN:OD1	2:B:344:LYS:HE3	1.70	0.92
3:F:153:CYS:SG	3:F:192:THR:HB	2.16	0.85
2:E:359:GLN:HE21	2:E:359:GLN:H	1.22	0.83
1:A:169:LEU:H	2:B:189:GLN:HE22	1.31	0.78
1:A:164:SER:HB3	3:C:137:GLU:O	1.85	0.76

There are no symmetry-related clashes.

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	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
1	D	55/66 (83%)	53 (96%)	2 (4%)	0	100	100
2	B	301/313 (96%)	280 (93%)	19 (6%)	2 (1%)	26	63
2	E	293/313 (94%)	271 (92%)	21 (7%)	1 (0%)	46	79
3	C	296/311 (95%)	271 (92%)	21 (7%)	4 (1%)	14	44
3	F	283/311 (91%)	264 (93%)	17 (6%)	2 (1%)	26	63
4	G	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
4	H	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
4	I	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
4	J	2/6 (33%)	0	2 (100%)	0	100	100
All	All	1299/1404 (92%)	1203 (93%)	86 (7%)	10 (1%)	24	60

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	198	LEU
3	C	240	SER
2	E	281	ASP
4	G	2	PRO
3	C	97	GLU

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	60/61 (98%)	56 (93%)	4 (7%)	20	50
1	D	53/61 (87%)	49 (92%)	4 (8%)	17	44
2	B	261/271 (96%)	250 (96%)	11 (4%)	36	73
2	E	253/271 (93%)	233 (92%)	20 (8%)	15	41
3	C	251/259 (97%)	235 (94%)	16 (6%)	22	53
3	F	239/259 (92%)	226 (95%)	13 (5%)	27	62
4	G	3/5 (60%)	2 (67%)	1 (33%)	0	1
4	H	3/5 (60%)	2 (67%)	1 (33%)	0	1
4	I	3/5 (60%)	2 (67%)	1 (33%)	0	1
4	J	3/5 (60%)	3 (100%)	0	100	100
All	All	1129/1202 (94%)	1058 (94%)	71 (6%)	22	54

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	175	LEU
2	E	195	THR
3	F	374	THR
1	D	176	LYS
2	E	184	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	317	ASN
2	E	253	GLN
3	F	317	ASN
3	C	319	ASN
3	C	365	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 ⓘ

6 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$
5	NAG	B	3	2,5	14,14,15	0.69	0	15,19,21	0.71	1 (6%)
5	NAG	B	4	5	14,14,15	0.75	1 (7%)	15,19,21	0.78	1 (6%)
5	FUC	B	5	5	10,10,11	0.63	0	14,14,16	0.51	0
5	NAG	E	3	2,5	14,14,15	0.63	0	15,19,21	1.31	2 (13%)
5	NAG	E	4	5	14,14,15	0.58	0	15,19,21	0.66	0
5	FUC	E	5	5	10,10,11	0.77	0	14,14,16	0.97	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
5	NAG	B	3	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	4	5	-	0/6/23/26	0/1/1/1
5	FUC	B	5	5	-	0/0/17/20	0/1/1/1
5	NAG	E	3	2,5	-	0/6/23/26	0/1/1/1
5	NAG	E	4	5	-	0/6/23/26	0/1/1/1
5	FUC	E	5	5	-	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4	NAG	C1-C2	2.05	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	3	NAG	C2-N2-C7	-2.45	119.89	123.04
5	B	4	NAG	C2-N2-C7	-2.07	120.39	123.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3	NAG	C2-N2-C7	-2.04	120.42	123.04
5	E	3	NAG	C3-C4-C5	2.67	114.85	110.20
5	E	5	FUC	C1-C2-C3	2.73	112.77	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	3	NAG	2	0
5	E	3	NAG	4	0
5	E	5	FUC	4	0

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	65/66 (98%)	0.11	1 (1%) 76 74	26, 53, 78, 81	0
1	D	57/66 (86%)	0.42	7 (12%) 5 3	27, 56, 96, 99	0
2	B	303/313 (96%)	-0.23	7 (2%) 64 59	22, 35, 55, 82	0
2	E	295/313 (94%)	-0.40	6 (2%) 68 64	14, 23, 53, 88	0
3	C	298/311 (95%)	-0.13	4 (1%) 79 78	25, 41, 65, 82	0
3	F	285/311 (91%)	-0.22	11 (3%) 43 36	17, 29, 50, 84	0
4	G	4/6 (66%)	1.03	0 100 100	72, 72, 72, 73	0
4	H	4/6 (66%)	-0.37	0 100 100	31, 31, 32, 33	0
4	I	4/6 (66%)	0.04	0 100 100	33, 34, 34, 37	0
4	J	4/6 (66%)	0.26	0 100 100	53, 54, 54, 55	0
All	All	1319/1404 (93%)	-0.19	36 (2%) 58 52	14, 33, 72, 99	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	393	THR	5.1
3	F	394	ILE	4.2
1	D	187	GLN	4.2
1	A	126	VAL	4.0
3	F	112	GLU	3.9

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
5	NAG	B	4	14/15	0.36	0.64	-	100,102,103,103	0
5	FUC	B	5	10/11	0.58	0.48	-	96,97,98,99	0
5	FUC	E	5	10/11	0.68	0.53	-	71,72,72,73	0
5	NAG	E	3	14/15	0.78	0.31	-	53,58,69,70	0
5	NAG	B	3	14/15	0.78	0.40	-	85,88,95,96	0
5	NAG	E	4	14/15	0.74	0.49	-	76,78,79,81	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
6	CA	E	602	1/1	0.97	0.12	-0.99	28,28,28,28	0
6	CA	F	603	1/1	0.94	0.07	-2.36	24,24,24,24	0
6	CA	C	601	1/1	0.97	0.04	-2.44	33,33,33,33	0
6	CA	B	600	1/1	0.95	0.12	-	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.