



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 09:29 PM UTC

PDB ID : 2FT3 / pdb_00002ft3
Title : Crystal structure of the biglycan dimer core protein
Authors : Scott, P.G.; Dodd, C.M.; Bergmann, E.M.
Deposited on : 2006-01-23
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

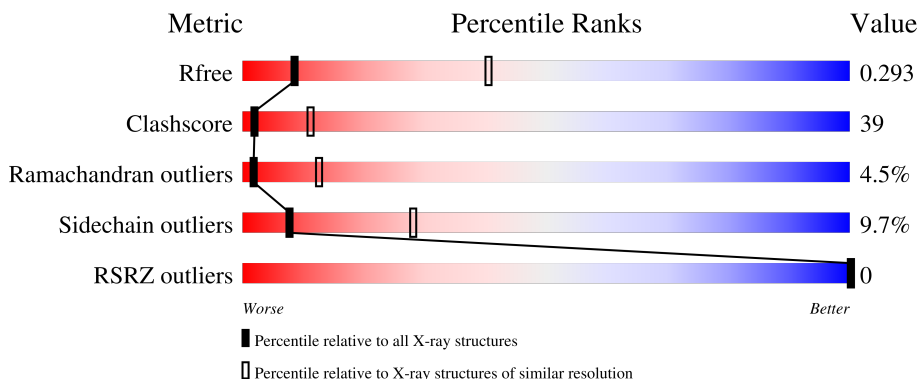
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	332	
1	B	332	
1	C	332	
1	D	332	
1	E	332	

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Mol	Chain	Length	Quality of chain
1	F	332	

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
3	FLC	D	2193	-	-	X	-

2 Entry composition [i](#)

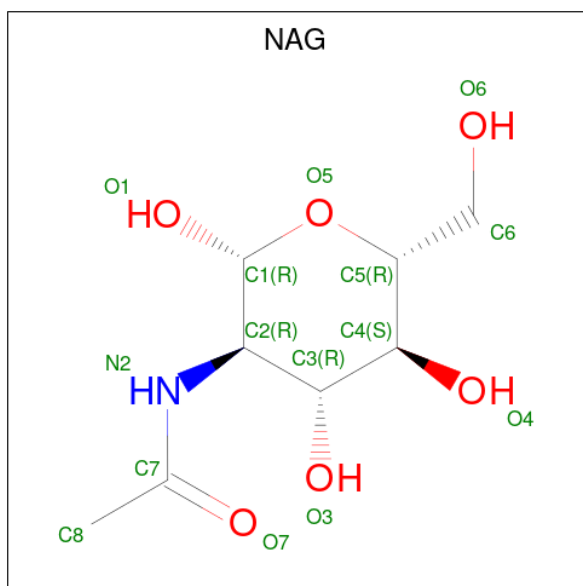
There are 3 unique types of molecules in this entry. The entry contains 14674 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Biglycan.

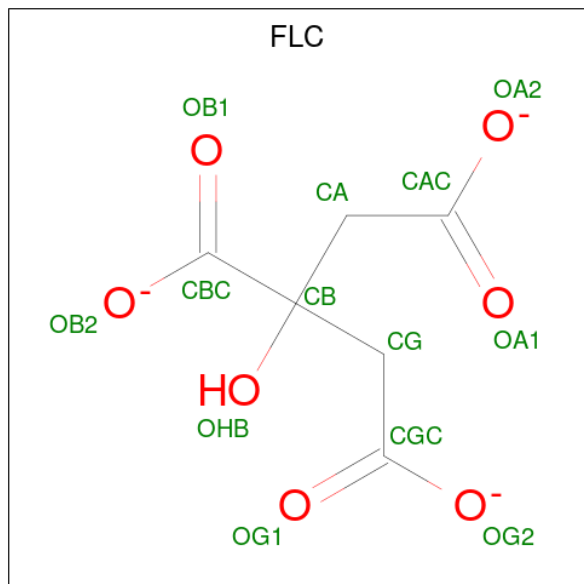
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	303	Total 2416	C 1545	N 428	O 432	S 11	0	0	0
1	B	303	Total 2416	C 1545	N 428	O 432	S 11	0	0	0
1	C	303	Total 2416	C 1545	N 428	O 432	S 11	0	0	0
1	D	304	Total 2420	C 1547	N 429	O 433	S 11	0	0	0
1	E	303	Total 2416	C 1545	N 428	O 432	S 11	0	0	0
1	F	305	Total 2428	C 1551	N 431	O 435	S 11	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7^-$).



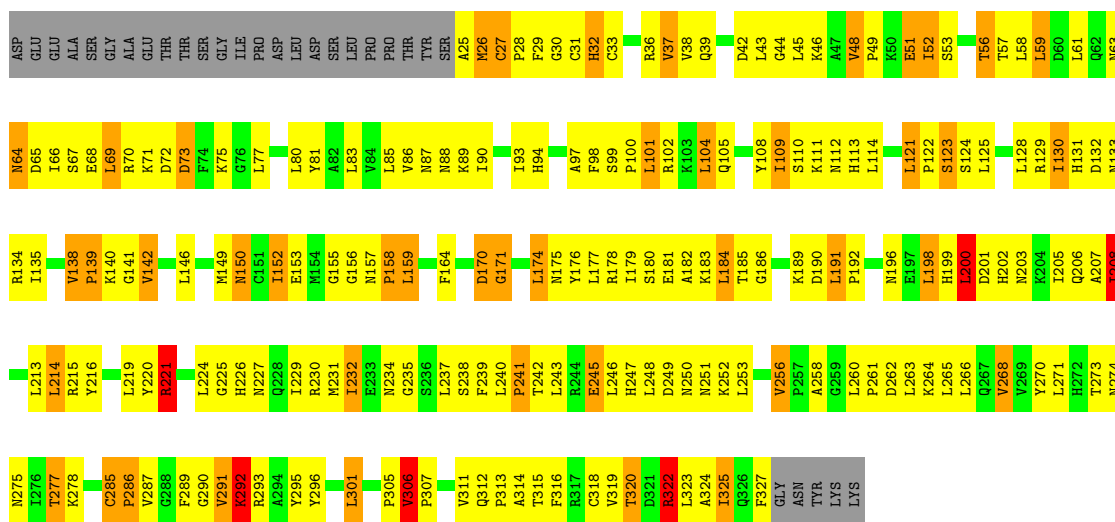
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			13	6 7		
3	B	1	Total	C O	0	0
			13	6 7		
3	C	1	Total	C O	0	0
			13	6 7		
3	D	1	Total	C O	0	0
			13	6 7		
3	E	1	Total	C O	0	0
			13	6 7		
3	F	1	Total	C O	0	0
			13	6 7		

3 Residue-property plots


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

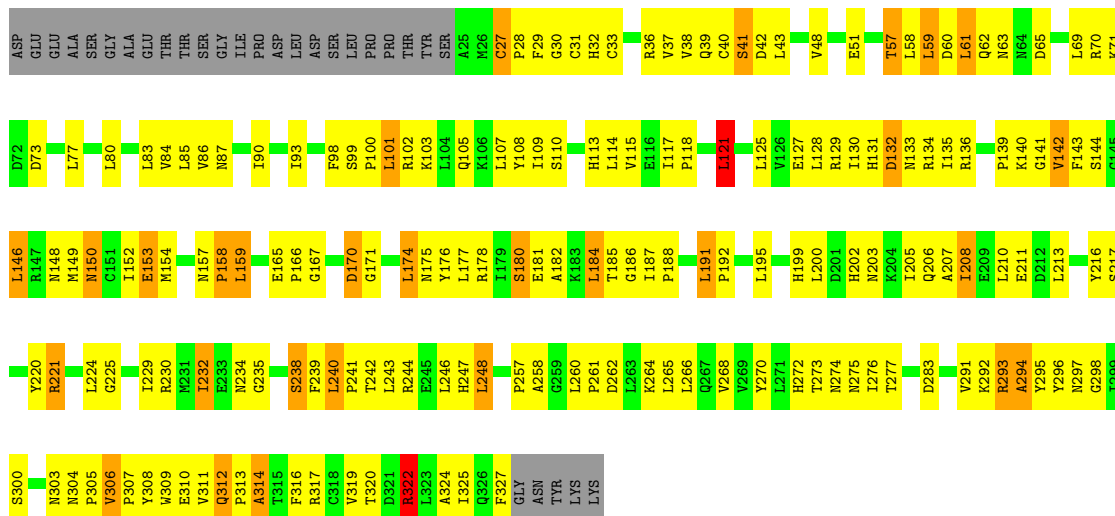
- Molecule 1: Biglycan

Chain A: 



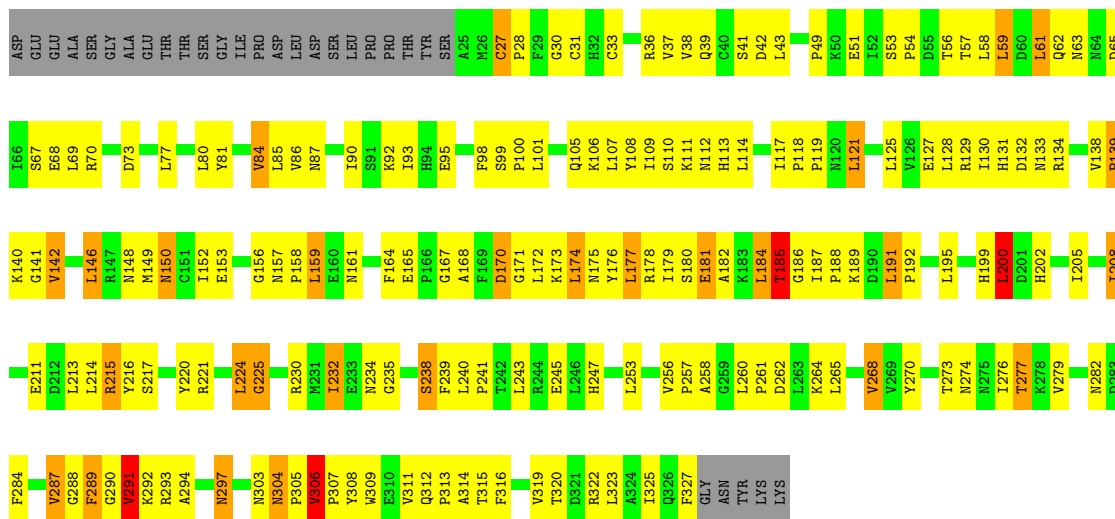
- Molecule 1: Biglycan

Chain B: 



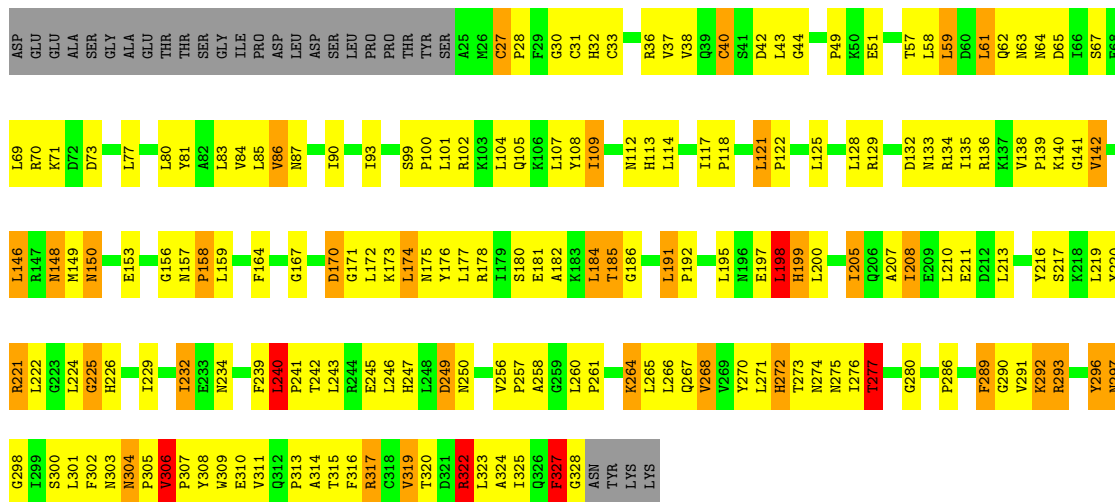
- Molecule 1: Biglycan

Chain C: 37% 45% 8% 9%



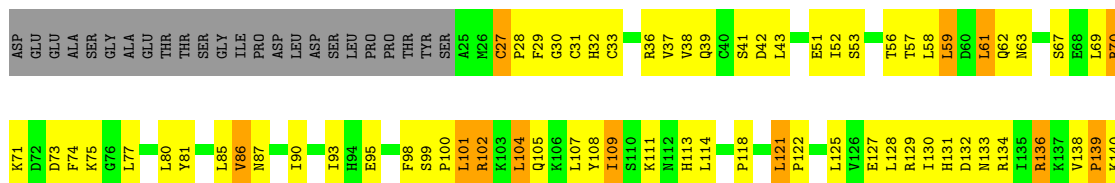
- Molecule 1: Biglycan

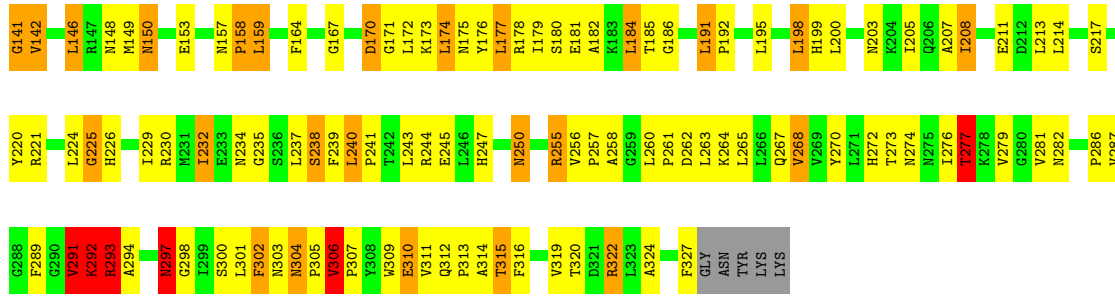
Chain D: 37% 42% 11% 8%



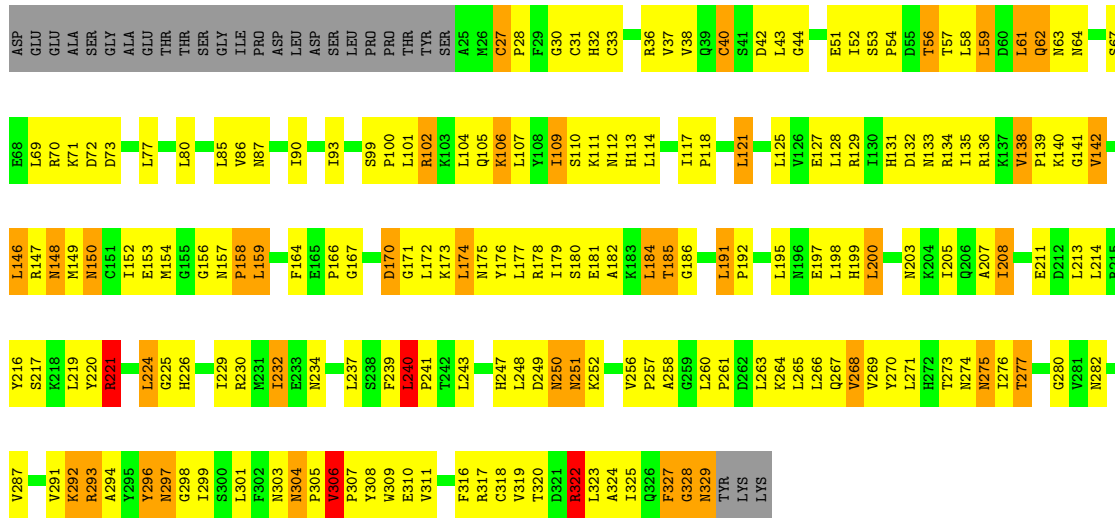
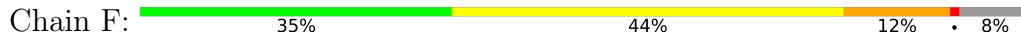
- Molecule 1: Biglycan

Chain E: 36% 42% 11% 9%





• Molecule 1: Biglycan



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	206.51Å 119.22Å 140.62Å 90.00° 116.61° 90.00°	Depositor
Resolution (Å)	23.00 – 3.40 23.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (23.00-3.40) 96.5 (23.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.37Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.258 , 0.291 (Not available) , 0.293	Depositor DCC
R_{free} test set	2040 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.098 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-1$ 0.090 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-1$	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14674	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, 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	1.39	11/2468 (0.4%)	1.49	21/3342 (0.6%)
1	B	1.32	8/2468 (0.3%)	1.47	20/3342 (0.6%)
1	C	1.29	7/2468 (0.3%)	1.46	23/3342 (0.7%)
1	D	1.34	12/2472 (0.5%)	1.45	25/3347 (0.7%)
1	E	1.32	11/2468 (0.4%)	1.50	31/3342 (0.9%)
1	F	1.36	14/2480 (0.6%)	1.42	16/3358 (0.5%)
All	All	1.34	63/14824 (0.4%)	1.47	136/20073 (0.7%)

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	62	GLN	CD-NE2	-9.05	1.14	1.33
1	B	291	VAL	CA-CB	8.89	1.66	1.54
1	C	291	VAL	CA-CB	8.53	1.66	1.54
1	A	64	ASN	CA-C	-7.37	1.46	1.53
1	D	205	ILE	CA-CB	7.31	1.63	1.54

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	27	CYS	N-CA-C	12.81	124.87	110.13
1	A	27	CYS	N-CA-C	11.86	125.93	110.40
1	D	27	CYS	N-CA-C	11.59	123.46	110.13
1	E	244	ARG	NE-CZ-NH2	11.33	129.40	119.20
1	C	27	CYS	N-CA-C	10.84	122.60	110.13

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	2416	0	2466	229	0
1	B	2416	0	2466	169	0
1	C	2416	0	2466	190	0
1	D	2420	0	2469	175	0
1	E	2416	0	2466	181	0
1	F	2428	0	2475	200	0
2	A	14	0	13	5	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	1	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
3	A	13	0	5	0	0
3	B	13	0	5	3	0
3	C	13	0	5	3	0
3	D	13	0	5	7	0
3	E	13	0	5	2	0
3	F	13	0	5	2	0
All	All	14674	0	14916	1144	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 39.

The worst 5 of 1144 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:D:225:GLY:CA	3:D:2193:FLC:OB2	1.87	1.23
1:B:153:GLU:OE1	1:B:178:ARG:HD3	1.39	1.21
1:D:225:GLY:HA3	3:D:2193:FLC:OB2	1.00	1.15
1:E:27:CYS:HB2	1:E:28:PRO:HD2	1.33	1.10
1:C:121:LEU:HD12	1:C:121:LEU:H	1.15	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	301/332 (91%)	216 (72%)	70 (23%)	15 (5%)	1	10
1	B	301/332 (91%)	225 (75%)	68 (23%)	8 (3%)	4	20
1	C	301/332 (91%)	219 (73%)	68 (23%)	14 (5%)	2	12
1	D	302/332 (91%)	230 (76%)	59 (20%)	13 (4%)	2	13
1	E	301/332 (91%)	229 (76%)	53 (18%)	19 (6%)	1	7
1	F	303/332 (91%)	223 (74%)	67 (22%)	13 (4%)	2	13
All	All	1809/1992 (91%)	1342 (74%)	385 (21%)	82 (4%)	2	12

5 of 82 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	MET
1	A	291	VAL
1	B	150	ASN
1	C	150	ASN
1	C	291	VAL

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	273/297 (92%)	243 (89%)	30 (11%)	6	22
1	B	273/297 (92%)	251 (92%)	22 (8%)	11	36
1	C	273/297 (92%)	250 (92%)	23 (8%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	273/297 (92%)	247 (90%)	26 (10%)	8	29
1	E	273/297 (92%)	244 (89%)	29 (11%)	6	23
1	F	274/297 (92%)	245 (89%)	29 (11%)	6	23
All	All	1639/1782 (92%)	1480 (90%)	159 (10%)	8	28

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	191	LEU
1	F	185	THR
1	E	232	ILE
1	F	56	THR
1	F	240	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	113	HIS
1	F	148	ASN
1	F	297	ASN
1	C	175	ASN
1	C	131	HIS

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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 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
3	FLC	F	2195	-	12,12,12	1.81	3 (25%)	17,17,17	3.01	9 (52%)
3	FLC	A	2190	-	12,12,12	1.12	1 (8%)	17,17,17	1.59	3 (17%)
2	NAG	A	801	1	14,14,15	1.22	1 (7%)	17,19,21	1.89	5 (29%)
2	NAG	B	803	1	14,14,15	1.06	1 (7%)	17,19,21	1.65	3 (17%)
2	NAG	F	811	1	14,14,15	1.11	1 (7%)	17,19,21	1.92	6 (35%)
3	FLC	C	2192	-	12,12,12	1.69	2 (16%)	17,17,17	2.91	7 (41%)
3	FLC	B	2191	-	12,12,12	1.31	1 (8%)	17,17,17	1.87	3 (17%)
3	FLC	D	2193	-	12,12,12	1.26	0	17,17,17	2.29	6 (35%)
3	FLC	E	2194	-	12,12,12	2.21	1 (8%)	17,17,17	2.99	8 (47%)
2	NAG	E	809	1	14,14,15	1.33	2 (14%)	17,19,21	2.26	4 (23%)
2	NAG	D	807	1	14,14,15	0.97	0	17,19,21	1.76	5 (29%)
2	NAG	C	805	1	14,14,15	1.36	3 (21%)	17,19,21	1.78	5 (29%)

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	FLC	F	2195	-	-	4/16/16/16	-
3	FLC	A	2190	-	-	9/16/16/16	-
2	NAG	A	801	1	-	4/6/23/26	0/1/1/1
2	NAG	B	803	1	-	3/6/23/26	0/1/1/1
2	NAG	F	811	1	-	3/6/23/26	0/1/1/1
3	FLC	C	2192	-	-	8/16/16/16	-
3	FLC	B	2191	-	-	8/16/16/16	-
3	FLC	D	2193	-	-	9/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FLC	E	2194	-	-	5/16/16/16	-
2	NAG	E	809	1	-	3/6/23/26	0/1/1/1
2	NAG	D	807	1	-	5/6/23/26	0/1/1/1
2	NAG	C	805	1	-	3/6/23/26	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2194	FLC	CB-CBC	6.56	1.60	1.53
3	C	2192	FLC	CB-CBC	4.33	1.58	1.53
3	F	2195	FLC	CG-CB	4.12	1.59	1.54
2	C	805	NAG	C3-C2	3.10	1.59	1.52
2	E	809	NAG	C1-C2	2.99	1.56	1.52

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2192	FLC	OHB-CB-CG	-6.37	94.86	109.38
3	F	2195	FLC	CB-CG-CGC	6.11	130.64	113.92
3	C	2192	FLC	OHB-CB-CBC	5.98	117.44	108.96
3	E	2194	FLC	OHB-CB-CG	-5.97	95.75	109.38
3	F	2195	FLC	OB2-CBC-CB	5.87	124.40	113.14

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAG	C8-C7-N2-C2
2	A	801	NAG	O7-C7-N2-C2
2	B	803	NAG	C8-C7-N2-C2
2	B	803	NAG	O7-C7-N2-C2
2	C	805	NAG	C8-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2195	FLC	2	0
2	A	801	NAG	5	0
3	C	2192	FLC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2191	FLC	3	0
3	D	2193	FLC	7	0
3	E	2194	FLC	2	0
2	D	807	NAG	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	303/332 (91%)	-1.71	0 100 100	8, 38, 52, 57	0
1	B	303/332 (91%)	-1.66	0 100 100	8, 38, 53, 70	0
1	C	303/332 (91%)	-1.66	0 100 100	8, 38, 53, 67	0
1	D	304/332 (91%)	-1.68	0 100 100	8, 38, 52, 57	0
1	E	303/332 (91%)	-1.67	0 100 100	8, 37, 53, 64	0
1	F	305/332 (91%)	-1.68	0 100 100	6, 38, 52, 58	0
All	All	1821/1992 (91%)	-1.68	0 100 100	6, 38, 53, 70	0

There are no RSRZ outliers to report.

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](#)

There are no oligosaccharides in this entry.

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. 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	B-factors(Å ²)	Q<0.9
2	NAG	D	807	14/15	0.96	0.04	58,59,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	A	801	14/15	0.97	0.05	51,53,55,55	0
2	NAG	C	805	14/15	0.98	0.04	53,56,57,58	0
2	NAG	B	803	14/15	0.98	0.05	46,50,51,51	0
2	NAG	E	809	14/15	0.98	0.04	59,61,62,62	0
2	NAG	F	811	14/15	0.98	0.03	49,50,51,51	0
3	FLC	A	2190	13/13	0.99	0.04	47,50,53,53	0
3	FLC	B	2191	13/13	0.99	0.06	49,53,56,57	0
3	FLC	C	2192	13/13	0.99	0.03	38,43,46,46	0
3	FLC	F	2195	13/13	0.99	0.04	38,42,42,43	0
3	FLC	E	2194	13/13	1.00	0.04	36,44,47,48	0
3	FLC	D	2193	13/13	1.00	0.02	38,40,44,45	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.