



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 20, 2024 – 05:34 PM EDT

PDB ID : 1M1J
Title : Crystal structure of native chicken fibrinogen with two different bound ligands
Authors : Yang, Z.; Kollman, J.M.; Pandi, L.; Doolittle, R.F.
Deposited on : 2002-06-19
Resolution : 2.70 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

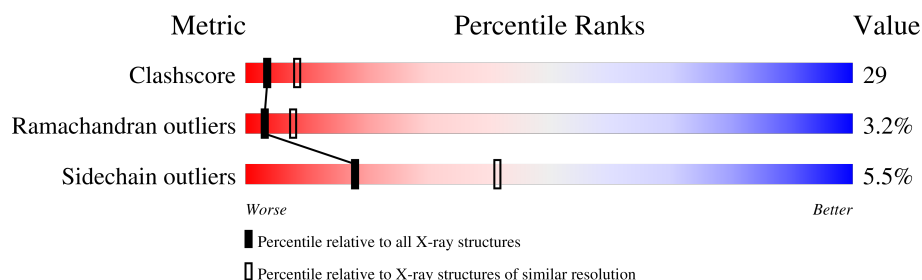
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	491	20% 16% • 61%
1	D	491	18% 19% • 60%
2	B	464	53% 31% • 13%
2	E	464	50% 33% • 14%
3	C	409	56% 32% 6% 5%
3	F	409	54% 36% 5% 5%
4	G	4	75% 25%
4	H	4	50% 50%

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Mol	Chain	Length	Quality of chain
5	I	4	<div><div></div><div>50%</div><div></div><div>50%</div></div>
5	J	4	<div><div></div><div>25%</div><div></div><div>75%</div></div>

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
6	NDG	B	470	-	-	X	-
6	NDG	C	420	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16117 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 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1544	947	282	305	10			
1	D	194	Total	C	N	O	S	0	0	0
			1565	962	286	307	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	GLY	CYS	SEE REMARK 999	UNP P14448
D	49	GLY	CYS	SEE REMARK 999	UNP P14448

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			3225	2023	554	623	25			
2	E	401	Total	C	N	O	S	0	0	0
			3216	2019	553	619	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLN	-	SEE REMARK 999	UNP Q02020
E	1	GLN	-	SEE REMARK 999	UNP Q02020

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	390	Total	C	N	O	S	0	0	0
			3162	1987	539	620	16			
3	F	389	Total	C	N	O	S	0	0	0
			3155	1983	538	618	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	286	ALA	ARG	SEE REMARK 999	UNP O93568
F	286	ALA	ARG	SEE REMARK 999	UNP O93568

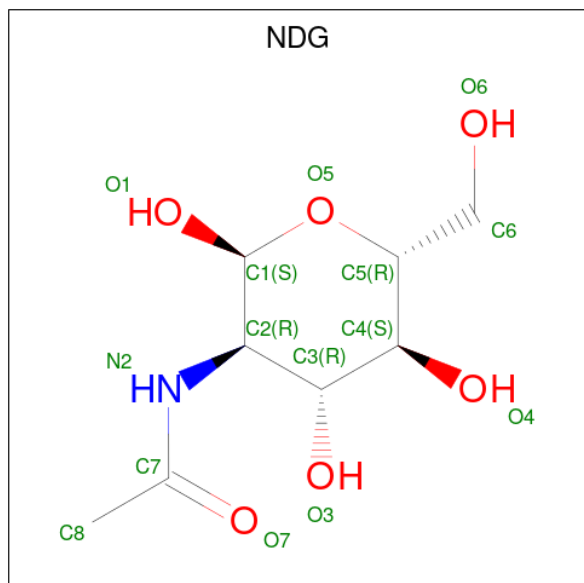
- Molecule 4 is a protein called GLY-PRO-ARG-PRO peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			30	18	7	5			
4	H	4	Total	C	N	O	0	0	0
			30	18	7	5			

- Molecule 5 is a protein called GLY-HIS-ARG-PRO peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	4	Total	C	N	O	0	0	0
			33	19	9	5			
5	J	4	Total	C	N	O	0	0	0
			33	19	9	5			

- Molecule 6 is 2-acetamido-2-deoxy- α -D-glucopyranose (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			15	8	1	6		

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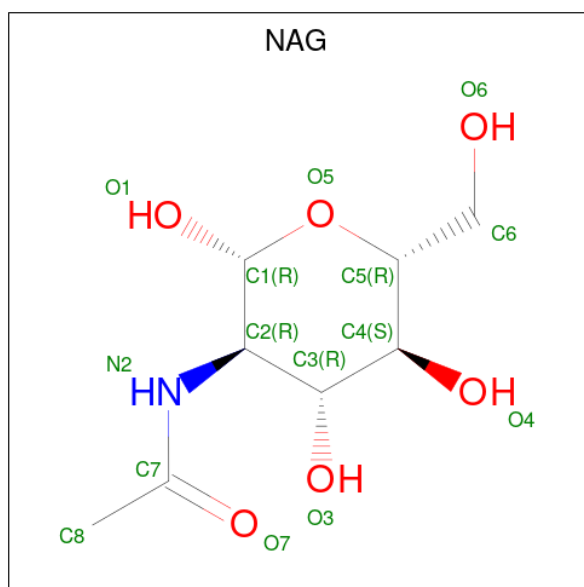
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			15	8	1	6		
6	E	1	Total	C	N	O	0	0
			15	8	1	6		
6	F	1	Total	C	N	O	0	0
			15	8	1	6		
6	J	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			15	8	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	F	1	Total	C	N	O	0	0
			15	8	1	6		
8	I	1	Total	C	N	O	0	0
			15	8	1	6		

[illegible]

- Molecule 2: Fibrinogen beta chain

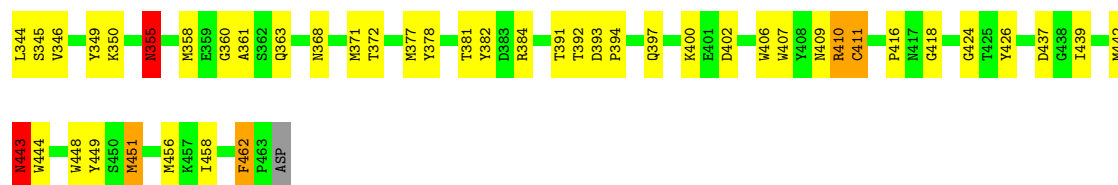
Chain B: 53% 31% • 13%

I458	D235	Q136	PRO	GLN
N355	T238	R137	ILE	ALA
M358	T239	K138	SER	VAL
E359		D139	G64	GLU
G360	D246	N140	P65	TYR
A361		D141	D66	ASP
S362	W254	I142	A67	ASN
Q363	T255	I143	G68	GLU
		L144	G69	GLU
N368	Q258	S145	C70	ASP
M371	N259	E146	K71	GLU
T372	R260	Y147	H72	SER
T373	G261	N148	P73	PRO
M377	D262	T149	L74	GLN
Y378	G263	E150	D75	ILE
		M151	E76	ASP
		E152	L77	ALA
T381	N266	L153		ARG
	F267	H154	L80	ALA
R384	G268		C81	HIS
T391	W271	Y157	P82	ARG
T392		I158	T83	PRO
D393	K275	K159	G84	LEU
P394	R276	D160	C85	ASP
		M161		LYS
	K288	L162	Q88	ARG
Q397			T89	GLN
K400	W297	N165	T90	GLU
E401		I166	L91	ALA
D402	N300	P167	L92	ALA
G403	D301		K93	PRO
	K302	L170	Q94	THR
W406	I303			LEU
W407	S304	L173	V98	ARG
Y408	Q305		K99	PRO
N409	L306	V176	P100	VAL
R410	T307	I177	L101	ALA
	K308	D178	L102	PRO
C411				PRO
	I316	L187	L105	ILE
G418	F317		K106	SER
	M318	I191		GLY
G424		T195	F112	THR
Y426	G332		T115	TYR
	F333	R199	S116	GLN
D429	T334			PRO
	I335	V203	M119	ARG
K432	H336	A204	Y120	PRO
		S205		PRO
M443	K341	C206	M125	LYS
	Y342	N207	I126	GLN
	Q343	L208	D127	ASP
W448	L344		M128	LYS
Y449	S345	E215	K129	GLN
S450	V346	C216	L130	ALA
M451	S347		V131	MET
	N348	M229	K132	LYS
W456	Y349		T133	LYS
	V350	P324		CYS

- Molecule 2: Fibrinogen beta chain

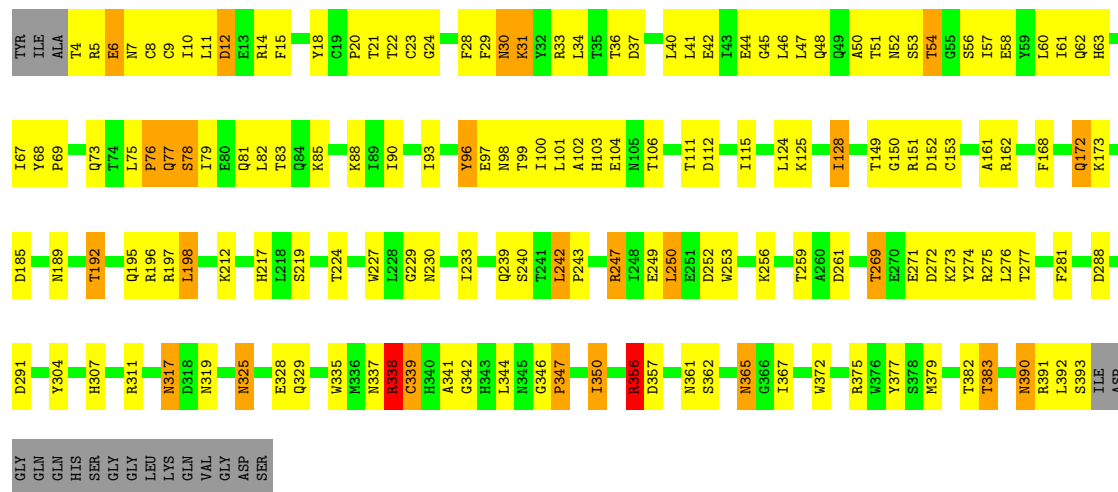
Chain E: 50% 33% • 14%

R221	R234	D235	T238	D246	W254	Q258	N259	Q261	D262	G263	N266	F267	G268	W271	K275	R276	K288	W297	L298	G299	N300	D301	K302	I303	Q305	L306	K308	V314	L315	I316	E317	N318	E319	K325	G332	F333	T334	H336	K341	R342																							
K129	L130	V131	K132	T133	Q134	K135	N140	I143	E146	T149	E150	M151	E152	L153	H154	Y155	N156	Y157	I158	K159	M160	N161	M164	N165	I166	P167	S168	S169	L170	R171	V172	V176	S179	L180	I184	D196	Y197	G198	R199	V203	A204	I208	P209	E215	G216	E217																	
PRO	ILE	IG3	Y64	P65	D66	A67	G68	G69	C70	ASP	K71	H72	P73	L74	D75	E76	L77	ARG	ALA	HIS	T83	G84	C85	E86	L87	Q88	T89	T90	L91	L92	K93	Q94	E95	V98	K99	P100	R103	D104	I105	K106	V109	A110	K111	F112	S113	T118	M119	Y120	Q121	Y122	V123	N124	M125	I126	D127	N128							
GLN	ALA	SER	VAL	GIJ	TVR	ASP	ASN	GIJ	GIJ	ASP	SER	PRO	GLN	ILE	ASP	ALA	ARG	ALA	HIS	ARG	PRO	LEU	ASP	LYS	GLN	GIJ	ALA	ALA	ALA	PRO	THR	THR	LEU	ARG	PRO	VAL	ALA	PRO	PRO	ILE	SER	GLY	THR	GLY	TYR	TVR	GLN	PRO	PRO	ARG	PRO	LYS	GLN	ASP	LYS	GLN	LYS	GLN	LYS	GLN	LYS	VAL	GLY



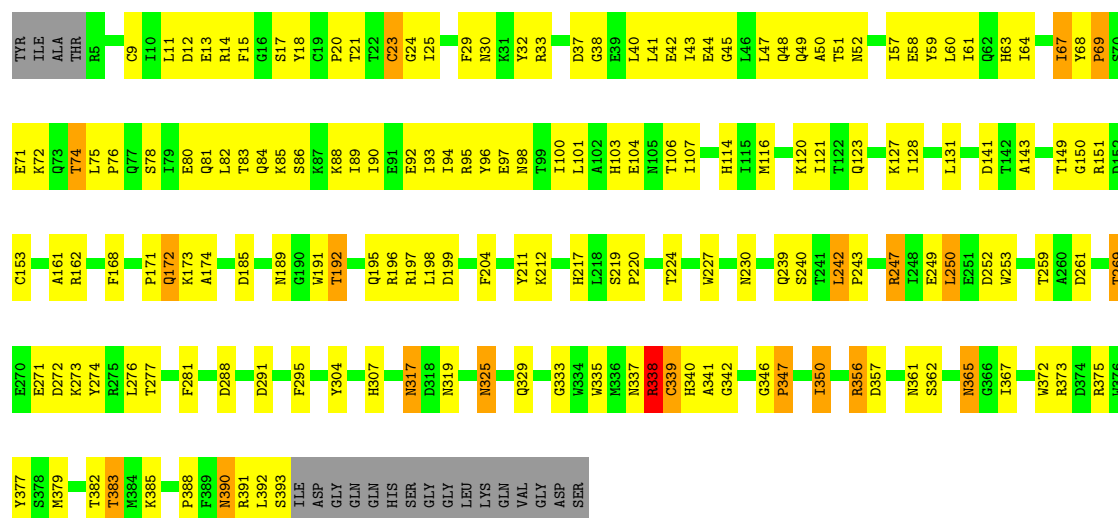
• Molecule 3: Fibrinogen gamma chain

Chain C: 56% 32% 6% 5%



• Molecule 3: Fibrinogen gamma chain

Chain F: 54% 36% 5% 5%



• Molecule 4: GLY-PRO-ARG-PRO peptide

Chain G: 75% 25%



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

Chain H:  50% 50%

G1	P2	R3	P4
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- Molecule 5: GLY-HIS-ARG-PRO peptide

Chain I:  50% 50%

G1	H2	R3	P4
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- Molecule 5: GLY-HIS-ARG-PRO peptide

Chain J:  25% 75%

G1	H2	R3	P4
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.09Å 100.02Å 200.09Å 90.00° 105.79° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	93.1 (20.00-2.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.227 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16117	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

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: CA, NDG, 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	0.33	0/1564	0.57	0/2108
1	D	0.30	0/1587	0.58	0/2139
2	B	0.39	0/3304	0.63	1/4467 (0.0%)
2	E	0.34	0/3295	0.61	1/4456 (0.0%)
3	C	0.42	0/3236	0.65	1/4374 (0.0%)
3	F	0.39	0/3229	0.65	1/4364 (0.0%)
4	G	0.62	0/31	0.80	0/40
4	H	0.60	0/31	0.69	0/40
5	I	0.55	0/34	0.69	0/43
5	J	0.46	0/34	0.52	0/43
All	All	0.37	0/16345	0.63	4/22074 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	338	ARG	N-CA-C	-6.79	92.66	111.00
3	C	338	ARG	N-CA-C	-6.79	92.67	111.00
2	B	403	GLY	N-CA-C	5.09	125.82	113.10
2	E	410	ARG	N-CA-C	-5.09	97.26	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	1544	0	1532	133	0
1	D	1565	0	1548	161	0
2	B	3225	0	3081	179	0
2	E	3216	0	3077	233	0
3	C	3162	0	2992	189	0
3	F	3155	0	2985	190	0
4	G	30	0	32	1	0
4	H	30	0	32	2	0
5	I	33	0	32	1	0
5	J	33	0	32	4	0
6	B	15	0	12	8	0
6	C	15	0	12	10	0
6	E	15	0	12	4	0
6	F	15	0	12	3	0
6	J	15	0	12	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
8	C	15	0	15	1	0
8	F	15	0	15	0	0
8	I	15	0	15	3	0
All	All	16117	0	15448	913	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 29.

The worst 5 of 913 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:216:VAL:HG22	2:B:129:LYS:HE3	1.24	1.15
3:F:52:ASN:HD21	6:F:520:NDG:H8C3	1.01	1.13
2:E:443:ASN:HD22	2:E:443:ASN:H	1.05	1.01
2:E:371:MET:HB2	2:E:410:ARG:CB	1.92	0.99
3:F:356:ARG:NH1	3:F:356:ARG:HB3	1.79	0.97

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	190/491 (39%)	159 (84%)	24 (13%)	7 (4%)	2	6
1	D	192/491 (39%)	147 (77%)	32 (17%)	13 (7%)	1	1
2	B	400/464 (86%)	353 (88%)	39 (10%)	8 (2%)	6	16
2	E	399/464 (86%)	335 (84%)	52 (13%)	12 (3%)	3	9
3	C	388/409 (95%)	350 (90%)	27 (7%)	11 (3%)	4	10
3	F	387/409 (95%)	342 (88%)	34 (9%)	11 (3%)	4	10
4	G	2/4 (50%)	2 (100%)	0	0	100	100
4	H	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
5	I	2/4 (50%)	2 (100%)	0	0	100	100
5	J	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1964/2744 (72%)	1693 (86%)	209 (11%)	62 (3%)	3	8

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	LEU
1	A	210	PRO
1	A	211	LEU
2	B	65	PRO
2	B	411	CYS

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	177/430 (41%)	164 (93%)	13 (7%)	11	29
1	D	179/430 (42%)	167 (93%)	12 (7%)	13	33
2	B	350/402 (87%)	335 (96%)	15 (4%)	25	52
2	E	349/402 (87%)	335 (96%)	14 (4%)	27	55
3	C	341/355 (96%)	317 (93%)	24 (7%)	12	31
3	F	340/355 (96%)	322 (95%)	18 (5%)	19	43
4	G	3/3 (100%)	3 (100%)	0	100	100
4	H	3/3 (100%)	3 (100%)	0	100	100
5	I	3/3 (100%)	3 (100%)	0	100	100
5	J	3/3 (100%)	3 (100%)	0	100	100
All	All	1748/2386 (73%)	1652 (94%)	96 (6%)	18	41

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	115	GLU
2	E	288	LYS
1	D	151	LEU
2	E	124	ASN
2	E	443	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	173	GLN
2	E	322	ASN
1	D	215	ASN
2	E	189	ASN
2	E	368	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z > 2$
8	NAG	C	421	-	15,15,15	0.48	0	21,21,21	0.61	0
6	NDG	B	470	-	15,15,15	0.47	0	21,21,21	0.79	0
6	NDG	F	520	-	15,15,15	0.45	0	21,21,21	0.59	0
6	NDG	C	420	-	15,15,15	0.42	0	21,21,21	0.55	0
8	NAG	I	471	-	15,15,15	0.49	0	21,21,21	0.55	0
8	NAG	F	521	-	15,15,15	0.43	0	21,21,21	0.55	0
6	NDG	J	571	-	15,15,15	0.56	0	21,21,21	0.56	0
6	NDG	E	570	-	15,15,15	0.45	0	21,21,21	0.58	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	NAG	C	421	-	-	2/6/26/26	0/1/1/1
6	NDG	B	470	-	-	4/6/26/26	0/1/1/1
6	NDG	F	520	-	-	2/6/26/26	0/1/1/1
6	NDG	C	420	-	-	2/6/26/26	0/1/1/1
8	NAG	I	471	-	-	3/6/26/26	0/1/1/1
8	NAG	F	521	-	-	2/6/26/26	0/1/1/1
6	NDG	J	571	-	-	3/6/26/26	0/1/1/1
6	NDG	E	570	-	-	2/6/26/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	470	NDG	C8-C7-N2-C2
6	B	470	NDG	O7-C7-N2-C2
6	C	420	NDG	C8-C7-N2-C2
6	C	420	NDG	O7-C7-N2-C2
6	F	520	NDG	C8-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	421	NAG	1	0
6	B	470	NDG	8	0
6	F	520	NDG	3	0
6	C	420	NDG	10	0
8	I	471	NAG	3	0
6	E	570	NDG	4	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](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.