



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2024 – 11:58 AM EDT

PDB ID : 6CYM
Title : Reversible Covalent Direct Thrombin Inhibitors
Authors : Sivaraja, M.; Williams, D.C.
Deposited on : 2018-04-06
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

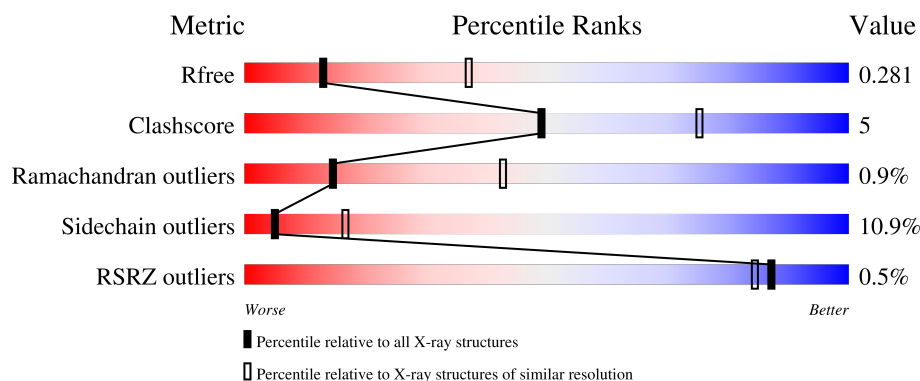
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (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 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	259	
1	C	259	
2	B	28	
2	D	28	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4614 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.

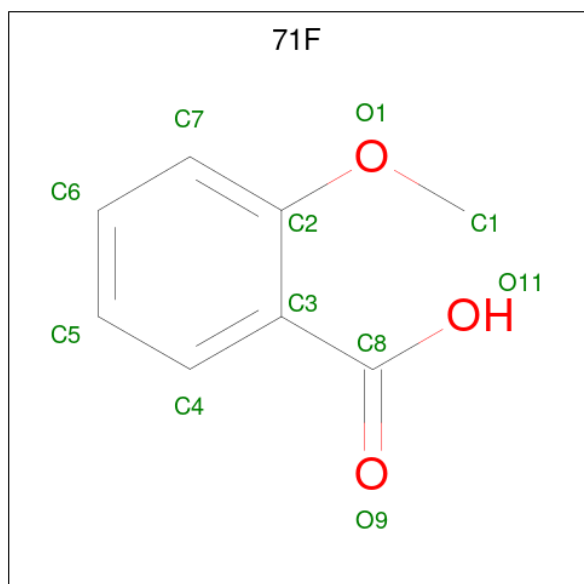
- Molecule 1 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			2025	1292	358	361	14			
1	C	257	Total	C	N	O	S	0	0	0
			2079	1327	368	370	14			

- Molecule 2 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	27	Total	C	N	O	S	0	0	0
			222	140	36	45	1			
2	D	28	Total	C	N	O	S	0	0	0
			230	144	37	48	1			

- Molecule 3 is 2-methoxybenzoic acid (three-letter code: 71F) (formula: C₈H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	8	2		
3	C	1	Total	C	O	0	0
			10	8	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	C	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	15	Total	O	0	0
			15	15		
6	C	6	Total	O	0	0
			6	6		

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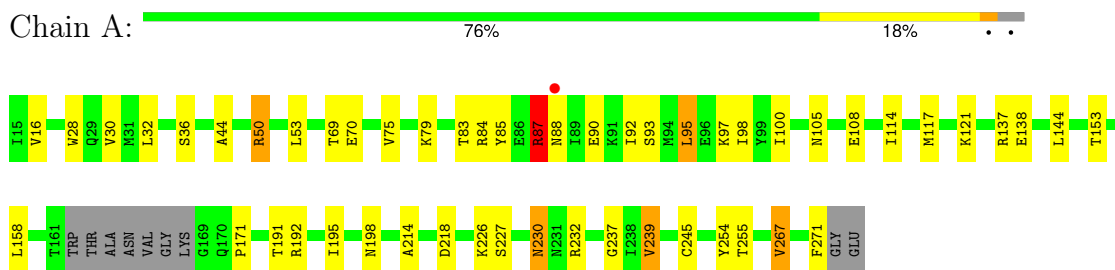
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	O	0	0
			1	1		

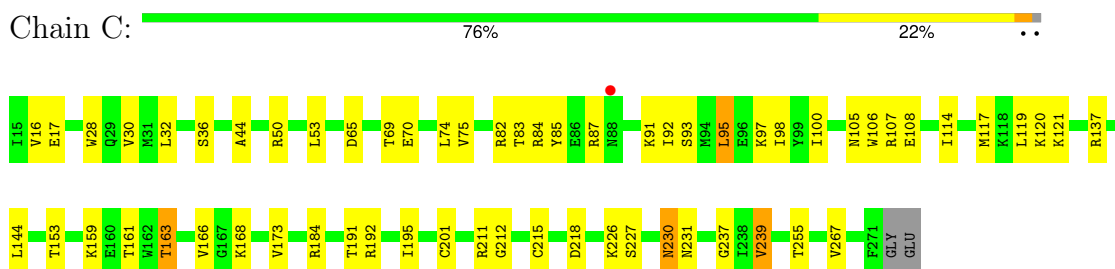
3 Residue-property plots [i](#)

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.

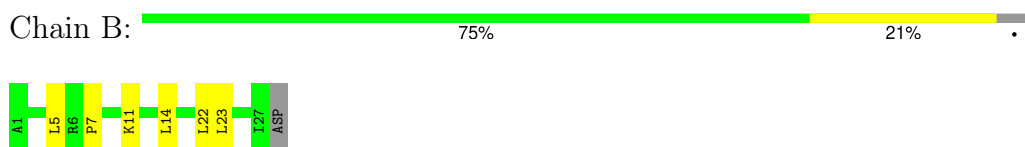
- Molecule 1: Prothrombin



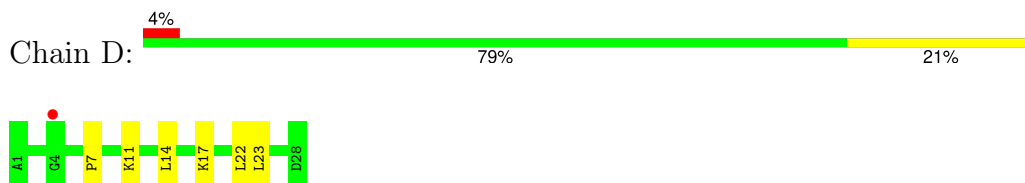
- Molecule 1: Prothrombin



- Molecule 2: Prothrombin



- Molecule 2: Prothrombin



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	91.67Å 99.73Å 146.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	72.1 (30.00-2.90) 72.0 (30.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.176 , 0.254 0.190 , 0.281	Depositor DCC
R_{free} test set	566 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 75.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4614	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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: NAG, 71F, NA

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	0.52	0/2077	0.74	0/2806
1	C	0.50	0/2134	0.74	0/2886
2	B	0.49	0/224	0.77	0/298
2	D	0.53	0/232	0.83	0/309
All	All	0.51	0/4667	0.74	0/6299

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 [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	2025	0	1999	24	0
1	C	2079	0	2054	22	0
2	B	222	0	225	3	0
2	D	230	0	229	2	0
3	A	10	0	0	3	0
3	C	10	0	0	1	0
4	A	14	0	13	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	15	0	0	1	0
6	C	6	0	0	0	0
6	D	1	0	0	0	0
All	All	4614	0	4520	48	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 5.

All (48) 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:C:163:THR:HG23	1:C:166:VAL:HG12	1.56	0.86
1:A:70:GLU:HG2	1:A:97:LYS:HA	1.69	0.74
1:C:70:GLU:HG2	1:C:97:LYS:HA	1.70	0.74
1:C:163:THR:HG23	1:C:166:VAL:CG1	2.16	0.73
1:A:158:LEU:HD21	1:A:171:PRO:HB3	1.83	0.60
1:A:214:ALA:HB1	1:A:218:ASP:HB2	1.84	0.60
1:A:226:LYS:HD3	2:B:23:LEU:HD21	1.83	0.60
1:C:191:THR:HG21	1:C:195:ILE:HD11	1.86	0.58
1:A:87:ARG:HD2	1:A:88:ASN:H	1.69	0.57
1:C:184:ARG:HH21	1:C:195:ILE:HG22	1.69	0.56
1:A:105:ASN:OD1	1:A:108:GLU:HB3	2.06	0.55
1:A:191:THR:HG21	1:A:195:ILE:HD11	1.88	0.54
1:C:105:ASN:OD1	1:C:108:GLU:HB3	2.08	0.54
1:C:227:SER:HB3	1:C:230:ASN:ND2	2.23	0.53
1:A:239:VAL:CG1	3:A:300:71F:C5	2.86	0.53
1:A:239:VAL:HG12	3:A:300:71F:C4	2.38	0.52
1:C:226:LYS:HD3	2:D:23:LEU:HD21	1.91	0.52
1:A:227:SER:HB3	1:A:230:ASN:ND2	2.26	0.50
1:A:53:LEU:HD11	1:A:114:ILE:HD11	1.93	0.50
1:A:239:VAL:HG22	1:A:254:TYR:HE2	1.77	0.50
1:C:239:VAL:HG12	3:C:301:71F:C4	2.42	0.49
1:C:53:LEU:HD11	1:C:114:ILE:HD11	1.95	0.48
1:A:95:LEU:HD22	1:A:117:MET:HB3	1.96	0.47
1:A:239:VAL:HG13	3:A:300:71F:C5	2.45	0.47
1:C:95:LEU:HD22	1:C:117:MET:HB3	1.96	0.47
1:C:106:TRP:CE3	1:C:107:ARG:HG3	2.50	0.46
1:A:267:VAL:O	1:A:271:PHE:HD2	1.98	0.46
1:C:70:GLU:HG2	1:C:97:LYS:CA	2.45	0.45
1:A:70:GLU:HG2	1:A:97:LYS:CA	2.44	0.45
1:A:239:VAL:HG22	1:A:254:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:VAL:O	1:C:212:GLY:HA2	2.16	0.45
1:C:237:GLY:HA2	1:C:255:THR:O	2.17	0.44
1:C:30:VAL:HB	1:C:44:ALA:HB3	2.00	0.44
1:C:215:CYS:O	1:C:218:ASP:HB2	2.18	0.44
1:C:85:TYR:HE1	1:C:92:ILE:HD11	1.82	0.43
1:A:16:VAL:HG21	1:A:245:CYS:HB3	2.00	0.43
2:B:7:PRO:HA	2:B:11:LYS:HG3	1.99	0.43
1:A:232:ARG:HE	2:B:5:LEU:HD11	1.83	0.43
2:D:7:PRO:HA	2:D:11:LYS:HG3	2.00	0.43
1:A:237:GLY:HA2	1:A:255:THR:O	2.19	0.42
1:A:85:TYR:HE1	1:A:92:ILE:HD11	1.84	0.42
1:A:30:VAL:HB	1:A:44:ALA:HB3	2.02	0.42
1:A:79:LYS:HE3	1:A:90:GLU:OE1	2.20	0.42
1:C:50:ARG:HA	1:C:119:LEU:HD12	2.02	0.41
1:A:50:ARG:HB2	6:A:413:HOH:O	2.22	0.40
1:C:159:LYS:HG3	1:C:168:LYS:HG3	2.03	0.40
1:C:106:TRP:CD2	1:C:107:ARG:HG3	2.56	0.40
1:C:17:GLU:HG3	1:C:211:ARG:HB2	2.04	0.40

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	246/259 (95%)	226 (92%)	18 (7%)	2 (1%)	16	45
1	C	255/259 (98%)	232 (91%)	21 (8%)	2 (1%)	16	45
2	B	25/28 (89%)	21 (84%)	4 (16%)	0	100	100
2	D	26/28 (93%)	20 (77%)	5 (19%)	1 (4%)	2	11
All	All	552/574 (96%)	499 (90%)	48 (9%)	5 (1%)	14	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ARG
1	C	87	ARG
2	D	17	LYS
1	C	239	VAL
1	A	239	VAL

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	219/225 (97%)	197 (90%)	22 (10%)	6	20
1	C	224/225 (100%)	196 (88%)	28 (12%)	3	12
2	B	25/26 (96%)	23 (92%)	2 (8%)	10	30
2	D	26/26 (100%)	24 (92%)	2 (8%)	10	31
All	All	494/502 (98%)	440 (89%)	54 (11%)	5	17

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	TRP
1	A	32	LEU
1	A	36	SER
1	A	50	ARG
1	A	69	THR
1	A	75	VAL
1	A	83	THR
1	A	84	ARG
1	A	87	ARG
1	A	93	SER
1	A	95	LEU
1	A	98	ILE
1	A	100	ILE
1	A	121	LYS
1	A	137	ARG
1	A	138	GLU
1	A	144	LEU

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Mol	Chain	Res	Type
1	A	153	THR
1	A	192	ARG
1	A	198	ASN
1	A	230	ASN
1	A	267	VAL
2	B	14	LEU
2	B	22	LEU
1	C	28	TRP
1	C	32	LEU
1	C	36	SER
1	C	65	ASP
1	C	69	THR
1	C	74	LEU
1	C	75	VAL
1	C	82	ARG
1	C	83	THR
1	C	84	ARG
1	C	91	LYS
1	C	93	SER
1	C	95	LEU
1	C	98	ILE
1	C	100	ILE
1	C	120	LYS
1	C	121	LYS
1	C	137	ARG
1	C	144	LEU
1	C	153	THR
1	C	161	THR
1	C	163	THR
1	C	173	VAL
1	C	192	ARG
1	C	201	CYS
1	C	230	ASN
1	C	231	ASN
1	C	267	VAL
2	D	14	LEU
2	D	22	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	ASN

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Mol	Chain	Res	Type
1	A	230	ASN
1	A	265	GLN
1	A	270	GLN
1	C	230	ASN
1	C	265	GLN
1	C	270	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	71F	C	301	1	10,10,11	1.86	1 (10%)	12,12,14	2.39	4 (33%)
4	NAG	A	301	1	14,14,15	0.38	0	17,19,21	0.92	1 (5%)
3	71F	A	300	1	10,10,11	1.72	1 (10%)	12,12,14	2.82	5 (41%)

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	71F	C	301	1	-	4/4/4/6	0/1/1/1
4	NAG	A	301	1	-	1/6/23/26	0/1/1/1
3	71F	A	300	1	-	2/4/4/6	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	71F	C3-C2	5.34	1.51	1.41
3	A	300	71F	C3-C2	4.73	1.50	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	300	71F	C2-C3-C8	5.88	127.42	121.13
3	C	301	71F	O1-C2-C3	4.91	122.20	115.92
3	A	300	71F	C1-O1-C2	4.90	124.70	117.51
3	C	301	71F	C2-C3-C8	4.33	125.77	121.13
3	A	300	71F	O1-C2-C3	3.65	120.59	115.92
3	C	301	71F	O1-C2-C7	-3.28	118.77	124.30
3	C	301	71F	C1-O1-C2	3.01	121.92	117.51
3	A	300	71F	O1-C2-C7	-2.49	120.10	124.30
4	A	301	NAG	C1-C2-N2	2.46	114.31	110.43
3	A	300	71F	C6-C5-C4	2.42	123.22	120.24

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	300	71F	C2-C3-C8-O9
3	A	300	71F	C4-C3-C8-O9
3	C	301	71F	C2-C3-C8-O9
3	C	301	71F	C7-C2-O1-C1
4	A	301	NAG	O5-C5-C6-O6
3	C	301	71F	C3-C2-O1-C1
3	C	301	71F	C4-C3-C8-O9

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	71F	1	0
3	A	300	71F	3	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	250/259 (96%)	-0.57	1 (0%) 89 86	19, 50, 88, 129	0
1	C	257/259 (99%)	-0.17	1 (0%) 89 86	21, 79, 140, 202	0
2	B	27/28 (96%)	-0.44	0 100 100	44, 58, 82, 85	0
2	D	28/28 (100%)	-0.28	1 (3%) 46 40	53, 80, 106, 116	0
All	All	562/574 (97%)	-0.37	3 (0%) 87 84	19, 61, 123, 202	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	4	GLY	2.4
1	A	88	ASN	2.4
1	C	88	ASN	2.1

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 monosaccharides 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(\AA^2)	Q<0.9
3	71F	A	300	10/11	0.68	0.27	85,87,92,93	0
3	71F	C	301	10/11	0.80	0.17	88,95,98,98	0
4	NAG	A	301	14/15	0.80	0.11	80,83,85,85	0
5	NA	C	302	1/1	0.92	0.07	27,27,27,27	0
5	NA	A	302	1/1	0.97	0.08	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.