wwPDB X-ray Structure Validation Summary Report (i)

Dec 15, 2016 – 03:03 PM EST

PDB ID	:	1DX5
Title	:	Crystal structure of the thrombin-thrombomodulin complex
Authors	:	Fuentes-Prior, P.; Iwanaga, Y.; Huber, R.; Pagila, R.; Rumennik, G.; Seto, M.; Morser, J.; Light, D.R.; Bode, W.
Deposited on	:	1999-12-20
Resolution	:	2.30 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 (i) symbol.

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

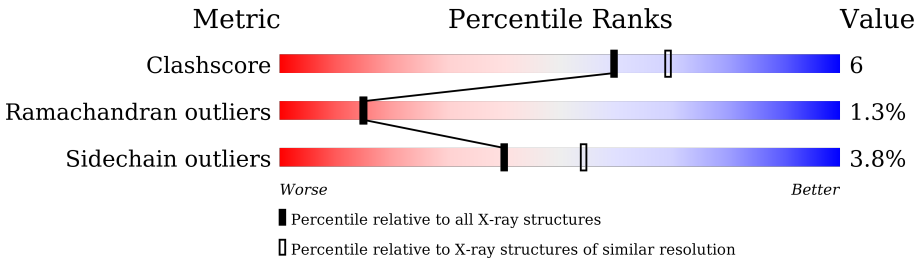
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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 <=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	36	72% 25% ·
1	B	36	69% 31%
1	C	36	69% 25% 6%
1	D	36	69% 28% ·
2	E	4	75% 25%
2	F	4	75% 25%
2	G	4	75% 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	4	75% 25%
3	I	118	81% 19%
3	J	118	78% 22%
3	K	118	82% 17%
3	L	118	82% 16%
4	M	259	75% 20%
4	N	259	76% 21%
4	O	259	80% 17%
4	P	259	80% 15% 5%

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
8	NAG	M	600	X	-	-	-
8	NAG	N	600	X	-	-	-
8	NAG	O	600	X	-	-	-
8	NAG	P	600	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14018 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 THROMBIN LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	36	Total	C	N	O	S	46	0	0
			287	177	48	61	1			
1	B	36	Total	C	N	O	S	38	0	0
			287	177	48	61	1			
1	C	36	Total	C	N	O	S	47	0	0
			287	177	48	61	1			
1	D	36	Total	C	N	O	S	39	0	0
			287	177	48	61	1			

- Molecule 2 is a protein called THROMBIN INHIBITOR GLU-GLY-ARG-0QE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	1
			25	14	6	5			
2	F	4	Total	C	N	O	0	0	1
			25	14	6	5			
2	G	4	Total	C	N	O	0	0	1
			25	14	6	5			
2	H	4	Total	C	N	O	0	0	1
			25	14	6	5			

- Molecule 3 is a protein called THROMBOMODULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	118	Total	C	N	O	S	61	0	0
			874	531	142	182	19			
3	J	118	Total	C	N	O	S	81	0	0
			874	531	142	182	19			
3	K	118	Total	C	N	O	S	74	0	0
			874	531	142	182	19			
3	L	118	Total	C	N	O	S	69	0	0
			874	531	142	182	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	364	ASP	ASN	RESULT OF DEGLYCOSYLA	UNP P07204
I	456	GLY	ARG	ENGINEERED	UNP P07204
I	457	GLN	HIS	ENGINEERED	UNP P07204
J	364	ASP	ASN	RESULT OF DEGLYCOSYLA	UNP P07204
J	456	GLY	ARG	ENGINEERED	UNP P07204
J	457	GLN	HIS	ENGINEERED	UNP P07204
K	364	ASP	ASN	RESULT OF DEGLYCOSYLA	UNP P07204
K	456	GLY	ARG	ENGINEERED	UNP P07204
K	457	GLN	HIS	ENGINEERED	UNP P07204
L	364	ASP	ASN	RESULT OF DEGLYCOSYLA	UNP P07204
L	456	GLY	ARG	ENGINEERED	UNP P07204
L	457	GLN	HIS	ENGINEERED	UNP P07204

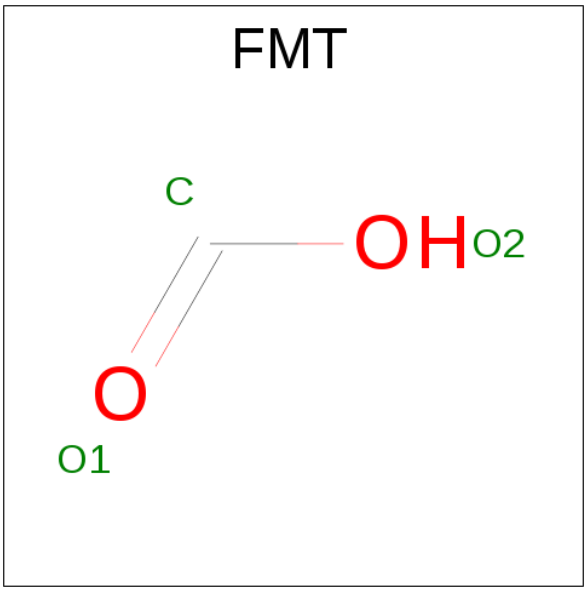
- Molecule 4 is a protein called THROMBIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	259	Total	C	N	O	S	72	0	0
			2094	1336	370	374	14			
4	N	259	Total	C	N	O	S	70	0	0
			2094	1336	370	374	14			
4	O	259	Total	C	N	O	S	76	0	0
			2094	1336	370	374	14			
4	P	259	Total	C	N	O	S	69	0	0
			2094	1336	370	374	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	60I	ILE	THR	CONFLICT	UNP P00734
N	60I	ILE	THR	CONFLICT	UNP P00734
O	60I	ILE	THR	CONFLICT	UNP P00734
P	60I	ILE	THR	CONFLICT	UNP P00734

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C O 3 1 2	0	0
5	I	1	Total C O 3 1 2	0	0
5	J	1	Total C O 3 1 2	0	0
5	K	1	Total C O 3 1 2	0	0
5	L	1	Total C O 3 1 2	0	0

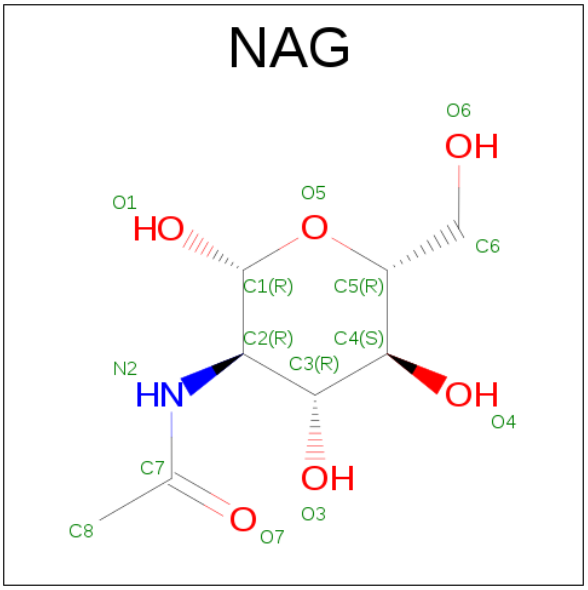
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total Ca 1 1	0	0
6	I	1	Total Ca 1 1	0	0
6	L	1	Total Ca 1 1	0	0
6	K	1	Total Ca 1 1	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	P	1	Total Na 1 1	0	0
7	J	1	Total Na 1 1	0	0
7	K	1	Total Na 1 1	0	0
7	I	1	Total Na 1 1	0	0
7	N	1	Total Na 1 1	0	0
7	O	1	Total Na 1 1	0	0
7	L	1	Total Na 1 1	0	0
7	M	1	Total Na 1 1	0	0

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	13	Total	O	0	0
			13	13		
9	B	12	Total	O	0	0
			12	12		
9	C	17	Total	O	0	0
			17	17		
9	D	4	Total	O	0	0
			4	4		
9	E	5	Total	O	0	0
			5	5		
9	F	5	Total	O	0	0
			5	5		
9	G	1	Total	O	0	0
			1	1		
9	H	2	Total	O	0	0
			2	2		
9	I	71	Total	O	0	0
			71	71		
9	J	66	Total	O	0	0
			66	66		
9	K	64	Total	O	0	0
			64	64		
9	L	60	Total	O	0	0
			60	60		
9	M	123	Total	O	0	0
			123	123		
9	N	129	Total	O	0	0
			129	129		
9	O	121	Total	O	0	0
			121	121		
9	P	122	Total	O	0	0
			122	122		

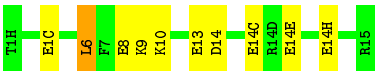
3 Residue-property plots (i)

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.

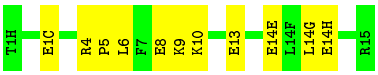
- Molecule 1: THROMBIN LIGHT CHAIN

Chain A:



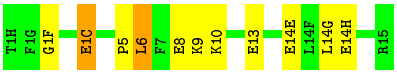
- Molecule 1: THROMBIN LIGHT CHAIN

Chain B:



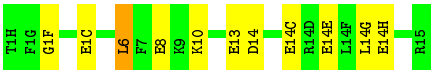
- Molecule 1: THROMBIN LIGHT CHAIN

Chain C:



- Molecule 1: THROMBIN LIGHT CHAIN

Chain D:



- Molecule 2: THROMBIN INHIBITOR GLU-GLY-ARG-0QE

Chain E:

- Molecule 2: THROMBIN INHIBITOR GLU-GLY-ARG-0QE

Chain F:

• Molecule 2: THROMBIN INHIBITOR GLU-GLY-ARG-0QE

Chain G:

• Molecule 2: THROMBIN INHIBITOR GLU-GLY-ARG-0QE

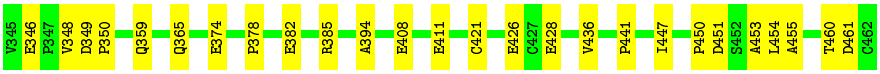
Chain H:

• Molecule 3: THROMBOMODULIN

Chain I:

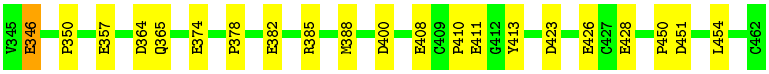
• Molecule 3: THROMBOMODULIN

Chain J:



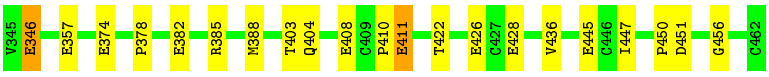
• Molecule 3: THROMBOMODULIN

Chain K:



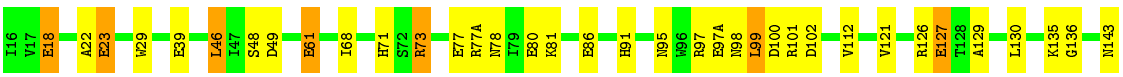
• Molecule 3: THROMBOMODULIN

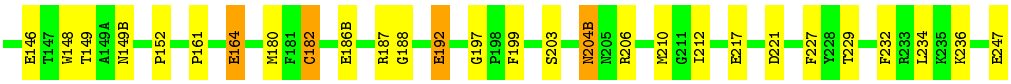
Chain L:



• Molecule 4: THROMBIN HEAVY CHAIN

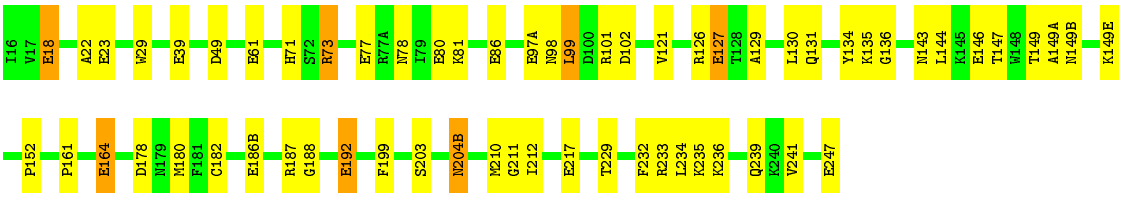
Chain M:





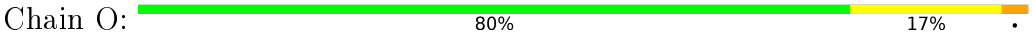
• Molecule 4: THROMBIN HEAVY CHAIN

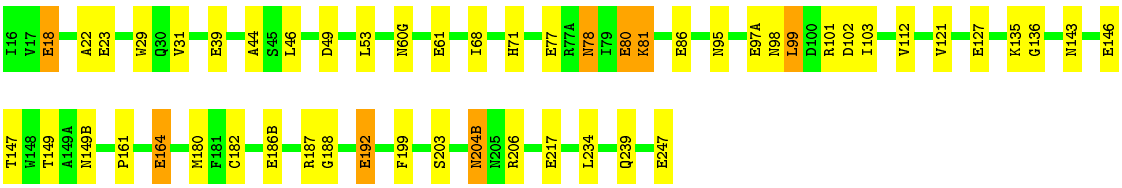
Chain N:



• Molecule 4: THROMBIN HEAVY CHAIN

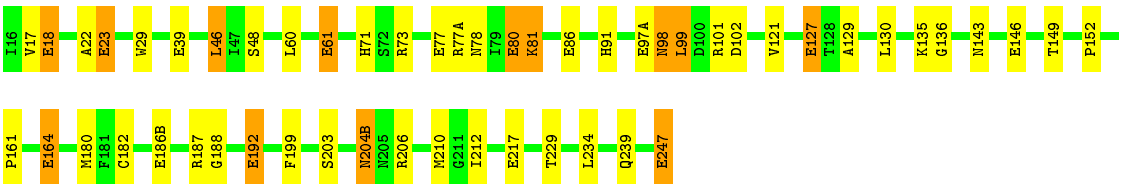
Chain O:





• Molecule 4: THROMBIN HEAVY CHAIN

Chain P:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	214.40Å 214.40Å 131.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	99.7 (10.00-2.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.200 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14018	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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: NAG, AR7, NA, FMT, CA, 0QE

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	1.07	6/290 (2.1%)	0.60	0/384
1	B	1.07	5/290 (1.7%)	0.61	0/384
1	C	1.06	5/290 (1.7%)	0.60	0/384
1	D	1.08	6/290 (2.1%)	0.58	0/384
2	E	1.98	1/12 (8.3%)	0.67	0/14
2	F	2.04	1/12 (8.3%)	0.45	0/14
2	G	1.97	1/12 (8.3%)	0.55	0/14
2	H	2.11	1/12 (8.3%)	0.51	0/14
3	I	0.99	9/896 (1.0%)	0.73	0/1222
3	J	0.98	7/896 (0.8%)	0.71	0/1222
3	K	0.98	10/896 (1.1%)	0.74	0/1222
3	L	0.98	9/896 (1.0%)	0.72	0/1222
4	M	0.85	18/2149 (0.8%)	0.69	0/2904
4	N	0.85	16/2149 (0.7%)	0.69	0/2904
4	O	0.86	18/2149 (0.8%)	0.69	0/2904
4	P	0.85	15/2149 (0.7%)	0.70	0/2904
All	All	0.92	128/13388 (1.0%)	0.70	0/18096

The worst 5 of 128 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	164	GLU	CG-CD	7.29	1.62	1.51
2	H	1	GLU	CG-CD	7.08	1.62	1.51
4	P	164	GLU	CG-CD	7.06	1.62	1.51
4	M	164	GLU	CG-CD	7.01	1.62	1.51
4	P	97(A)	GLU	CG-CD	6.92	1.62	1.51

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	287	0	278	2	0
1	B	287	0	278	2	0
1	C	287	0	278	3	0
1	D	287	0	278	3	0
2	E	25	0	23	0	0
2	F	25	0	23	0	0
2	G	25	0	23	0	0
2	H	25	0	23	0	0
3	I	874	0	754	6	0
3	J	874	0	754	8	0
3	K	874	0	754	5	0
3	L	874	0	754	8	0
4	M	2094	0	2066	28	0
4	N	2094	0	2066	26	0
4	O	2094	0	2066	20	0
4	P	2094	0	2066	33	0
5	H	3	0	1	0	0
5	I	3	0	1	0	0
5	J	3	0	1	0	0
5	K	3	0	1	0	0
5	L	3	0	1	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
7	O	1	0	0	0	0
7	P	1	0	0	0	0
8	M	14	0	13	0	0
8	N	14	0	13	0	0
8	O	14	0	13	0	0
8	P	14	0	13	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	13	0	0	0	0
9	B	12	0	0	0	0
9	C	17	0	0	0	0
9	D	4	0	0	0	0
9	E	5	0	0	0	0
9	F	5	0	0	0	0
9	G	1	0	0	0	0
9	H	2	0	0	0	0
9	I	71	0	0	1	0
9	J	66	0	0	2	0
9	K	64	0	0	0	0
9	L	60	0	0	0	0
9	M	123	0	0	4	0
9	N	129	0	0	1	0
9	O	121	0	0	0	0
9	P	122	0	0	3	0
All	All	14018	0	12541	137	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 6.

The worst 5 of 137 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)
4:P:60:LEU:HD11	8:P:600:NAG:H82	1.57	0.85
3:I:448:CYS:SG	3:I:457:GLN:NE2	2.56	0.78
4:P:247:GLU:HG2	9:P:2023:HOH:O	1.86	0.76
1:C:1(F):GLY:HA3	4:O:239:GLN:HE21	1.58	0.67
4:O:18:GLU:HB2	4:O:188:GLY:HA2	1.80	0.64

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	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
1	B	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
1	C	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
1	D	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
2	E	1/4 (25%)	1 (100%)	0	0	100	100
2	F	1/4 (25%)	1 (100%)	0	0	100	100
2	G	1/4 (25%)	1 (100%)	0	0	100	100
2	H	1/4 (25%)	1 (100%)	0	0	100	100
3	I	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	11	10
3	J	116/118 (98%)	105 (90%)	6 (5%)	5 (4%)	3	1
3	K	116/118 (98%)	107 (92%)	6 (5%)	3 (3%)	7	4
3	L	116/118 (98%)	105 (90%)	7 (6%)	4 (3%)	5	2
4	M	257/259 (99%)	243 (95%)	12 (5%)	2 (1%)	24	27
4	N	257/259 (99%)	241 (94%)	13 (5%)	3 (1%)	16	16
4	O	257/259 (99%)	243 (95%)	12 (5%)	2 (1%)	24	27
4	P	257/259 (99%)	245 (95%)	11 (4%)	1 (0%)	39	48
All	All	1632/1668 (98%)	1528 (94%)	82 (5%)	22 (1%)	15	15

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	346	GLU
3	K	346	GLU
3	L	346	GLU
3	L	451	ASP
4	M	149	THR

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	31/31 (100%)	29 (94%)	2 (6%)	21 27
1	B	31/31 (100%)	28 (90%)	3 (10%)	10 12
1	C	31/31 (100%)	27 (87%)	4 (13%)	5 5
1	D	31/31 (100%)	29 (94%)	2 (6%)	21 27
2	E	1/1 (100%)	1 (100%)	0	100 100
2	F	1/1 (100%)	1 (100%)	0	100 100
2	G	1/1 (100%)	1 (100%)	0	100 100
2	H	1/1 (100%)	1 (100%)	0	100 100
3	I	100/100 (100%)	99 (99%)	1 (1%)	82 91
3	J	100/100 (100%)	100 (100%)	0	100 100
3	K	100/100 (100%)	99 (99%)	1 (1%)	82 91
3	L	100/100 (100%)	99 (99%)	1 (1%)	82 91
4	M	225/225 (100%)	214 (95%)	11 (5%)	31 41
4	N	225/225 (100%)	214 (95%)	11 (5%)	31 41
4	O	225/225 (100%)	217 (96%)	8 (4%)	42 57
4	P	225/225 (100%)	215 (96%)	10 (4%)	35 46
All	All	1428/1428 (100%)	1374 (96%)	54 (4%)	40 54

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	M	204(B)	ASN
4	N	149(B)	ASN
4	P	99	LEU
4	N	73	ARG
4	N	81	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
4	M	204(B)	ASN
4	N	204(B)	ASN
4	O	244	GLN
4	M	78	ASN
4	P	78	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

4 non-standard protein/DNA/RNA residues 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	AR7	E	3	2,4	7,10,11	1.71	1 (14%)	5,11,13	1.00	1 (20%)
2	AR7	F	3	2,4	7,10,11	1.69	1 (14%)	5,11,13	1.00	1 (20%)
2	AR7	G	3	2,4	7,10,11	1.68	1 (14%)	5,11,13	1.03	1 (20%)
2	AR7	H	3	2,4	7,10,11	1.70	1 (14%)	5,11,13	1.01	1 (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	AR7	E	3	2,4	-	0/7/9/11	0/0/0/0
2	AR7	F	3	2,4	-	0/7/9/11	0/0/0/0
2	AR7	G	3	2,4	-	0/7/9/11	0/0/0/0
2	AR7	H	3	2,4	-	0/7/9/11	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	AR7	O-C	-4.37	1.23	1.42
2	F	3	AR7	O-C	-4.33	1.23	1.42
2	H	3	AR7	O-C	-4.32	1.23	1.42
2	G	3	AR7	O-C	-4.28	1.23	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	3	AR7	O-C-CA	2.02	117.12	111.77
2	F	3	AR7	O-C-CA	2.07	117.24	111.77
2	G	3	AR7	O-C-CA	2.13	117.42	111.77
2	H	3	AR7	O-C-CA	2.15	117.46	111.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 12 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
5	FMT	H	502	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	I	501	7	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	J	501	7	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	K	501	7	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	L	501	7	0,2,2	0.00	-	0,1,1	0.00	-
8	NAG	M	600	4	14,14,15	0.79	0	15,19,21	1.00	1 (6%)
8	NAG	N	600	4	14,14,15	0.81	0	15,19,21	0.92	0
8	NAG	O	600	4	14,14,15	0.70	0	15,19,21	1.02	1 (6%)
8	NAG	P	600	4	14,14,15	0.82	1 (7%)	15,19,21	1.04	2 (13%)

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	FMT	H	502	-	-	0/0/0/0	0/0/0/0
5	FMT	I	501	7	-	0/0/0/0	0/0/0/0
5	FMT	J	501	7	-	0/0/0/0	0/0/0/0
5	FMT	K	501	7	-	0/0/0/0	0/0/0/0
5	FMT	L	501	7	-	0/0/0/0	0/0/0/0
8	NAG	M	600	4	1/1/5/7	0/6/23/26	0/1/1/1
8	NAG	N	600	4	1/1/5/7	0/6/23/26	0/1/1/1
8	NAG	O	600	4	1/1/5/7	0/6/23/26	0/1/1/1
8	NAG	P	600	4	1/1/5/7	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	600	NAG	O5-C1	-2.03	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	600	NAG	C2-N2-C7	-2.40	119.99	123.11
8	O	600	NAG	C2-N2-C7	-2.29	120.12	123.11
8	M	600	NAG	C2-N2-C7	-2.25	120.17	123.11
8	P	600	NAG	C1-O5-C5	2.03	115.12	112.14

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	N	600	NAG	C1
8	M	600	NAG	C1
8	O	600	NAG	C1
8	P	600	NAG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	P	600	NAG	2	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.