wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2016 – 04:16 PM EDT

PDB ID	:	5E8E
Title	:	Crystal structure of thrombin bound to an exosite 1-specific IgA Fab
Authors	:	Baglin, T.P.; Langdown, J.; Frasson, R.; Huntington, J.A.
Deposited on	:	2015-10-14
Resolution	:	1.90 Å(reported)

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)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

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 1.90 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	Percentile Ranks	Value
Rfree		0.246
Clashscore		9
Ramachandran outliers		0
Sidechain outliers		2.1%
RSRZ outliers		0.5%

Worse .... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
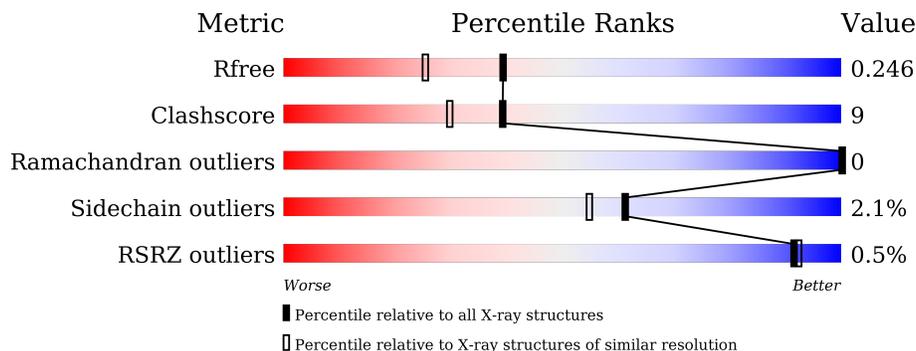
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 <=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	215	84% 15% ·
2	B	229	% 79% 20% ·
3	H	259	89% 11%
4	L	36	75% 11% 6% 8%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CIT	H	608	-	-	-	X
5	NAG	H	602	-	-	X	-
6	PEG	H	616	-	-	-	X
7	PO4	B	301	-	-	X	-
7	PO4	H	613	-	-	-	X
8	BMA	H	603	-	-	X	-

2 Entry composition ⓘ

There are 15 unique types of molecules in this entry. The entry contains 6373 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 IGA FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total 1670	C 1048	N 280	O 337	S 5	0	5	0

- Molecule 2 is a protein called IGA FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total 1722	C 1088	N 283	O 340	S 11	0	3	0

- Molecule 3 is a protein called THROMBIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	259	Total 2091	C 1332	N 370	O 375	S 14	0	1	0

- Molecule 4 is a protein called THROMBIN LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	33	Total 270	C 169	N 42	O 58	S 1	0	1	0

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
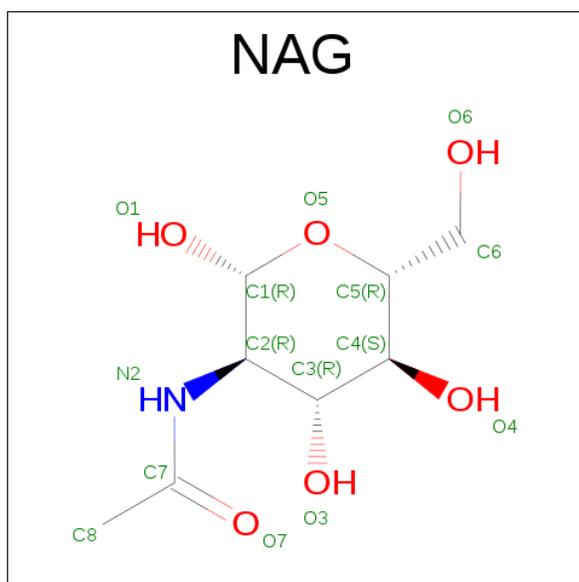
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 14	C 8	N 1	O 5	0	0
5	A	1	Total 14	C 8	N 1	O 5	0	0
5	H	1	Total 14	C 8	N 1	O 5	0	0
5	H	1	Total 14	C 8	N 1	O 5	0	0
5	H	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
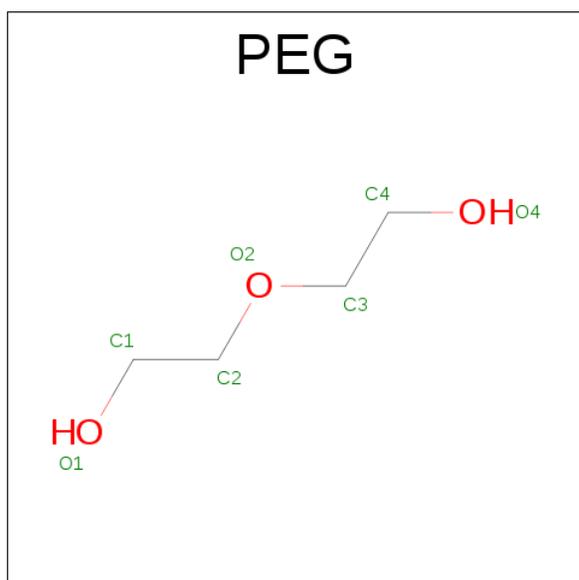
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 7	C 4	O 3	0	0
6	H	1	Total 7	C 4	O 3	0	0
6	H	1	Total 7	C 4	O 3	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
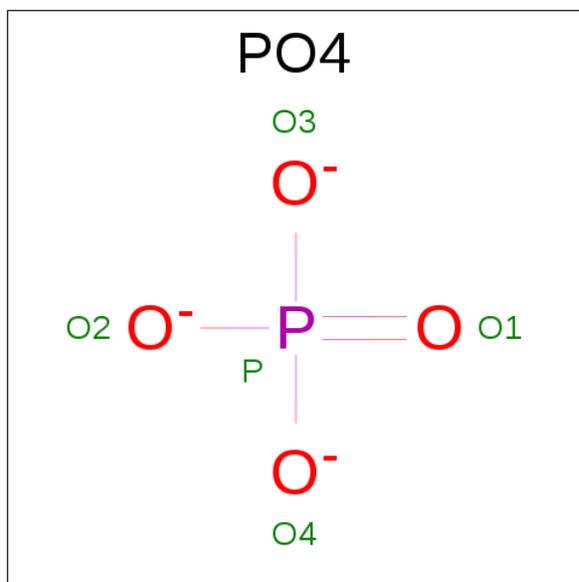
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 5	O 4	P 1	0	0
7	H	1	Total 5	O 4	P 1	0	0
7	H	1	Total 5	O 4	P 1	0	0
7	H	1	Total 5	O 4	P 1	0	0
7	H	1	Total 5	O 4	P 1	0	0

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).
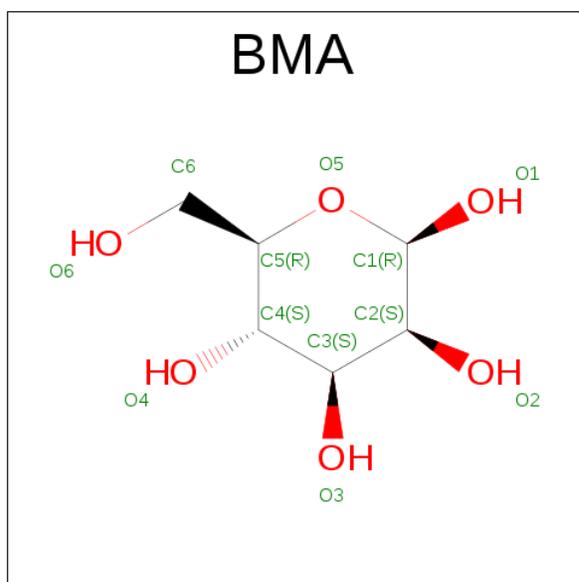
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	H	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).
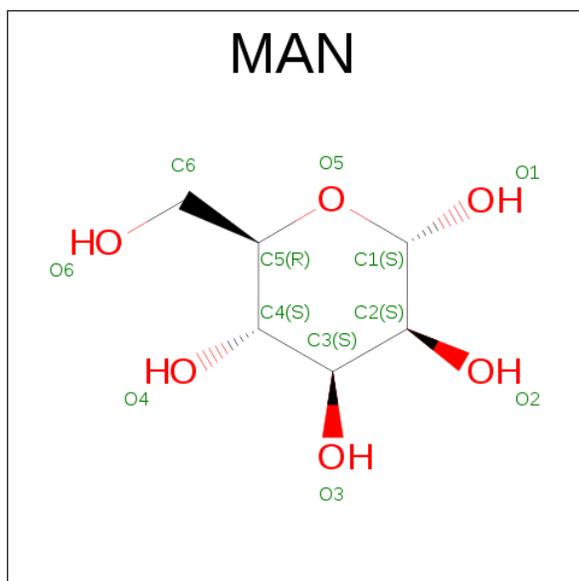
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	H	1	Total	C	O	0	0
			11	6	5		

- Molecule 10 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).
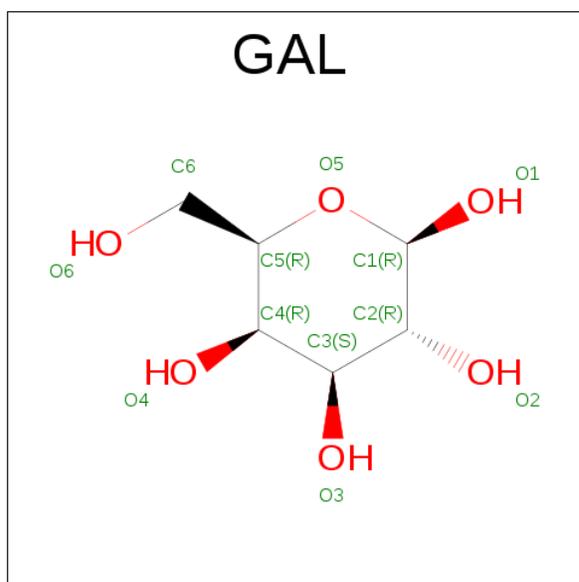
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total 11	C 6	O 5	0	0

- Molecule 11 is O-SIALIC ACID (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).
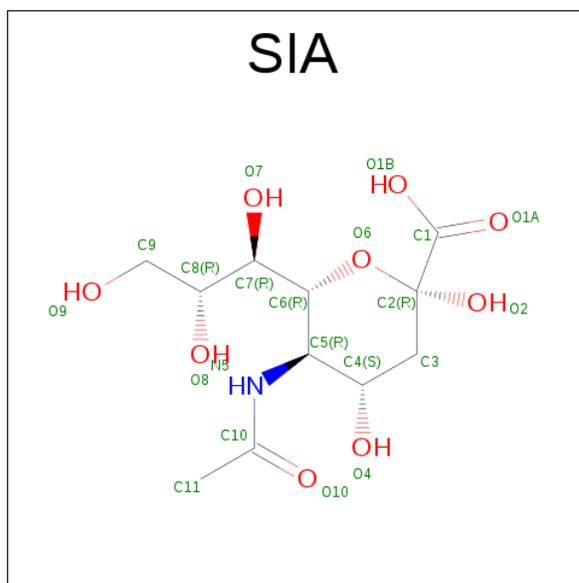
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	H	1	Total 20	C 11	N 1	O 8	0	0

- Molecule 12 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).
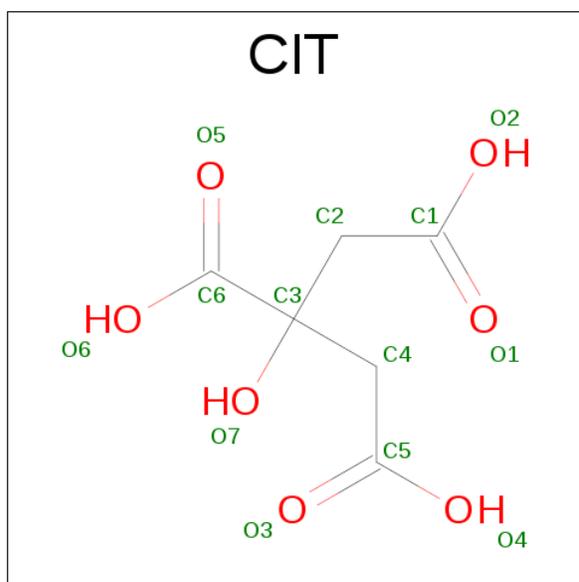
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
12	H	1	13	6	7	0	0

- Molecule 13 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
13	H	1	1	1	0	0

- Molecule 14 is D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydro xyhexan-3-yl]-L-prolinamide (three-letter code: 0G6) (formula: $C_{21}H_{34}ClN_6O_3$).
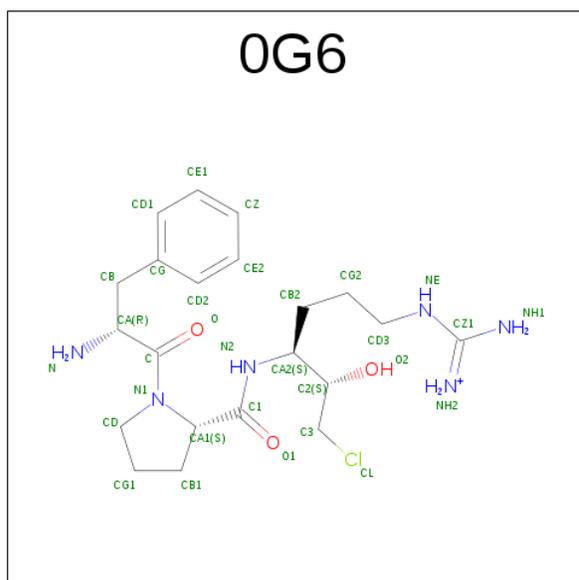
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	H	1	Total 30	C 21	N 6	O 3	0	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	95	Total 95	O 95	0	0
15	B	105	Total 105	O 105	0	0
15	H	189	Total 189	O 189	0	0
15	L	18	Total 18	O 18	0	0

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: IGA FAB LIGHT CHAIN
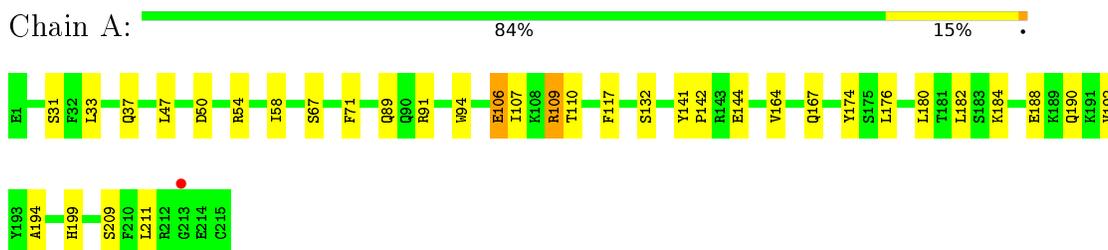
- Molecule 2: IGA FAB HEAVY CHAIN
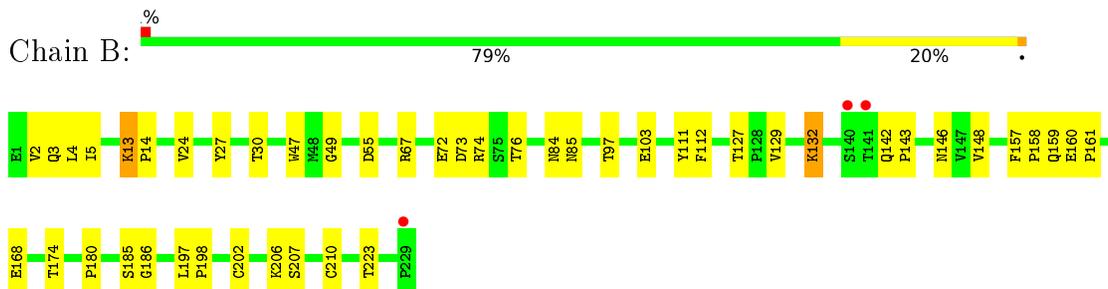
- Molecule 3: THROMBIN HEAVY CHAIN

- Molecule 4: THROMBIN LIGHT CHAIN
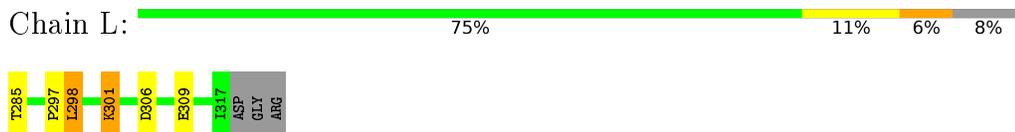
4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.77Å 92.23Å 147.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.83 – 1.90 60.83 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (60.83-1.90) 99.6 (60.83-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.201 , 0.244 0.204 , 0.246	Depositor DCC
R_{free} test set	3744 reflections (5.47%)	DCC
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6373	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \|L\| >$, $< L^2 >$ 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: BMA, NAG, NA, PO4, 0G6, SIA, GAL, CIT, PEG, PCA, MAN

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	0.31	0/1707	0.52	0/2326
2	B	0.32	0/1761	0.48	0/2415
3	H	0.34	0/2146	0.54	0/2903
4	L	0.33	0/273	0.55	0/364
All	All	0.33	0/5887	0.52	0/8008

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	1670	0	1583	30	0
2	B	1722	0	1594	42	0
3	H	2091	0	2045	19	0
4	L	270	0	253	4	0
5	A	28	0	25	1	0
5	H	42	0	36	9	0
6	A	7	0	10	0	0
6	H	14	0	20	0	0
7	B	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	20	0	0	1	0
8	H	11	0	9	6	0
9	H	11	0	9	1	0
10	H	11	0	9	0	0
11	H	20	0	17	2	0
12	H	13	0	5	4	0
13	H	1	0	0	0	0
14	H	30	0	31	0	0
15	A	95	0	0	2	0
15	B	105	0	0	5	0
15	H	189	0	0	5	1
15	L	18	0	0	0	0
All	All	6373	0	5646	103	1

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 9.

The worst 5 of 103 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)
12:H:608:CIT:O2	12:H:608:CIT:H42	1.54	1.02
1:A:91[A]:ARG:NH1	2:B:111:TYR:CE2	2.37	0.93
15:H:755:HOH:O	4:L:285:THR:HG22	1.71	0.91
5:H:602:NAG:H3	8:H:603:BMA:H2	1.60	0.83
1:A:192:VAL:HG22	1:A:211:LEU:CD2	2.11	0.80

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:874:HOH:O	15:H:888:HOH:O[4_466]	2.14	0.06

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	218/215 (101%)	208 (95%)	10 (5%)	0	100	100
2	B	230/229 (100%)	219 (95%)	11 (5%)	0	100	100
3	H	258/259 (100%)	247 (96%)	11 (4%)	0	100	100
4	L	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
All	All	738/739 (100%)	705 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	182/187 (97%)	178 (98%)	4 (2%)	60	53
2	B	184/196 (94%)	178 (97%)	6 (3%)	45	34
3	H	223/225 (99%)	222 (100%)	1 (0%)	93	94
4	L	29/31 (94%)	27 (93%)	2 (7%)	19	8
All	All	618/639 (97%)	605 (98%)	13 (2%)	61	55

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	67	ARG
2	B	132	LYS
3	H	507	CYS
2	B	13	LYS
2	B	210	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	200	GLN
2	B	146	ASN
2	B	217	ASN
3	H	537	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	PCA	B	1	2	7,8,9	0.54	0	9,10,12	1.38	1 (11%)

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	PCA	B	1	2	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	PCA	CB-CA-C	-2.90	108.50	112.80

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	NAG	A	301	1,5	14,14,15	0.55	0	15,19,21	0.80	0
5	NAG	A	302	5	14,14,15	0.50	0	15,19,21	0.63	0
6	PEG	A	303	-	6,6,6	0.47	0	5,5,5	0.36	0
7	PO4	B	301	-	4,4,4	0.62	0	6,6,6	0.23	0
5	NAG	H	601	3,5	14,14,15	0.47	0	15,19,21	1.80	3 (20%)
5	NAG	H	602	8,5	14,14,15	0.49	0	15,19,21	0.69	0
8	BMA	H	603	9,5	11,11,12	0.31	0	15,15,17	0.58	0
9	MAN	H	604	8,5	11,11,12	0.61	0	15,15,17	0.82	0
5	NAG	H	605	9,10	14,14,15	0.59	0	15,19,21	0.94	0
10	GAL	H	606	11,5	11,11,12	0.63	0	15,15,17	0.82	0
11	SIA	H	607	10	17,20,21	0.28	0	18,28,31	0.71	1 (5%)
12	CIT	H	608	-	3,12,12	0.98	0	3,17,17	2.97	2 (66%)
6	PEG	H	609	-	6,6,6	0.52	0	5,5,5	0.32	0
7	PO4	H	611	-	4,4,4	0.56	0	6,6,6	0.24	0
7	PO4	H	612	-	4,4,4	0.46	0	6,6,6	0.23	0
7	PO4	H	613	-	4,4,4	0.65	0	6,6,6	0.23	0
7	PO4	H	614	-	4,4,4	0.63	0	6,6,6	0.23	0
14	0G6	H	615	-	27,31,32	0.45	0	34,41,42	0.85	2 (5%)
6	PEG	H	616	-	6,6,6	0.43	0	5,5,5	0.40	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
5	NAG	A	301	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	302	5	-	0/6/23/26	0/1/1/1
6	PEG	A	303	-	-	0/4/4/4	0/0/0/0
7	PO4	B	301	-	-	0/0/0/0	0/0/0/0
5	NAG	H	601	3,5	-	0/6/23/26	0/1/1/1
5	NAG	H	602	8,5	-	0/6/23/26	0/1/1/1
8	BMA	H	603	9,5	-	0/2/19/22	0/1/1/1
9	MAN	H	604	8,5	-	0/2/19/22	1/1/1/1
5	NAG	H	605	9,10	-	0/6/23/26	0/1/1/1
10	GAL	H	606	11,5	-	0/2/19/22	0/1/1/1
11	SIA	H	607	10	-	1/14/34/38	0/1/1/1
12	CIT	H	608	-	-	0/6/16/16	0/0/0/0
6	PEG	H	609	-	-	0/4/4/4	0/0/0/0
7	PO4	H	611	-	-	0/0/0/0	0/0/0/0
7	PO4	H	612	-	-	0/0/0/0	0/0/0/0
7	PO4	H	613	-	-	0/0/0/0	0/0/0/0
7	PO4	H	614	-	-	0/0/0/0	0/0/0/0
14	0G6	H	615	-	-	0/29/41/43	0/2/2/2
6	PEG	H	616	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	601	NAG	C4-C3-C2	-4.77	103.93	111.34
12	H	608	CIT	C3-C4-C5	-4.45	108.00	114.95
14	H	615	0G6	O1-C1-N2	-2.82	117.42	122.91
12	H	608	CIT	C3-C2-C1	-2.43	111.16	114.95
11	H	607	SIA	C7-C6-C5	-2.02	111.28	114.06

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	H	607	SIA	O10-C10-N5-C5

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	H	604	MAN	C1-C2-C3-C4-C5-O5

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	301	NAG	1	0
7	B	301	PO4	2	0
5	H	601	NAG	3	0
5	H	602	NAG	8	0
8	H	603	BMA	6	0
9	H	604	MAN	1	0
5	H	605	NAG	1	0
11	H	607	SIA	2	0
12	H	608	CIT	4	0
7	H	613	PO4	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	215/215 (100%)	-0.05	1 (0%)	91	92	26, 35, 51, 63	0
2	B	228/229 (99%)	0.00	3 (1%)	79	82	26, 37, 56, 69	0
3	H	259/259 (100%)	-0.02	0	100	100	19, 27, 39, 51	0
4	L	33/36 (91%)	0.01	0	100	100	27, 35, 47, 54	0
All	All	735/739 (99%)	-0.02	4 (0%)	91	92	19, 33, 51, 69	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	141	THR	3.4
2	B	140	SER	3.3
1	A	213	GLY	2.9
2	B	229	PRO	2.4

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	PCA	B	1	8/9	0.87	0.14	-	54,55,58,59	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. 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
7	PO4	H	613	5/5	0.92	0.16	4.53	77,79,81,83	0
12	CIT	H	608	13/13	0.70	0.17	4.15	50,55,63,66	0
6	PEG	H	616	7/7	0.88	0.13	3.69	52,53,55,56	0
6	PEG	A	303	7/7	0.83	0.14	1.19	50,52,53,53	0
7	PO4	B	301	5/5	0.79	0.19	1.03	100,104,105,106	0
14	0G6	H	615	30/31	0.97	0.12	0.87	19,21,22,23	0
5	NAG	A	301	14/15	0.91	0.13	0.28	46,50,56,66	0
6	PEG	H	609	7/7	0.87	0.13	0.26	34,43,47,51	0
7	PO4	H	611	5/5	0.97	0.11	-0.23	53,54,57,58	0
13	NA	H	610	1/1	0.97	0.09	-0.71	34,34,34,34	0
10	GAL	H	606	11/12	0.93	0.09	-0.78	43,44,45,46	0
7	PO4	H	612	5/5	0.99	0.07	-2.98	32,33,33,34	0
9	MAN	H	604	11/12	0.77	0.17	-	80,85,87,88	0
7	PO4	H	614	5/5	0.71	0.17	-	94,96,99,100	0
5	NAG	H	602	14/15	0.73	0.25	-	86,91,96,103	0
5	NAG	H	605	14/15	0.87	0.14	-	50,63,74,75	0
8	BMA	H	603	11/12	0.55	0.29	-	90,103,106,109	0
11	SIA	H	607	20/21	0.90	0.14	-	47,61,68,69	0
5	NAG	A	302	14/15	0.76	0.24	-	75,80,84,87	0
5	NAG	H	601	14/15	0.84	0.14	-	54,61,66,76	0

6.5 Other polymers (i)

There are no such residues in this entry.