



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2016 – 08:57 PM EDT

PDB ID : 5AMB
Title : Crystal structure of the Angiotensin-1 converting enzyme N-domain in complex with amyloid-beta 35-42
Authors : Masuyer, G.; Larmuth, K.M.; Douglas, R.G.; Sturrock, E.D.; Acharya, K.R.
Deposited on : 2015-03-10
Resolution : 1.55 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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-20027107
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-20027107

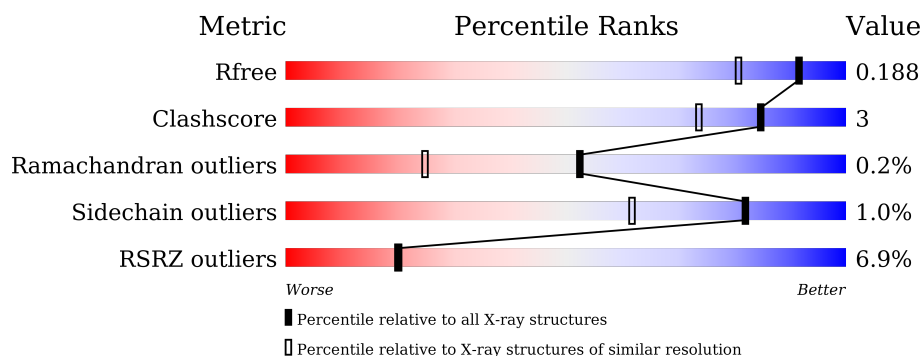
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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}	91344	1665 (1.58-1.54)
Clashscore	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

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 $\leq 5\%$. 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	629	<div> <div>5%</div> <div>89%</div> <div>7%</div> <div>..</div> </div>
1	B	629	<div> <div>9%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>
2	P	8	<div> <div>25%</div> <div>75%</div> </div>
2	Q	8	<div> <div>25%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	P6G	A	1205	-	-	-	X
10	P6G	B	1201	-	-	-	X
10	P6G	B	1202	-	-	-	X
11	NAG	B	1104	-	-	-	X
5	NAG	A	1100	-	-	-	X
5	NAG	B	1100	-	-	-	X
6	NAG	A	1102	-	-	-	X
6	NAG	B	1102	-	-	-	X
8	PEG	A	1201	-	-	-	X
8	PEG	A	1204	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 11095 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 ANGIOTENSIN-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	2	0
			4964	3187	852	906	19			
1	B	607	Total	C	N	O	S	0	0	0
			4940	3174	848	899	19			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	131	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	289	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	545	ARG	GLN	ENGINEERED MUTATION	UNP P12821
A	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821
A	629	LEU	ARG	ENGINEERED MUTATION	UNP P12821
B	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	131	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	289	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	545	ARG	GLN	ENGINEERED MUTATION	UNP P12821
B	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821
B	629	LEU	ARG	ENGINEERED MUTATION	UNP P12821

- Molecule 2 is a protein called AMYLOID BETA A4 PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	2	Total	C	N	O	0	0	0
			14	9	2	3			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	2	Total	C	N	O	0	0	0
			14	9	2	3			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			24	14	1	9		
5	B	2	Total	C	N	O	0	0
			24	14	1	9		

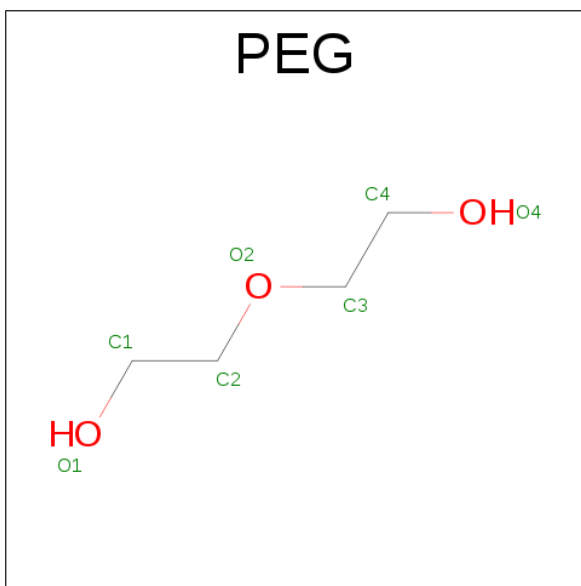
- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

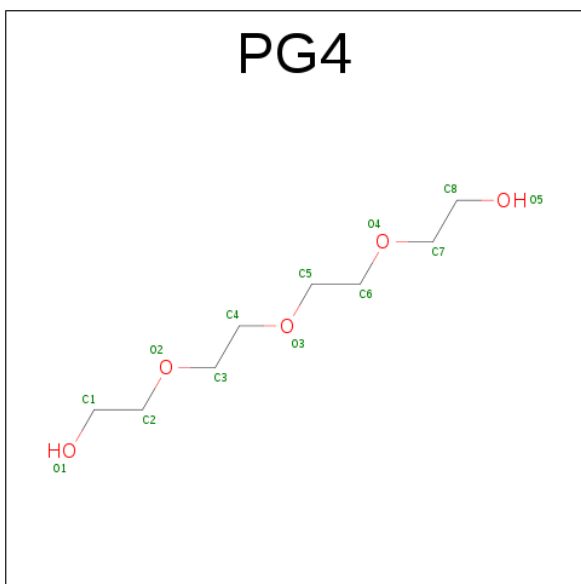
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



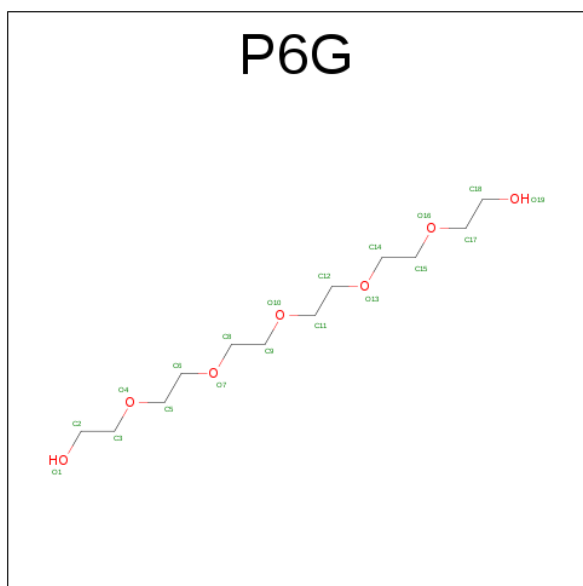
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			19	12	7		
10	B	1	Total	C	O	0	0
			19	12	7		
10	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 11 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	3	Total	C	N	O	0	0
			39	22	2	15		

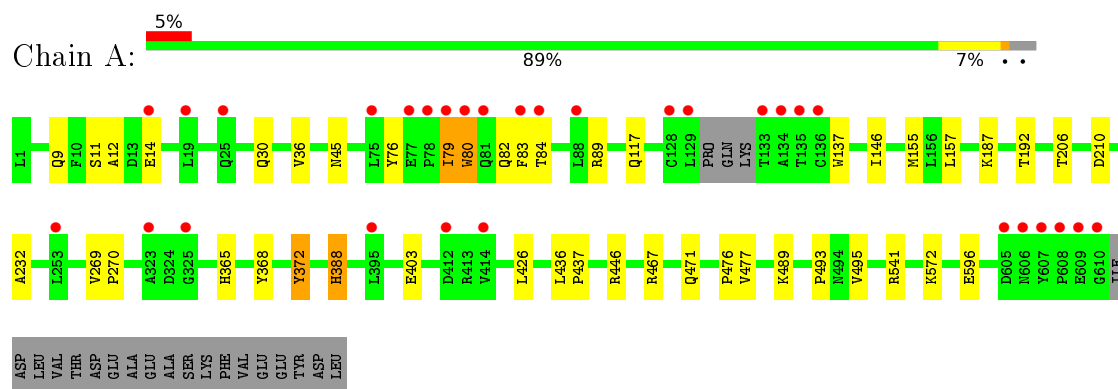
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	513	Total	O	0	0
			513	513		
12	B	359	Total	O	0	0
			359	359		

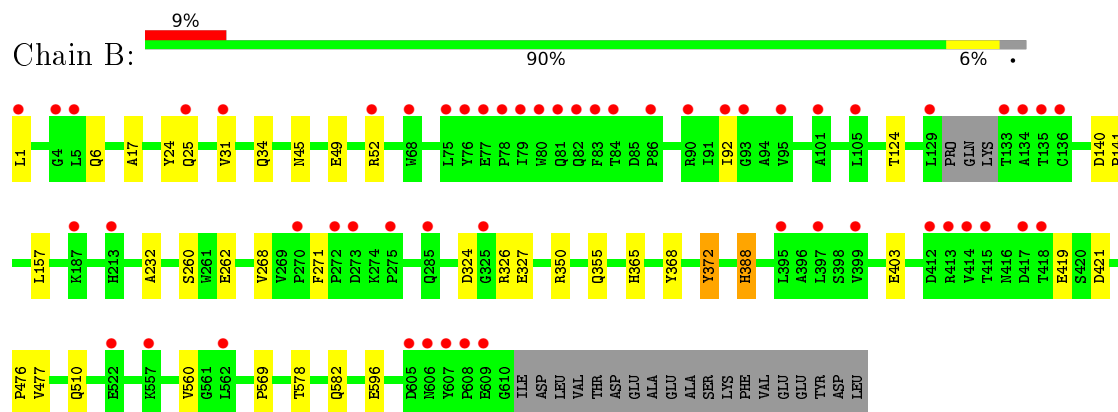
3 Residue-property plots [i](#)

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.

• Molecule 1: ANGIOTENSIN-CONVERTING ENZYME



• Molecule 1: ANGIOTENSIN-CONVERTING ENZYME



• Molecule 2: AMYLOID BETA A4 PROTEIN



• Molecule 2: AMYLOID BETA A4 PROTEIN



MET	VAL	GLY	GLY	VAL	VAL	I41
						A42

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.98Å 76.95Å 83.22Å 88.63° 64.14° 75.22°	Depositor
Resolution (Å)	74.51 – 1.55 29.60 – 1.55	Depositor EDS
% Data completeness (in resolution range)	87.8 (74.51-1.55) 86.8 (29.60-1.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.158 , 0.181 0.167 , 0.188	Depositor DCC
R_{free} test set	9791 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 200050 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11095	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CL, PG4, FUC, P6G, PEG

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	0.70	0/5125	0.74	3/6980 (0.0%)
1	B	0.63	0/5095	0.69	0/6940
2	P	0.90	0/13	0.54	0/15
2	Q	0.75	0/13	0.45	0/15
All	All	0.67	0/10246	0.71	3/13950 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	TRP	N-CA-C	5.69	126.37	111.00
1	A	541	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	446	ARG	NE-CZ-NH2	-5.56	117.52	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	79	ILE	Peptide

5.2 Too-close contacts ⓘ

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	4964	0	4741	31	0
1	B	4940	0	4707	24	0
2	P	14	0	15	0	0
2	Q	14	0	15	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	24	0	22	1	0
5	B	24	0	22	1	0
6	A	28	0	25	0	0
6	B	28	0	25	0	0
7	A	49	0	43	0	0
8	A	21	0	30	2	0
8	B	7	0	10	0	0
9	A	10	0	13	0	0
10	A	19	0	26	3	0
10	B	38	0	52	0	0
11	B	39	0	34	0	0
12	A	513	0	0	6	0
12	B	359	0	0	1	0
All	All	11095	0	9780	57	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 3.

All (57) 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:B:260:SER:OG	1:B:262:GLU:OE1	1.87	0.93
1:A:365:HIS:HD1	1:A:388:HIS:HD2	1.26	0.84
1:B:124:THR:HG22	1:B:327:GLU:HG2	1.60	0.81
1:A:365:HIS:HD1	1:A:388:HIS:CD2	2.00	0.80
1:B:365:HIS:HD1	1:B:388:HIS:HD2	1.30	0.78
1:A:270:PRO:HD3	1:A:426:LEU:HD23	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:HIS:HD1	1:B:388:HIS:CD2	2.05	0.73
1:A:467:ARG:HH11	1:A:471:GLN:HE22	1.38	0.72
1:A:12:ALA:O	12:A:2005:HOH:O	2.12	0.68
1:A:14:GLU:HG2	1:A:83:PHE:CD1	2.30	0.66
1:B:350:ARG:H	1:B:355:GLN:HE21	1.43	0.64
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.79	0.64
1:A:596:GLU:OE2	5:B:1100:NAG:O7	2.16	0.63
1:A:187:LYS:HE2	1:A:192:THR:O	1.98	0.63
1:A:206:THR:HG23	1:A:210:ASP:OD2	1.99	0.62
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.83	0.59
1:A:14:GLU:OE2	1:A:83:PHE:HA	2.03	0.58
1:A:372:TYR:OH	1:A:388:HIS:HE1	1.87	0.57
1:B:24:TYR:HD2	1:B:25:GLN:HG3	1.69	0.57
1:B:419:GLU:O	1:B:421:ASP:N	2.36	0.56
1:A:79:ILE:HD12	1:A:80:TRP:HA	1.87	0.56
1:B:124:THR:HG22	1:B:327:GLU:CG	2.34	0.56
1:B:49:GLU:OE2	1:B:52:ARG:NH2	2.39	0.53
1:A:467:ARG:NH1	1:A:471:GLN:HE22	2.07	0.53
10:A:1205:P6G:H31	12:A:2124:HOH:O	2.09	0.51
1:A:84:THR:HB	12:A:2006:HOH:O	2.09	0.51
10:A:1205:P6G:H81	12:A:2358:HOH:O	2.11	0.50
5:A:1100:NAG:O7	1:B:596:GLU:OE2	2.29	0.50
1:A:157:LEU:HD13	1:A:476:PRO:HB2	1.93	0.49
1:B:271:PHE:CE2	1:B:419:GLU:HG2	2.47	0.49
1:B:560:VAL:CG2	12:B:2313:HOH:O	2.61	0.49
1:A:572:LYS:HD2	8:A:1201:PEG:H11	1.94	0.48
1:A:436:LEU:N	1:A:437:PRO:HD2	2.29	0.48
1:A:76:TYR:HB3	1:A:80:TRP:HB3	1.95	0.48
1:B:17:ALA:HB1	1:B:92:ILE:HD11	1.94	0.48
1:B:31:VAL:O	1:B:34:GLN:HG3	2.14	0.47
1:B:1:LEU:HD23	1:B:6:GLN:HG2	1.97	0.47
1:A:232:ALA:HB2	8:A:1204:PEG:H22	1.96	0.45
1:B:578:THR:O	1:B:582:GLN:HG3	2.16	0.45
1:B:510:GLN:HG2	1:B:569:PRO:HG2	1.98	0.45
1:A:117[A]:GLN:NE2	12:A:2050:HOH:O	2.40	0.45
1:B:124:THR:CG2	1:B:327:GLU:HG2	2.41	0.44
1:A:146:ILE:HD13	1:A:155:MET:HE2	2.01	0.43
1:B:232:ALA:CB	1:B:268:VAL:HG12	2.49	0.43
1:B:157:LEU:HD13	1:B:476:PRO:HB2	2.01	0.43
1:A:30:GLN:NE2	12:A:2018:HOH:O	2.52	0.43
1:B:372:TYR:OH	1:B:388:HIS:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TRP:CH2	1:A:155:MET:HE1	2.55	0.42
1:A:83:PHE:HB2	1:A:89:ARG:CG	2.50	0.42
1:A:269:VAL:HA	1:A:270:PRO:HD3	1.91	0.42
1:B:324:ASP:OD1	1:B:326:ARG:HB2	2.20	0.41
1:A:489:LYS:O	1:A:493:PRO:HD2	2.20	0.41
1:A:79:ILE:O	1:A:82:GLN:OE1	2.38	0.41
1:B:140:ASP:HA	1:B:141:PRO:HA	1.88	0.41
1:A:495:VAL:O	1:A:495:VAL:HG12	2.21	0.41
1:A:146:ILE:HD13	1:A:155:MET:CE	2.51	0.41
1:A:36:VAL:HA	10:A:1205:P6G:H172	2.03	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	605/629 (96%)	593 (98%)	11 (2%)	1 (0%)	52	25
1	B	603/629 (96%)	591 (98%)	11 (2%)	1 (0%)	52	25
All	All	1208/1258 (96%)	1184 (98%)	22 (2%)	2 (0%)	52	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	B	45	ASN

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	522/541 (96%)	516 (99%)	6 (1%)	80	58
1	B	516/541 (95%)	512 (99%)	4 (1%)	86	71
2	P	1/5 (20%)	1 (100%)	0	100	100
2	Q	1/5 (20%)	1 (100%)	0	100	100
All	All	1040/1092 (95%)	1030 (99%)	10 (1%)	82	62

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	11	SER
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	A	403	GLU
1	B	368	TYR
1	B	372	TYR
1	B	388	HIS
1	B	403	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	371	GLN
1	A	388	HIS
1	A	471	GLN
1	B	188	GLN
1	B	355	GLN
1	B	371	GLN
1	B	388	HIS

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 ⓘ

15 carbohydrates 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	$\# Z > 2$
5	NAG	A	1100	1,5	14,14,15	0.59	0	15,19,21	0.75	0
5	FUC	A	1101	5	10,10,11	0.37	0	13,14,16	0.91	1 (7%)
6	NAG	A	1102	1,6	14,14,15	0.80	1 (7%)	15,19,21	1.33	1 (6%)
6	NAG	A	1103	6	14,14,15	0.47	0	15,19,21	1.51	2 (13%)
7	NAG	A	1104	1,7	14,14,15	0.96	1 (7%)	15,19,21	0.99	0
7	NAG	A	1105	7	14,14,15	0.36	0	15,19,21	1.04	0
7	BMA	A	1106	7	11,11,12	0.58	0	15,15,17	2.14	3 (20%)
7	FUC	A	1107	7	10,10,11	0.71	0	13,14,16	1.96	1 (7%)
5	NAG	B	1100	1,5	14,14,15	0.52	0	15,19,21	1.07	1 (6%)
5	FUC	B	1101	5	10,10,11	0.57	0	13,14,16	1.72	3 (23%)
6	NAG	B	1102	1,6	14,14,15	0.37	0	15,19,21	0.94	0
6	NAG	B	1103	6	14,14,15	0.47	0	15,19,21	1.79	2 (13%)
11	NAG	B	1104	1,11	14,14,15	0.37	0	15,19,21	0.89	0
11	NAG	B	1105	11	14,14,15	0.36	0	15,19,21	1.13	1 (6%)
11	BMA	B	1106	11	11,11,12	0.73	0	15,15,17	1.91	3 (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
5	NAG	A	1100	1,5	-	0/6/23/26	0/1/1/1
5	FUC	A	1101	5	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1102	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1103	6	-	0/6/23/26	0/1/1/1
7	NAG	A	1104	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1105	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1106	7	-	0/2/19/22	0/1/1/1
7	FUC	A	1107	7	-	0/0/17/20	0/1/1/1
5	NAG	B	1100	1,5	-	0/6/23/26	0/1/1/1
5	FUC	B	1101	5	-	0/0/17/20	0/1/1/1
6	NAG	B	1102	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1103	6	-	0/6/23/26	0/1/1/1
11	NAG	B	1104	1,11	-	0/6/23/26	0/1/1/1
11	NAG	B	1105	11	-	0/6/23/26	0/1/1/1
11	BMA	B	1106	11	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1104	NAG	O5-C1	-2.47	1.39	1.43
6	A	1102	NAG	O5-C1	2.64	1.48	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1100	NAG	O5-C5-C4	-2.24	106.42	110.13
5	A	1101	FUC	O5-C5-C6	2.21	110.24	106.28
11	B	1105	NAG	C3-C4-C5	2.45	114.59	110.23
5	B	1101	FUC	O5-C1-C2	2.53	114.94	110.89
5	B	1101	FUC	C1-C2-C3	2.89	113.06	109.55
7	A	1106	BMA	C2-C3-C4	2.90	116.11	111.05
11	B	1106	BMA	C1-O5-C5	3.16	116.78	112.14
11	B	1106	BMA	C2-C3-C4	3.27	116.76	111.05
6	A	1103	NAG	O4-C4-C3	3.37	117.96	110.36
6	A	1103	NAG	C3-C4-C5	3.58	116.61	110.23
5	B	1101	FUC	C3-C4-C5	3.61	115.05	109.66
6	B	1103	NAG	C3-C4-C5	4.28	117.86	110.23
7	A	1106	BMA	C1-O5-C5	4.42	118.64	112.14
6	A	1102	NAG	O5-C5-C4	4.42	117.46	110.13
6	B	1103	NAG	O4-C4-C3	4.56	120.63	110.36
11	B	1106	BMA	O3-C3-C2	5.11	119.38	110.01
7	A	1106	BMA	O3-C3-C2	5.84	120.72	110.01
7	A	1107	FUC	O2-C2-C1	6.27	121.79	109.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1100	NAG	1	0
5	B	1100	NAG	1	0

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	PEG	A	1201	-	6,6,6	0.51	0	5,5,5	0.60	0
8	PEG	A	1202	-	6,6,6	0.49	0	5,5,5	0.37	0
9	PG4	A	1203	-	9,9,12	0.55	0	8,8,11	0.51	0
8	PEG	A	1204	-	6,6,6	0.60	0	5,5,5	0.40	0
10	P6G	A	1205	-	18,18,18	0.46	0	17,17,17	0.53	0
8	PEG	B	1200	-	6,6,6	0.56	0	5,5,5	0.26	0
10	P6G	B	1201	-	18,18,18	0.68	0	17,17,17	0.38	0
10	P6G	B	1202	-	18,18,18	0.53	0	17,17,17	0.25	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	PEG	A	1201	-	-	0/4/4/4	0/0/0/0
8	PEG	A	1202	-	-	0/4/4/4	0/0/0/0
9	PG4	A	1203	-	-	0/7/7/10	0/0/0/0
8	PEG	A	1204	-	-	0/4/4/4	0/0/0/0
10	P6G	A	1205	-	-	0/16/16/16	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PEG	B	1200	-	-	0/4/4/4	0/0/0/0
10	P6G	B	1201	-	-	0/16/16/16	0/0/0/0
10	P6G	B	1202	-	-	0/16/16/16	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1201	PEG	1	0
8	A	1204	PEG	1	0
10	A	1205	P6G	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

6.1 Protein, DNA and RNA chains

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	607/629 (96%)	0.20	30 (4%) 33 34	20, 30, 53, 87	0
1	B	607/629 (96%)	0.45	54 (8%) 12 12	21, 36, 58, 87	0
2	P	2/8 (25%)	0.27	0 100 100	26, 26, 26, 30	0
2	Q	2/8 (25%)	0.16	0 100 100	27, 27, 27, 31	0
All	All	1218/1274 (95%)	0.33	84 (6%) 20 20	20, 33, 56, 87	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	ALA	8.5
1	A	78	PRO	8.5
1	B	135	THR	7.6
1	B	133	THR	7.2
1	A	80	TRP	6.7
1	A	325	GLY	6.3
1	A	79	ILE	6.3
1	A	135	THR	5.7
1	B	415	THR	5.7
1	B	1	LEU	5.5
1	A	606	ASN	5.5
1	B	78	PRO	5.3
1	A	607	TYR	5.3
1	B	325	GLY	5.2
1	A	19	LEU	4.9
1	B	129	LEU	4.9
1	B	414	VAL	4.8
1	B	80	TRP	4.7
1	A	14	GLU	4.7
1	A	133	THR	4.6
1	B	413	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	323	ALA	4.3
1	B	81	GLN	4.3
1	A	134	ALA	4.3
1	A	83	PHE	4.2
1	B	82	GLN	4.2
1	A	609	GLU	4.0
1	B	609	GLU	4.0
1	A	605	ASP	3.7
1	A	610	GLY	3.7
1	B	606	ASN	3.7
1	A	129	LEU	3.6
1	B	607	TYR	3.5
1	B	4	GLY	3.5
1	B	418	THR	3.4
1	B	84	THR	3.4
1	A	414	VAL	3.2
1	B	605	ASP	3.1
1	B	412	ASP	3.1
1	B	75	LEU	3.1
1	B	83	PHE	3.1
1	B	562	LEU	3.0
1	A	81	GLN	3.0
1	B	76	TYR	3.0
1	A	608	PRO	2.9
1	B	275	PRO	2.8
1	A	395	LEU	2.8
1	B	5	LEU	2.8
1	A	77	GLU	2.8
1	A	412	ASP	2.7
1	B	93	GLY	2.7
1	A	75	LEU	2.7
1	A	136	CYS	2.7
1	B	273	ASP	2.7
1	B	397	LEU	2.6
1	B	522	GLU	2.6
1	B	92	ILE	2.6
1	B	77	GLU	2.5
1	B	136	CYS	2.5
1	A	88	LEU	2.4
1	B	68	TRP	2.3
1	A	253	LEU	2.3
1	B	86	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	608	PRO	2.3
1	B	52	ARG	2.3
1	B	25	GLN	2.3
1	B	79	ILE	2.3
1	A	25	GLN	2.3
1	B	285	GLN	2.3
1	B	105	LEU	2.2
1	B	95	VAL	2.2
1	B	417	ASP	2.2
1	B	187	LYS	2.2
1	B	399	VAL	2.1
1	B	90	ARG	2.1
1	A	128	CYS	2.1
1	B	557	LYS	2.1
1	A	84	THR	2.1
1	B	101	ALA	2.1
1	B	395	LEU	2.1
1	B	31	VAL	2.1
1	B	272	PRO	2.1
1	B	213	HIS	2.1
1	B	270	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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
6	NAG	A	1102	14/15	0.88	0.26	5.11	50,57,64,71	0
11	NAG	B	1104	14/15	0.94	0.28	4.21	56,63,75,88	0
6	NAG	B	1102	14/15	0.80	0.31	2.86	47,55,73,74	0
5	NAG	B	1100	14/15	0.89	0.12	2.42	44,51,60,75	0
5	NAG	A	1100	14/15	0.89	0.15	2.42	36,46,55,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	NAG	A	1104	14/15	0.98	0.12	1.25	34,40,45,50	0
7	NAG	A	1105	14/15	0.95	0.19	-	44,56,66,66	0
6	NAG	A	1103	14/15	0.85	0.41	-	58,71,85,92	0
11	NAG	B	1105	14/15	0.91	0.39	-	78,81,96,106	0
5	FUC	A	1101	10/11	0.73	0.35	-	64,75,79,93	0
5	FUC	B	1101	10/11	0.79	0.30	-	65,81,88,91	0
7	FUC	A	1107	10/11	0.89	0.22	-	46,57,66,68	0
6	NAG	B	1103	14/15	0.54	0.59	-	84,92,109,116	0
11	BMA	B	1106	11/12	0.75	0.42	-	91,99,101,103	0
7	BMA	A	1106	11/12	0.87	0.20	-	63,66,79,84	0

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(\AA^2)	Q<0.9
8	PEG	A	1201	7/7	0.90	0.25	9.91	50,52,62,68	0
10	P6G	B	1202	19/19	0.67	0.20	5.32	47,52,58,59	0
10	P6G	A	1205	19/19	0.70	0.21	5.02	46,52,56,56	0
10	P6G	B	1201	19/19	0.78	0.14	3.61	44,55,62,63	0
8	PEG	A	1204	7/7	0.88	0.20	2.59	31,40,46,72	0
9	PG4	A	1203	10/13	0.94	0.11	0.99	43,54,56,60	0
4	CL	B	1002	1/1	1.00	0.08	0.75	29,29,29,29	0
4	CL	A	1002	1/1	1.00	0.08	-0.19	23,23,23,23	0
3	ZN	B	1001	1/1	1.00	0.06	-1.72	25,25,25,25	0
3	ZN	A	1001	1/1	1.00	0.06	-2.47	25,25,25,25	0
8	PEG	B	1200	7/7	0.95	0.11	-	38,44,50,55	0
8	PEG	A	1202	7/7	0.89	0.16	-	50,52,65,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.