



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:03 AM GMT

PDB ID : 3NXQ
Title : Angiotensin Converting Enzyme N domain glycosylation mutant (Ndom389)
in complex with RXP407
Authors : Anthony, C.S.; Corradi, H.R.; Schwager, S.L.U.; Redelinghuys, P.; Georgiadis,
D.; Dive, V.; Acharya, K.R.; Sturrock, E.D.
Deposited on : 2010-07-14
Resolution : 1.99 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 ⓘ 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

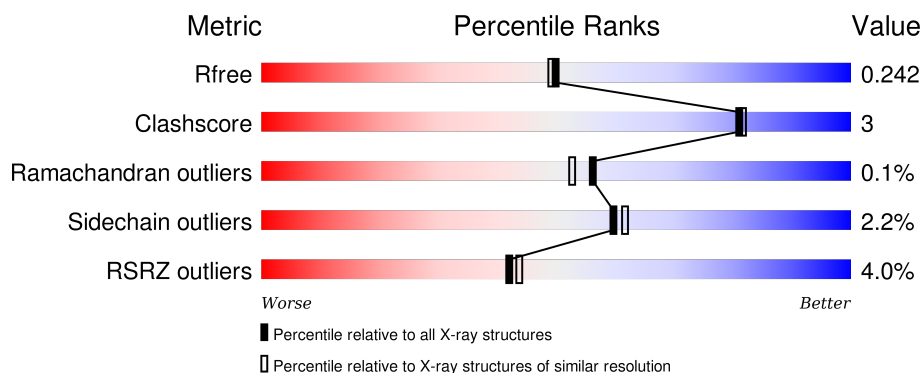
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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>3%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	B	629	<div> <div>5%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	P6G	B	709	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 10796 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	6	0
			4955	3189	850	897	19			
1	B	610	Total	C	N	O	S	0	3	0
			4935	3181	841	894	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 ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0

- RX4
-
- The chemical structure of RX4 is a complex molecule. It features a central phosphorus atom (P1) bonded to a hydroxyl group (OH), a carboxylate group (COO-), and a complex organic moiety. The organic moiety includes a benzene ring (C1-C6) and a carboxylate group (COO-). The molecule is labeled with RX4.

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



WORLD WIDE
PDB
PROTEIN DATA BANK

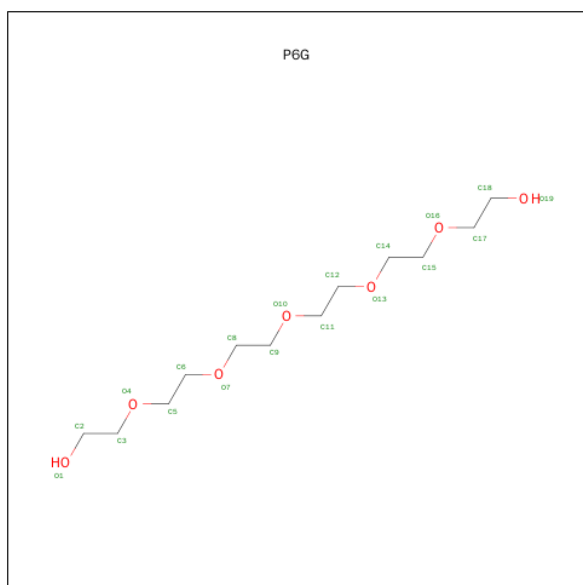
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 7 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).

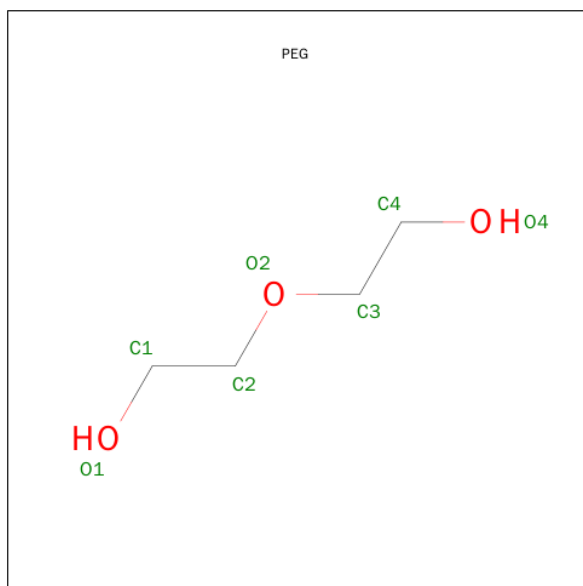


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

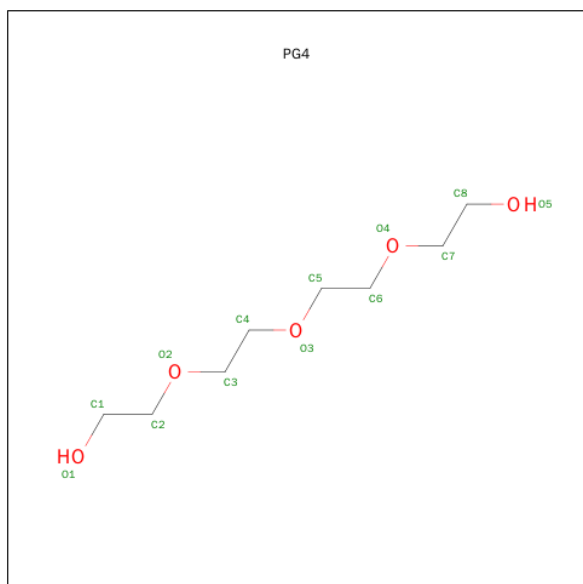
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			13	8	5		

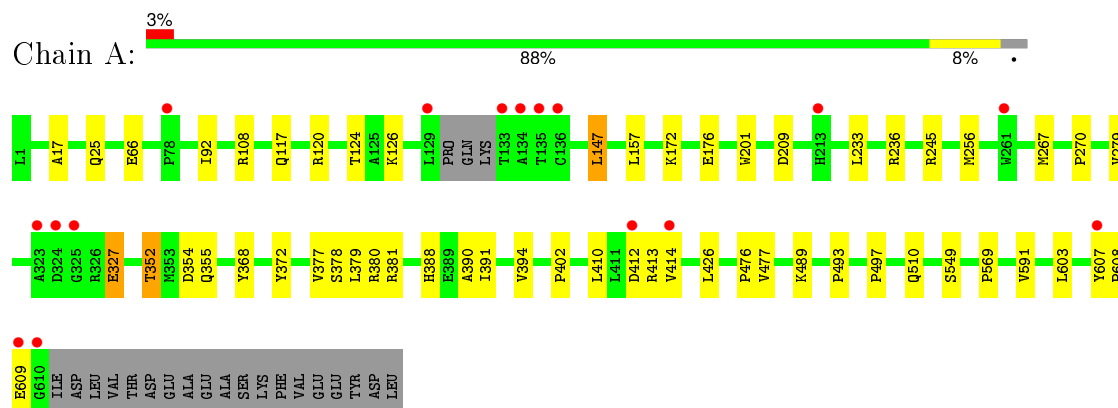
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	303	Total	O	0	0
			303	303		
11	B	260	Total	O	0	0
			260	260		

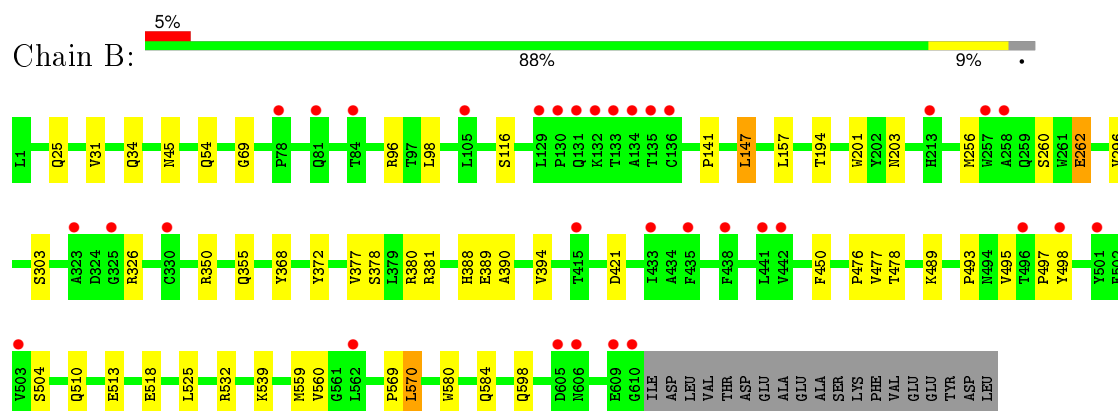
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.88Å 76.69Å 82.65Å 88.63° 64.17° 75.70°	Depositor
Resolution (Å)	40.81 – 1.99 40.81 – 1.99	Depositor EDS
% Data completeness (in resolution range)	95.6 (40.81-1.99) 92.8 (40.81-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.194 , 0.237 0.202 , 0.242	Depositor DCC
R_{free} test set	1025 reflections (1.02%)	DCC
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 101705 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10796	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CL, PG4, FUC, P6G, PEG, RX4

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	0.39	0/5129	0.51	0/6989
1	B	0.39	0/5101	0.51	1/6959 (0.0%)
All	All	0.39	0/10230	0.51	1/13948 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	570	LEU	CB-CG-CD1	5.66	120.62	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4955	0	4715	34	0
1	B	4935	0	4677	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	34	0	29	3	0
3	B	34	0	29	3	0
4	A	24	0	22	0	0
4	B	24	0	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	28	0	25	0	0
5	B	28	0	25	0	0
6	A	49	0	43	0	0
6	B	49	0	43	0	0
7	A	13	0	17	0	0
7	B	19	0	26	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	7	0	10	0	0
9	B	7	0	10	0	0
10	B	23	0	31	0	0
11	A	303	0	0	0	0
11	B	260	0	0	3	0
All	All	10796	0	9724	66	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.

The worst 5 of 66 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:THR:HG22	1:A:355:GLN:H	1.37	0.89
1:B:69:GLY:HA3	1:B:98[B]:LEU:HD21	1.57	0.86
1:B:518:GLU:HG3	1:B:539:LYS:HD2	1.69	0.74
1:B:350:ARG:H	1:B:355:GLN:HE21	1.36	0.73
1:A:236:ARG:HD2	1:A:267:MET:HE3	1.73	0.70

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	609/629 (97%)	598 (98%)	11 (2%)	0	100	100
1	B	611/629 (97%)	596 (98%)	14 (2%)	1 (0%)	52	48
All	All	1220/1258 (97%)	1194 (98%)	25 (2%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	45	ASN

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	515/541 (95%)	506 (98%)	9 (2%)	68	71
1	B	508/541 (94%)	495 (97%)	13 (3%)	54	54
All	All	1023/1082 (94%)	1001 (98%)	22 (2%)	60	62

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	96	ARG
1	B	203	ASN
1	B	560	VAL
1	B	116	SER
1	B	147	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	598	GLN
1	B	25	GLN
1	B	491	HIS
1	A	491	HIS
1	B	406	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 ⓘ

16 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	$\# Z > 2$
4	NAG	A	630	1,4	14,14,15	0.51	0	15,19,21	0.98	1 (6%)
4	FUC	A	631	4	10,10,11	0.61	0	14,14,16	1.73	4 (28%)
5	NAG	A	632	1,5	14,14,15	0.52	0	15,19,21	0.84	1 (6%)
5	NAG	A	633	5	14,14,15	0.45	0	15,19,21	0.94	1 (6%)
6	NAG	A	634	1,6	14,14,15	0.59	0	15,19,21	0.81	0
6	NAG	A	635	6	14,14,15	0.51	0	15,19,21	0.72	0
6	BMA	A	636	6	11,11,12	0.36	0	14,15,17	1.00	1 (7%)
6	FUC	A	637	6	10,10,11	0.57	0	14,14,16	0.80	1 (7%)
4	NAG	B	630	1,4	14,14,15	0.49	0	15,19,21	1.29	1 (6%)
4	FUC	B	631	4	10,10,11	0.59	0	14,14,16	1.17	2 (14%)
5	NAG	B	632	1,5	14,14,15	0.57	0	15,19,21	0.79	0
5	NAG	B	633	5	14,14,15	0.41	0	15,19,21	1.20	1 (6%)
6	NAG	B	634	1,6	14,14,15	0.55	0	15,19,21	0.85	1 (6%)
6	NAG	B	635	6	14,14,15	0.50	0	15,19,21	0.67	0
6	BMA	B	636	6	11,11,12	0.46	0	14,15,17	1.41	2 (14%)
6	FUC	B	637	6	10,10,11	0.45	0	14,14,16	0.84	1 (7%)

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
4	NAG	A	630	1,4	-	0/6/23/26	0/1/1/1
4	FUC	A	631	4	-	0/0/17/20	0/1/1/1
5	NAG	A	632	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	633	5	-	0/6/23/26	0/1/1/1
6	NAG	A	634	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	635	6	-	0/6/23/26	0/1/1/1
6	BMA	A	636	6	-	0/2/19/22	0/1/1/1
6	FUC	A	637	6	-	0/0/17/20	0/1/1/1
4	NAG	B	630	1,4	-	0/6/23/26	0/1/1/1
4	FUC	B	631	4	-	0/0/17/20	0/1/1/1
5	NAG	B	632	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	633	5	-	0/6/23/26	0/1/1/1
6	NAG	B	634	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	635	6	-	0/6/23/26	0/1/1/1
6	BMA	B	636	6	-	0/2/19/22	0/1/1/1
6	FUC	B	637	6	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	637	FUC	O5-C5-C6	2.04	109.50	106.13
4	B	631	FUC	C1-O5-C5	2.19	115.76	112.38
6	B	634	NAG	C1-O5-C5	2.21	115.06	112.25
5	A	632	NAG	C1-O5-C5	2.26	115.12	112.25
4	B	631	FUC	O5-C5-C6	2.28	109.91	106.13

There are no chirality outliers.

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
4	B	631	FUC	2	0

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	RX4	A	700	2	27,34,34	0.60	0	30,47,47	0.89	1 (3%)
9	PEG	A	706	-	6,6,6	0.42	0	5,5,5	0.36	0
7	P6G	A	708	-	12,12,18	0.46	0	11,11,17	0.35	0
3	RX4	B	700	2	27,34,34	0.63	1 (3%)	30,47,47	0.77	1 (3%)
10	PG4	B	704	-	9,9,12	0.42	0	8,8,11	0.41	0
10	PG4	B	705	-	12,12,12	0.45	0	11,11,11	0.31	0
7	P6G	B	709	-	18,18,18	0.51	0	17,17,17	0.29	0
9	PEG	B	710	-	6,6,6	0.41	0	5,5,5	0.37	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
3	RX4	A	700	2	-	0/36/43/43	0/1/1/1
9	PEG	A	706	-	-	0/4/4/4	0/0/0/0
7	P6G	A	708	-	-	0/10/10/16	0/0/0/0
3	RX4	B	700	2	-	0/36/43/43	0/1/1/1
10	PG4	B	704	-	-	0/7/7/10	0/0/0/0
10	PG4	B	705	-	-	0/10/10/10	0/0/0/0
7	P6G	B	709	-	-	0/16/16/16	0/0/0/0
9	PEG	B	710	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	RX4	P1-CAT	2.07	1.81	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	700	RX4	CAR-CBF-NAU	-2.72	105.10	110.80
3	B	700	RX4	CAR-CBF-NAU	-2.40	105.78	110.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	700	RX4	3	0
3	B	700	RX4	3	0
7	B	709	P6G	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	607/629 (96%)	0.07	16 (2%) 59 60	19, 31, 43, 66	0
1	B	610/629 (96%)	0.26	33 (5%) 29 31	21, 33, 51, 66	0
All	All	1217/1258 (96%)	0.17	49 (4%) 42 44	19, 31, 48, 66	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	PRO	8.6
1	B	135	THR	6.9
1	B	134	ALA	5.4
1	A	610	GLY	5.3
1	A	323	ALA	5.0

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](#)

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
5	NAG	B	632	14/15	0.87	0.23	1.44	38,44,47,51	0
4	NAG	B	630	14/15	0.84	0.13	1.16	40,46,49,54	0
4	NAG	A	630	14/15	0.87	0.13	0.28	38,45,48,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	A	632	14/15	0.92	0.14	0.06	39,43,45,48	0
4	FUC	B	631	10/11	0.76	0.37	-	58,60,60,60	0
6	BMA	A	636	11/12	0.78	0.23	-	61,62,63,63	0
6	BMA	B	636	11/12	0.81	0.32	-	66,67,67,67	0
6	NAG	B	635	14/15	0.90	0.26	-	62,64,65,65	0
5	NAG	A	633	14/15	0.85	0.28	-	51,53,56,56	0
6	NAG	A	634	14/15	0.92	0.11	-	43,47,51,51	0
4	FUC	A	631	10/11	0.74	0.32	-	56,58,59,59	0
6	FUC	B	637	10/11	0.91	0.28	-	63,63,64,64	0
6	NAG	B	634	14/15	0.89	0.19	-	52,56,59,62	0
6	NAG	A	635	14/15	0.88	0.17	-	54,56,57,60	0
6	FUC	A	637	10/11	0.79	0.16	-	53,55,55,56	0
5	NAG	B	633	14/15	0.79	0.40	-	55,58,59,60	0

6.4 Ligands ⓘ

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	P6G	B	709	19/19	0.73	0.20	2.93	60,60,61,61	0
7	P6G	A	708	13/19	0.83	0.17	1.47	46,47,49,49	0
10	PG4	B	705	13/13	0.89	0.10	1.11	52,53,54,55	0
10	PG4	B	704	10/13	0.87	0.15	0.94	52,52,52,53	0
9	PEG	A	706	7/7	0.93	0.13	0.61	51,52,52,52	0
3	RX4	A	700	34/34	0.94	0.14	0.50	20,26,35,39	0
3	RX4	B	700	34/34	0.96	0.17	0.23	19,23,37,38	0
8	CL	B	900	1/1	1.00	0.10	-1.67	28,28,28,28	0
8	CL	A	900	1/1	0.99	0.07	-1.90	23,23,23,23	0
2	ZN	B	650	1/1	1.00	0.10	-	21,21,21,21	0
9	PEG	B	710	7/7	0.83	0.24	-	66,67,67,67	0
2	ZN	A	650	1/1	1.00	0.11	-	23,23,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.