



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 14, 2018 – 12:05 AM EST

PDB ID : 6EN5
Title : Crystal structure A of the Angiotensin-1 converting enzyme N-domain in complex with a diprolyl inhibitor.
Authors : Cozier, G.E.; Acharya, K.R.; Fienberg, S.; Chibale, K.; Sturrock, E.D.
Deposited on : 2017-10-04
Resolution : 1.75 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030736

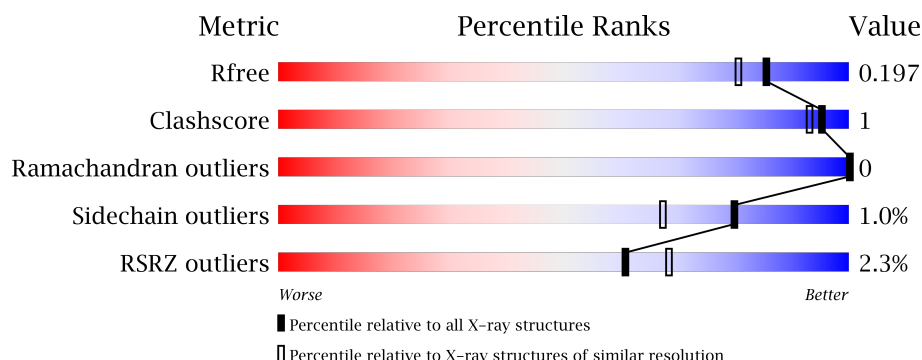
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	100719	1762 (1.76-1.76)
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (1.76-1.76)

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>2%</div> <div>92%</div> <div>• •</div> </div>
1	B	629	<div> <div>4%</div> <div>93%</div> <div>• •</div> </div>
1	C	629	<div> <div>2%</div> <div>93%</div> <div>• •</div> </div>
1	D	629	<div> <div>•%</div> <div>94%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	EDO	A	717	-	-	-	X
10	EDO	A	719	-	-	-	X
10	EDO	A	720	-	-	-	X
10	EDO	B	720	-	-	-	X
10	EDO	C	718	-	-	-	X
10	EDO	C	719	-	-	-	X
10	EDO	C	720	-	-	-	X
10	EDO	C	721	-	-	-	X
10	EDO	C	722	-	-	-	X
10	EDO	D	719	-	-	-	X
10	EDO	D	721	-	-	-	X
11	ACT	A	724	-	-	-	X
11	ACT	C	723	-	-	-	X
12	PE3	A	726	-	-	-	X
14	PG4	B	726	-	-	-	X
4	CL	A	703	-	-	-	X
4	CL	B	703	-	-	-	X
4	CL	C	703	-	-	-	X
4	CL	D	703	-	-	-	X
6	NAG	A	705	-	-	-	X
6	NAG	C	707	-	-	-	X
8	FUC	A	708	-	-	-	X
8	FUC	A	713	-	-	-	X
8	FUC	B	713	-	-	-	X
8	FUC	C	710	-	-	-	X
8	FUC	D	716	-	-	-	X
9	PEG	A	714	-	-	-	X
9	PEG	A	715	-	-	-	X
9	PEG	A	716	-	-	-	X
9	PEG	B	715	-	-	-	X
9	PEG	B	716	-	-	-	X
9	PEG	B	718	-	-	-	X
9	PEG	C	713	-	-	-	X
9	PEG	C	714	-	-	-	X
9	PEG	D	717	-	-	-	X

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 43786 atoms, of which 20257 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	605	Total	C	H	N	O	S	0	11	0
			9849	3228	4811	870	920	20			
1	B	608	Total	C	H	N	O	S	0	9	0
			9851	3231	4810	867	923	20			
1	C	606	Total	C	H	N	O	S	0	9	0
			9789	3213	4779	862	916	19			
1	D	614	Total	C	H	N	O	S	0	14	0
			9957	3264	4865	874	934	20			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	conflict	UNP P12821
A	25	GLN	ASN	conflict	UNP P12821
A	82	GLN	ASN	conflict	UNP P12821
A	117	GLN	ASN	conflict	UNP P12821
A	131	GLN	ASN	conflict	UNP P12821
A	289	GLN	ASN	conflict	UNP P12821
A	545	ARG	GLN	conflict	UNP P12821
A	576	LEU	PRO	conflict	UNP P12821
A	629	LEU	-	expression tag	UNP P12821
B	9	GLN	ASN	conflict	UNP P12821
B	25	GLN	ASN	conflict	UNP P12821
B	82	GLN	ASN	conflict	UNP P12821
B	117	GLN	ASN	conflict	UNP P12821
B	131	GLN	ASN	conflict	UNP P12821
B	289	GLN	ASN	conflict	UNP P12821
B	545	ARG	GLN	conflict	UNP P12821
B	576	LEU	PRO	conflict	UNP P12821
B	629	LEU	-	expression tag	UNP P12821
C	9	GLN	ASN	conflict	UNP P12821
C	25	GLN	ASN	conflict	UNP P12821
C	82	GLN	ASN	conflict	UNP P12821

Continued on next page...

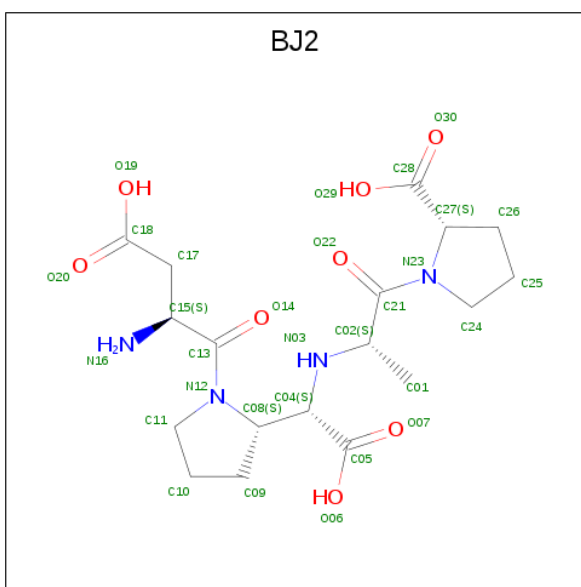
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	117	GLN	ASN	conflict	UNP P12821
C	131	GLN	ASN	conflict	UNP P12821
C	289	GLN	ASN	conflict	UNP P12821
C	545	ARG	GLN	conflict	UNP P12821
C	576	LEU	PRO	conflict	UNP P12821
C	629	LEU	-	expression tag	UNP P12821
D	9	GLN	ASN	conflict	UNP P12821
D	25	GLN	ASN	conflict	UNP P12821
D	82	GLN	ASN	conflict	UNP P12821
D	117	GLN	ASN	conflict	UNP P12821
D	131	GLN	ASN	conflict	UNP P12821
D	289	GLN	ASN	conflict	UNP P12821
D	545	ARG	GLN	conflict	UNP P12821
D	576	LEU	PRO	conflict	UNP P12821
D	629	LEU	-	expression tag	UNP P12821

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is (2 {S})-1-[(2 {S})-2-[(1 {S})-1-[(2 {S})-1-[(2 {S})-2-azanyl-4-oxidanyl-4-oxidanylidene-butanoyl]pyrrolidin-2-yl]-2-oxidanyl-2-oxidanylidene-ethyl]amino]propanoyl]pyrrolidine-2-carboxylic acid (three-letter code: BJ2) (formula: C₁₈H₂₈N₄O₈).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			55	18	25	4	8		
3	B	1	Total	C	H	N	O	0	0
			55	18	25	4	8		
3	C	1	Total	C	H	N	O	0	0
			55	18	25	4	8		
3	D	1	Total	C	H	N	O	0	0
			55	18	25	4	8		

- 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		
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

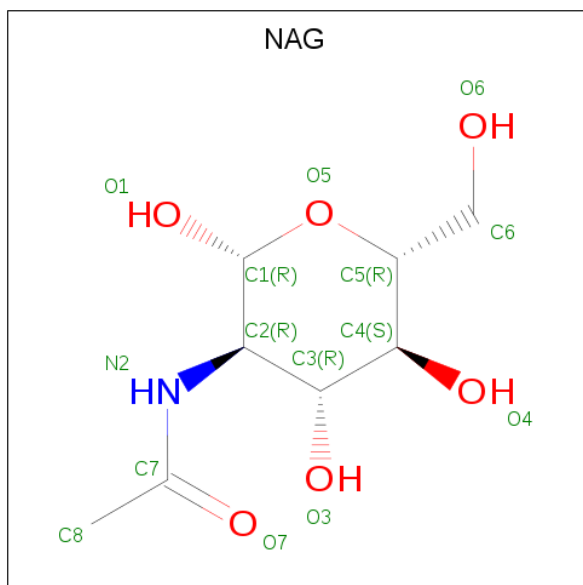
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



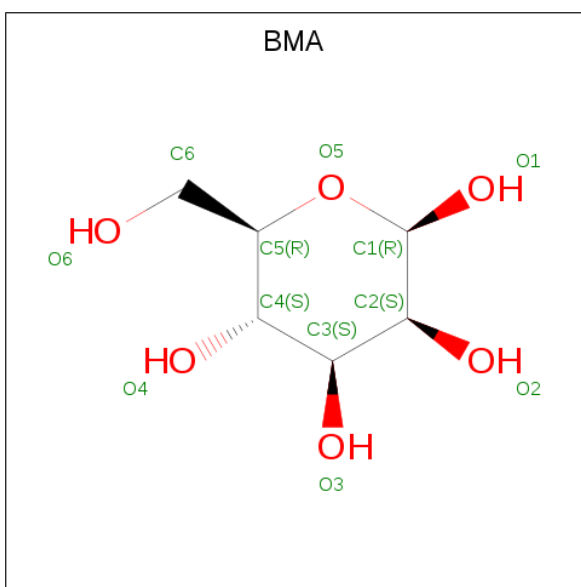
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
6	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
6	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
6	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
6	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

Continued on next page...

Continued from previous page...

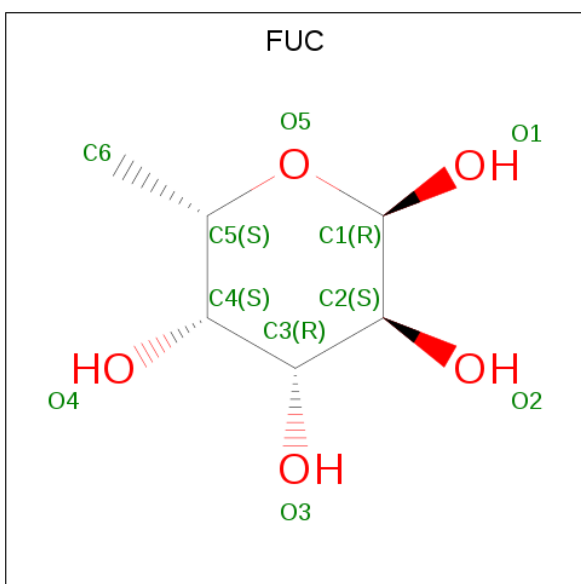
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
6	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
6	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
6	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
6	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
6	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
6	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
6	C	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
6	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
6	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
6	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
6	D	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
6	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 7 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



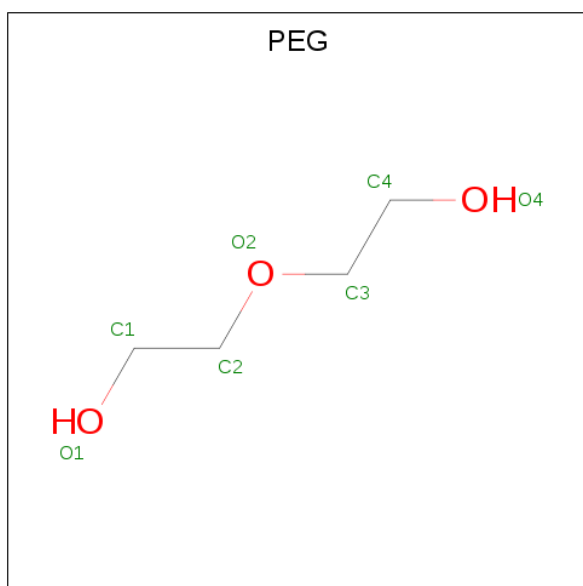
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			22	6	11	5		
7	B	1	Total	C	H	O	0	0
			21	6	10	5		
7	C	1	Total	C	H	O	0	0
			21	6	10	5		
7	D	1	Total	C	H	O	0	0
			21	6	10	5		
7	D	1	Total	C	H	O	0	0
			19	6	8	5		

- Molecule 8 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			20	6	10	4		
8	A	1	Total	C	H	O	0	0
			20	6	10	4		
8	B	1	Total	C	H	O	0	0
			21	6	11	4		
8	B	1	Total	C	H	O	0	0
			20	6	10	4		
8	C	1	Total	C	H	O	0	0
			21	6	11	4		
8	D	1	Total	C	H	O	0	0
			21	6	11	4		
8	D	1	Total	C	H	O	0	0
			19	6	9	4		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



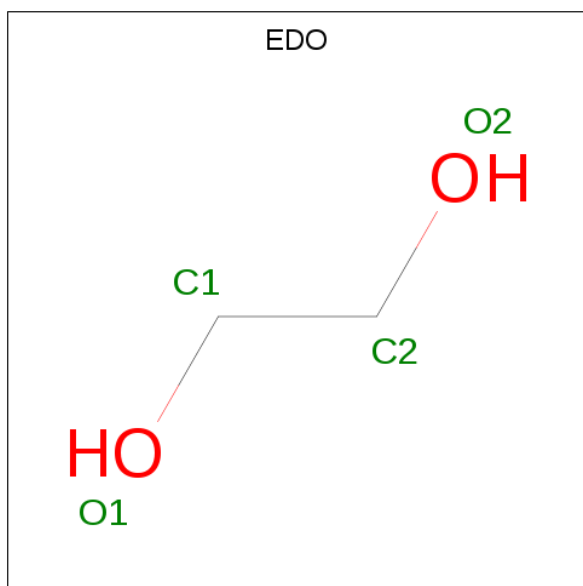
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			17	4	10	3		
9	A	1	Total	C	H	O	0	0
			17	4	10	3		
9	A	1	Total	C	H	O	0	0
			17	4	10	3		
9	B	1	Total	C	H	O	0	0
			17	4	10	3		
9	B	1	Total	C	H	O	0	0
			17	4	10	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	H	O	0	0
			17	4	10	3		
9	B	1	Total	C	H	O	0	0
			17	4	10	3		
9	B	1	Total	C	H	O	0	0
			17	4	10	3		
9	C	1	Total	C	H	O	0	0
			17	4	10	3		
9	C	1	Total	C	H	O	0	0
			17	4	10	3		
9	D	1	Total	C	H	O	0	0
			17	4	10	3		
9	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			10	2	6	2		
10	A	1	Total	C	H	O	0	0
			10	2	6	2		
10	A	1	Total	C	H	O	0	0
			10	2	6	2		
10	A	1	Total	C	H	O	0	0
			10	2	6	2		

Continued on next page...

Continued from previous page...

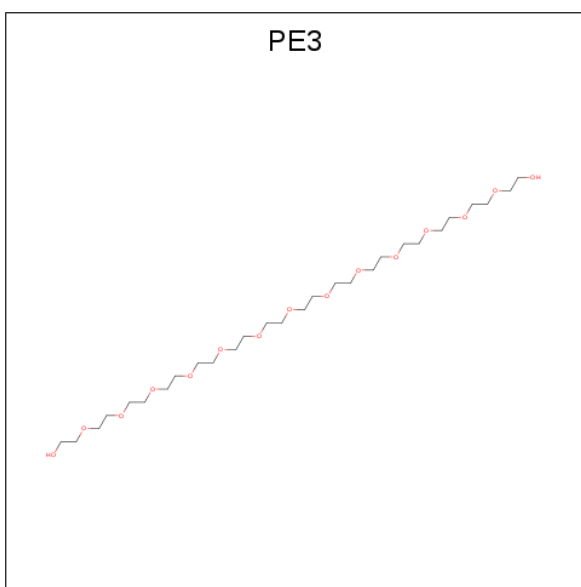
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			10	2	6	2		
10	A	1	Total	C	H	O	0	0
			10	2	6	2		
10	A	1	Total	C	H	O	0	0
			10	2	6	2		
10	B	1	Total	C	H	O	0	0
			10	2	6	2		
10	B	1	Total	C	H	O	0	0
			10	2	6	2		
10	B	1	Total	C	H	O	0	0
			10	2	6	2		
10	B	1	Total	C	H	O	0	0
			10	2	6	2		
10	B	1	Total	C	H	O	0	0
			10	2	6	2		
10	C	1	Total	C	H	O	0	0
			10	2	6	2		
10	C	1	Total	C	H	O	0	0
			10	2	6	2		
10	C	1	Total	C	H	O	0	0
			10	2	6	2		
10	C	1	Total	C	H	O	0	0
			10	2	6	2		
10	C	1	Total	C	H	O	0	0
			10	2	6	2		
10	C	1	Total	C	H	O	0	0
			10	2	6	2		
10	C	1	Total	C	H	O	0	0
			10	2	6	2		
10	D	1	Total	C	H	O	0	0
			10	2	6	2		
10	D	1	Total	C	H	O	0	0
			10	2	6	2		
10	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 11 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			7	2	3	2		
11	A	1	Total	C	H	O	0	0
			7	2	3	2		
11	B	1	Total	C	H	O	0	0
			7	2	3	2		
11	C	1	Total	C	H	O	0	0
			7	2	3	2		
11	D	1	Total	C	H	O	0	0
			7	2	3	2		
11	D	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 12 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAOXAHENTETRACONTANE-1,41-DIOL (three-letter code: PE3) (formula: C₂₈H₅₈O₁₅).



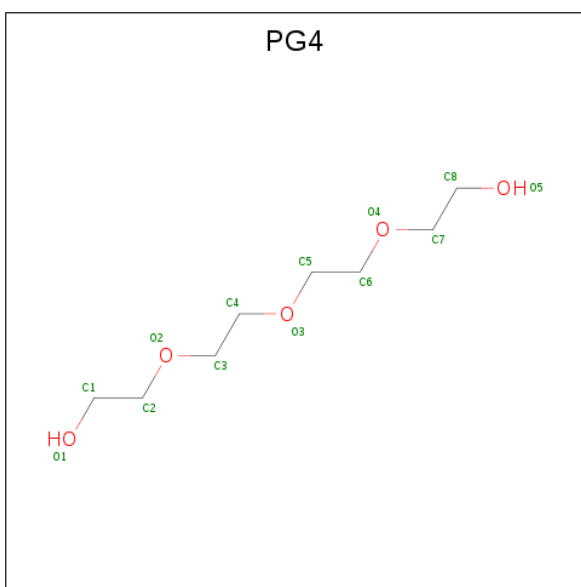
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	H	O	0	0
			101	28	58	15		

- Molecule 13 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



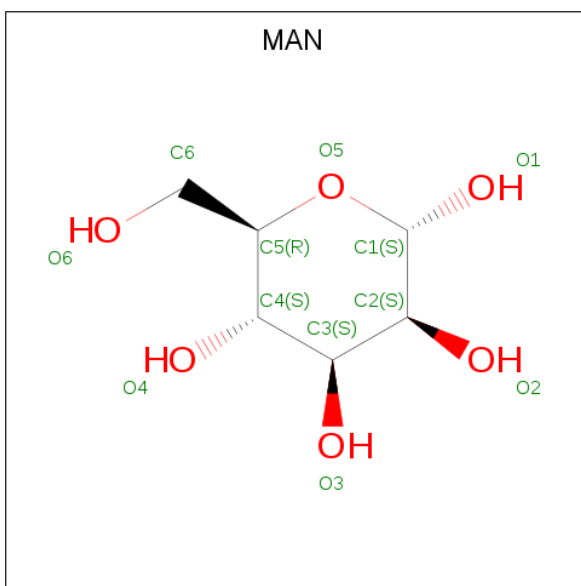
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 14 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



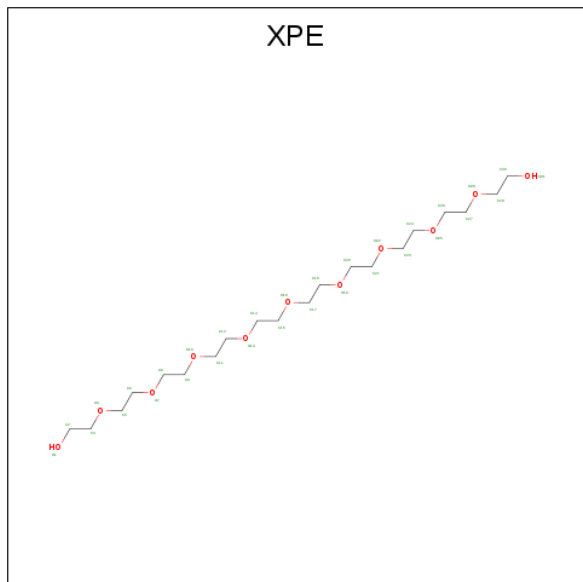
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	1	Total	C	H	O	0	0
			31	8	18	5		
14	C	1	Total	C	H	O	0	1
			62	16	36	10		

- Molecule 15 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	D	1	Total	C	H	O	0	0
			21	6	10	5		
15	D	1	Total	C	H	O	0	0
			21	6	10	5		

- Molecule 16 is 3,6,9,12,15,18,21,24,27-NONAOXANONACOSANE-1,29-DIOL (three-letter code: XPE) (formula: C₂₀H₄₂O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	D	1	Total	C	H	O	0	0
			73	20	42	11		

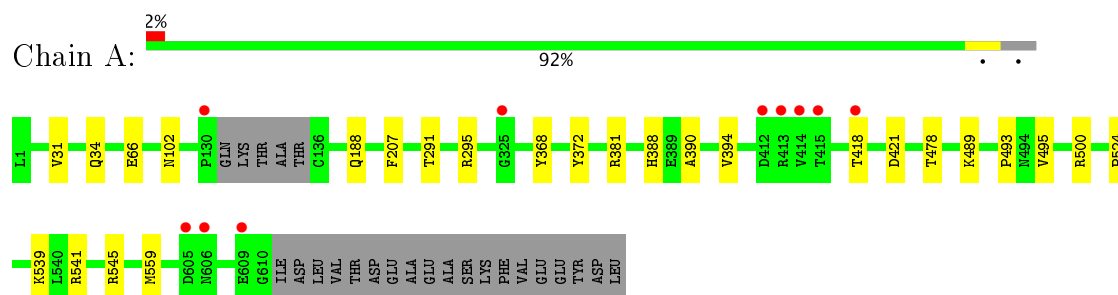
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	584	Total	O	0	4
			588	588		
17	B	580	Total	O	0	2
			581	581		
17	C	547	Total	O	0	4
			551	551		
17	D	682	Total	O	0	8
			690	690		

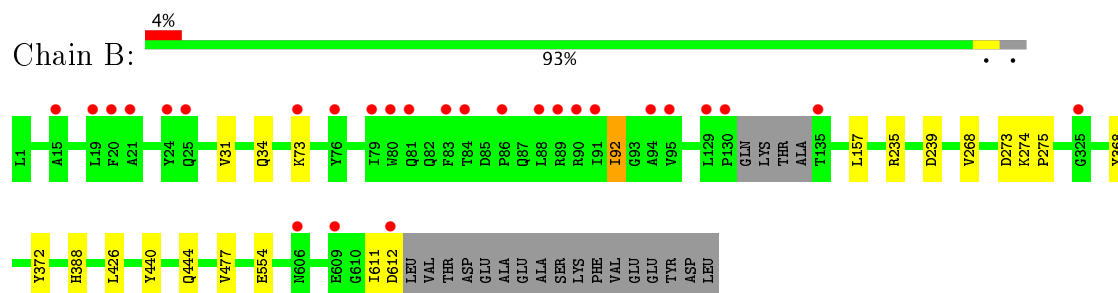
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

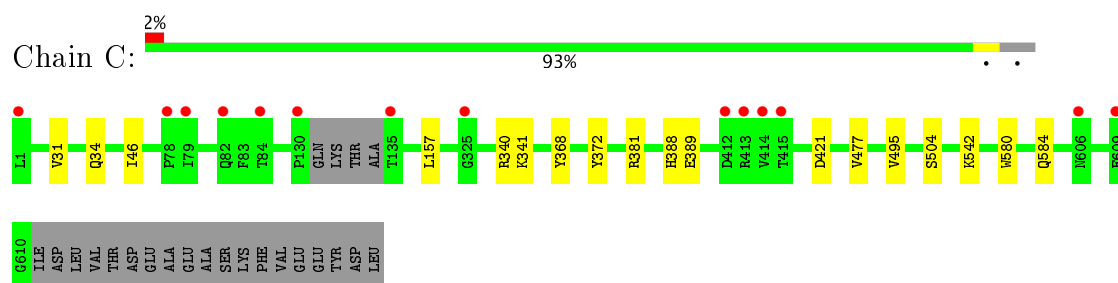
- Molecule 1: Angiotensin-converting enzyme



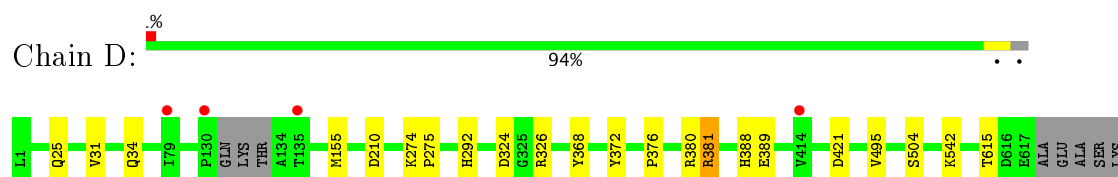
- Molecule 1: Angiotensin-converting enzyme



- Molecule 1: Angiotensin-converting enzyme



- Molecule 1: Angiotensin-converting enzyme



PHE
VAL
GLU
GLU
TYR
ASP
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.17Å 103.45Å 115.45Å 84.86° 85.49° 81.99°	Depositor
Resolution (Å)	79.48 – 1.75 102.11 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.0 (79.48-1.75) 94.8 (102.11-1.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.75Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.173 , 0.198 0.173 , 0.197	Depositor DCC
R_{free} test set	3206 reflections (0.97%)	DCC
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	43786	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.30 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.3807e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, NAG, CL, ZN, XPE, EDO, FUC, PG4, PGE, BJ2, ACT, PEG, PE3, 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	0.45	0/5194	0.56	0/7070
1	B	0.44	0/5197	0.57	0/7076
1	C	0.41	0/5181	0.56	0/7055
1	D	0.49	0/5280	0.60	0/7190
All	All	0.45	0/20852	0.57	0/28391

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	5038	4811	4799	15	0
1	B	5041	4810	4802	13	0
1	C	5010	4779	4758	9	0
1	D	5092	4865	4820	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	30	25	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	30	25	0	0	0
3	C	30	25	0	1	0
3	D	30	25	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	84	78	72	2	0
6	B	84	76	72	0	0
6	C	84	77	73	0	0
6	D	84	76	71	1	0
7	A	11	11	10	0	0
7	B	11	10	10	0	0
7	C	11	10	10	0	0
7	D	22	18	18	0	0
8	A	20	20	20	3	0
8	B	20	21	20	0	0
8	C	10	11	10	0	0
8	D	20	20	20	2	0
9	A	21	30	30	2	0
9	B	35	50	50	0	0
9	C	14	20	20	3	0
9	D	14	20	20	0	0
10	A	28	42	42	3	0
10	B	20	30	30	0	0
10	C	32	48	48	0	0
10	D	12	18	18	0	0
11	A	8	6	6	0	0
11	B	4	3	3	0	0
11	C	4	3	3	0	0
11	D	8	6	6	1	0
12	A	43	58	58	4	0
13	B	10	14	14	0	0
14	B	13	18	18	2	0
14	C	26	36	36	0	0
15	D	22	20	20	0	0
16	D	31	42	42	0	0
17	A	588	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	B	581	0	0	3	0
17	C	551	0	0	2	0
17	D	690	0	0	4	0
All	All	23529	20257	20049	59	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 1.

All (59) 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)
11:D:723:ACT:H1	17:D:1087:HOH:O	1.89	0.71
1:D:542:LYS:NZ	17:D:804:HOH:O	2.25	0.69
1:C:542:LYS:NZ	17:C:804:HOH:O	2.27	0.67
1:C:340[A]:ARG:O	1:C:341:LYS:HE2	1.99	0.62
1:C:340[B]:ARG:O	1:C:341:LYS:HE2	1.99	0.62
1:A:381[B]:ARG:NH1	17:A:803:HOH:O	2.34	0.61
6:A:712:NAG:H83	6:A:712:NAG:H3	1.81	0.61
1:D:324:ASP:OD1	1:D:326:ARG:HB2	2.01	0.60
1:B:554:GLU:OE2	17:B:801:HOH:O	2.17	0.58
1:A:31:VAL:O	1:A:34:GLN:HG3	2.05	0.56
1:A:295:ARG:HG3	12:A:726:PE3:H381	1.86	0.55
3:C:702:BJ2:N16	9:C:713:PEG:O1	2.39	0.55
1:D:155[A]:MET:SD	1:D:615:THR:HG22	2.47	0.54
12:A:726:PE3:H392	12:A:726:PE3:O31	2.08	0.54
1:B:73:LYS:HE3	17:B:1097:HOH:O	2.09	0.53
1:C:31:VAL:O	1:C:34:GLN:HG3	2.10	0.51
1:B:31:VAL:O	1:B:34:GLN:HG3	2.10	0.51
1:A:418:THR:HG22	8:A:708:FUC:O4	2.12	0.50
6:A:711:NAG:H61	8:A:713:FUC:O2	2.11	0.50
6:D:714:NAG:H61	8:D:716:FUC:O2	2.12	0.49
1:A:539:LYS:HE3	1:A:559:MET:O	2.11	0.49
1:B:440:TYR:O	1:B:444[B]:GLN:HG2	2.13	0.48
1:D:25:GLN:OE1	1:D:376:PRO:HA	2.15	0.46
9:A:716:PEG:H31	17:A:827:HOH:O	2.15	0.46
1:D:31:VAL:O	1:D:34:GLN:HG3	2.15	0.46
1:D:274:LYS:HB3	1:D:275:PRO:CD	2.45	0.46
1:B:611:ILE:O	1:B:612:ASP:HB2	2.15	0.46
10:A:723:EDO:H22	17:A:1009:HOH:O	2.16	0.45
1:B:92:ILE:CD1	1:B:92:ILE:N	2.80	0.45
1:C:580:TRP:O	1:C:584:GLN:HG2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ARG:HH11	14:B:726:PG4:C6	2.30	0.44
1:A:541:ARG:HG2	1:A:545:ARG:HD2	1.99	0.44
1:B:274:LYS:HB3	1:B:275:PRO:CD	2.48	0.44
1:C:157:LEU:HD11	1:C:477:VAL:HG13	1.98	0.43
9:C:713:PEG:H31	17:C:1234:HOH:O	2.16	0.43
1:C:495:VAL:HG12	1:C:495:VAL:O	2.18	0.43
1:C:46:ILE:HG22	9:C:714:PEG:H31	1.99	0.43
1:B:73:LYS:HG3	17:B:1097:HOH:O	2.18	0.43
1:D:210:ASP:OD2	17:D:801:HOH:O	2.22	0.43
1:A:524:PRO:HB3	10:A:719:EDO:H12	2.00	0.43
1:D:380:ARG:O	1:D:381[A]:ARG:HD2	2.19	0.42
8:D:716:FUC:O4	8:D:716:FUC:C1	2.66	0.42
1:B:235:ARG:HH11	14:B:726:PG4:H62	1.83	0.42
1:B:92:ILE:HD12	1:B:92:ILE:N	2.34	0.42
1:A:390:ALA:O	1:A:394:VAL:HG23	2.20	0.41
1:A:500:ARG:HH12	10:A:723:EDO:C1	2.32	0.41
1:D:495:VAL:HG12	1:D:495:VAL:O	2.20	0.41
1:A:495:VAL:O	1:A:495:VAL:HG12	2.21	0.41
1:A:291:THR:HG21	12:A:726:PE3:H391	2.01	0.41
1:A:478:THR:HB	8:A:713:FUC:H63	2.02	0.41
1:B:157:LEU:HD11	1:B:477:VAL:HG13	2.02	0.41
1:D:389:GLU:HB2	1:D:504:SER:HB2	2.03	0.41
1:A:489:LYS:O	1:A:493:PRO:HD2	2.21	0.41
1:D:292:HIS:HD2	17:D:1316:HOH:O	2.04	0.41
12:A:726:PE3:H382	12:A:726:PE3:H271	2.02	0.40
1:C:389:GLU:HB2	1:C:504:SER:HB2	2.02	0.40
1:A:102:ASN:HB3	1:A:188:GLN:HG3	2.02	0.40
1:B:268:VAL:HG23	1:B:426:LEU:HD11	2.02	0.40
1:A:207:PHE:HB3	9:A:716:PEG:H12	2.03	0.40

There are no symmetry-related clashes.

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	612/629 (97%)	603 (98%)	9 (2%)	0	100	100
1	B	613/629 (98%)	605 (99%)	8 (1%)	0	100	100
1	C	611/629 (97%)	603 (99%)	8 (1%)	0	100	100
1	D	624/629 (99%)	615 (99%)	9 (1%)	0	100	100
All	All	2460/2516 (98%)	2426 (99%)	34 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	531/541 (98%)	526 (99%)	5 (1%)	82	71
1	B	532/541 (98%)	526 (99%)	6 (1%)	78	64
1	C	530/541 (98%)	525 (99%)	5 (1%)	82	71
1	D	542/541 (100%)	536 (99%)	6 (1%)	78	64
All	All	2135/2164 (99%)	2113 (99%)	22 (1%)	80	67

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	GLU
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	A	421	ASP
1	B	92	ILE
1	B	239	ASP
1	B	273	ASP
1	B	368	TYR
1	B	372	TYR
1	B	388	HIS
1	C	368	TYR
1	C	372	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	381	ARG
1	C	388	HIS
1	C	421	ASP
1	D	368	TYR
1	D	372	TYR
1	D	381[A]	ARG
1	D	381[B]	ARG
1	D	388	HIS
1	D	421	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 101 ligands modelled in this entry, 12 are monoatomic - leaving 89 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	BJ2	A	702	2	22,31,31	4.17	9 (40%)	28,44,44	1.56	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	705	1,6	14,14,15	0.42	0	15,19,21	0.65	0
6	NAG	A	706	6	14,14,15	0.27	0	15,19,21	0.56	0
7	BMA	A	707	6	11,11,12	0.53	0	13,15,17	0.76	0
8	FUC	A	708	6	9,10,11	0.75	0	13,14,16	0.87	0
6	NAG	A	709	1,8,6	14,14,15	0.21	0	15,19,21	0.58	0
6	NAG	A	710	7,6	14,14,15	0.29	0	15,19,21	0.44	0
6	NAG	A	711	1,8,6	14,14,15	0.50	0	15,19,21	0.97	1 (6%)
6	NAG	A	712	6	14,14,15	0.38	0	15,19,21	1.09	1 (6%)
8	FUC	A	713	6	9,10,11	1.01	0	13,14,16	1.67	2 (15%)
9	PEG	A	714	-	6,6,6	0.51	0	5,5,5	0.28	0
9	PEG	A	715	-	6,6,6	0.47	0	5,5,5	0.36	0
9	PEG	A	716	-	6,6,6	0.40	0	5,5,5	0.45	0
10	EDO	A	717	-	3,3,3	0.57	0	2,2,2	0.31	0
10	EDO	A	718	-	3,3,3	0.47	0	2,2,2	0.36	0
10	EDO	A	719	-	3,3,3	0.54	0	2,2,2	0.25	0
10	EDO	A	720	-	3,3,3	0.48	0	2,2,2	0.09	0
10	EDO	A	721	-	3,3,3	0.48	0	2,2,2	0.45	0
10	EDO	A	722	-	3,3,3	0.46	0	2,2,2	0.30	0
10	EDO	A	723	-	3,3,3	0.42	0	2,2,2	0.22	0
11	ACT	A	724	-	1,3,3	7.80	1 (100%)	0,3,3	0.00	-
11	ACT	A	725	-	1,3,3	6.72	1 (100%)	0,3,3	0.00	-
12	PE3	A	726	-	42,42,42	0.55	0	41,41,41	0.47	0
3	BJ2	B	702	2	22,31,31	4.17	9 (40%)	28,44,44	1.43	3 (10%)
6	NAG	B	705	1,6	14,14,15	0.24	0	15,19,21	0.69	1 (6%)
6	NAG	B	706	6	14,14,15	0.32	0	15,19,21	0.56	0
8	FUC	B	707	6	9,10,11	0.66	0	13,14,16	0.84	0
6	NAG	B	708	1,8,6	14,14,15	0.56	0	15,19,21	0.71	0
6	NAG	B	709	7,6	14,14,15	0.25	0	15,19,21	0.42	0
7	BMA	B	710	6	11,11,12	0.73	0	13,15,17	0.69	0
6	NAG	B	711	1,8,6	14,14,15	0.47	0	15,19,21	0.65	0
6	NAG	B	712	6	14,14,15	0.33	0	15,19,21	0.44	0
8	FUC	B	713	6	9,10,11	0.97	0	13,14,16	1.00	1 (7%)
9	PEG	B	714	-	6,6,6	0.48	0	5,5,5	0.36	0
9	PEG	B	715	-	6,6,6	0.50	0	5,5,5	0.31	0
9	PEG	B	716	-	6,6,6	0.50	0	5,5,5	0.32	0
9	PEG	B	717	-	6,6,6	0.49	0	5,5,5	0.49	0
9	PEG	B	718	-	6,6,6	0.47	0	5,5,5	0.40	0
10	EDO	B	719	-	3,3,3	0.51	0	2,2,2	0.24	0
10	EDO	B	720	-	3,3,3	0.52	0	2,2,2	0.28	0
10	EDO	B	721	-	3,3,3	0.46	0	2,2,2	0.32	0
10	EDO	B	722	-	3,3,3	0.44	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	EDO	B	723	-	3,3,3	0.47	0	2,2,2	0.33	0
11	ACT	B	724	-	1,3,3	6.91	1 (100%)	0,3,3	0.00	-
13	PGE	B	725	-	9,9,9	0.32	0	8,8,8	0.31	0
14	PG4	B	726	-	12,12,12	0.60	0	11,11,11	0.55	0
3	BJ2	C	702	2	22,31,31	4.38	9 (40%)	28,44,44	1.37	2 (7%)
6	NAG	C	705	1,6	14,14,15	0.31	0	15,19,21	0.57	0
6	NAG	C	706	6	14,14,15	0.29	0	15,19,21	0.54	0
6	NAG	C	707	1,6	14,14,15	0.16	0	15,19,21	0.56	0
6	NAG	C	708	7,6	14,14,15	0.39	0	15,19,21	0.62	0
7	BMA	C	709	6	11,11,12	0.70	0	13,15,17	0.98	1 (7%)
8	FUC	C	710	6	9,10,11	1.13	1 (11%)	13,14,16	1.38	2 (15%)
6	NAG	C	711	1,8,6	14,14,15	0.25	0	15,19,21	0.77	0
6	NAG	C	712	6	14,14,15	0.32	0	15,19,21	0.44	0
9	PEG	C	713	-	6,6,6	0.49	0	5,5,5	0.55	0
9	PEG	C	714	-	6,6,6	0.49	0	5,5,5	0.30	0
10	EDO	C	715	-	3,3,3	0.48	0	2,2,2	0.28	0
10	EDO	C	716	-	3,3,3	0.50	0	2,2,2	0.17	0
10	EDO	C	717	-	3,3,3	0.50	0	2,2,2	0.26	0
10	EDO	C	718	-	3,3,3	0.53	0	2,2,2	0.26	0
10	EDO	C	719	-	3,3,3	0.48	0	2,2,2	0.28	0
10	EDO	C	720	-	3,3,3	0.43	0	2,2,2	0.44	0
10	EDO	C	721	-	3,3,3	0.49	0	2,2,2	0.27	0
10	EDO	C	722	-	3,3,3	0.50	0	2,2,2	0.02	0
11	ACT	C	723	-	1,3,3	6.00	1 (100%)	0,3,3	0.00	-
14	PG4	C	724[A]	-	12,12,12	0.53	0	11,11,11	0.38	0
14	PG4	C	724[B]	-	12,12,12	0.53	0	11,11,11	0.33	0
3	BJ2	D	702	2	22,31,31	4.08	10 (45%)	28,44,44	1.52	5 (17%)
6	NAG	D	705	1,6	14,14,15	0.36	0	15,19,21	0.72	0
6	NAG	D	706	7,6	14,14,15	0.30	0	15,19,21	0.54	0
7	BMA	D	707	6	11,11,12	0.62	0	13,15,17	0.73	0
8	FUC	D	708	6	9,10,11	0.97	0	13,14,16	0.73	0
6	NAG	D	709	1,8,6	14,14,15	0.65	0	15,19,21	0.85	0
6	NAG	D	710	7,6	14,14,15	0.46	0	15,19,21	0.58	0
7	BMA	D	711	15,6	11,11,12	0.78	0	13,15,17	0.92	0
15	MAN	D	712	7	11,11,12	0.89	1 (9%)	13,15,17	1.01	1 (7%)
15	MAN	D	713	7	11,11,12	1.05	1 (9%)	13,15,17	1.28	2 (15%)
6	NAG	D	714	1,8,6	14,14,15	0.36	0	15,19,21	0.84	0
6	NAG	D	715	6	14,14,15	0.51	0	15,19,21	0.42	0
8	FUC	D	716	6	9,10,11	1.52	1 (11%)	13,14,16	1.12	1 (7%)
9	PEG	D	717	-	6,6,6	0.47	0	5,5,5	0.26	0
9	PEG	D	718	-	6,6,6	0.44	0	5,5,5	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	EDO	D	719	-	3,3,3	0.51	0	2,2,2	0.22	0
10	EDO	D	720	-	3,3,3	0.49	0	2,2,2	0.32	0
10	EDO	D	721	-	3,3,3	0.41	0	2,2,2	0.40	0
11	ACT	D	722	-	1,3,3	3.18	1 (100%)	0,3,3	0.00	-
11	ACT	D	723	-	1,3,3	5.07	1 (100%)	0,3,3	0.00	-
16	XPE	D	724	-	30,30,30	0.54	0	29,29,29	0.51	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	BJ2	A	702	2	-	0/26/56/56	0/2/2/2
6	NAG	A	705	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	706	6	-	0/6/23/26	0/1/1/1
7	BMA	A	707	6	-	0/2/19/22	0/1/1/1
8	FUC	A	708	6	-	0/0/17/20	0/1/1/1
6	NAG	A	709	1,8,6	-	0/6/23/26	0/1/1/1
6	NAG	A	710	7,6	-	0/6/23/26	0/1/1/1
6	NAG	A	711	1,8,6	-	0/6/23/26	0/1/1/1
6	NAG	A	712	6	-	0/6/23/26	0/1/1/1
8	FUC	A	713	6	-	0/0/17/20	0/1/1/1
9	PEG	A	714	-	-	0/4/4/4	0/0/0/0
9	PEG	A	715	-	-	0/4/4/4	0/0/0/0
9	PEG	A	716	-	-	0/4/4/4	0/0/0/0
10	EDO	A	717	-	-	0/1/1/1	0/0/0/0
10	EDO	A	718	-	-	0/1/1/1	0/0/0/0
10	EDO	A	719	-	-	0/1/1/1	0/0/0/0
10	EDO	A	720	-	-	0/1/1/1	0/0/0/0
10	EDO	A	721	-	-	0/1/1/1	0/0/0/0
10	EDO	A	722	-	-	0/1/1/1	0/0/0/0
10	EDO	A	723	-	-	0/1/1/1	0/0/0/0
11	ACT	A	724	-	-	0/0/0/0	0/0/0/0
11	ACT	A	725	-	-	0/0/0/0	0/0/0/0
12	PE3	A	726	-	-	0/40/40/40	0/0/0/0
3	BJ2	B	702	2	-	0/26/56/56	0/2/2/2
6	NAG	B	705	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	706	6	-	0/6/23/26	0/1/1/1
8	FUC	B	707	6	-	0/0/17/20	0/1/1/1
6	NAG	B	708	1,8,6	-	0/6/23/26	0/1/1/1
6	NAG	B	709	7,6	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	B	710	6	-	0/2/19/22	0/1/1/1
6	NAG	B	711	1,8,6	-	0/6/23/26	0/1/1/1
6	NAG	B	712	6	-	0/6/23/26	0/1/1/1
8	FUC	B	713	6	-	0/0/17/20	0/1/1/1
9	PEG	B	714	-	-	0/4/4/4	0/0/0/0
9	PEG	B	715	-	-	0/4/4/4	0/0/0/0
9	PEG	B	716	-	-	0/4/4/4	0/0/0/0
9	PEG	B	717	-	-	0/4/4/4	0/0/0/0
9	PEG	B	718	-	-	0/4/4/4	0/0/0/0
10	EDO	B	719	-	-	0/1/1/1	0/0/0/0
10	EDO	B	720	-	-	0/1/1/1	0/0/0/0
10	EDO	B	721	-	-	0/1/1/1	0/0/0/0
10	EDO	B	722	-	-	0/1/1/1	0/0/0/0
10	EDO	B	723	-	-	0/1/1/1	0/0/0/0
11	ACT	B	724	-	-	0/0/0/0	0/0/0/0
13	PGE	B	725	-	-	0/7/7/7	0/0/0/0
14	PG4	B	726	-	-	0/10/10/10	0/0/0/0
3	BJ2	C	702	2	-	0/26/56/56	0/2/2/2
6	NAG	C	705	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	706	6	-	0/6/23/26	0/1/1/1
6	NAG	C	707	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	708	7,6	-	0/6/23/26	0/1/1/1
7	BMA	C	709	6	-	0/2/19/22	0/1/1/1
8	FUC	C	710	6	-	0/0/17/20	0/1/1/1
6	NAG	C	711	1,8,6	-	0/6/23/26	0/1/1/1
6	NAG	C	712	6	-	0/6/23/26	0/1/1/1
9	PEG	C	713	-	-	0/4/4/4	0/0/0/0
9	PEG	C	714	-	-	0/4/4/4	0/0/0/0
10	EDO	C	715	-	-	0/1/1/1	0/0/0/0
10	EDO	C	716	-	-	0/1/1/1	0/0/0/0
10	EDO	C	717	-	-	0/1/1/1	0/0/0/0
10	EDO	C	718	-	-	0/1/1/1	0/0/0/0
10	EDO	C	719	-	-	0/1/1/1	0/0/0/0
10	EDO	C	720	-	-	0/1/1/1	0/0/0/0
10	EDO	C	721	-	-	0/1/1/1	0/0/0/0
10	EDO	C	722	-	-	0/1/1/1	0/0/0/0
11	ACT	C	723	-	-	0/0/0/0	0/0/0/0
14	PG4	C	724[A]	-	-	0/10/10/10	0/0/0/0
14	PG4	C	724[B]	-	-	0/10/10/10	0/0/0/0
3	BJ2	D	702	2	-	0/26/56/56	0/2/2/2
6	NAG	D	705	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	706	7,6	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	D	707	6	-	0/2/19/22	0/1/1/1
8	FUC	D	708	6	-	0/0/17/20	0/1/1/1
6	NAG	D	709	1,8,6	-	0/6/23/26	0/1/1/1
6	NAG	D	710	7,6	-	0/6/23/26	0/1/1/1
7	BMA	D	711	15,6	-	0/2/19/22	0/1/1/1
15	MAN	D	712	7	-	0/2/19/22	0/1/1/1
15	MAN	D	713	7	-	0/2/19/22	1/1/1/1
6	NAG	D	714	1,8,6	-	0/6/23/26	0/1/1/1
6	NAG	D	715	6	-	0/6/23/26	0/1/1/1
8	FUC	D	716	6	-	0/0/17/20	0/1/1/1
9	PEG	D	717	-	-	0/4/4/4	0/0/0/0
9	PEG	D	718	-	-	0/4/4/4	0/0/0/0
10	EDO	D	719	-	-	0/1/1/1	0/0/0/0
10	EDO	D	720	-	-	0/1/1/1	0/0/0/0
10	EDO	D	721	-	-	0/1/1/1	0/0/0/0
11	ACT	D	722	-	-	0/0/0/0	0/0/0/0
11	ACT	D	723	-	-	0/0/0/0	0/0/0/0
16	XPE	D	724	-	-	0/28/28/28	0/0/0/0

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	BJ2	C09-C08	-7.41	1.40	1.53
3	D	702	BJ2	C09-C08	-7.22	1.40	1.53
3	C	702	BJ2	C09-C08	-7.21	1.40	1.53
3	A	702	BJ2	C09-C08	-7.16	1.40	1.53
3	A	702	BJ2	C26-C27	-6.37	1.38	1.54
3	D	702	BJ2	C24-N23	-6.25	1.35	1.47
3	C	702	BJ2	C26-C27	-6.24	1.38	1.54
3	A	702	BJ2	C24-N23	-6.20	1.35	1.47
3	C	702	BJ2	C24-N23	-6.19	1.35	1.47
3	B	702	BJ2	C26-C27	-6.17	1.38	1.54
3	B	702	BJ2	C24-N23	-5.96	1.36	1.47
3	D	702	BJ2	C26-C27	-5.94	1.39	1.54
3	A	702	BJ2	C11-N12	-5.66	1.36	1.47
3	C	702	BJ2	C11-N12	-5.59	1.36	1.47
3	B	702	BJ2	C11-N12	-5.32	1.37	1.47
3	D	702	BJ2	C11-N12	-4.52	1.39	1.47
15	D	712	MAN	O5-C1	-2.15	1.40	1.43
8	C	710	FUC	O5-C1	-2.08	1.40	1.43
3	D	702	BJ2	C25-C24	2.14	1.59	1.51
15	D	713	MAN	C1-C2	2.65	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	722	ACT	CH3-C	3.18	1.52	1.48
3	D	702	BJ2	C04-C08	3.81	1.58	1.54
8	D	716	FUC	C1-C2	4.06	1.61	1.52
3	D	702	BJ2	C13-N12	4.16	1.43	1.34
3	A	702	BJ2	C13-N12	4.31	1.43	1.34
3	B	702	BJ2	C13-N12	4.48	1.44	1.34
3	B	702	BJ2	C04-C08	4.56	1.59	1.54
3	C	702	BJ2	C13-N12	4.71	1.44	1.34
3	C	702	BJ2	C04-C08	4.80	1.60	1.54
3	A	702	BJ2	C04-C08	4.95	1.60	1.54
11	D	723	ACT	CH3-C	5.07	1.55	1.48
3	A	702	BJ2	C21-N23	5.50	1.46	1.34
3	D	702	BJ2	C21-N23	5.69	1.46	1.34
11	C	723	ACT	CH3-C	6.00	1.56	1.48
3	C	702	BJ2	C21-N23	6.01	1.47	1.34
3	B	702	BJ2	C21-N23	6.04	1.47	1.34
11	A	725	ACT	CH3-C	6.72	1.57	1.48
11	B	724	ACT	CH3-C	6.91	1.57	1.48
3	B	702	BJ2	C08-N12	7.60	1.57	1.47
11	A	724	ACT	CH3-C	7.80	1.58	1.48
3	D	702	BJ2	C08-N12	7.84	1.58	1.47
3	A	702	BJ2	C08-N12	7.97	1.58	1.47
3	A	702	BJ2	C27-N23	8.39	1.59	1.47
3	C	702	BJ2	C08-N12	8.48	1.58	1.47
3	B	702	BJ2	C27-N23	8.82	1.59	1.47
3	D	702	BJ2	C27-N23	8.94	1.59	1.47
3	C	702	BJ2	C27-N23	9.62	1.60	1.47

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	BJ2	C08-C04-N03	-4.15	101.90	109.80
3	C	702	BJ2	C08-C04-N03	-3.67	102.81	109.80
3	B	702	BJ2	C08-C04-N03	-3.01	104.06	109.80
3	D	702	BJ2	C08-C04-N03	-2.81	104.45	109.80
3	B	702	BJ2	C24-N23-C27	-2.52	109.55	111.81
15	D	713	MAN	O2-C2-C3	-2.47	105.33	110.17
15	D	712	MAN	O2-C2-C3	-2.20	105.86	110.17
3	D	702	BJ2	C02-C21-N23	-2.15	114.80	118.00
3	D	702	BJ2	C11-N12-C08	-2.03	108.41	111.70
3	A	702	BJ2	O22-C21-C02	2.03	123.81	120.19
6	B	705	NAG	C1-O5-C5	2.04	114.97	112.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	710	FUC	O5-C5-C4	2.13	113.13	109.62
8	B	713	FUC	C1-C2-C3	2.25	112.50	109.65
6	A	711	NAG	C1-O5-C5	2.29	115.33	112.17
7	C	709	BMA	C1-O5-C5	2.38	115.44	112.17
3	A	702	BJ2	C05-C04-C08	2.40	114.99	111.17
8	C	710	FUC	O2-C2-C1	2.47	114.20	109.18
8	A	713	FUC	O2-C2-C1	2.70	114.66	109.18
8	D	716	FUC	O2-C2-C1	2.72	114.70	109.18
15	D	713	MAN	C1-O5-C5	2.73	115.93	112.17
3	D	702	BJ2	O22-C21-C02	3.12	125.75	120.19
6	A	712	NAG	C2-N2-C7	3.19	127.60	122.94
8	A	713	FUC	O5-C5-C4	3.48	115.36	109.62
3	A	702	BJ2	C26-C27-N23	3.77	105.97	102.05
3	C	702	BJ2	C26-C27-N23	4.04	106.25	102.05
3	D	702	BJ2	C26-C27-N23	4.07	106.27	102.05
3	B	702	BJ2	C26-C27-N23	4.65	106.88	102.05

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	D	713	MAN	C1-C2-C3-C4-C5-O5

15 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	708	FUC	1	0
6	A	711	NAG	1	0
6	A	712	NAG	1	0
8	A	713	FUC	2	0
9	A	716	PEG	2	0
10	A	719	EDO	1	0
10	A	723	EDO	2	0
12	A	726	PE3	4	0
14	B	726	PG4	2	0
3	C	702	BJ2	1	0
9	C	713	PEG	2	0
9	C	714	PEG	1	0
6	D	714	NAG	1	0
8	D	716	FUC	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	723	ACT	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 ⓘ

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	605/629 (96%)	-0.18	10 (1%) 70 78	17, 26, 46, 98	0
1	B	608/629 (96%)	-0.04	27 (4%) 35 42	17, 26, 47, 75	50 (8%)
1	C	606/629 (96%)	-0.10	14 (2%) 61 68	18, 30, 53, 83	0
1	D	614/629 (97%)	-0.19	4 (0%) 87 91	16, 24, 41, 69	0
All	All	2433/2516 (96%)	-0.13	55 (2%) 61 68	16, 26, 48, 98	50 (2%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	414	VAL	6.9
1	C	130	PRO	5.5
1	D	135	THR	5.4
1	C	135	THR	4.9
1	A	413	ARG	4.7
1	B	325	GLY	4.6
1	B	90	ARG	4.4
1	C	606	ASN	4.3
1	B	129	LEU	4.2
1	A	130	PRO	4.1
1	B	21	ALA	4.0
1	B	135	THR	3.8
1	B	73	LYS	3.5
1	C	414	VAL	3.5
1	A	325	GLY	3.4
1	C	413	ARG	3.4
1	A	606	ASN	3.4
1	C	79	ILE	3.3
1	B	95	VAL	3.3
1	A	415	THR	3.2
1	B	20	PHE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	91	ILE	3.1
1	C	415	THR	3.1
1	A	609	GLU	3.1
1	B	24	TYR	2.9
1	D	414	VAL	2.9
1	B	25	GLN	2.9
1	B	612	ASP	2.9
1	B	89	ARG	2.9
1	B	81	GLN	2.8
1	B	19	LEU	2.6
1	C	609	GLU	2.5
1	C	1	LEU	2.5
1	B	80	TRP	2.5
1	B	88	LEU	2.5
1	C	78	PRO	2.5
1	B	86	PRO	2.4
1	B	76	TYR	2.4
1	B	130	PRO	2.3
1	B	83	PHE	2.3
1	A	418	THR	2.3
1	B	606	ASN	2.2
1	C	325	GLY	2.2
1	B	609	GLU	2.2
1	B	79	ILE	2.2
1	B	15	ALA	2.2
1	C	412	ASP	2.2
1	B	94	ALA	2.1
1	C	82	GLN	2.1
1	C	84	THR	2.1
1	A	605	ASP	2.1
1	D	79	ILE	2.1
1	B	84	THR	2.0
1	A	412	ASP	2.0
1	D	130	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 ⓘ

There are no carbohydrates in this entry.

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
8	FUC	D	716	10/11	0.69	0.30	54.02	52,65,78,82	19
8	FUC	B	713	10/11	0.73	0.25	34.84	53,65,78,81	20
8	FUC	A	713	10/11	0.81	0.23	15.80	48,66,76,80	20
10	EDO	C	721	4/4	0.83	0.18	11.84	49,59,65,67	0
9	PEG	B	716	7/7	0.73	0.18	11.78	39,47,63,63	17
10	EDO	A	717	4/4	0.87	0.18	10.51	17,30,36,38	10
9	PEG	A	716	7/7	0.83	0.18	9.88	30,36,42,48	17
10	EDO	A	720	4/4	0.81	0.15	7.56	33,43,51,59	10
4	CL	D	703	1/1	1.00	0.12	6.63	18,18,18,18	0
12	PE3	A	726	43/43	0.84	0.15	5.26	28,42,56,63	101
14	PG4	B	726	13/13	0.87	0.14	4.90	26,42,54,55	0
8	FUC	C	710	10/11	0.73	0.14	4.75	51,62,71,79	21
9	PEG	A	715	7/7	0.91	0.12	4.70	26,41,49,52	17
4	CL	B	703	1/1	0.99	0.12	4.68	20,20,20,20	0
10	EDO	B	720	4/4	0.81	0.18	4.51	31,38,43,48	10
9	PEG	C	714	7/7	0.78	0.20	4.38	31,42,51,51	17
4	CL	A	703	1/1	1.00	0.11	3.98	19,19,19,19	0
4	CL	C	703	1/1	1.00	0.13	3.95	22,22,22,22	0
10	EDO	C	720	4/4	0.83	0.14	3.94	38,48,58,63	10
10	EDO	C	722	4/4	0.78	0.23	3.93	36,44,60,60	10
10	EDO	D	719	4/4	0.88	0.16	3.77	29,38,43,49	10
10	EDO	A	719	4/4	0.68	0.30	3.77	36,44,46,48	10
10	EDO	C	718	4/4	0.68	0.19	3.65	46,56,58,58	10
6	NAG	A	705	14/15	0.76	0.18	3.57	44,61,76,80	0
11	ACT	A	724	4/4	0.85	0.19	3.37	30,36,44,46	0
9	PEG	A	714	7/7	0.88	0.10	3.32	35,46,55,55	17
9	PEG	B	715	7/7	0.79	0.21	3.24	33,43,52,55	17
8	FUC	A	708	10/11	0.77	0.22	3.13	42,51,63,72	20
9	PEG	C	713	7/7	0.88	0.10	2.96	39,47,54,55	17

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	PEG	D	717	7/7	0.87	0.10	2.86	32,42,51,51	17
10	EDO	C	719	4/4	0.75	0.13	2.80	46,57,69,69	10
9	PEG	B	718	7/7	0.86	0.14	2.47	41,50,68,68	0
10	EDO	D	721	4/4	0.90	0.14	2.38	38,46,52,53	10
6	NAG	C	707	14/15	0.83	0.18	2.30	56,70,88,88	0
11	ACT	C	723	4/4	0.64	0.17	2.22	34,41,51,52	0
10	EDO	A	723	4/4	0.86	0.15	1.90	31,37,49,58	10
6	NAG	A	711	14/15	0.85	0.10	1.83	30,43,57,61	0
6	NAG	D	714	14/15	0.84	0.11	1.59	37,50,65,74	0
6	NAG	C	705	14/15	0.82	0.15	1.58	36,53,63,67	0
6	NAG	C	708	14/15	0.89	0.19	1.50	67,82,93,95	27
14	PG4	C	724[A]	13/13	0.84	0.15	1.47	30,37,42,53	31
6	NAG	B	711	14/15	0.83	0.12	1.42	35,46,60,66	0
14	PG4	C	724[B]	13/13	0.84	0.15	1.42	27,34,41,42	31
13	PGE	B	725	10/10	0.84	0.13	1.41	30,43,49,51	24
6	NAG	B	705	14/15	0.78	0.13	1.38	33,50,60,68	0
10	EDO	D	720	4/4	0.74	0.15	1.24	49,63,65,78	0
16	XPE	D	724	31/31	0.85	0.11	1.22	31,47,60,71	0
10	EDO	B	719	4/4	0.89	0.08	1.19	40,48,55,60	0
11	ACT	D	722	4/4	0.77	0.13	1.02	24,29,37,46	0
6	NAG	A	709	14/15	0.90	0.13	0.91	40,48,60,60	26
6	NAG	C	711	14/15	0.88	0.10	0.61	37,50,65,69	0
10	EDO	C	716	4/4	0.76	0.12	0.60	56,67,80,80	0
11	ACT	D	723	4/4	0.93	0.15	0.46	27,33,35,39	0
3	BJ2	B	702	30/30	0.96	0.08	0.36	16,23,28,31	0
3	BJ2	D	702	30/30	0.97	0.09	0.23	13,20,24,28	0
10	EDO	A	718	4/4	0.84	0.10	0.01	49,59,60,63	0
3	BJ2	A	702	30/30	0.97	0.08	-0.14	14,21,28,29	0
6	NAG	D	709	14/15	0.92	0.09	-0.30	29,40,46,52	0
6	NAG	D	705	14/15	0.87	0.09	-0.39	30,45,54,59	0
10	EDO	B	721	4/4	0.88	0.11	-0.58	48,58,70,71	0
11	ACT	B	724	4/4	0.92	0.07	-0.61	32,41,42,47	0
6	NAG	B	708	14/15	0.95	0.09	-0.64	32,41,49,50	0
3	BJ2	C	702	30/30	0.96	0.08	-0.66	17,24,31,31	0
9	PEG	B	714	7/7	0.87	0.10	-0.74	45,55,66,76	0
2	ZN	A	701	1/1	1.00	0.13	-	17,17,17,17	0
6	NAG	C	712	14/15	0.68	0.24	-	52,79,101,112	27
9	PEG	D	718	7/7	0.93	0.08	-	44,53,63,73	0
6	NAG	A	710	14/15	0.90	0.15	-	44,55,64,64	27
7	BMA	D	711	11/12	0.80	0.20	-	63,70,84,84	0
10	EDO	A	722	4/4	0.89	0.06	-	43,52,57,61	0
2	ZN	D	701	1/1	1.00	0.12	-	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	B	706	14/15	0.70	0.17	-	57,68,87,95	27
5	MG	A	704	1/1	0.97	0.12	-	23,23,23,23	0
10	EDO	C	717	4/4	0.76	0.10	-	64,76,83,92	0
6	NAG	A	706	14/15	0.68	0.26	-	66,86,105,126	28
5	MG	C	704	1/1	0.95	0.06	-	31,31,31,31	0
7	BMA	A	707	11/12	0.70	0.24	-	57,70,85,88	22
10	EDO	B	722	4/4	0.86	0.14	-	29,38,46,48	10
10	EDO	C	715	4/4	0.79	0.10	-	42,50,55,59	0
2	ZN	B	701	1/1	1.00	0.13	-	18,18,18,18	0
6	NAG	B	709	14/15	0.90	0.11	-	41,55,68,68	0
6	NAG	D	706	14/15	0.71	0.20	-	44,64,87,96	27
7	BMA	D	707	11/12	0.64	0.23	-	84,102,122,126	0
10	EDO	B	723	4/4	0.78	0.19	-	48,61,63,75	0
6	NAG	D	710	14/15	0.90	0.15	-	39,49,70,71	0
15	MAN	D	713	11/12	0.46	0.31	-	75,92,108,116	0
9	PEG	B	717	7/7	0.85	0.15	-	46,55,62,62	17
5	MG	D	704	1/1	0.99	0.16	-	17,17,17,17	0
15	MAN	D	712	11/12	0.30	0.37	-	71,86,101,106	21
6	NAG	C	706	14/15	0.62	0.28	-	56,71,86,94	27
7	BMA	C	709	11/12	0.67	0.25	-	76,95,114,115	0
8	FUC	D	708	10/11	0.84	0.15	-	42,53,64,67	0
6	NAG	D	715	14/15	0.56	0.39	-	59,79,102,109	27
2	ZN	C	701	1/1	1.00	0.11	-	20,20,20,20	0
6	NAG	B	712	14/15	0.48	0.35	-	52,70,88,93	27
6	NAG	A	712	14/15	0.57	0.21	-	53,80,99,111	28
10	EDO	A	721	4/4	0.79	0.11	-	40,49,55,59	10
7	BMA	B	710	11/12	0.72	0.21	-	64,74,89,90	0
8	FUC	B	707	10/11	0.90	0.10	-	45,55,65,67	0
11	ACT	A	725	4/4	0.91	0.19	-	46,49,59,59	0
5	MG	B	704	1/1	0.99	0.07	-	29,29,29,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.