

Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 08:39 am GMT

PDB ID : 2XEJ

Title : Human glutamate carboxypeptidase II in complex with ARM-M4, urea- based

inhibitor

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Deposited on : 2010-05-14

Resolution : 1.78 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

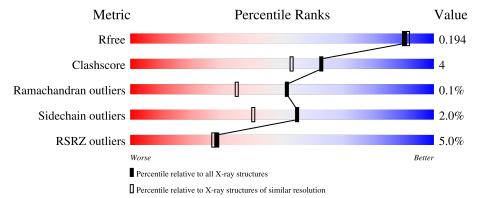
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.78 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
R_{free}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	- +						
1	A	709	87%	11%						
2	В	2	100%							
2	С	2	50% 50%							
2	D	2	100%							



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Mol	Chain	Length	Quality of chain	
3	Е	4	75%	25%



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6557 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 GLUTAMATE CARBOXYPEPTIDASE 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	694	Total 5773	C 3713	N 960	O 1077	S 23	0	48	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ARG	-	expression tag	UNP Q04609
A	43	SER	-	expression tag	UNP Q04609
A	593	GLN	LEU	conflict	UNP Q04609

• Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	В	2	Total C N O 28 16 2 10	0	0	0
2	С	2	Total C N O 28 16 2 10	0	0	0
2	D	2	Total C N O 28 16 2 10	0	0	0

• Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Е	4	Total 50	C 28	N 2	O 20	0	0	0

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

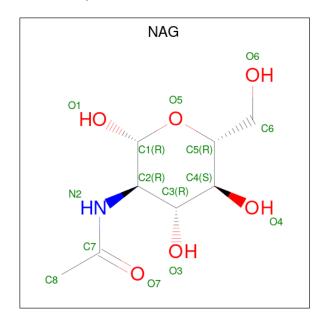
• Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0

• Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0

• Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



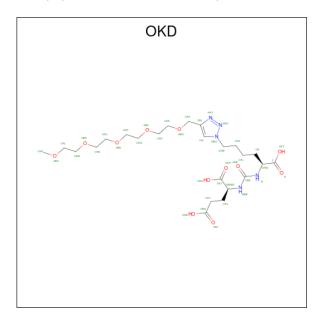
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 14	C 8	N 1	O 5	0	0



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Mol	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf
7	A	1	Total 14				0	0
7	A	1	Total 14	C 8		O 5	0	0

• Molecule 8 is N-({(1S)-1-CARBOXY-5-[4-(2,5,8,11,14-PENTAOXAPENTADEC-1-YL)-1H -1,2,3-TRIAZOL-1-YL]PENTYL}CARBAMOYL)-L-GLUTAMIC ACID (three-letter code: OKD) (formula: $C_{24}H_{41}N_5O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total 41	C 24	N 5	O 12	11	0

• Molecule 9 is water.

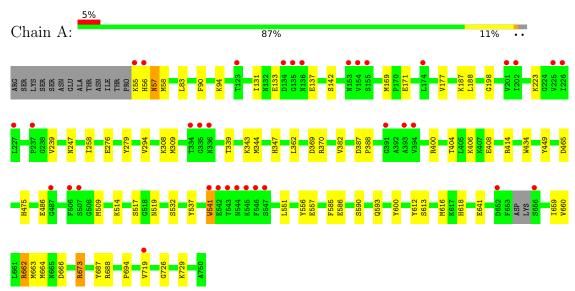
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	563	Total O 563 563	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 100%

NAG1 NAG2

 $\bullet \ \, \text{Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2$

Chain C: 50% 50%



 $\bullet \ \, \text{Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose} \\$

Chain D: 100%





 $\bullet \ \, Molecule \ 3: \ alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyrano$

Chain E: 75% 25%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	101.51Å 129.96Å 159.25Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 - 1.78	Depositor
Resolution (A)	28.53 - 1.78	EDS
% Data completeness	99.6 (20.00-1.78)	Depositor
(in resolution range)	99.6 (28.53-1.78)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.44 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.5.0104	Depositor
D D.	0.157 , 0.185	Depositor
R, R_{free}	0.166 , 0.194	DCC
R_{free} test set	1488 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 47.3	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6557	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, OKD, CL, CA, MAN, ZN, NAG

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		Boı	nd lengths	Bond angles	
MOI	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.97	3/6057 (0.0%)	0.84	6/8203 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
1	A	557	GLU	CB-CG	-6.61	1.39	1.52
1	A	434	TRP	CE3-CZ3	5.11	1.47	1.38
1	A	83	LEU	CG-CD2	5.01	1.70	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^o)$
1	A	673	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	A	673	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	465	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	370	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	309[A]	MET	CA-CB-CG	-5.14	104.57	113.30
1	A	309[B]	MET	CA-CB-CG	-5.14	104.57	113.30

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	5773	0	5635	49	1
2	В	28	0	25	2	0
2	С	28	0	25	0	0
2	D	28	0	25	0	0
3	Е	50	0	43	0	1
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	42	0	39	0	0
8	A	41	0	38	0	0
9	A	563	0	0	17	2
All	All	6557	0	5830	51	3

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 4.

All (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ (\rm \mathring{A}) \end{array}$	Clash overlap (Å)
1:A:541[B]:TRP:CH2	9:A:2308:HOH:O	1.64	1.21
1:A:660[A]:VAL:O	1:A:664[A]:MET:HG2	1.35	1.21
1:A:541[B]:TRP:CZ2	9:A:2308:HOH:O	1.70	1.12
1:A:541[B]:TRP:CZ3	9:A:2356:HOH:O	2.17	0.96
1:A:541[B]:TRP:CH2	9:A:2356:HOH:O	2.22	0.93
1:A:641:GLU:HG3	9:A:2436:HOH:O	1.80	0.80
1:A:688[B]:ARG:NH2	9:A:2480:HOH:O	2.17	0.77
1:A:131:ILE:HG22	1:A:137:GLU:HG2	1.71	0.72
1:A:400:ARG:O	1:A:404[B]:THR:HG23	1.92	0.70
1:A:414:ARG:CZ	1:A:593[A]:GLN:HE22	2.07	0.68
1:A:56:HIS:HE1	1:A:408:GLU:OE2	1.76	0.68
1:A:90[B]:PHE:HE2	1:A:94:LYS:HZ3	1.42	0.65
1:A:666:ASP:OD2	9:A:2456:HOH:O	2.16	0.63
1:A:90[B]:PHE:CE2	1:A:94:LYS:NZ	2.69	0.61
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.36	0.60
9:A:2544:HOH:O	2:B:2:NAG:H83	2.03	0.59
1:A:414:ARG:NE	1:A:593[A]:GLN:HE22	2.01	0.58
1:A:613[B]:SER:OG	9:A:2408:HOH:O	2.18	0.56
1:A:198:GLY:O	1:A:223:LYS:HE2	2.05	0.55
9:A:2031:HOH:O	2:B:2:NAG:H81	2.06	0.55
1:A:369:ASP:OD2	1:A:662[B]:ARG:NH2	2.39	0.55
1:A:58[B]:MET:HG3	1:A:585:PHE:CG	2.43	0.54
1:A:475:HIS:CE1	1:A:509[B]:MET:CE	2.91	0.54



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Atom-1	Atom-2	Interatomic	Clash
		${f distance}({ m \AA})$	overlap (Å)
1:A:239[A]:VAL:HG22	1:A:247:ASN:ND2	2.22	0.53
1:A:618:HIS:HD2	9:A:2416:HOH:O	1.93	0.51
1:A:133:GLU:HG3	1:A:339:THR:HB	1.93	0.51
1:A:369:ASP:CG	1:A:662[B]:ARG:HH22	2.15	0.49
1:A:90[B]:PHE:CE2	1:A:94:LYS:HE2	2.47	0.49
1:A:659[B]:ILE:O	1:A:663[B]:MET:HG3	2.13	0.49
1:A:177:VAL:HG12	1:A:188:LEU:HD11	1.95	0.48
1:A:688[B]:ARG:CZ	9:A:2476:HOH:O	2.62	0.47
1:A:90[B]:PHE:CE2	1:A:94:LYS:CE	2.97	0.47
1:A:258:ILE:HD13	1:A:294:VAL:HB	1.96	0.47
1:A:347:HIS:HE1	9:A:2064:HOH:O	1.97	0.47
1:A:586[B]:GLU:OE2	1:A:590[B]:SER:OG	2.33	0.46
1:A:308:LYS:HB2	9:A:2228:HOH:O	2.16	0.46
1:A:171[A]:GLU:HG2	1:A:343:LYS:HG3	1.99	0.45
1:A:726:GLY:HA2	1:A:729[C]:LYS:HE3	1.97	0.45
1:A:517:SER:HB2	1:A:694:PRO:HG3	1.99	0.44
1:A:618:HIS:HE1	9:A:2507:HOH:O	2.01	0.43
1:A:57:ASN:C	1:A:57:ASN:HD22	2.22	0.43
1:A:541[B]:TRP:HH2	9:A:2308:HOH:O	1.41	0.42
1:A:387:ASP:HA	1:A:388:PRO:HA	1.93	0.42
1:A:239[A]:VAL:HG22	1:A:247:ASN:CG	2.40	0.41
1:A:362:LEU:HD11	1:A:406:LYS:HG3	2.03	0.41
1:A:514[A]:LYS:HG3	9:A:2344:HOH:O	2.20	0.41
1:A:687:TYR:CZ	1:A:694:PRO:HG2	2.56	0.41
1:A:169:MET:HA	1:A:344:MET:O	2.21	0.40
1:A:551:LEU:HD22	1:A:556:TYR:HB2	2.03	0.40
1:A:449:TYR:O	1:A:532:SER:HA	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
9:A:2456:HOH:O	9:A:2456:HOH:O[2_565]	1.19	1.01
9:A:2301:HOH:O	9:A:2457:HOH:O[2_565]	1.91	0.29
1:A:276[A]:GLU:OE1	3:E:3:BMA:O2[2_565]	2.02	0.18



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	735/709 (104%)	717 (98%)	17 (2%)	1 (0%)	51 35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	VAL

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	Analysed Rotameric		Percentiles	
1	A	637/605 (105%)	622 (98%)	15 (2%)	49 33	

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	57	ASN
1	A	142[A]	SER
1	A	142[B]	SER
1	A	187	LYS
1	A	486	GLU
1	A	519	ASN
1	A	537	TYR
1	A	541[A]	TRP
1	A	541[B]	TRP



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Mol	Chain	Res	Type
1	A	600	TYR
1	A	662[A]	ARG
1	A	662[B]	ARG
1	A	673	ARG
1	A	719	VAL

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

Mol	Chain	Res	Type
1	A	56	HIS
1	A	57	ASN
1	A	91	GLN
1	A	136	ASN
1	A	303	GLN
1	A	345	HIS
1	A	544	ASN
1	A	618	HIS

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)

10 monosaccharides 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).

Mal	Type	Chain	Res	Link	Bond lengths			Bond angles		
IVIOI	туре			Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	В	1	2,1	14,14,15	0.52	0	17,19,21	1.08	1 (5%)



Mol	Trino	Chain	Res	Link	Во	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	В	2	2	14,14,15	0.71	0	17,19,21	1.21	0
2	NAG	С	1	2,1	14,14,15	0.69	0	17,19,21	0.94	0
2	NAG	С	2	2	14,14,15	0.52	0	17,19,21	1.27	2 (11%)
2	NAG	D	1	2,1	14,14,15	0.94	0	17,19,21	1.14	2 (11%)
2	NAG	D	2	2	14,14,15	0.67	0	17,19,21	1.21	1 (5%)
3	NAG	Е	1	3,1	14,14,15	0.74	0	17,19,21	1.36	4 (23%)
3	NAG	Е	2	3	14,14,15	0.83	1 (7%)	17,19,21	1.19	2 (11%)
3	BMA	Е	3	3	11,11,12	0.64	0	15,15,17	1.28	1 (6%)
3	MAN	Е	4	3	11,11,12	0.66	0	15,15,17	1.50	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	В	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	В	2	2	-	2/6/23/26	0/1/1/1
2	NAG	С	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	С	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	Е	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Е	2	3	-	4/6/23/26	0/1/1/1
3	BMA	Е	3	3	-	0/2/19/22	0/1/1/1
3	MAN	Е	4	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
3	Е	2	NAG	O5-C1	-2.49	1.39	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^{o})$
3	Ε	3	BMA	O3-C3-C2	-3.41	103.46	109.99
3	Е	2	NAG	C1-O5-C5	3.05	116.32	112.19
3	Е	1	NAG	O5-C1-C2	-2.98	106.58	111.29
2	В	1	NAG	O5-C1-C2	-2.86	106.77	111.29



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
2	С	2	NAG	O5-C5-C6	2.79	111.58	107.20
2	D	2	NAG	C8-C7-N2	2.72	120.70	116.10
3	Ε	4	MAN	O5-C5-C6	2.63	111.33	107.20
2	С	2	NAG	O4-C4-C5	2.40	115.26	109.30
2	D	1	NAG	O3-C3-C2	-2.31	104.69	109.47
2	D	1	NAG	O5-C5-C4	-2.26	105.34	110.83
3	Ε	1	NAG	C2-N2-C7	-2.24	119.72	122.90
3	${ m E}$	1	NAG	O4-C4-C5	-2.12	104.03	109.30
3	Е	1	NAG	C6-C5-C4	-2.09	108.10	113.00
3	Ε	2	NAG	C8-C7-N2	2.07	119.60	116.10

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	2	NAG	C8-C7-N2-C2
2	В	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
3	Е	2	NAG	C8-C7-N2-C2
3	Е	2	NAG	O7-C7-N2-C2
3	Е	2	NAG	C4-C5-C6-O6
2	С	2	NAG	C4-C5-C6-O6
3	Е	2	NAG	O5-C5-C6-O6
2	С	2	NAG	O5-C5-C6-O6

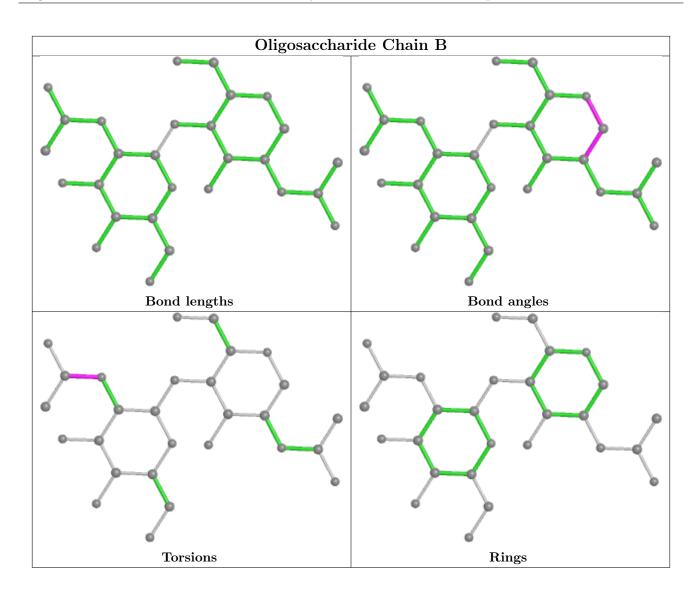
There are no ring outliers.

2 monomers are involved in 3 short contacts:

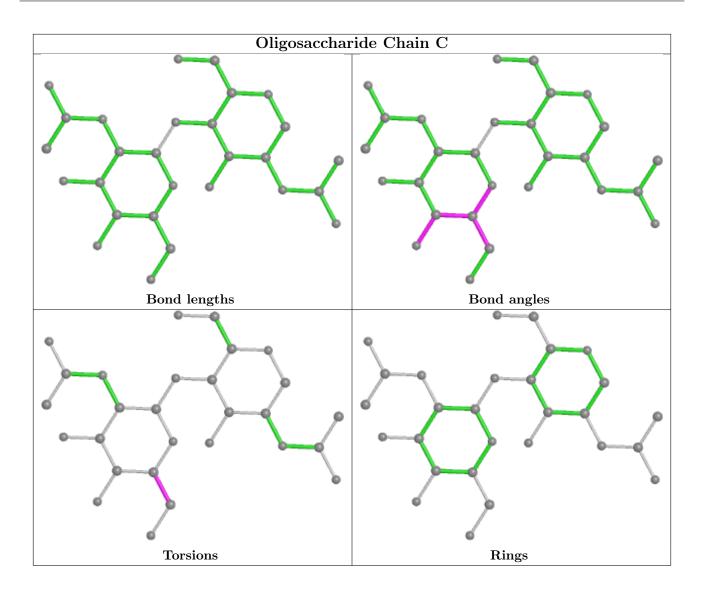
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Ε	3	BMA	0	1
2	В	2	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

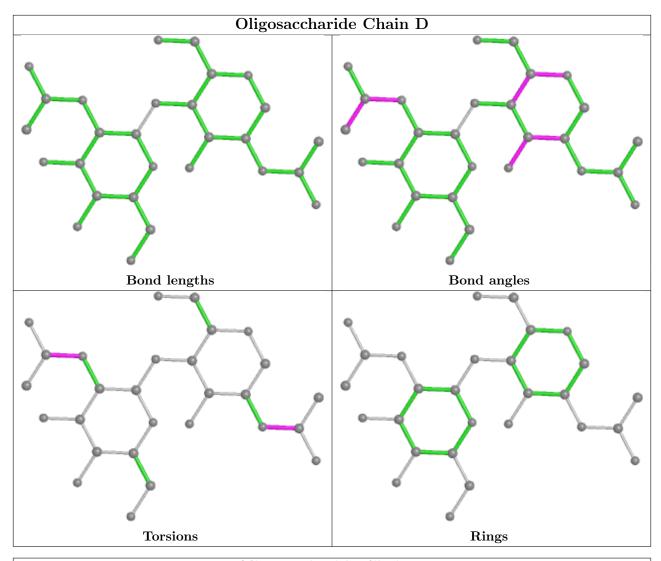


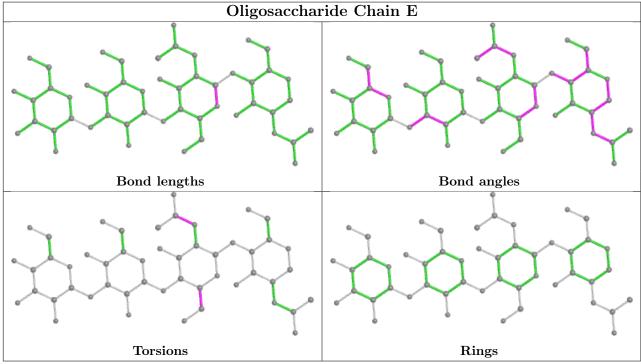














5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	Clasia	Res	Link	Вс	ond leng	ths	Bond angles		
MIOI	Moi Type C	Chain	nes	es Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	1760	1	14,14,15	0.78	1 (7%)	17,19,21	1.65	5 (29%)
7	NAG	A	1759	1	14,14,15	0.56	0	17,19,21	2.72	5 (29%)
7	NAG	A	1757	1	14,14,15	0.78	0	17,19,21	1.77	3 (17%)
8	OKD	A	1768	4	41,41,41	1.63	5 (12%)	44,49,49	1.91	11 (25%)

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.

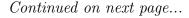
Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1760	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1759	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1757	1	-	0/6/23/26	0/1/1/1
8	OKD	A	1768	4	-	9/41/43/43	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\textup{\AA})$	Ideal(A)
8	A	1768	OKD	NAY-NAZ	-4.74	1.25	1.34
8	A	1768	OKD	NAZ-NBO	-4.60	1.25	1.34
8	A	1768	OKD	OBG-CAX	3.02	1.53	1.42
8	A	1768	OKD	CAX-CBL	-2.70	1.43	1.50
8	A	1768	OKD	CAT-CBH	2.33	1.56	1.50
7	A	1760	NAG	C1-C2	2.17	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
7	A	1759	NAG	C1-O5-C5	9.02	124.42	112.19





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Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
8	A	1768	OKD	OBG-CAX-CBL	5.21	125.78	110.94
8	A	1768	OKD	CB-CA-N	-4.48	101.82	110.88
8	A	1768	OKD	OBF-CAR-CAS	-4.47	90.25	110.39
8	A	1768	OKD	NAY-NAZ-NBO	4.45	110.67	107.31
7	A	1757	NAG	C1-C2-N2	-3.89	103.85	110.49
7	A	1757	NAG	O5-C5-C6	3.69	112.99	107.20
7	A	1760	NAG	C1-O5-C5	3.59	117.05	112.19
8	A	1768	OKD	CAW-NBO-CAI	-3.45	121.71	129.82
7	A	1759	NAG	C8-C7-N2	3.11	121.37	116.10
7	A	1760	NAG	O3-C3-C4	-3.04	103.32	110.35
8	A	1768	OKD	CAI-CBL-NAY	-2.92	107.00	111.34
7	A	1759	NAG	C4-C3-C2	-2.91	106.75	111.02
7	A	1759	NAG	C6-C5-C4	-2.63	106.85	113.00
7	A	1760	NAG	O5-C1-C2	-2.49	107.35	111.29
7	A	1759	NAG	C1-C2-N2	2.39	114.58	110.49
7	A	1760	NAG	O5-C5-C6	2.32	110.84	107.20
8	A	1768	OKD	OAD-CBJ-CBN	2.20	120.72	113.40
8	A	1768	OKD	CAV-CBN-CBJ	-2.18	105.10	110.35
7	A	1757	NAG	C2-N2-C7	-2.17	119.81	122.90
8	A	1768	OKD	OAH-CBJ-CBN	-2.11	115.32	122.26
8	A	1768	OKD	CAK-CAJ-CB	-2.05	106.36	113.62
7	A	1760	NAG	C8-C7-N2	2.01	119.50	116.10
8	A	1768	OKD	CAX-CBL-CAI	-2.00	124.67	128.45

There are no chirality outliers.

All (13) torsion outliers are listed below:

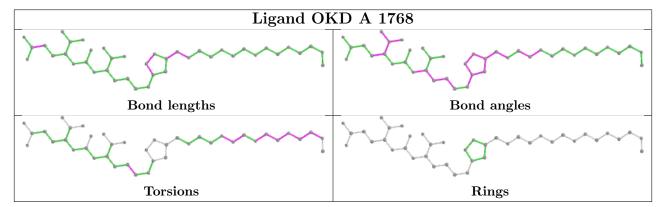
Mol	Chain	Res	Type	Atoms
7	A	1759	NAG	C8-C7-N2-C2
7	A	1759	NAG	O7-C7-N2-C2
7	A	1759	NAG	C4-C5-C6-O6
8	A	1768	OKD	OBD-CAN-CAO-OBE
8	A	1768	OKD	CB-CAJ-CAK-CAW
8	A	1768	OKD	CAM-CAL-OBC-CAA
8	A	1768	OKD	OBE-CAP-CAQ-OBF
8	A	1768	OKD	CAL-CAM-OBD-CAN
7	A	1759	NAG	O5-C5-C6-O6
8	A	1768	OKD	CAN-CAO-OBE-CAP
8	A	1768	OKD	CAP-CAQ-OBF-CAR
8	A	1768	OKD	CAO-CAN-OBD-CAM
8	A	1768	OKD	OBC-CAL-CAM-OBD



There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95^{th} 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	$OWAB(A^2)$	Q < 0.9
1	A	694/709 (97%)	0.04	35 (5%) 28 27	14, 24, 43, 66	1 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	544	ASN	6.6
1	A	545	LYS	6.5
1	A	543	THR	6.0
1	A	541[A]	TRP	5.8
1	A	546	PHE	5.3
1	A	656[A]	SER	4.9
1	A	542	GLU	4.7
1	A	55	LYS	4.0
1	A	153	ASN	3.8
1	A	134	ASP	3.8
1	A	506	PHE	3.7
1	A	335	GLY	3.3
1	A	336	ASN	3.2
1	A	155	SER	3.1
1	A	154	VAL	3.0
1	A	227	LEU	3.0
1	A	507	SER	2.9
1	A	136	ASN	2.7
1	A	135	GLY	2.6
1	A	652	ASP	2.5
1	A	201	VAL	2.5
1	A	123	THR	2.5
1	A	56	HIS	2.5
1	A	202	ILE	2.5
1	A	174[A]	LEU	2.5
1	A	393	ALA	2.4
1	A	487	GLY	2.4



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Mol	Chain	Res	Type	RSRZ
1	A	719	VAL	2.4
1	A	226	ILE	2.3
1	A	334	THR	2.3
1	A	225	VAL	2.2
1	A	237	PRO	2.2
1	A	547	SER	2.1
1	A	394	VAL	2.1
1	A	391	GLY	2.1

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)

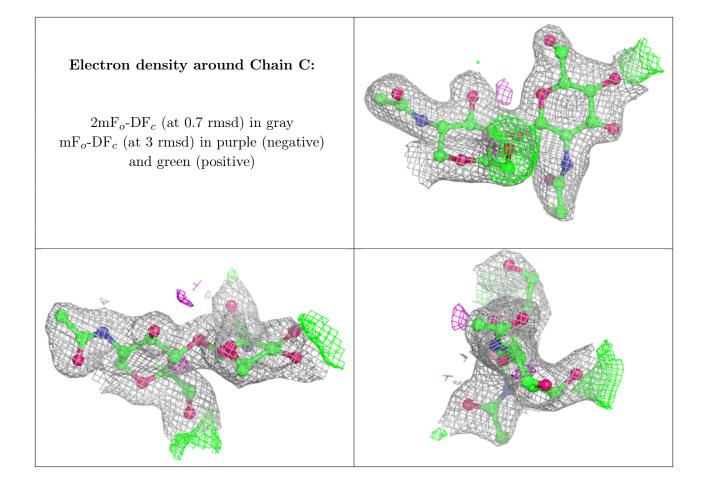
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	NAG	В	2	14/15	0.72	0.25	39,47,52,56	0
2	NAG	С	2	14/15	0.79	0.27	53,57,61,63	0
2	NAG	С	1	14/15	0.86	0.15	36,40,43,49	0
3	NAG	Е	2	14/15	0.88	0.21	35,38,48,50	0
2	NAG	D	2	14/15	0.90	0.18	31,37,43,45	0
3	BMA	Е	3	11/12	0.91	0.14	35,38,41,41	0
2	NAG	D	1	14/15	0.92	0.11	24,28,33,37	0
3	NAG	Е	1	14/15	0.92	0.09	20,27,37,45	0
3	MAN	Е	4	11/12	0.92	0.14	43,46,49,49	0
2	NAG	В	1	14/15	0.94	0.10	29,38,41,46	0

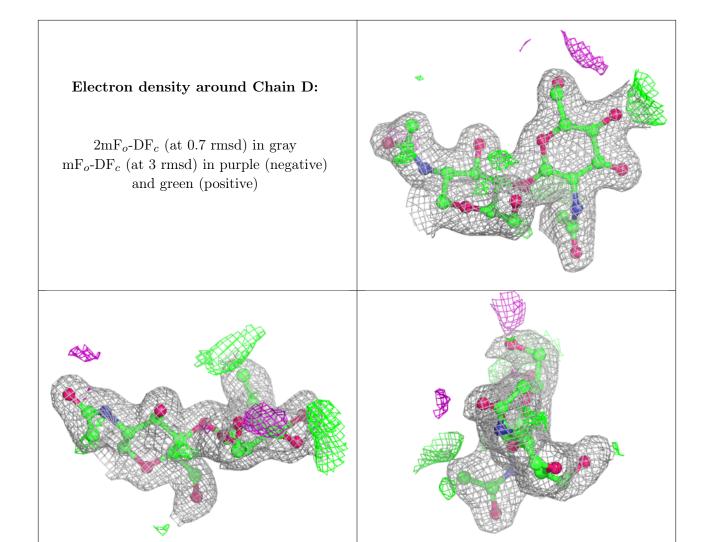
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



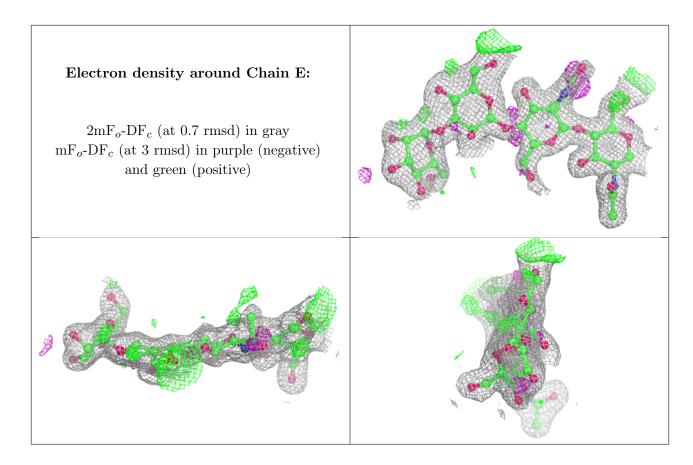












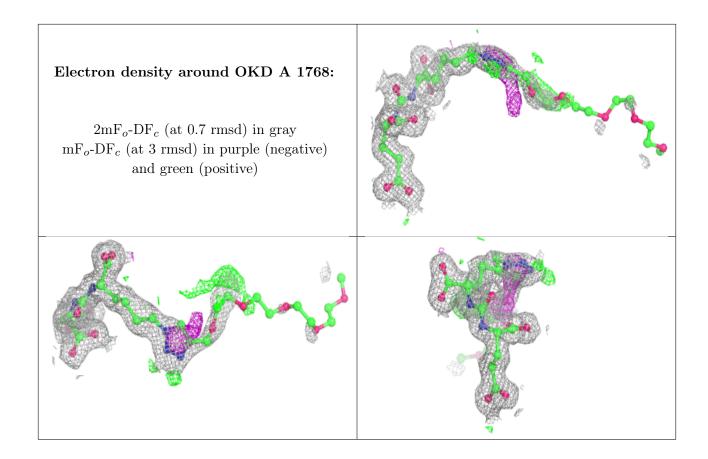
6.4 Ligands (i)

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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
7	NAG	A	1757	14/15	0.78	0.25	40,48,54,54	0
7	NAG	A	1759	14/15	0.79	0.17	52,60,64,65	0
7	NAG	A	1760	14/15	0.89	0.15	28,43,46,50	0
8	OKD	A	1768	41/41	0.94	0.12	14,32,101,104	11
4	ZN	A	1751	1/1	1.00	0.07	19,19,19,19	0
4	ZN	A	1752	1/1	1.00	0.06	18,18,18,18	0
5	CA	A	1753	1/1	1.00	0.08	16,16,16,16	0
6	CL	A	1754	1/1	1.00	0.08	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers (i)

There are no such residues in this entry.

