



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 08:37 PM UTC

PDB ID : 9EZ6 / pdb_00009ez6
Title : Complex of a mutant of the SARS-CoV-2 main protease Mpro with the nsp14/15 substrate peptide.
Authors : Battistutta, R.; Fornasier, E.; Giachin, G.
Deposited on : 2024-04-10
Resolution : 1.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

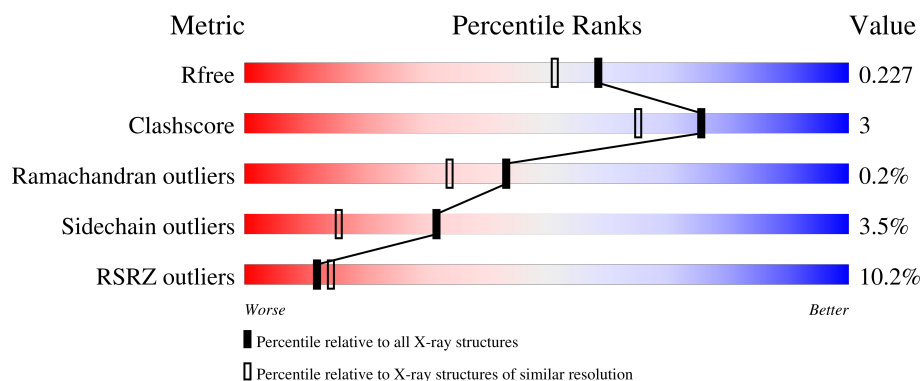
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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 $\leq 5\%$. 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	306	8% 92% 7%
1	B	306	12% 87% 10%
2	C	11	73% 18% 9%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9780 atoms, of which 4765 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 Replicase polypeptide 1a.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	302	Total	C	H	N	O	S	0	6	0
			4661	1487	2308	401	443	22			
1	B	299	Total	C	H	N	O	S	0	0	0
			4572	1465	2263	392	432	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ALA	HIS	conflict	UNP A0A8B1KJN1
A	145	ALA	CYS	conflict	UNP A0A8B1KJN1
B	41	ALA	HIS	conflict	UNP A0A8B1KJN1
B	145	ALA	CYS	conflict	UNP A0A8B1KJN1

- Molecule 2 is a protein called THR-PHE-THR-ARG-LEU-GLN-SER-LEU-GLU-ASN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	H	N	O	0	0	0
			170	54	83	15	18			

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



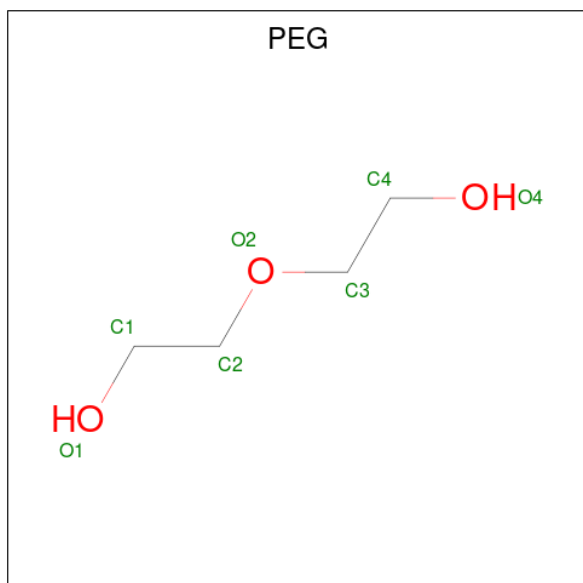
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		

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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

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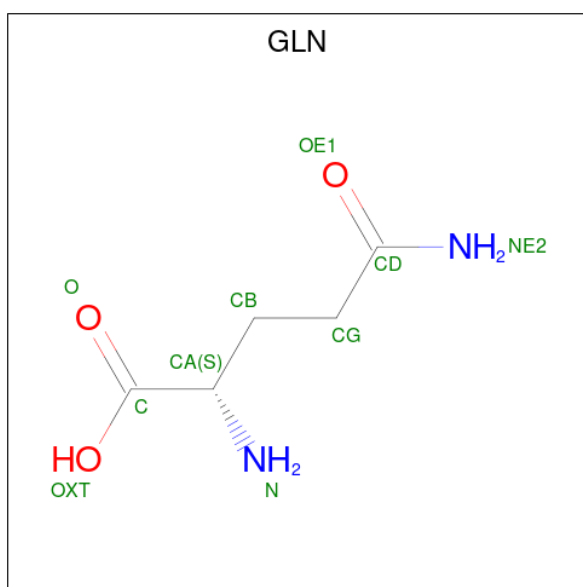
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	B	1	Total	Na	0	0
			1	1		

- Molecule 7 is GLUTAMINE (CCD ID: GLN) (formula: C₅H₁₀N₂O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	H	N	O	0	0
			16	5	7	2	2		

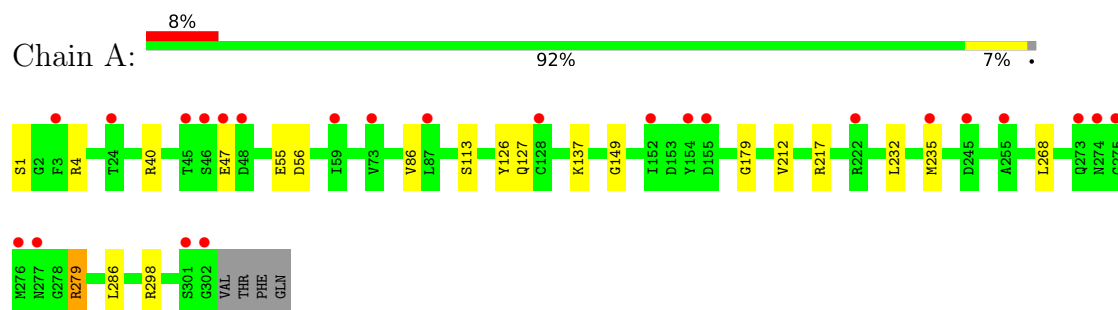
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	118	Total	O	0	0
			118	118		
8	B	60	Total	O	0	0
			60	60		
8	C	7	Total	O	0	0
			7	7		

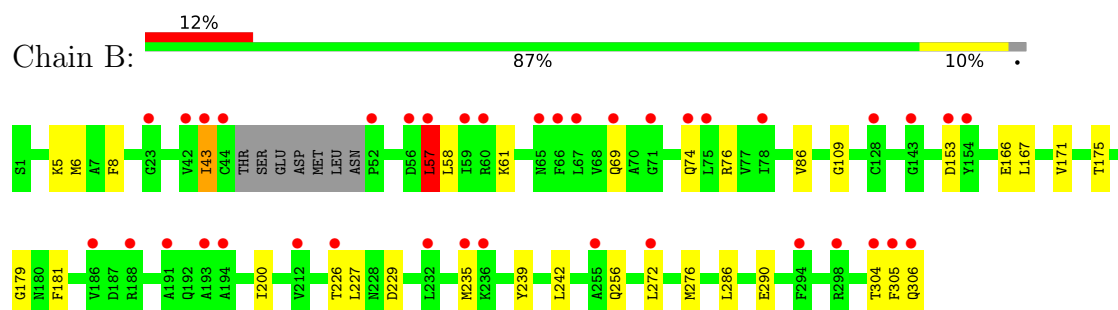
3 Residue-property plots

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.

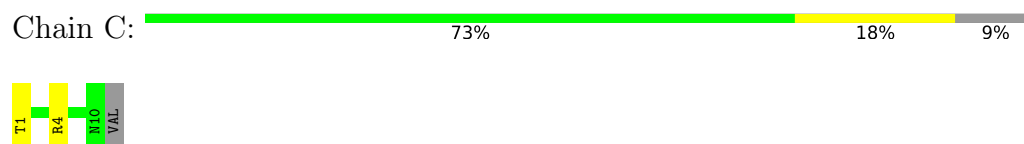
- Molecule 1: Replicase polypeptide 1a



- Molecule 1: Replicase polypeptide 1a



- Molecule 2: THR-PHE-THR-ARG-LEU-GLN-SER-LEU-GLU-ASN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.80Å 99.03Å 100.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.95 – 1.87 55.95 – 1.87	Depositor EDS
% Data completeness (in resolution range)	98.2 (55.95-1.87) 98.3 (55.95-1.87)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.87Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.195 , 0.228 0.194 , 0.227	Depositor DCC
R_{free} test set	2743 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9780	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, THC, CSD, DMS, PEG, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/2436	0.43	0/3311
1	B	0.27	0/2352	0.40	0/3195
2	C	0.24	0/77	0.51	0/102
All	All	0.29	0/4865	0.41	0/6608

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

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	2353	2308	2274	14	0
1	B	2309	2263	2264	17	0
2	C	87	83	81	0	0
3	A	8	12	12	2	0
4	A	36	54	54	3	0
4	B	12	18	18	0	0
5	A	14	20	20	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	B	9	7	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	118	0	0	4	0
8	B	60	0	0	1	0
8	C	7	0	0	0	0
All	All	5015	4765	4730	29	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (29) 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:56:ASP:OD1	8:A:501:HOH:O	1.84	0.94
1:B:43:ILE:HG23	1:B:57:LEU:HD12	1.75	0.66
1:A:55:GLU:H	3:A:401:DMS:H13	1.62	0.65
1:B:43:ILE:HD11	1:B:58:LEU:HD13	1.80	0.64
1:B:239:TYR:CZ	1:B:272:LEU:HD21	2.42	0.55
1:A:217[A]:ARG:NH2	8:A:509:HOH:O	2.42	0.52
1:A:232:LEU:HA	1:A:235:MET:HE2	1.91	0.52
1:B:57:LEU:O	1:B:61:LYS:HG2	2.14	0.48
1:A:4:ARG:HD2	4:A:411:EDO:H11	1.96	0.48
1:B:86:VAL:HG13	1:B:179:GLY:HA2	1.95	0.48
1:A:126:TYR:CD2	1:B:6:MET:HE2	2.48	0.47
1:A:279:ARG:NH1	8:A:511:HOH:O	2.47	0.47
1:B:227:LEU:HD11	1:B:242:LEU:HB3	1.96	0.47
1:A:127:GLN:NE2	8:A:510:HOH:O	2.44	0.46
1:B:290:GLU:OE1	8:B:501:HOH:O	2.21	0.46
1:B:109:GLY:HA2	1:B:200:ILE:HD13	1.98	0.46
1:A:86:VAL:HG23	1:A:179:GLY:HA2	2.00	0.44
1:A:113:SER:O	1:A:149:GLY:HA2	2.18	0.44
1:A:1:SER:OG	1:B:166:GLU:OE2	2.36	0.43
1:A:212:VAL:O	1:A:217[B]:ARG:NH2	2.51	0.43
1:A:40:ARG:HH12	3:A:401:DMS:H23	1.83	0.43
1:B:226:THR:HG23	1:B:229:ASP:H	1.84	0.43
1:B:167:LEU:HD12	1:B:171:VAL:HG23	2.01	0.42
4:A:411:EDO:H22	1:B:5:LYS:HD2	2.01	0.42
1:B:226:THR:CG2	1:B:229:ASP:H	2.32	0.42
1:B:175:THR:HG22	1:B:181:PHE:HA	2.02	0.41
4:A:411:EDO:C2	1:B:5:LYS:HD2	2.51	0.41
1:A:137:LYS:HD3	5:A:410:PEG:H11	2.04	0.40
1:B:8:PHE:HE1	1:B:305:PHE:CZ	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/306 (100%)	293 (96%)	12 (4%)	0	100	100
1	B	294/306 (96%)	286 (97%)	7 (2%)	1 (0%)	36	26
2	C	8/11 (73%)	7 (88%)	1 (12%)	0	100	100
All	All	607/623 (97%)	586 (96%)	20 (3%)	1 (0%)	43	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	57	LEU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/260 (101%)	257 (98%)	5 (2%)	50	36
1	B	253/260 (97%)	241 (95%)	12 (5%)	23	8
2	C	9/10 (90%)	8 (89%)	1 (11%)	6	0
All	All	524/530 (99%)	506 (97%)	18 (3%)	32	16

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLU
1	A	268	LEU
1	A	279	ARG
1	A	286	LEU
1	A	298	ARG
1	B	43	ILE
1	B	57	LEU
1	B	69	GLN
1	B	74	GLN
1	B	76	ARG
1	B	153	ASP
1	B	235	MET
1	B	256	GLN
1	B	276	MET
1	B	286	LEU
1	B	304	THR
1	B	306	GLN
2	C	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSD	B	156	1	4,7,8	0.89	0	1,8,10	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	THC	C	1	2	8,9,10	0.48	0	10,11,13	1.07	1 (10%)
1	CSD	A	156	1	4,7,8	0.90	0	1,8,10	0.22	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
1	CSD	B	156	1	-	1/2/6/8	-
2	THC	C	1	2	-	0/9/10/12	-
1	CSD	A	156	1	-	2/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	THC	CB-CA-C	-2.07	108.12	111.55

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	156	CSD	N-CA-CB-SG
1	A	156	CSD	CA-CB-SG-OD1
1	B	156	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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$
4	EDO	B	403	-	3,3,3	0.42	0	2,2,2	0.36	0
4	EDO	A	404	-	3,3,3	0.51	0	2,2,2	0.42	0
4	EDO	B	404	-	3,3,3	0.48	0	2,2,2	0.35	0
4	EDO	A	412	-	3,3,3	0.51	0	2,2,2	0.41	0
4	EDO	A	411	-	3,3,3	0.35	0	2,2,2	0.28	0
4	EDO	A	409	-	3,3,3	0.43	0	2,2,2	0.39	0
4	EDO	B	401	-	3,3,3	0.50	0	2,2,2	0.43	0
4	EDO	A	408	-	3,3,3	0.58	0	2,2,2	0.46	0
5	PEG	A	407	-	6,6,6	0.20	0	5,5,5	0.18	0
7	GLN	B	402	-	7,8,9	0.43	0	4,9,11	0.09	0
5	PEG	A	410	-	6,6,6	0.10	0	5,5,5	0.11	0
4	EDO	A	405	-	3,3,3	0.46	0	2,2,2	0.43	0
4	EDO	A	402	-	3,3,3	0.51	0	2,2,2	0.32	0
3	DMS	A	401	-	3,3,3	0.70	0	3,3,3	0.56	0
4	EDO	A	413	-	3,3,3	0.48	0	2,2,2	0.42	0
3	DMS	A	403	-	3,3,3	0.69	0	3,3,3	0.54	0
4	EDO	A	406	-	3,3,3	0.56	0	2,2,2	0.42	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
4	EDO	B	403	-	-	0/1/1/1	-
4	EDO	A	404	-	-	0/1/1/1	-
4	EDO	B	404	-	-	0/1/1/1	-
4	EDO	A	412	-	-	1/1/1/1	-
4	EDO	A	411	-	-	1/1/1/1	-
4	EDO	A	409	-	-	1/1/1/1	-
4	EDO	B	401	-	-	1/1/1/1	-
4	EDO	A	408	-	-	0/1/1/1	-
5	PEG	A	407	-	-	4/4/4/4	-
7	GLN	B	402	-	-	1/6/7/9	-
5	PEG	A	410	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	405	-	-	1/1/1/1	-
4	EDO	A	402	-	-	0/1/1/1	-
4	EDO	A	413	-	-	0/1/1/1	-
4	EDO	A	406	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	402	GLN	O-C-CA-CB
5	A	410	PEG	O1-C1-C2-O2
5	A	410	PEG	O2-C3-C4-O4
5	A	407	PEG	O2-C3-C4-O4
4	A	405	EDO	O1-C1-C2-O2
5	A	407	PEG	O1-C1-C2-O2
4	A	411	EDO	O1-C1-C2-O2
4	A	406	EDO	O1-C1-C2-O2
4	A	412	EDO	O1-C1-C2-O2
5	A	407	PEG	C1-C2-O2-C3
5	A	407	PEG	C4-C3-O2-C2
5	A	410	PEG	C4-C3-O2-C2
4	A	409	EDO	O1-C1-C2-O2
4	B	401	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	411	EDO	3	0
5	A	410	PEG	1	0
3	A	401	DMS	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	301/306 (98%)	0.48	24 (7%) 18 20	18, 48, 74, 122	3 (0%)
1	B	298/306 (97%)	0.93	38 (12%) 7 8	32, 58, 98, 126	0
2	C	9/11 (81%)	0.80	0 100 100	35, 46, 80, 90	0
All	All	608/623 (97%)	0.70	62 (10%) 12 14	18, 53, 89, 126	3 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	PRO	6.3
1	A	154	TYR	4.9
1	A	59	ILE	3.9
1	B	43	ILE	3.6
1	A	301	SER	3.6
1	A	46	SER	3.5
1	A	275	GLY	3.5
1	B	194	ALA	3.4
1	B	57	LEU	3.3
1	A	302	GLY	3.2
1	B	59	ILE	3.1
1	B	154	TYR	3.1
1	B	67	LEU	3.0
1	A	273	GLN	2.9
1	B	56	ASP	2.9
1	B	272	LEU	2.9
1	A	48	ASP	2.8
1	B	255	ALA	2.8
1	B	153	ASP	2.8
1	A	274	ASN	2.7
1	B	191	ALA	2.7
1	B	44	CYS	2.6
1	B	294	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	235	MET	2.6
1	A	245	ASP	2.6
1	B	23	GLY	2.5
1	A	277	ASN	2.5
1	A	152	ILE	2.5
1	B	298	ARG	2.5
1	A	47	GLU	2.5
1	B	186	VAL	2.5
1	B	128	CYS	2.5
1	A	87	LEU	2.5
1	A	276	MET	2.5
1	B	305	PHE	2.4
1	B	304	THR	2.4
1	A	255	ALA	2.3
1	A	3	PHE	2.3
1	B	42	VAL	2.3
1	A	235	MET	2.3
1	A	128	CYS	2.3
1	B	60	ARG	2.2
1	B	306	GLN	2.2
1	A	73	VAL	2.2
1	A	24	THR	2.2
1	B	74	GLN	2.2
1	A	45	THR	2.2
1	B	71	GLY	2.2
1	B	193	ALA	2.2
1	B	212	VAL	2.1
1	B	226	THR	2.1
1	A	222	ARG	2.1
1	B	66	PHE	2.1
1	B	78	ILE	2.1
1	B	143	GLY	2.1
1	B	75	LEU	2.1
1	B	232	LEU	2.0
1	A	155	ASP	2.0
1	B	236	LYS	2.0
1	B	69	GLN	2.0
1	B	65	ASN	2.0
1	B	188	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
1	CSD	A	156	8/9	0.84	0.16	48,63,80,80	0
1	CSD	B	156	8/9	0.88	0.12	38,54,62,65	0
2	THC	C	1	10/11	0.88	0.12	41,49,56,56	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
3	DMS	A	401	4/4	0.76	0.19	58,70,79,89	0
4	EDO	A	406	4/4	0.77	0.16	74,89,97,102	0
4	EDO	A	404	4/4	0.78	0.21	72,87,89,95	0
6	NA	B	405	1/1	0.78	0.23	58,58,58,58	0
3	DMS	A	403	4/4	0.79	0.17	72,86,87,96	0
4	EDO	A	405	4/4	0.79	0.20	51,62,75,83	0
4	EDO	B	401	4/4	0.81	0.17	62,75,85,91	0
7	GLN	B	402	9/10	0.83	0.14	56,72,84,87	0
4	EDO	A	402	4/4	0.84	0.13	50,61,73,74	0
6	NA	A	414	1/1	0.85	0.15	63,63,63,63	0
5	PEG	A	407	7/7	0.87	0.13	62,74,87,87	0
4	EDO	A	411	4/4	0.87	0.15	48,58,68,69	0
5	PEG	A	410	7/7	0.90	0.12	66,80,91,91	0
4	EDO	A	408	4/4	0.90	0.13	53,66,79,82	0
4	EDO	B	403	4/4	0.91	0.11	44,53,64,64	0
4	EDO	A	409	4/4	0.91	0.14	59,71,74,74	0
4	EDO	B	404	4/4	0.92	0.12	73,88,94,98	0
4	EDO	A	412	4/4	0.92	0.13	55,66,80,80	0
4	EDO	A	413	4/4	0.92	0.13	64,77,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.