



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:12 PM UTC

PDB ID : 6C09 / pdb_00006c09
Title : Ternary crystal structure of the 3C8 TCR-CD1c-monoacylglycerol complex
Authors : Wun, K.S.; Rossjohn, J.
Deposited on : 2017-12-28
Resolution : 2.95 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 ⓘ 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

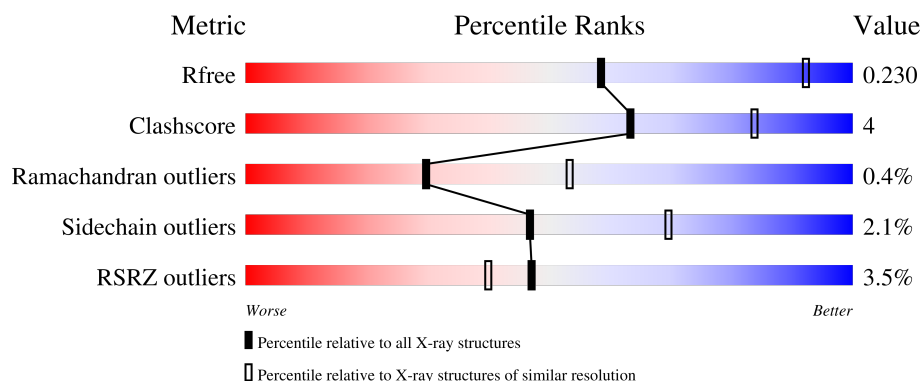
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	287	5% 80% 13% 6%
2	B	108	81% 10% 9%
3	C	205	3% 75% 17% 6%
4	D	247	3% 91% 7%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6245 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 T-cell surface glycoprotein CD1c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	2	0
			2107	1359	366	375	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLU	-	expression tag	UNP P29017
A	-1	THR	-	expression tag	UNP P29017
A	0	GLY	-	expression tag	UNP P29017
A	280	SER	-	expression tag	UNP P29017
A	281	LEU	-	expression tag	UNP P29017
A	282	VAL	-	expression tag	UNP P29017
A	283	PRO	-	expression tag	UNP P29017
A	284	ARG	-	expression tag	UNP P29017

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			773	494	130	146	3			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLU	-	expression tag	UNP P61769
B	-1	THR	-	expression tag	UNP P61769
B	0	GLY	-	expression tag	UNP P61769
B	100	GLY	-	expression tag	UNP P61769
B	101	SER	-	expression tag	UNP P61769
B	102	LEU	-	expression tag	UNP P61769
B	103	VAL	-	expression tag	UNP P61769
B	104	PRO	-	expression tag	UNP P61769

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	105	ARG	-	expression tag	UNP P61769

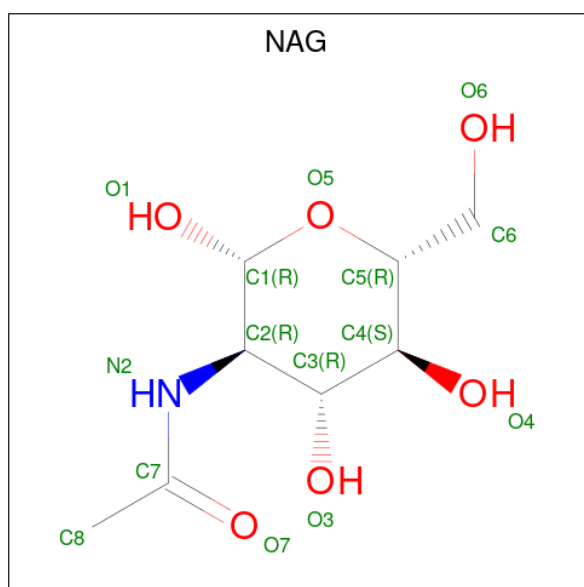
- Molecule 3 is a protein called 3C8 T cell receptor alpha-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	192	Total	C	N	O	S	0	0	0
			1427	912	234	272	9			

- Molecule 4 is a protein called 3C8 T cell receptor beta-chain.

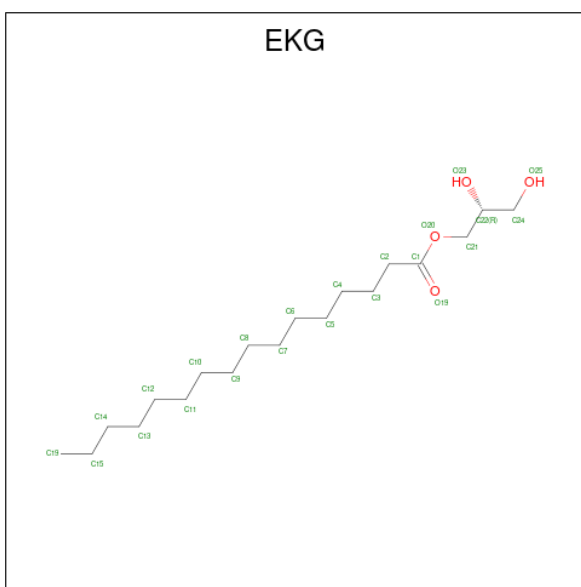
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	244	Total	C	N	O	S	0	1	0
			1846	1165	327	348	6			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



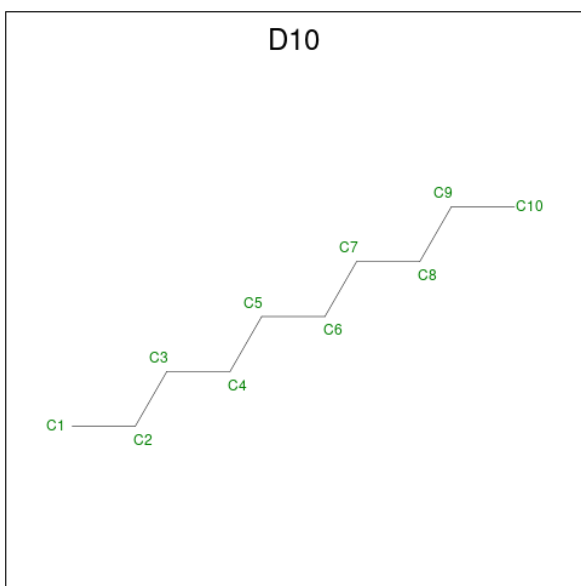
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is (2R)-2,3-dihydroxypropyl hexadecanoate (CCD ID: EKG) (formula: $C_{19}H_{38}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			23	19	4		

- Molecule 7 is DECANE (CCD ID: D10) (formula: $\text{C}_{10}\text{H}_{22}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 10 10	0	0
7	A	1	Total C 10 10	0	0

- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total K 2 2	0	0
8	D	1	Total K 1 1	0	0

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			7	4	3		

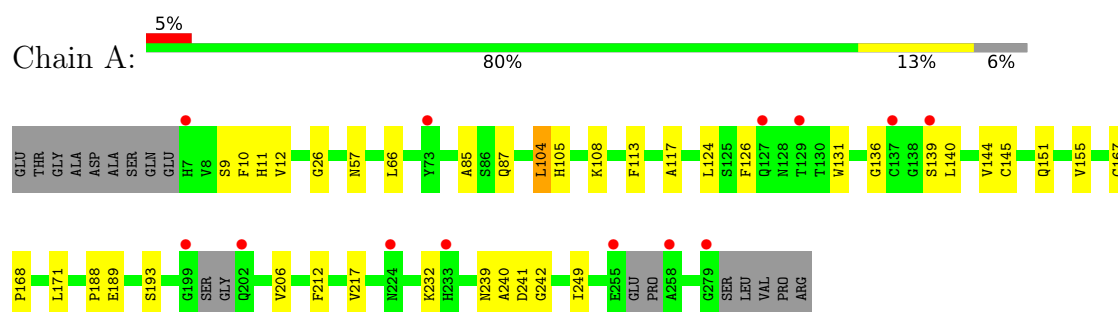
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	3	Total	O	0	0
			3	3		
11	B	1	Total	O	0	0
			1	1		
11	C	6	Total	O	0	0
			6	6		
11	D	3	Total	O	0	0
			3	3		

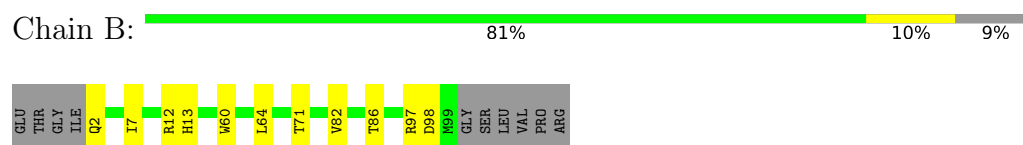
3 Residue-property plots [i](#)

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.

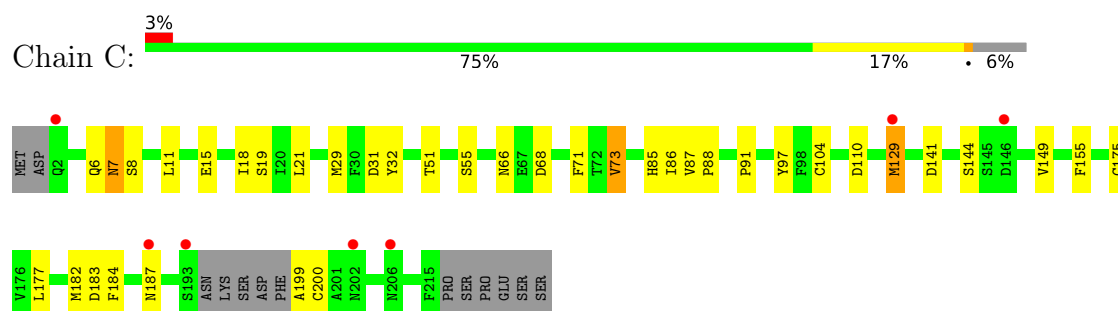
- Molecule 1: T-cell surface glycoprotein CD1c



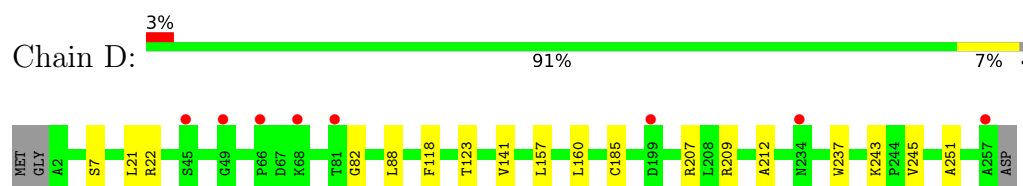
- Molecule 2: Beta-2-microglobulin



- Molecule 3: 3C8 T cell receptor alpha-chain



- Molecule 4: 3C8 T cell receptor beta-chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.17Å 173.17Å 82.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.53 – 2.95 37.53 – 2.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.53-2.95) 99.9 (37.53-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.174 , 0.208 0.186 , 0.230	Depositor DCC
R_{free} test set	1532 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	82.0	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 79.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6245	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: EKG, EDO, K, NAG, PEG, D10

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	0.83	0/2171	1.28	11/2955 (0.4%)
2	B	0.87	0/796	1.25	3/1089 (0.3%)
3	C	0.99	1/1460 (0.1%)	1.34	9/1990 (0.5%)
4	D	0.77	0/1899	1.17	2/2594 (0.1%)
All	All	0.86	1/6326 (0.0%)	1.26	25/8628 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	182	MET	SD-CE	7.94	1.99	1.79

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	SER	N-CA-C	-8.90	102.55	113.41
3	C	183	ASP	CA-CB-CG	7.15	119.75	112.60
2	B	97	ARG	N-CA-C	-6.94	98.63	109.25
1	A	57	ASN	CA-CB-CG	6.86	119.45	112.60
3	C	199	ALA	CA-C-N	6.71	129.60	120.54
3	C	199	ALA	C-N-CA	6.71	129.60	120.54
3	C	31	ASP	CA-CB-CG	6.48	119.08	112.60
3	C	110	ASP	CA-CB-CG	6.47	119.07	112.60
2	B	64	LEU	N-CA-CB	-6.31	101.20	111.24
3	C	7	ASN	N-CA-C	-6.29	102.05	110.55
1	A	242	GLY	N-CA-C	-6.06	106.67	114.85
3	C	88	PRO	CA-C-N	-5.97	113.25	122.09
3	C	88	PRO	C-N-CA	-5.97	113.25	122.09
3	C	68	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	139	SER	CA-C-N	5.68	128.36	120.29
1	A	139	SER	C-N-CA	5.68	128.36	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ALA	CA-C-N	5.67	128.15	120.38
1	A	240	ALA	C-N-CA	5.67	128.15	120.38
2	B	71	THR	CB-CA-C	5.35	117.30	110.34
4	D	212	ALA	CA-C-N	5.24	127.82	120.28
4	D	212	ALA	C-N-CA	5.24	127.82	120.28
1	A	239	ASN	N-CA-C	-5.22	101.61	109.85
1	A	9	SER	N-CA-C	5.16	117.03	109.24
1	A	189	GLU	N-CA-C	-5.03	100.53	108.73
1	A	241	ASP	CB-CA-C	-5.01	102.16	110.68

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	2107	0	1948	17	0
2	B	773	0	683	5	0
3	C	1427	0	1303	20	0
4	D	1846	0	1694	13	0
5	A	14	0	13	0	0
6	A	23	0	0	1	0
7	A	20	0	44	0	0
8	A	2	0	0	0	0
8	D	1	0	0	0	0
9	C	12	0	18	2	0
10	C	7	0	10	1	0
11	A	3	0	0	0	0
11	B	1	0	0	0	0
11	C	6	0	0	0	0
11	D	3	0	0	0	0
All	All	6245	0	5713	47	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 4.

All (47) 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:105:HIS:HB2	1:A:108:LYS:HB2	1.70	0.73
1:A:188:PRO:HB3	1:A:212:PHE:HB3	1.71	0.71
4:D:243:LYS:HG2	4:D:245:VAL:HG13	1.74	0.70
1:A:104:LEU:HD12	1:A:171:LEU:HD23	1.82	0.62
1:A:66:LEU:HG	3:C:29:MET:HE2	1.83	0.60
4:D:21:LEU:HD22	4:D:123:THR:HG21	1.83	0.60
1:A:124:LEU:HD21	1:A:144:VAL:HG13	1.84	0.59
1:A:124:LEU:HD22	1:A:145:CYS:SG	2.41	0.59
1:A:193:SER:HB2	2:B:98:ASP:HB2	1.85	0.58
3:C:15:GLU:HG3	3:C:91:PRO:HD3	1.86	0.58
3:C:51:THR:HA	9:C:301:EDO:H22	1.86	0.58
9:C:301:EDO:H21	4:D:118:PHE:HA	1.86	0.58
4:D:237:TRP:CB	4:D:243:LYS:HD3	2.36	0.56
3:C:175:CYS:HG	4:D:185:CYS:HG	0.84	0.55
1:A:11:HIS:HB3	1:A:113:PHE:HZ	1.72	0.54
4:D:237:TRP:HB3	4:D:243:LYS:HD3	1.90	0.54
3:C:18:ILE:HG13	3:C:87:VAL:HG22	1.91	0.53
1:A:10:PHE:HB2	1:A:171:LEU:HD13	1.91	0.52
2:B:7:ILE:HG12	2:B:82:VAL:HG21	1.91	0.51
2:B:2:GLN:HG2	2:B:86:THR:HG22	1.93	0.51
3:C:155:PHE:CE1	3:C:187:ASN:HB3	2.46	0.50
4:D:141:VAL:HG23	4:D:251:ALA:HB3	1.94	0.49
3:C:141:ASP:HB3	3:C:144:SER:O	2.12	0.49
3:C:71:PHE:CE2	3:C:86:ILE:HG12	2.47	0.48
1:A:26:GLY:HA3	6:A:302:EKG:C24	2.43	0.48
3:C:184:PHE:HD2	4:D:209:ARG:HG2	1.81	0.46
1:A:140:LEU:O	1:A:144:VAL:HG12	2.16	0.45
4:D:21:LEU:HD12	4:D:88:LEU:HD23	1.98	0.45
1:A:126:PHE:HB2	1:A:131:TRP:CZ3	2.52	0.44
1:A:212:PHE:CZ	1:A:217:VAL:HG11	2.52	0.44
3:C:18:ILE:HD11	3:C:85:HIS:ND1	2.32	0.44
3:C:19:SER:HB2	3:C:86:ILE:HB	2.00	0.44
3:C:21:LEU:HD22	3:C:97:TYR:HB2	1.99	0.44
3:C:7:ASN:HB2	10:C:304:PEG:H41	1.99	0.43
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.54	0.43
1:A:85:ALA:C	1:A:87:GLN:H	2.27	0.43
3:C:177:LEU:HA	4:D:185:CYS:CB	2.49	0.43
3:C:177:LEU:HA	4:D:185:CYS:HB3	2.01	0.43
3:C:184:PHE:CD2	4:D:209:ARG:HG2	2.55	0.42
3:C:66:ASN:HB3	3:C:73:VAL:HG23	2.01	0.42
2:B:12:ARG:HG3	2:B:13:HIS:CD2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:VAL:HG22	1:A:249:ILE:HG12	2.02	0.41
4:D:7:SER:HB2	4:D:22:ARG:HB3	2.02	0.41
3:C:129:MET:HE1	3:C:187:ASN:OD1	2.21	0.41
1:A:167:CYS:HB3	1:A:168:PRO:HD3	2.02	0.41
3:C:6:GLN:HG3	3:C:104:CYS:SG	2.61	0.40
3:C:32:TYR:CE2	3:C:55:SER:HB2	2.56	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	265/287 (92%)	252 (95%)	12 (4%)	1 (0%)	30	53
2	B	96/108 (89%)	94 (98%)	2 (2%)	0	100	100
3	C	188/205 (92%)	179 (95%)	8 (4%)	1 (0%)	24	49
4	D	243/247 (98%)	227 (93%)	15 (6%)	1 (0%)	30	53
All	All	792/847 (94%)	752 (95%)	37 (5%)	3 (0%)	30	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	8	SER
1	A	136	GLY
4	D	82	GLY

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	213/247 (86%)	208 (98%)	5 (2%)	44	67
2	B	80/101 (79%)	80 (100%)	0	100	100
3	C	147/187 (79%)	142 (97%)	5 (3%)	32	58
4	D	186/212 (88%)	183 (98%)	3 (2%)	55	75
All	All	626/747 (84%)	613 (98%)	13 (2%)	47	69

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	104	LEU
1	A	151	GLN
1	A	155	VAL
1	A	232	LYS
3	C	11	LEU
3	C	73	VAL
3	C	129	MET
3	C	149	VAL
3	C	200	CYS
4	D	157	LEU
4	D	160	LEU
4	D	207	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	115	GLN
4	D	48	GLN
4	D	94	GLN
4	D	189	GLN
4	D	221	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	EDO	C	302	-	3,3,3	0.75	0	2,2,2	0.14	0
7	D10	A	304	-	9,9,9	0.40	0	8,8,8	0.35	0
7	D10	A	303	-	9,9,9	0.32	0	8,8,8	0.31	0
9	EDO	C	303	-	3,3,3	0.47	0	2,2,2	0.28	0
6	EKG	A	302	-	22,22,22	1.12	1 (4%)	23,23,23	1.14	3 (13%)
5	NAG	A	301	1	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
10	PEG	C	304	-	6,6,6	0.54	0	5,5,5	0.16	0
9	EDO	C	301	-	3,3,3	0.51	0	2,2,2	0.33	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
9	EDO	C	302	-	-	1/1/1/1	-
7	D10	A	304	-	-	6/7/7/7	-
7	D10	A	303	-	-	5/7/7/7	-
9	EDO	C	303	-	-	1/1/1/1	-
6	EKG	A	302	-	-	13/22/22/22	-
5	NAG	A	301	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PEG	C	304	-	-	1/4/4/4	-
9	EDO	C	301	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	302	EKG	O20-C1	4.90	1.47	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	302	EKG	O20-C1-C2	3.43	122.30	111.83
5	A	301	NAG	O5-C1-C2	-2.99	106.67	111.29
5	A	301	NAG	C1-O5-C5	2.93	116.11	112.19
6	A	302	EKG	C21-O20-C1	2.63	126.72	117.12
6	A	302	EKG	O20-C1-O19	-2.36	117.72	123.63

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	302	EKG	O19-C1-O20-C21
6	A	302	EKG	C2-C1-O20-C21
6	A	302	EKG	O20-C21-C22-O23
6	A	302	EKG	O20-C21-C22-C24
6	A	302	EKG	C3-C4-C5-C6
7	A	304	D10	C6-C7-C8-C9
6	A	302	EKG	C6-C7-C8-C9
6	A	302	EKG	C1-C2-C3-C4
6	A	302	EKG	C2-C3-C4-C5
7	A	303	D10	C4-C5-C6-C7
6	A	302	EKG	C5-C6-C7-C8
10	C	304	PEG	O2-C3-C4-O4
6	A	302	EKG	C10-C11-C12-C13
9	C	303	EDO	O1-C1-C2-O2
7	A	304	D10	C5-C6-C7-C8
7	A	303	D10	C6-C7-C8-C9
6	A	302	EKG	C11-C12-C13-C14
6	A	302	EKG	C12-C13-C14-C15
7	A	304	D10	C1-C2-C3-C4
7	A	304	D10	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

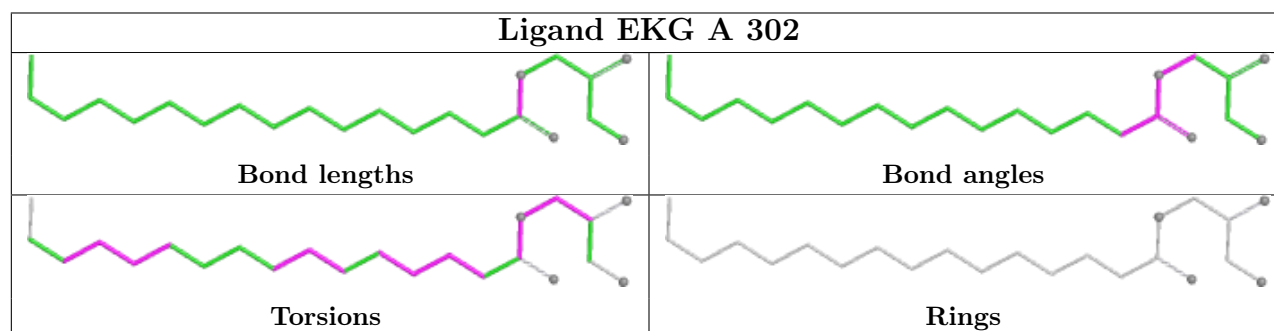
Mol	Chain	Res	Type	Atoms
9	C	302	EDO	O1-C1-C2-O2
7	A	304	D10	C2-C3-C4-C5
7	A	304	D10	C3-C4-C5-C6
7	A	303	D10	C7-C8-C9-C10
7	A	303	D10	C1-C2-C3-C4
6	A	302	EKG	C22-C21-O20-C1
7	A	303	D10	C2-C3-C4-C5

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	302	EKG	1	0
10	C	304	PEG	1	0
9	C	301	EDO	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 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 than 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 ⓘ

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	269/287 (93%)	-0.06	13 (4%) 35 30	35, 88, 143, 168	3 (1%)
2	B	98/108 (90%)	-0.13	0 100 100	67, 95, 135, 151	0
3	C	192/205 (93%)	0.00	7 (3%) 46 38	51, 76, 160, 171	0
4	D	244/247 (98%)	-0.05	8 (3%) 49 42	45, 94, 128, 152	1 (0%)
All	All	803/847 (94%)	-0.05	28 (3%) 47 40	35, 89, 145, 171	4 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	GLU	6.1
4	D	257	ALA	4.0
1	A	73[A]	TYR	3.9
1	A	7	HIS	3.8
1	A	129	THR	3.4
1	A	139	SER	3.2
1	A	137	CYS	2.9
3	C	187	ASN	2.8
1	A	224	ASN	2.7
3	C	206	ASN	2.7
1	A	258	ALA	2.7
1	A	279	GLY	2.6
3	C	2	GLN	2.6
1	A	199	GLY	2.6
1	A	127	GLN	2.5
1	A	202	GLN	2.3
4	D	234	ASN	2.3
3	C	202	ASN	2.2
3	C	193	SER	2.2
1	A	233[A]	HIS	2.2
3	C	146	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	66	PRO	2.2
4	D	45	SER	2.2
4	D	199	ASP	2.1
3	C	129	MET	2.1
4	D	49	GLY	2.1
4	D	81	THR	2.1
4	D	68	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

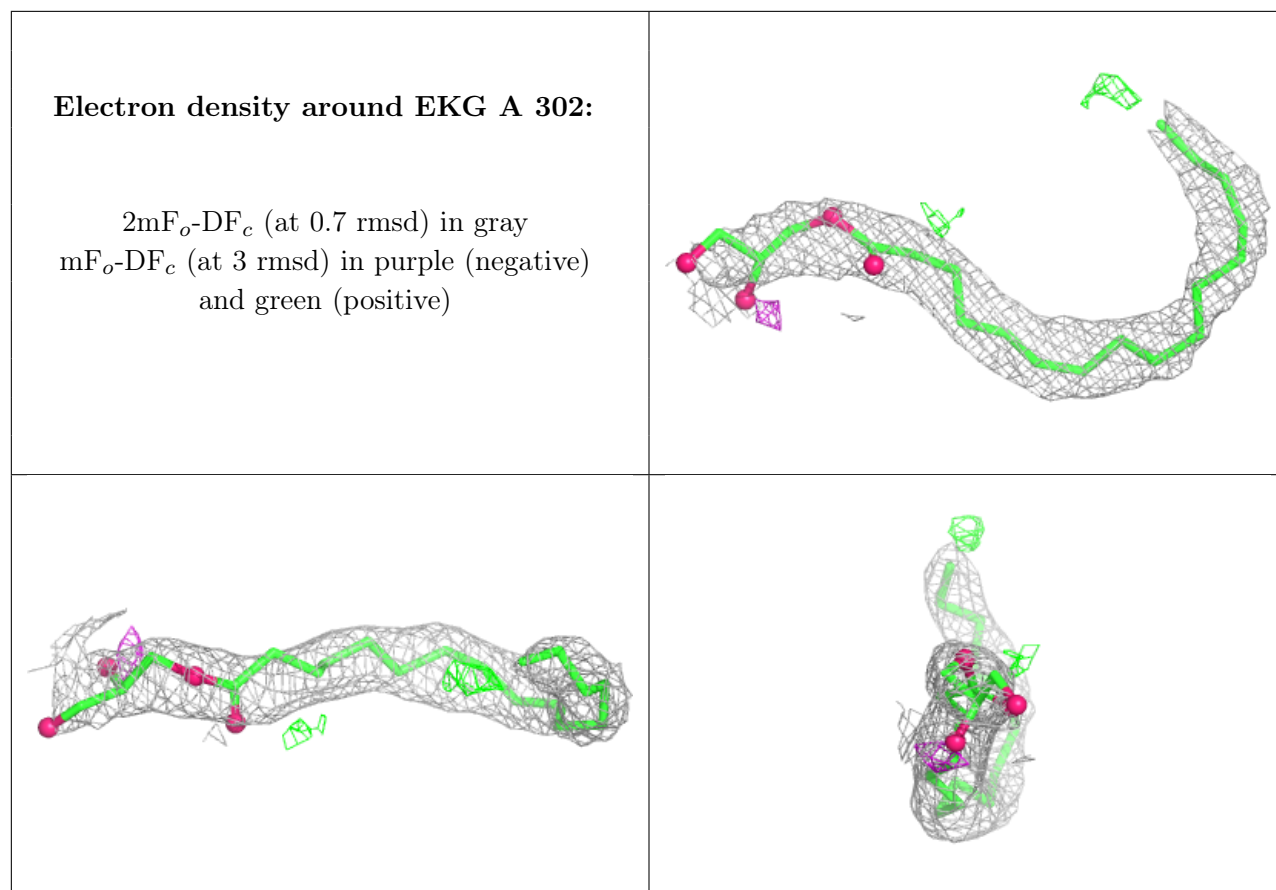
There are no oligosaccharides in this entry.

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
5	NAG	A	301	14/15	0.71	0.11	129,135,140,140	0
9	EDO	C	302	4/4	0.76	0.14	97,97,99,100	0
8	K	D	301	1/1	0.77	0.20	135,135,135,135	0
10	PEG	C	304	7/7	0.84	0.15	105,111,113,114	7
7	D10	A	303	10/10	0.91	0.25	75,79,93,95	0
8	K	A	305	1/1	0.92	0.13	83,83,83,83	0
7	D10	A	304	10/10	0.92	0.18	74,77,80,83	0
6	EKG	A	302	23/23	0.93	0.16	62,76,119,120	0
9	EDO	C	301	4/4	0.93	0.22	72,73,73,74	0
8	K	A	306	1/1	0.94	0.10	87,87,87,87	0
9	EDO	C	303	4/4	0.95	0.12	72,74,80,85	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 ⓘ

There are no such residues in this entry.