



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:43 AM UTC

PDB ID : 6A2S / pdb_00006a2s
Title : Mycobacterium tuberculosis LexA C-domain S160A
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Deposited on : 2018-06-12
Resolution : 2.50 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

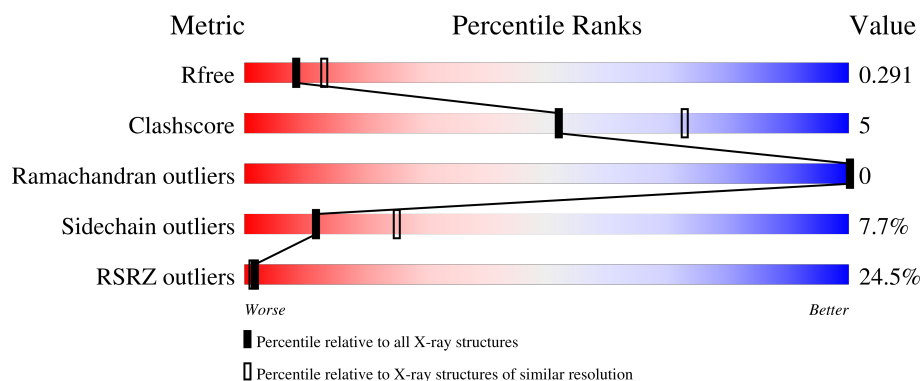
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	111	3% 74% 16% 10%
1	B	111	9% 76% 14% 10%
1	C	111	6% 77% 12% 10%
1	D	111	13% 77% 13% 10%
1	E	111	16% 76% 14% 10%

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Mol	Chain	Length	Quality of chain
1	F	111	41% 76% 14% 10%
1	G	111	56% 77% 11% 10%
1	H	111	32% 77% 10% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6045 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 LexA repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	0	0	0
			739	476	125	133	5			
1	B	100	Total	C	N	O	S	0	0	0
			744	476	127	136	5			
1	C	100	Total	C	N	O	S	0	0	0
			746	479	125	137	5			
1	D	100	Total	C	N	O	S	0	0	0
			743	477	127	134	5			
1	E	100	Total	C	N	O	S	0	0	0
			731	467	127	133	4			
1	F	100	Total	C	N	O	S	0	0	0
			691	442	120	124	5			
1	G	100	Total	C	N	O	S	0	0	0
			677	426	121	126	4			
1	H	100	Total	C	N	O	S	0	0	0
			707	456	117	130	4			

There are 8 discrepancies between the modelled and reference sequences:

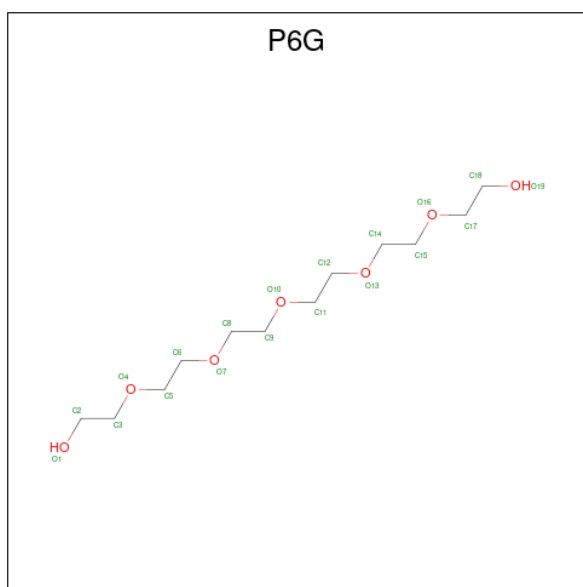
Chain	Residue	Modelled	Actual	Comment	Reference
A	160	ALA	SER	engineered mutation	UNP P9WHR7
B	160	ALA	SER	engineered mutation	UNP P9WHR7
C	160	ALA	SER	engineered mutation	UNP P9WHR7
D	160	ALA	SER	engineered mutation	UNP P9WHR7
E	160	ALA	SER	engineered mutation	UNP P9WHR7
F	160	ALA	SER	engineered mutation	UNP P9WHR7
G	160	ALA	SER	engineered mutation	UNP P9WHR7
H	160	ALA	SER	engineered mutation	UNP P9WHR7

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			19	12	7		
3	C	1	Total	C	O	0	0
			19	12	7		

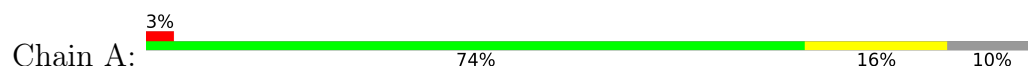
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total	O	0	0
			38	38		
4	B	26	Total	O	0	0
			26	26		
4	C	37	Total	O	0	0
			37	37		
4	D	28	Total	O	0	0
			28	28		
4	E	17	Total	O	0	0
			17	17		
4	F	8	Total	O	0	0
			8	8		
4	G	6	Total	O	0	0
			6	6		
4	H	13	Total	O	0	0
			13	13		

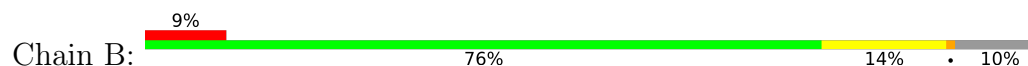
3 Residue-property plots [i](#)

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.

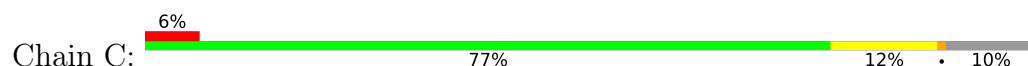
- Molecule 1: LexA repressor



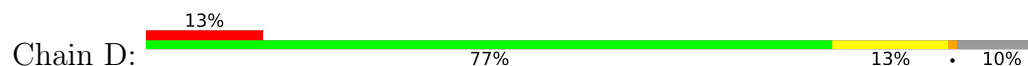
- Molecule 1: LexA repressor



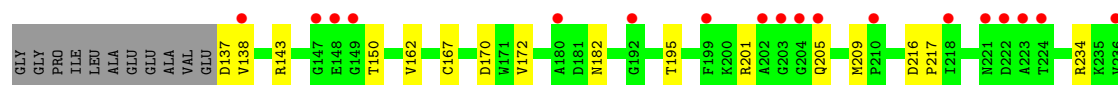
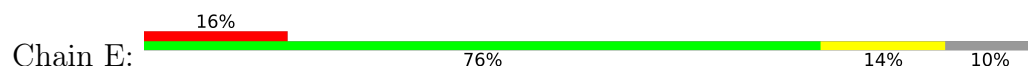
- Molecule 1: LexA repressor



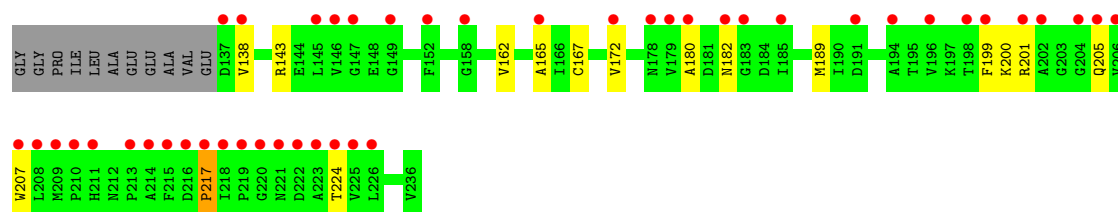
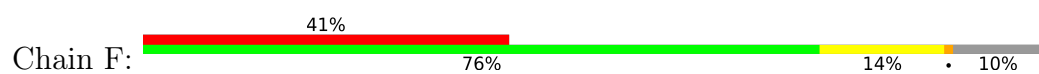
- Molecule 1: LexA repressor



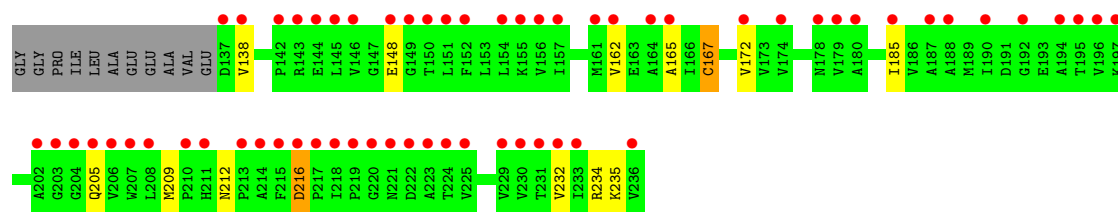
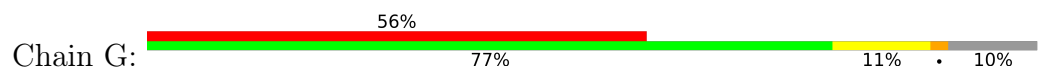
- Molecule 1: LexA repressor



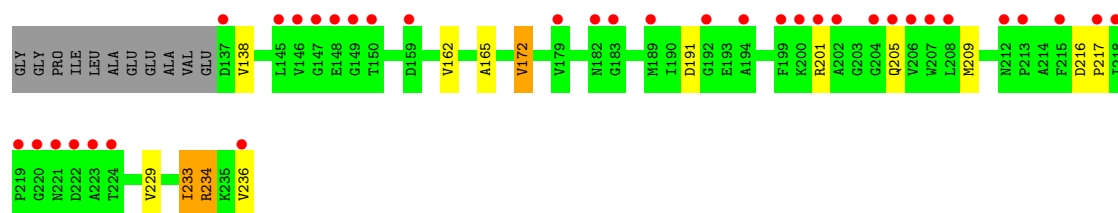
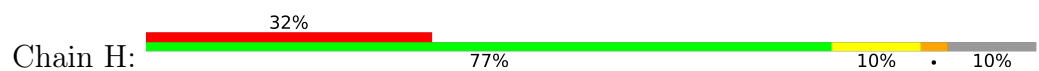
- Molecule 1: LexA repressor



- Molecule 1: LexA repressor



- Molecule 1: LexA repressor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.61Å 104.20Å 88.10Å 90.00° 104.08° 90.00°	Depositor
Resolution (Å)	66.16 – 2.50 66.16 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (66.16-2.50) 100.0 (66.16-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.241 , 0.290 0.243 , 0.291	Depositor DCC
R_{free} test set	1709 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6045	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: CME, PEG, P6G

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	0.77	1/742 (0.1%)	0.97	2/1012 (0.2%)
1	B	0.70	0/747	0.97	2/1017 (0.2%)
1	C	0.77	0/749	1.00	2/1021 (0.2%)
1	D	0.66	0/745	0.96	2/1014 (0.2%)
1	E	0.65	0/733	0.91	0/997
1	F	0.62	0/692	0.94	0/945
1	G	0.65	1/675 (0.1%)	0.98	2/914 (0.2%)
1	H	0.66	2/710 (0.3%)	0.89	0/971
All	All	0.69	4/5793 (0.1%)	0.95	10/7891 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	233	ILE	C-N	-6.39	1.25	1.33
1	A	234	ARG	C-N	-6.07	1.25	1.33
1	H	234	ARG	C-N	-5.63	1.25	1.33
1	G	234	ARG	C-N	-5.58	1.25	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	212	ASN	CA-C-N	5.77	126.16	119.47
1	G	212	ASN	C-N-CA	5.77	126.16	119.47
1	C	212	ASN	CA-C-N	5.53	125.36	119.28
1	C	212	ASN	C-N-CA	5.53	125.36	119.28
1	D	212	ASN	CA-C-N	5.47	126.68	119.84
1	D	212	ASN	C-N-CA	5.47	126.68	119.84
1	A	212	ASN	CA-C-N	5.38	125.20	119.28
1	A	212	ASN	C-N-CA	5.38	125.20	119.28
1	B	137	ASP	CA-C-N	5.06	130.14	122.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	ASP	C-N-CA	5.06	130.14	122.91

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	739	0	747	8	0
1	B	744	0	745	5	0
1	C	746	0	753	9	0
1	D	743	0	750	10	0
1	E	731	0	723	9	0
1	F	691	0	656	12	0
1	G	677	0	617	12	0
1	H	707	0	673	12	0
2	A	14	0	20	0	0
2	B	14	0	20	1	0
2	C	7	0	10	0	0
2	D	7	0	10	0	0
2	E	7	0	10	0	0
2	F	7	0	10	0	0
3	A	19	0	26	3	0
3	C	19	0	26	0	0
4	A	38	0	0	1	0
4	B	26	0	0	0	0
4	C	37	0	0	1	0
4	D	28	0	0	0	0
4	E	17	0	0	1	0
4	F	8	0	0	0	0
4	G	6	0	0	0	0
4	H	13	0	0	0	0
All	All	6045	0	5796	60	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 5.

All (60) 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:G:185:ILE:HB	1:H:236:VAL:HG11	1.51	0.92
1:H:201:ARG:HA	1:H:205:GLN:O	1.88	0.72
1:G:165:ALA:O	1:H:234:ARG:NH1	2.22	0.72
1:E:170:ASP:OD1	1:E:234:ARG:HD3	1.91	0.69
1:D:146:VAL:HG11	1:D:151:LEU:HG	1.74	0.69
1:C:189:MET:HB3	1:C:224:THR:OG1	1.97	0.64
1:A:189:MET:HB3	1:A:224:THR:OG1	1.98	0.64
1:A:204:GLY:HA3	4:A:404:HOH:O	2.03	0.58
1:D:146:VAL:HG11	1:D:151:LEU:CD1	2.35	0.57
1:E:182:ASN:OD1	1:E:201:ARG:N	2.35	0.57
1:H:201:ARG:CA	1:H:205:GLN:O	2.52	0.56
1:D:146:VAL:HG11	1:D:151:LEU:CG	2.36	0.56
1:F:182:ASN:ND2	1:F:200:LYS:O	2.38	0.55
1:F:189:MET:HB3	1:F:224:THR:OG1	2.07	0.54
1:A:160:ALA:HB2	1:A:215:PHE:CE2	2.44	0.53
1:G:167:CME:CE	1:H:165:ALA:HB2	2.39	0.53
1:B:217:PRO:HG3	1:C:209:MET:HE2	1.90	0.52
1:B:176:GLN:NE2	2:B:302:PEG:O1	2.43	0.52
1:C:182:ASN:OD1	1:C:200:LYS:HA	2.10	0.51
1:C:200:LYS:HG3	1:C:209:MET:HG3	1.93	0.51
1:C:204:GLY:HA3	4:C:410:HOH:O	2.09	0.51
1:G:232:VAL:O	1:H:233:ILE:HA	2.12	0.50
1:E:234:ARG:HH22	1:F:165:ALA:C	2.20	0.50
3:A:303:P6G:C18	1:C:167:CME:HE3	2.42	0.49
1:B:212:ASN:OD1	1:B:213:PRO:HD2	2.12	0.49
1:F:201:ARG:HA	1:F:205:GLN:O	2.13	0.49
1:F:217:PRO:HB2	1:G:209:MET:CE	2.43	0.48
1:B:189:MET:HB3	1:B:224:THR:OG1	2.13	0.48
1:C:189:MET:HE2	1:C:226:LEU:HD11	1.95	0.48
1:D:146:VAL:CG1	1:D:151:LEU:CD1	2.91	0.48
1:E:209:MET:HE3	1:H:217:PRO:HG2	1.95	0.48
1:F:180:ALA:HB3	1:F:199:PHE:CD1	2.49	0.48
1:D:178:ASN:OD1	1:D:178:ASN:N	2.46	0.48
1:G:232:VAL:HB	1:H:234:ARG:HB3	1.95	0.48
1:A:200:LYS:HG3	1:A:209:MET:HG3	1.95	0.47
1:F:217:PRO:HB2	1:G:209:MET:HE1	1.97	0.47
1:D:189:MET:HB3	1:D:224:THR:OG1	2.15	0.46
1:F:180:ALA:HB3	1:F:199:PHE:CE1	2.51	0.46
1:B:206:VAL:O	1:B:220:GLY:N	2.44	0.46
1:D:146:VAL:HG12	1:D:148:GLU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:PRO:HG3	1:H:209:MET:HE2	1.98	0.45
1:G:185:ILE:HB	1:H:236:VAL:CG1	2.35	0.45
1:F:200:LYS:CB	1:F:207:TRP:H	2.30	0.44
1:G:216:ASP:OD1	1:G:216:ASP:N	2.51	0.44
1:E:143:ARG:HD3	1:E:150:THR:OG1	2.18	0.43
1:F:217:PRO:CG	1:G:209:MET:HE3	2.48	0.43
1:A:209:MET:HE2	1:D:217:PRO:HG3	2.00	0.43
1:A:221:ASN:OD1	1:A:221:ASN:C	2.62	0.43
1:A:202:ALA:O	1:A:204:GLY:N	2.52	0.42
1:A:139:PHE:HB2	1:A:153:LEU:HB2	2.02	0.42
3:A:303:P6G:H182	1:C:167:CME:HE3	2.01	0.42
1:F:217:PRO:HG2	1:G:209:MET:HE3	2.01	0.42
1:G:185:ILE:CB	1:H:236:VAL:HG11	2.37	0.42
1:C:202:ALA:O	1:C:204:GLY:N	2.52	0.42
1:D:209:MET:SD	1:D:217:PRO:HB3	2.60	0.41
1:H:172:VAL:HG21	1:H:229:VAL:HG22	2.02	0.41
1:E:195:THR:HG22	4:E:417:HOH:O	2.21	0.41
1:E:170:ASP:OD1	1:E:234:ARG:CD	2.63	0.40
1:E:234:ARG:NH2	1:F:165:ALA:C	2.79	0.40
3:A:303:P6G:H141	1:D:167:CME:HE3	2.03	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	97/111 (87%)	92 (95%)	5 (5%)	0	100	100
1	B	97/111 (87%)	92 (95%)	5 (5%)	0	100	100
1	C	97/111 (87%)	92 (95%)	5 (5%)	0	100	100
1	D	97/111 (87%)	93 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	97/111 (87%)	89 (92%)	8 (8%)	0	100	100
1	F	97/111 (87%)	90 (93%)	7 (7%)	0	100	100
1	G	97/111 (87%)	90 (93%)	7 (7%)	0	100	100
1	H	97/111 (87%)	92 (95%)	5 (5%)	0	100	100
All	All	776/888 (87%)	730 (94%)	46 (6%)	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	75/86 (87%)	71 (95%)	4 (5%)	20	42
1	B	75/86 (87%)	68 (91%)	7 (9%)	8	18
1	C	77/86 (90%)	73 (95%)	4 (5%)	21	42
1	D	75/86 (87%)	70 (93%)	5 (7%)	15	31
1	E	72/86 (84%)	66 (92%)	6 (8%)	10	22
1	F	62/86 (72%)	57 (92%)	5 (8%)	11	23
1	G	59/86 (69%)	52 (88%)	7 (12%)	5	11
1	H	65/86 (76%)	60 (92%)	5 (8%)	12	25
All	All	560/688 (81%)	517 (92%)	43 (8%)	12	25

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	VAL
1	A	162	VAL
1	A	172	VAL
1	A	216	ASP
1	B	137	ASP
1	B	138	VAL

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Mol	Chain	Res	Type
1	B	162	VAL
1	B	172	VAL
1	B	201	ARG
1	B	205	GLN
1	B	235	LYS
1	C	138	VAL
1	C	162	VAL
1	C	172	VAL
1	C	205	GLN
1	D	138	VAL
1	D	162	VAL
1	D	172	VAL
1	D	179	VAL
1	D	216	ASP
1	E	137	ASP
1	E	138	VAL
1	E	162	VAL
1	E	172	VAL
1	E	205	GLN
1	E	216	ASP
1	F	138	VAL
1	F	143	ARG
1	F	162	VAL
1	F	172	VAL
1	F	217	PRO
1	G	138	VAL
1	G	148	GLU
1	G	162	VAL
1	G	172	VAL
1	G	205	GLN
1	G	216	ASP
1	G	235	LYS
1	H	138	VAL
1	H	162	VAL
1	H	172	VAL
1	H	191	ASP
1	H	216	ASP

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	176	GLN

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Mol	Chain	Res	Type
1	A	205	GLN
1	B	176	GLN
1	D	176	GLN
1	E	176	GLN
1	E	178	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	CME	C	167	1	8,9,10	0.68	0	6,9,11	1.91	2 (33%)
1	CME	A	167	1	8,9,10	0.76	0	6,9,11	1.85	2 (33%)
1	CME	F	167	1	8,9,10	0.80	0	6,9,11	1.53	2 (33%)
1	CME	E	167	1	8,9,10	0.89	0	6,9,11	1.41	1 (16%)
1	CME	B	167	1	8,9,10	1.02	1 (12%)	6,9,11	1.72	2 (33%)
1	CME	D	167	1	8,9,10	0.93	0	6,9,11	1.78	2 (33%)
1	CME	G	167	1	8,9,10	0.80	0	6,9,11	1.60	2 (33%)
1	CME	H	167	1	8,9,10	0.89	0	6,9,11	1.18	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	CME	C	167	1	-	3/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	A	167	1	-	3/5/8/10	-
1	CME	F	167	1	-	3/5/8/10	-
1	CME	E	167	1	-	2/5/8/10	-
1	CME	B	167	1	-	3/5/8/10	-
1	CME	D	167	1	-	3/5/8/10	-
1	CME	G	167	1	-	3/5/8/10	-
1	CME	H	167	1	-	3/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	167	CME	CB-SG	-2.19	1.74	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	167	CME	CB-SG-SD	-3.65	94.41	103.86
1	A	167	CME	CB-SG-SD	-3.61	94.51	103.86
1	D	167	CME	CB-SG-SD	-2.98	96.14	103.86
1	D	167	CME	CB-CA-C	-2.57	103.81	110.80
1	B	167	CME	CB-SG-SD	-2.57	97.20	103.86
1	G	167	CME	CB-SG-SD	-2.57	97.22	103.86
1	G	167	CME	CB-CA-C	-2.52	103.96	110.80
1	F	167	CME	CB-SG-SD	-2.48	97.44	103.86
1	E	167	CME	CB-CA-C	-2.44	104.17	110.80
1	F	167	CME	CB-CA-C	-2.36	104.40	110.80
1	C	167	CME	CB-CA-C	-2.36	104.40	110.80
1	B	167	CME	CB-CA-C	-2.34	104.46	110.80
1	A	167	CME	CB-CA-C	-2.01	105.35	110.80

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	167	CME	N-CA-CB-SG
1	A	167	CME	SD-CE-CZ-OH
1	B	167	CME	N-CA-CB-SG
1	B	167	CME	SD-CE-CZ-OH
1	C	167	CME	N-CA-CB-SG
1	C	167	CME	SD-CE-CZ-OH

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Mol	Chain	Res	Type	Atoms
1	D	167	CME	N-CA-CB-SG
1	D	167	CME	SD-CE-CZ-OH
1	E	167	CME	N-CA-CB-SG
1	E	167	CME	SD-CE-CZ-OH
1	F	167	CME	N-CA-CB-SG
1	F	167	CME	SD-CE-CZ-OH
1	G	167	CME	N-CA-CB-SG
1	G	167	CME	SD-CE-CZ-OH
1	H	167	CME	N-CA-CB-SG
1	H	167	CME	SD-CE-CZ-OH
1	A	167	CME	CZ-CE-SD-SG
1	B	167	CME	CZ-CE-SD-SG
1	C	167	CME	CZ-CE-SD-SG
1	D	167	CME	CZ-CE-SD-SG
1	F	167	CME	CZ-CE-SD-SG
1	G	167	CME	CZ-CE-SD-SG
1	H	167	CME	CZ-CE-SD-SG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	167	CME	2	0
1	D	167	CME	1	0
1	G	167	CME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands 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
2	PEG	C	301	-	6,6,6	0.49	0	5,5,5	0.39	0
2	PEG	B	302	-	6,6,6	0.43	0	5,5,5	0.31	0
2	PEG	D	301	-	6,6,6	0.59	0	5,5,5	0.34	0
2	PEG	E	301	-	6,6,6	0.53	0	5,5,5	0.24	0
2	PEG	A	301	-	6,6,6	0.51	0	5,5,5	0.20	0
2	PEG	F	301	-	6,6,6	0.50	0	5,5,5	0.21	0
3	P6G	C	302	-	18,18,18	0.58	0	17,17,17	0.39	0
3	P6G	A	303	-	18,18,18	0.57	0	17,17,17	0.46	0
2	PEG	B	301	-	6,6,6	0.51	0	5,5,5	0.30	0
2	PEG	A	302	-	6,6,6	0.80	0	5,5,5	0.68	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
2	PEG	C	301	-	-	2/4/4/4	-
2	PEG	B	302	-	-	0/4/4/4	-
2	PEG	D	301	-	-	3/4/4/4	-
2	PEG	E	301	-	-	3/4/4/4	-
2	PEG	A	301	-	-	1/4/4/4	-
2	PEG	F	301	-	-	2/4/4/4	-
3	P6G	C	302	-	-	11/16/16/16	-
3	P6G	A	303	-	-	11/16/16/16	-
2	PEG	B	301	-	-	3/4/4/4	-
2	PEG	A	302	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	P6G	O13-C14-C15-O16
2	B	301	PEG	O1-C1-C2-O2
2	C	301	PEG	O1-C1-C2-O2
2	D	301	PEG	O2-C3-C4-O4
2	A	302	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
2	D	301	PEG	O1-C1-C2-O2
2	E	301	PEG	O1-C1-C2-O2
3	A	303	P6G	O1-C2-C3-O4
3	C	302	P6G	O1-C2-C3-O4
3	A	303	P6G	C8-C9-O10-C11
2	C	301	PEG	O2-C3-C4-O4
3	A	303	P6G	O7-C8-C9-O10
3	C	302	P6G	C14-C15-O16-C17
3	A	303	P6G	O4-C5-C6-O7
3	C	302	P6G	O4-C5-C6-O7
3	C	302	P6G	C18-C17-O16-C15
3	A	303	P6G	O16-C17-C18-O19
3	C	302	P6G	O10-C11-C12-O13
3	C	302	P6G	C15-C14-O13-C12
3	A	303	P6G	C2-C3-O4-C5
3	A	303	P6G	C15-C14-O13-C12
3	A	303	P6G	C12-C11-O10-C9
2	D	301	PEG	C1-C2-O2-C3
3	C	302	P6G	O16-C17-C18-O19
2	A	301	PEG	O1-C1-C2-O2
3	A	303	P6G	C18-C17-O16-C15
2	E	301	PEG	C4-C3-O2-C2
2	F	301	PEG	C1-C2-O2-C3
3	A	303	P6G	O10-C11-C12-O13
3	C	302	P6G	C6-C5-O4-C3
2	B	301	PEG	C1-C2-O2-C3
2	E	301	PEG	C1-C2-O2-C3
3	C	302	P6G	O13-C14-C15-O16
2	F	301	PEG	O1-C1-C2-O2
3	C	302	P6G	C5-C6-O7-C8
3	C	302	P6G	C2-C3-O4-C5
2	B	301	PEG	C4-C3-O2-C2

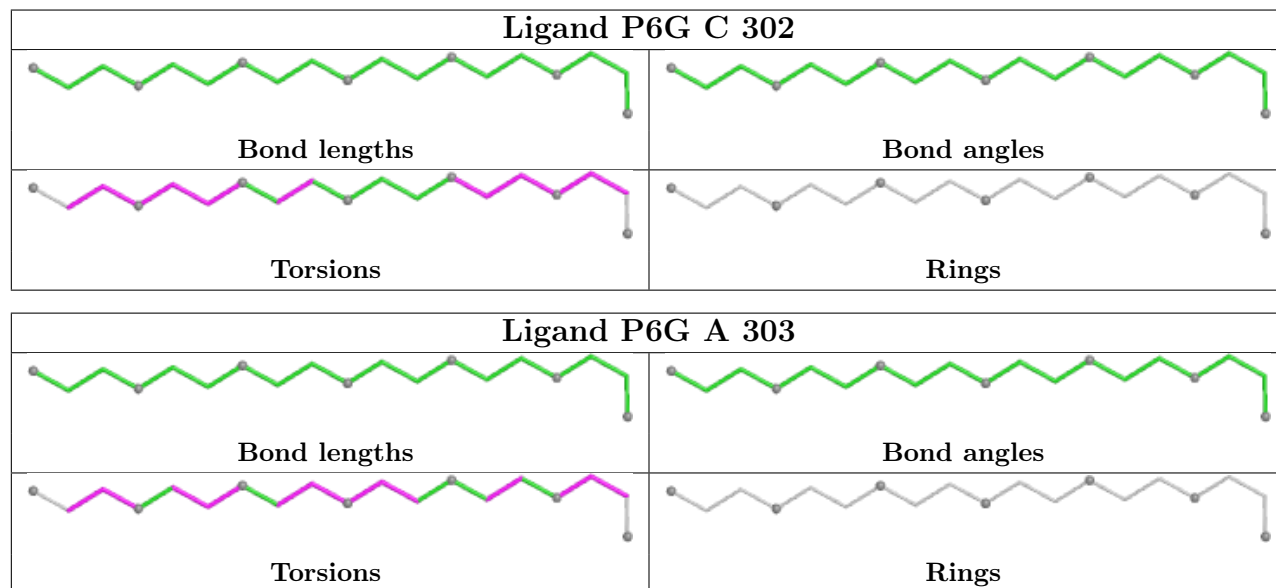
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	302	PEG	1	0
3	A	303	P6G	3	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 [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	99/111 (89%)	0.45	3 (3%) 52 48	28, 40, 73, 114	0
1	B	99/111 (89%)	0.75	10 (10%) 12 10	27, 48, 92, 119	0
1	C	99/111 (89%)	0.28	7 (7%) 22 19	26, 39, 78, 110	0
1	D	99/111 (89%)	0.78	14 (14%) 6 5	28, 48, 91, 126	0
1	E	99/111 (89%)	1.26	18 (18%) 3 2	42, 65, 109, 116	0
1	F	99/111 (89%)	1.87	45 (45%) 0 0	42, 79, 113, 140	0
1	G	99/111 (89%)	2.50	62 (62%) 0 0	46, 79, 110, 132	0
1	H	99/111 (89%)	1.68	35 (35%) 1 1	44, 72, 119, 134	0
All	All	792/888 (89%)	1.19	194 (24%) 2 1	26, 60, 109, 140	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	145	LEU	5.5
1	G	215	PHE	5.5
1	G	178	ASN	5.2
1	G	223	ALA	5.1
1	G	208	LEU	5.0
1	E	203	GLY	4.9
1	G	219	PRO	4.8
1	G	217	PRO	4.7
1	E	202	ALA	4.6
1	F	204	GLY	4.5
1	H	207	TRP	4.5
1	H	222	ASP	4.5
1	D	146	VAL	4.4
1	G	196	VAL	4.4
1	D	137	ASP	4.4
1	E	147	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	218	ILE	4.2
1	E	204	GLY	4.2
1	G	220	GLY	4.2
1	H	202	ALA	4.2
1	H	183	GLY	4.1
1	F	202	ALA	4.1
1	G	210	PRO	4.1
1	H	179	VAL	4.0
1	G	204	GLY	3.9
1	H	223	ALA	3.9
1	G	157	ILE	3.9
1	G	202	ALA	3.8
1	B	203	GLY	3.8
1	G	221	ASN	3.8
1	F	205	GLN	3.8
1	G	203	GLY	3.7
1	A	148	GLU	3.7
1	G	137	ASP	3.6
1	G	164	ALA	3.6
1	F	208	LEU	3.5
1	H	206	VAL	3.5
1	G	207	TRP	3.5
1	H	148	GLU	3.4
1	G	156	VAL	3.4
1	H	208	LEU	3.4
1	E	223	ALA	3.4
1	H	199	PHE	3.4
1	G	179	VAL	3.4
1	G	149	GLY	3.4
1	F	222	ASP	3.3
1	G	213	PRO	3.3
1	D	149	GLY	3.3
1	F	180	ALA	3.3
1	D	147	GLY	3.2
1	H	182	ASN	3.2
1	B	148	GLU	3.2
1	F	178	ASN	3.2
1	G	155	LYS	3.2
1	H	147	GLY	3.2
1	H	236	VAL	3.2
1	F	206	VAL	3.2
1	C	224	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	148	GLU	3.1
1	E	148	GLU	3.1
1	G	188	ALA	3.1
1	H	221	ASN	3.1
1	H	192	GLY	3.1
1	F	146	VAL	3.1
1	D	194	ALA	3.0
1	G	154	LEU	3.0
1	F	214	ALA	3.0
1	F	209	MET	3.0
1	F	213	PRO	3.0
1	E	221	ASN	3.0
1	B	149	GLY	3.0
1	F	147	GLY	3.0
1	H	220	GLY	3.0
1	F	179	VAL	3.0
1	B	147	GLY	3.0
1	B	146	VAL	3.0
1	G	206	VAL	3.0
1	E	224	THR	3.0
1	F	165	ALA	3.0
1	F	185	ILE	2.9
1	G	229	VAL	2.9
1	G	152	PHE	2.9
1	F	182	ASN	2.9
1	G	205	GLN	2.9
1	G	146	VAL	2.9
1	G	236	VAL	2.9
1	H	146	VAL	2.9
1	F	158	GLY	2.9
1	C	148	GLU	2.9
1	F	152	PHE	2.9
1	F	221	ASN	2.9
1	G	172	VAL	2.9
1	G	225	VAL	2.9
1	E	210	PRO	2.9
1	F	219	PRO	2.8
1	F	223	ALA	2.8
1	E	192	GLY	2.8
1	F	226	LEU	2.8
1	G	174	VAL	2.8
1	G	230	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	180	ALA	2.8
1	A	147	GLY	2.8
1	G	150	THR	2.8
1	F	216	ASP	2.8
1	F	149	GLY	2.7
1	F	220	GLY	2.7
1	G	233	ILE	2.7
1	F	210	PRO	2.7
1	B	179	VAL	2.7
1	F	225	VAL	2.7
1	C	145	LEU	2.7
1	F	198	THR	2.7
1	H	224	THR	2.7
1	F	183	GLY	2.7
1	H	212	ASN	2.7
1	F	137	ASP	2.6
1	G	138	VAL	2.6
1	H	205	GLN	2.6
1	F	207	TRP	2.6
1	H	200	LYS	2.6
1	E	149	GLY	2.6
1	H	213	PRO	2.6
1	G	144	GLU	2.6
1	G	148	GLU	2.6
1	D	138	VAL	2.6
1	E	138	VAL	2.6
1	F	224	THR	2.6
1	G	224	THR	2.6
1	F	196	VAL	2.6
1	G	211	HIS	2.6
1	G	161	MET	2.5
1	H	219	PRO	2.5
1	D	144	GLU	2.5
1	E	199	PHE	2.5
1	B	202	ALA	2.5
1	G	231	THR	2.5
1	G	143	ARG	2.5
1	E	222	ASP	2.5
1	F	211	HIS	2.5
1	H	189	MET	2.5
1	B	145	LEU	2.5
1	D	145	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	194	ALA	2.5
1	G	187	ALA	2.5
1	G	142	PRO	2.5
1	G	218	ILE	2.5
1	G	232	VAL	2.5
1	D	213	PRO	2.4
1	F	215	PHE	2.4
1	C	146	VAL	2.4
1	F	199	PHE	2.4
1	G	214	ALA	2.4
1	G	195	THR	2.4
1	F	217	PRO	2.4
1	C	147	GLY	2.4
1	E	218	ILE	2.4
1	D	205	GLN	2.4
1	F	191	ASP	2.4
1	D	202	ALA	2.4
1	G	190	ILE	2.3
1	B	137	ASP	2.3
1	H	159	ASP	2.3
1	H	150	THR	2.3
1	B	192	GLY	2.3
1	G	185	ILE	2.3
1	F	172	VAL	2.3
1	H	194	ALA	2.3
1	C	203	GLY	2.3
1	H	204	GLY	2.3
1	A	137	ASP	2.3
1	H	218	ILE	2.2
1	G	162	VAL	2.2
1	G	194	ALA	2.2
1	D	204	GLY	2.2
1	H	149	GLY	2.2
1	G	180	ALA	2.2
1	C	137	ASP	2.2
1	G	216	ASP	2.2
1	G	222	ASP	2.2
1	F	201	ARG	2.2
1	H	201	ARG	2.2
1	H	217	PRO	2.2
1	E	236	VAL	2.2
1	F	145	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	215	PHE	2.2
1	G	165	ALA	2.1
1	G	151	LEU	2.1
1	H	145	LEU	2.1
1	H	137	ASP	2.1
1	G	197	LYS	2.1
1	D	203	GLY	2.1
1	G	192	GLY	2.0
1	E	205	GLN	2.0
1	F	138	VAL	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	CME	G	167	10/11	0.83	0.17	66,73,89,105	0
1	CME	H	167	10/11	0.84	0.16	61,66,108,109	0
1	CME	F	167	10/11	0.85	0.17	52,64,105,109	0
1	CME	E	167	10/11	0.88	0.14	52,57,84,92	0
1	CME	B	167	10/11	0.90	0.15	34,39,74,84	0
1	CME	C	167	10/11	0.90	0.15	35,46,77,83	0
1	CME	A	167	10/11	0.94	0.12	30,37,69,80	0
1	CME	D	167	10/11	0.94	0.12	33,37,70,76	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

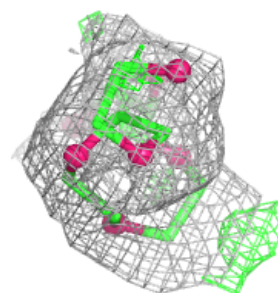
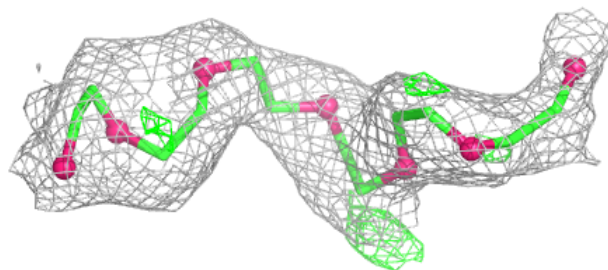
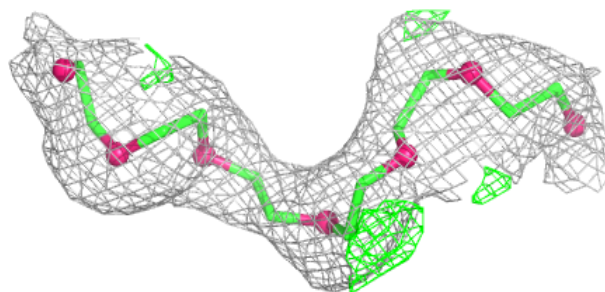
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PEG	F	301	7/7	0.62	0.18	95,97,102,105	0
2	PEG	B	302	7/7	0.71	0.15	76,84,90,92	0
2	PEG	D	301	7/7	0.78	0.17	74,84,90,91	0
3	P6G	C	302	19/19	0.79	0.19	79,88,95,98	0
2	PEG	C	301	7/7	0.80	0.19	65,69,74,74	0
2	PEG	A	302	7/7	0.83	0.17	36,47,59,59	0
2	PEG	E	301	7/7	0.83	0.16	72,78,85,86	0
3	P6G	A	303	19/19	0.86	0.20	68,91,101,106	0
2	PEG	B	301	7/7	0.86	0.21	81,86,91,91	0
2	PEG	A	301	7/7	0.90	0.13	59,63,72,73	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.

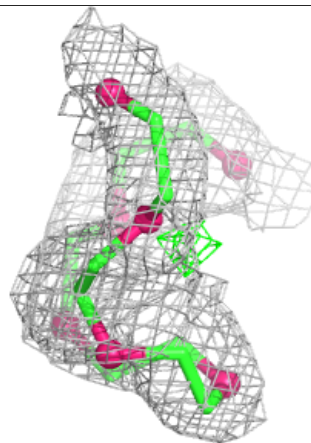
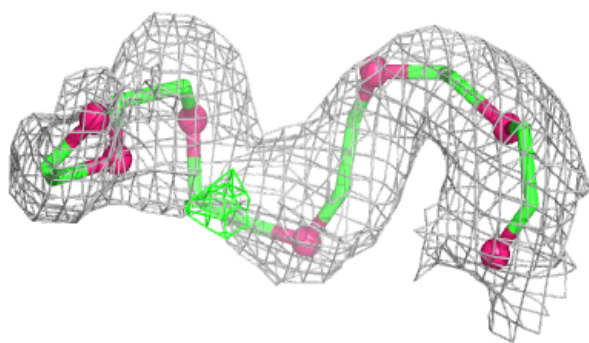
Electron density around P6G C 302:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around P6G A 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.