Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2023 – 02:45 PM EDT

PDB ID	:	8DEI
Title	:	Structure of the Cac1 KER domain
Authors	:	Rosas, R.; Churchill, M.E.A.
Deposited on	:	2022-06-20
Resolution	:	2.81 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:

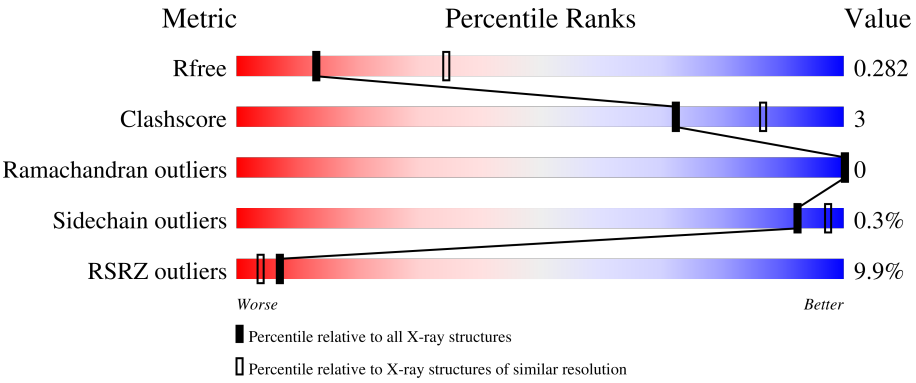
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.81 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}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	490	9% 85% 12% ·
1	B	490	8% 89% 8% ·
1	C	490	8% 86% 8% 7%
1	D	490	13% 86% 9% 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14757 atoms, of which 44 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 Maltodextrin-binding protein,Chromatin assembly factor 1 subunit p90 fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3741	2383	640	712	6			
1	B	476	Total	C	N	O	S	0	0	0
			3774	2403	641	724	6			
1	C	457	Total	C	N	O	S	0	0	0
			3569	2280	604	679	6			
1	D	462	Total	C	N	O	S	0	0	0
			3575	2283	602	684	6			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP C3SHQ8
A	-8	ARG	-	expression tag	UNP C3SHQ8
A	-7	SER	-	expression tag	UNP C3SHQ8
A	-6	HIS	-	expression tag	UNP C3SHQ8
A	-5	HIS	-	expression tag	UNP C3SHQ8
A	-4	HIS	-	expression tag	UNP C3SHQ8
A	-3	HIS	-	expression tag	UNP C3SHQ8
A	-2	HIS	-	expression tag	UNP C3SHQ8
A	-1	HIS	-	expression tag	UNP C3SHQ8
A	0	GLY	-	expression tag	UNP C3SHQ8
A	367	ASN	-	linker	UNP C3SHQ8
A	368	SER	-	linker	UNP C3SHQ8
A	369	GLY	-	linker	UNP C3SHQ8
A	370	SER	-	linker	UNP C3SHQ8
A	371	ASP	-	linker	UNP C3SHQ8
A	372	ILE	-	linker	UNP C3SHQ8
A	373	THR	-	linker	UNP C3SHQ8
A	374	SER	-	linker	UNP C3SHQ8
A	375	LEU	-	linker	UNP C3SHQ8
A	376	TYR	-	linker	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	377	LYS	-	linker	UNP C3SHQ8
A	378	LYS	-	linker	UNP C3SHQ8
A	379	ALA	-	linker	UNP C3SHQ8
A	380	GLY	-	linker	UNP C3SHQ8
A	381	PHE	-	linker	UNP C3SHQ8
A	382	LEU	-	linker	UNP C3SHQ8
A	383	GLU	-	linker	UNP C3SHQ8
A	384	VAL	-	linker	UNP C3SHQ8
A	385	LEU	-	linker	UNP C3SHQ8
A	386	PHE	-	linker	UNP C3SHQ8
A	387	GLN	-	linker	UNP C3SHQ8
A	388	GLY	-	linker	UNP C3SHQ8
A	389	PRO	-	linker	UNP C3SHQ8
A	390	LEU	-	linker	UNP C3SHQ8
B	-9	MET	-	initiating methionine	UNP C3SHQ8
B	-8	ARG	-	expression tag	UNP C3SHQ8
B	-7	SER	-	expression tag	UNP C3SHQ8
B	-6	HIS	-	expression tag	UNP C3SHQ8
B	-5	HIS	-	expression tag	UNP C3SHQ8
B	-4	HIS	-	expression tag	UNP C3SHQ8
B	-3	HIS	-	expression tag	UNP C3SHQ8
B	-2	HIS	-	expression tag	UNP C3SHQ8
B	-1	HIS	-	expression tag	UNP C3SHQ8
B	0	GLY	-	expression tag	UNP C3SHQ8
B	367	ASN	-	linker	UNP C3SHQ8
B	368	SER	-	linker	UNP C3SHQ8
B	369	GLY	-	linker	UNP C3SHQ8
B	370	SER	-	linker	UNP C3SHQ8
B	371	ASP	-	linker	UNP C3SHQ8
B	372	ILE	-	linker	UNP C3SHQ8
B	373	THR	-	linker	UNP C3SHQ8
B	374	SER	-	linker	UNP C3SHQ8
B	375	LEU	-	linker	UNP C3SHQ8
B	376	TYR	-	linker	UNP C3SHQ8
B	377	LYS	-	linker	UNP C3SHQ8
B	378	LYS	-	linker	UNP C3SHQ8
B	379	ALA	-	linker	UNP C3SHQ8
B	380	GLY	-	linker	UNP C3SHQ8
B	381	PHE	-	linker	UNP C3SHQ8
B	382	LEU	-	linker	UNP C3SHQ8
B	383	GLU	-	linker	UNP C3SHQ8
B	384	VAL	-	linker	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	385	LEU	-	linker	UNP C3SHQ8
B	386	PHE	-	linker	UNP C3SHQ8
B	387	GLN	-	linker	UNP C3SHQ8
B	388	GLY	-	linker	UNP C3SHQ8
B	389	PRO	-	linker	UNP C3SHQ8
B	390	LEU	-	linker	UNP C3SHQ8
C	-9	MET	-	initiating methionine	UNP C3SHQ8
C	-8	ARG	-	expression tag	UNP C3SHQ8
C	-7	SER	-	expression tag	UNP C3SHQ8
C	-6	HIS	-	expression tag	UNP C3SHQ8
C	-5	HIS	-	expression tag	UNP C3SHQ8
C	-4	HIS	-	expression tag	UNP C3SHQ8
C	-3	HIS	-	expression tag	UNP C3SHQ8
C	-2	HIS	-	expression tag	UNP C3SHQ8
C	-1	HIS	-	expression tag	UNP C3SHQ8
C	0	GLY	-	expression tag	UNP C3SHQ8
C	367	ASN	-	linker	UNP C3SHQ8
C	368	SER	-	linker	UNP C3SHQ8
C	369	GLY	-	linker	UNP C3SHQ8
C	370	SER	-	linker	UNP C3SHQ8
C	371	ASP	-	linker	UNP C3SHQ8
C	372	ILE	-	linker	UNP C3SHQ8
C	373	THR	-	linker	UNP C3SHQ8
C	374	SER	-	linker	UNP C3SHQ8
C	375	LEU	-	linker	UNP C3SHQ8
C	376	TYR	-	linker	UNP C3SHQ8
C	377	LYS	-	linker	UNP C3SHQ8
C	378	LYS	-	linker	UNP C3SHQ8
C	379	ALA	-	linker	UNP C3SHQ8
C	380	GLY	-	linker	UNP C3SHQ8
C	381	PHE	-	linker	UNP C3SHQ8
C	382	LEU	-	linker	UNP C3SHQ8
C	383	GLU	-	linker	UNP C3SHQ8
C	384	VAL	-	linker	UNP C3SHQ8
C	385	LEU	-	linker	UNP C3SHQ8
C	386	PHE	-	linker	UNP C3SHQ8
C	387	GLN	-	linker	UNP C3SHQ8
C	388	GLY	-	linker	UNP C3SHQ8
C	389	PRO	-	linker	UNP C3SHQ8
C	390	LEU	-	linker	UNP C3SHQ8
D	-9	MET	-	initiating methionine	UNP C3SHQ8
D	-8	ARG	-	expression tag	UNP C3SHQ8

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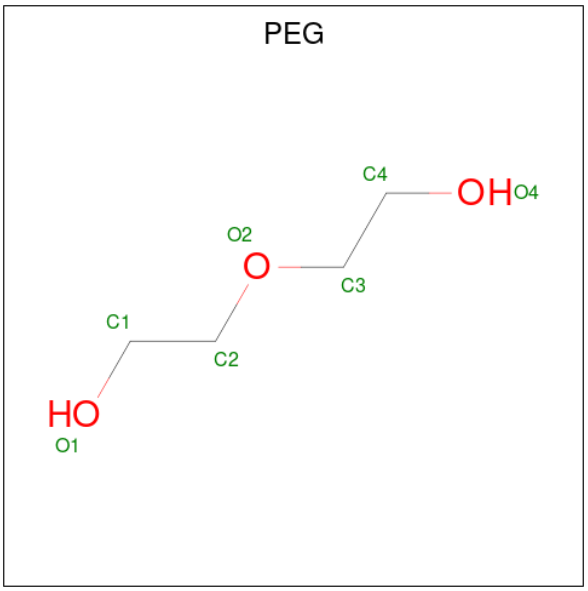
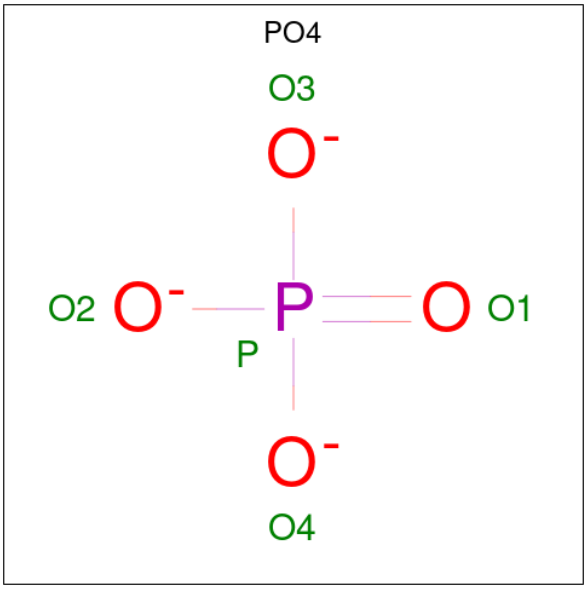
Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	SER	-	expression tag	UNP C3SHQ8
D	-6	HIS	-	expression tag	UNP C3SHQ8
D	-5	HIS	-	expression tag	UNP C3SHQ8
D	-4	HIS	-	expression tag	UNP C3SHQ8
D	-3	HIS	-	expression tag	UNP C3SHQ8
D	-2	HIS	-	expression tag	UNP C3SHQ8
D	-1	HIS	-	expression tag	UNP C3SHQ8
D	0	GLY	-	expression tag	UNP C3SHQ8
D	367	ASN	-	linker	UNP C3SHQ8
D	368	SER	-	linker	UNP C3SHQ8
D	369	GLY	-	linker	UNP C3SHQ8
D	370	SER	-	linker	UNP C3SHQ8
D	371	ASP	-	linker	UNP C3SHQ8
D	372	ILE	-	linker	UNP C3SHQ8
D	373	THR	-	linker	UNP C3SHQ8
D	374	SER	-	linker	UNP C3SHQ8
D	375	LEU	-	linker	UNP C3SHQ8
D	376	TYR	-	linker	UNP C3SHQ8
D	377	LYS	-	linker	UNP C3SHQ8
D	378	LYS	-	linker	UNP C3SHQ8
D	379	ALA	-	linker	UNP C3SHQ8
D	380	GLY	-	linker	UNP C3SHQ8
D	381	PHE	-	linker	UNP C3SHQ8
D	382	LEU	-	linker	UNP C3SHQ8
D	383	GLU	-	linker	UNP C3SHQ8
D	384	VAL	-	linker	UNP C3SHQ8
D	385	LEU	-	linker	UNP C3SHQ8
D	386	PHE	-	linker	UNP C3SHQ8
D	387	GLN	-	linker	UNP C3SHQ8
D	388	GLY	-	linker	UNP C3SHQ8
D	389	PRO	-	linker	UNP C3SHQ8
D	390	LEU	-	linker	UNP C3SHQ8

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



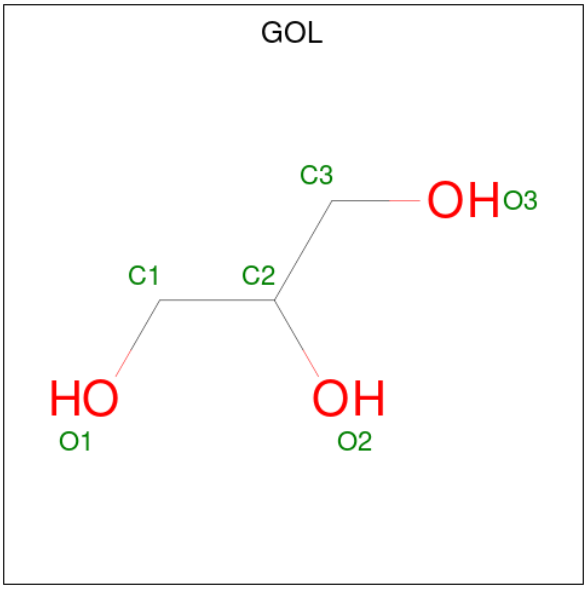
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C H O 15 4 9 2	0	0
2	B	1	Total C H O 17 4 10 3	0	0
2	C	1	Total C H O 10 3 5 2	0	0
2	C	1	Total C H O 17 4 10 3	0	0
2	D	1	Total C H O 17 4 10 3	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O P 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

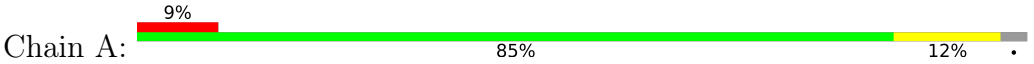
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	B	5	Total O 5 5	0	0
5	C	2	Total O 2 2	0	0
5	D	3	Total O 3 3	0	0

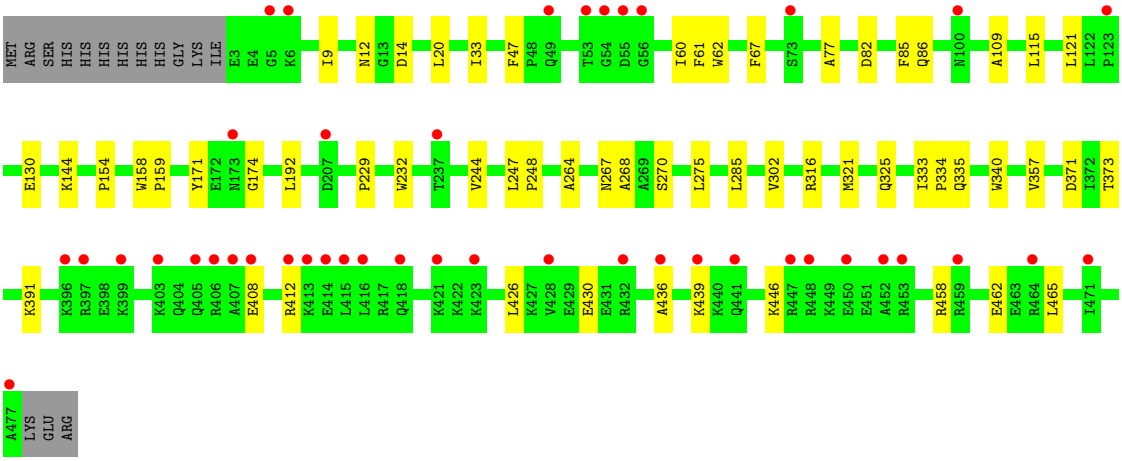
3 Residue-property plots (i)

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 1: Maltodextrin-binding protein,Chromatin assembly factor 1 subunit p90 fusion

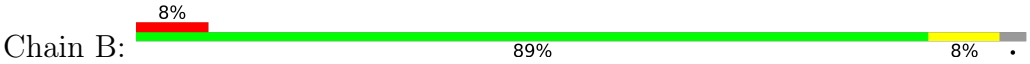
Chain A:

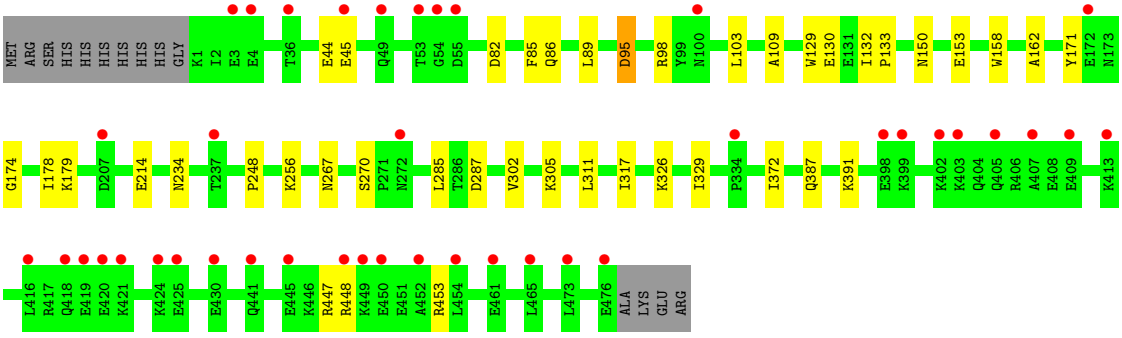




• Molecule 1: Maltodextrin-binding protein,Chromatin assembly factor 1 subunit p90 fusion

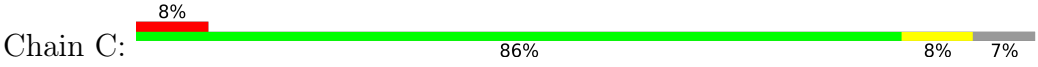
Chain B:

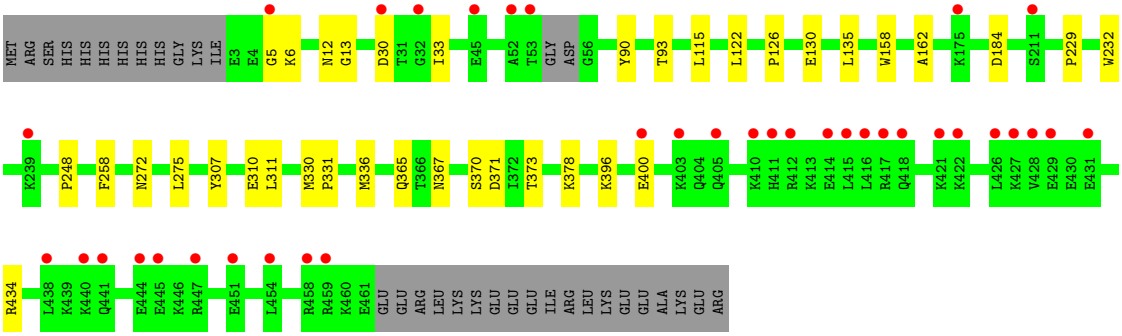




• Molecule 1: Maltodextrin-binding protein,Chromatin assembly factor 1 subunit p90 fusion

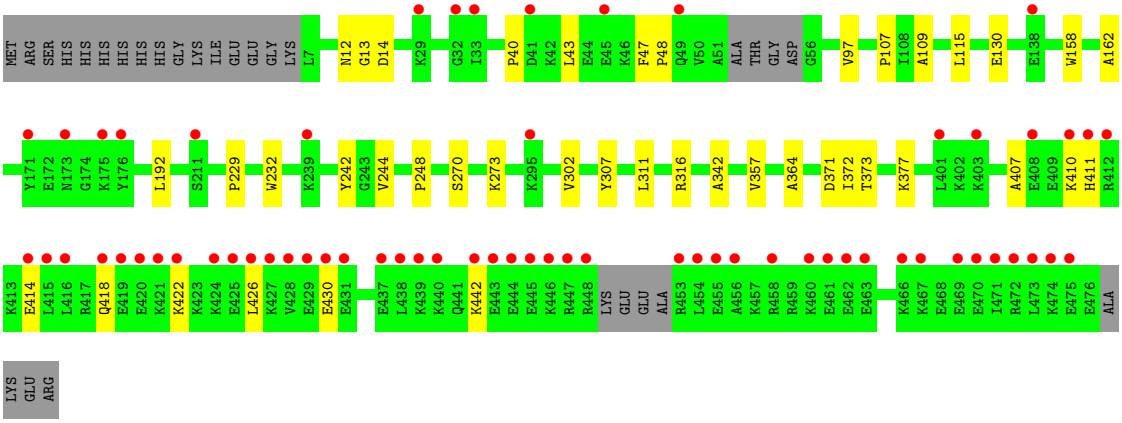
Chain C:





• Molecule 1: Maltodextrin-binding protein,Chromatin assembly factor 1 subunit p90 fusion

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.59Å 165.25Å 116.15Å 90.00° 96.47° 90.00°	Depositor
Resolution (Å)	28.68 – 2.81 28.68 – 2.81	Depositor EDS
% Data completeness (in resolution range)	97.9 (28.68-2.81) 97.9 (28.68-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.233 , 0.282 0.233 , 0.282	Depositor DCC
R_{free} test set	4768 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å^2)	46.8	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	14757	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GOL, PEG

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	0.23	0/3815	0.36	0/5142
1	B	0.24	0/3848	0.37	0/5183
1	C	0.24	0/3642	0.37	0/4917
1	D	0.24	0/3647	0.36	0/4926
All	All	0.24	0/14952	0.36	0/20168

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	3741	0	3734	35	0
1	B	3774	0	3780	24	0
1	C	3569	0	3541	20	0
1	D	3575	0	3496	23	0
2	B	13	19	17	0	0
2	C	12	15	15	0	0
2	D	7	10	10	0	0
3	C	5	0	0	0	0
4	C	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	5	0	0	0	0
5	C	2	0	0	0	0
5	D	3	0	0	0	0
All	All	14713	44	14601	100	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 (100) 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:33:ILE:HD13	1:A:275:LEU:HD13	1.67	0.75
1:B:372:ILE:H	1:B:372:ILE:HD12	1.52	0.73
1:D:372:ILE:HD12	1:D:372:ILE:H	1.53	0.72
1:B:150:ASN:HD21	1:B:153:GLU:HG2	1.59	0.67
1:A:391:LYS:HA	1:A:391:LYS:HE2	1.80	0.61
1:B:85:PHE:HZ	1:B:285:LEU:HD13	1.65	0.61
1:C:115:LEU:HD22	1:C:248:PRO:HD3	1.81	0.61
1:A:333:ILE:HG22	1:A:335:GLN:H	1.67	0.59
1:D:418:GLN:O	1:D:422:LYS:HG2	2.02	0.58
1:A:62:TRP:HB3	1:A:67:PHE:HE1	1.70	0.56
1:A:85:PHE:HZ	1:A:285:LEU:HD13	1.71	0.56
1:A:436:ALA:HA	1:A:439:LYS:HE2	1.87	0.56
1:C:184:ASP:HB2	1:C:365:GLN:HB2	1.87	0.55
1:A:130:GLU:N	1:A:130:GLU:OE1	2.40	0.55
1:A:371:ASP:OD2	1:A:373:THR:OG1	2.24	0.54
1:A:171:TYR:CZ	1:A:174:GLY:HA2	2.43	0.54
1:C:378:LYS:NZ	4:C:502:GOL:H2	2.23	0.53
1:A:12:ASN:ND2	1:A:14:ASP:OD1	2.38	0.53
1:C:371:ASP:OD2	1:C:373:THR:HB	2.10	0.51
1:D:410:LYS:O	1:D:414:GLU:HG3	2.10	0.51
1:A:244:VAL:HB	1:A:316:ARG:HA	1.91	0.51
1:B:447:ARG:HD2	1:B:448:ARG:HH11	1.75	0.51
1:C:331:PRO:O	1:C:336:MET:HG3	2.10	0.51
1:B:256:LYS:HE3	1:B:326:LYS:O	2.10	0.51
1:A:171:TYR:OH	1:A:174:GLY:HA2	2.11	0.50
1:A:121:LEU:HD11	1:A:144:LYS:HZ3	1.75	0.50
1:C:5:GLY:O	1:C:33:ILE:HG23	2.11	0.50
1:C:258:PHE:HB3	1:C:330:MET:HE2	1.92	0.50
1:C:122:LEU:HD21	1:C:126:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASN:ND2	1:B:153:GLU:HG2	2.24	0.50
1:A:109:ALA:HA	1:A:302:VAL:HA	1.95	0.49
1:D:40:PRO:HD2	1:D:43:LEU:HD21	1.95	0.48
1:D:242:TYR:OH	1:D:316:ARG:NH1	2.46	0.48
1:A:192:LEU:HD23	1:A:357:VAL:HG13	1.96	0.48
1:A:408:GLU:O	1:A:412:ARG:HG2	2.14	0.47
1:B:98:ARG:HG2	1:B:103:LEU:HD23	1.96	0.47
1:B:453:ARG:HD2	1:B:453:ARG:O	2.15	0.47
1:D:229:PRO:HA	1:D:232:TRP:CE2	2.50	0.47
1:A:426:LEU:O	1:A:430:GLU:HG3	2.14	0.47
1:B:158:TRP:CE2	1:B:162:ALA:HB2	2.50	0.47
1:B:178:ILE:HG13	1:B:179:LYS:HG3	1.96	0.47
1:A:115:LEU:HB2	1:A:247:LEU:HD23	1.97	0.46
1:A:267:ASN:HB3	1:A:270:SER:HB2	1.97	0.46
1:A:154:PRO:HG2	1:A:340:TRP:HE3	1.81	0.46
1:D:426:LEU:O	1:D:430:GLU:HG3	2.15	0.46
1:D:371:ASP:OD2	1:D:373:THR:HB	2.16	0.46
1:D:158:TRP:CE2	1:D:162:ALA:HB2	2.51	0.45
1:D:97:VAL:HG21	1:D:107:PRO:HD3	1.98	0.45
1:D:130:GLU:OE1	1:D:130:GLU:N	2.46	0.45
1:B:311:LEU:HB3	1:B:317:ILE:HG21	1.99	0.45
1:D:109:ALA:HA	1:D:302:VAL:HA	1.98	0.45
1:D:407:ALA:O	1:D:411:HIS:ND1	2.50	0.45
1:C:90:TYR:O	1:C:93:THR:OG1	2.33	0.45
1:C:272:ASN:HB3	1:C:275:LEU:HB2	1.97	0.45
1:A:321:MET:O	1:A:325:GLN:HG3	2.17	0.44
1:C:6:LYS:HA	1:C:33:ILE:HG23	1.99	0.44
1:A:158:TRP:N	1:A:159:PRO:CD	2.80	0.44
1:A:458:ARG:O	1:A:462:GLU:HG3	2.17	0.44
1:A:61:PHE:CE2	1:A:264:ALA:HB2	2.51	0.44
1:C:130:GLU:OE1	1:C:130:GLU:N	2.47	0.44
1:B:214:GLU:OE2	1:B:234:ASN:ND2	2.50	0.44
1:D:192:LEU:HD23	1:D:357:VAL:HG13	1.99	0.44
1:C:367:ASN:HA	1:C:370:SER:OG	2.18	0.44
1:A:47:PHE:CG	1:A:60:ILE:HD12	2.53	0.43
1:A:333:ILE:HG23	1:A:334:PRO:HD2	2.00	0.43
1:C:158:TRP:CE2	1:C:162:ALA:HB2	2.54	0.43
1:D:12:ASN:OD1	1:D:13:GLY:N	2.51	0.43
1:D:342:ALA:HB1	1:D:364:ALA:HA	2.00	0.43
1:A:85:PHE:CZ	1:A:285:LEU:HD13	2.53	0.43
1:A:115:LEU:HD22	1:A:248:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:LEU:HD21	1:C:135:LEU:HD21	2.01	0.43
1:C:307:TYR:CE2	1:C:311:LEU:HD11	2.54	0.43
1:D:270:SER:O	1:D:273:LYS:NZ	2.50	0.43
1:B:129:TRP:CD1	1:B:248:PRO:HB2	2.54	0.42
1:D:373:THR:HG22	1:D:377:LYS:HE3	2.00	0.42
1:D:307:TYR:CE2	1:D:311:LEU:HD11	2.54	0.42
1:B:85:PHE:CZ	1:B:285:LEU:HD13	2.51	0.42
1:C:12:ASN:OD1	1:C:13:GLY:N	2.52	0.42
1:B:130:GLU:OE1	1:B:130:GLU:N	2.40	0.42
1:A:232:TRP:CH2	1:A:316:ARG:HB3	2.54	0.42
1:C:229:PRO:HA	1:C:232:TRP:CE2	2.55	0.42
1:A:82:ASP:O	1:A:86:GLN:HG3	2.20	0.42
1:A:465:LEU:HB3	1:C:434:ARG:HG3	2.02	0.42
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.55	0.42
1:B:132:ILE:HB	1:B:133:PRO:HD3	2.02	0.42
1:D:115:LEU:HD22	1:D:248:PRO:HD3	2.01	0.42
1:A:9:ILE:HG21	1:A:20:LEU:HD21	2.01	0.41
1:B:44:GLU:HG3	1:B:45:GLU:HG2	2.01	0.41
1:B:89:LEU:O	1:B:305:LYS:HE3	2.19	0.41
1:B:82:ASP:O	1:B:86:GLN:HG3	2.20	0.41
1:B:95:ASP:HB2	1:B:329:ILE:HD13	2.02	0.41
1:B:387:GLN:HE21	1:B:391:LYS:HE3	1.85	0.41
1:C:396:LYS:HG2	1:C:400:GLU:OE1	2.20	0.41
1:D:244:VAL:HB	1:D:316:ARG:HA	2.03	0.41
1:A:77:ALA:HB2	1:A:268:ALA:HA	2.02	0.41
1:A:446:LYS:HE2	1:D:442:LYS:NZ	2.36	0.41
1:D:47:PHE:HB3	1:D:48:PRO:HD3	2.03	0.41
1:B:109:ALA:HA	1:B:302:VAL:HA	2.03	0.41
1:B:267:ASN:HB3	1:B:270:SER:HB2	2.02	0.40
1:B:171:TYR:OH	1:B:174:GLY:HA2	2.21	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	473/490 (96%)	457 (97%)	16 (3%)	0	100	100
1	B	474/490 (97%)	455 (96%)	19 (4%)	0	100	100
1	C	453/490 (92%)	437 (96%)	16 (4%)	0	100	100
1	D	456/490 (93%)	441 (97%)	15 (3%)	0	100	100
All	All	1856/1960 (95%)	1790 (96%)	66 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	381/406 (94%)	381 (100%)	0	100	100
1	B	389/406 (96%)	387 (100%)	2 (0%)	88	96
1	C	362/406 (89%)	360 (99%)	2 (1%)	86	95
1	D	357/406 (88%)	356 (100%)	1 (0%)	92	97
All	All	1489/1624 (92%)	1484 (100%)	5 (0%)	92	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	95	ASP
1	B	287	ASP
1	C	30	ASP
1	C	310	GLU
1	D	14	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	433	GLN
1	C	387	GLN
1	D	100	ASN
1	D	365	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
4	GOL	C	502	-	5,5,5	0.27	0	5,5,5	0.28	0
3	PO4	C	501	-	4,4,4	0.92	0	6,6,6	0.42	0
2	PEG	D	501	-	6,6,6	0.46	0	5,5,5	0.25	0
2	PEG	B	501	-	5,5,6	0.51	0	4,4,5	0.21	0
2	PEG	C	503	-	4,4,6	0.44	0	3,3,5	0.30	0
2	PEG	B	502	-	6,6,6	0.45	0	5,5,5	0.28	0
2	PEG	C	504	-	6,6,6	0.46	0	5,5,5	0.24	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	GOL	C	502	-	-	0/4/4/4	-
2	PEG	D	501	-	-	0/4/4/4	-
2	PEG	B	501	-	-	0/3/3/4	-
2	PEG	C	503	-	-	0/2/2/4	-
2	PEG	B	502	-	-	1/4/4/4	-
2	PEG	C	504	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	502	PEG	O1-C1-C2-O2

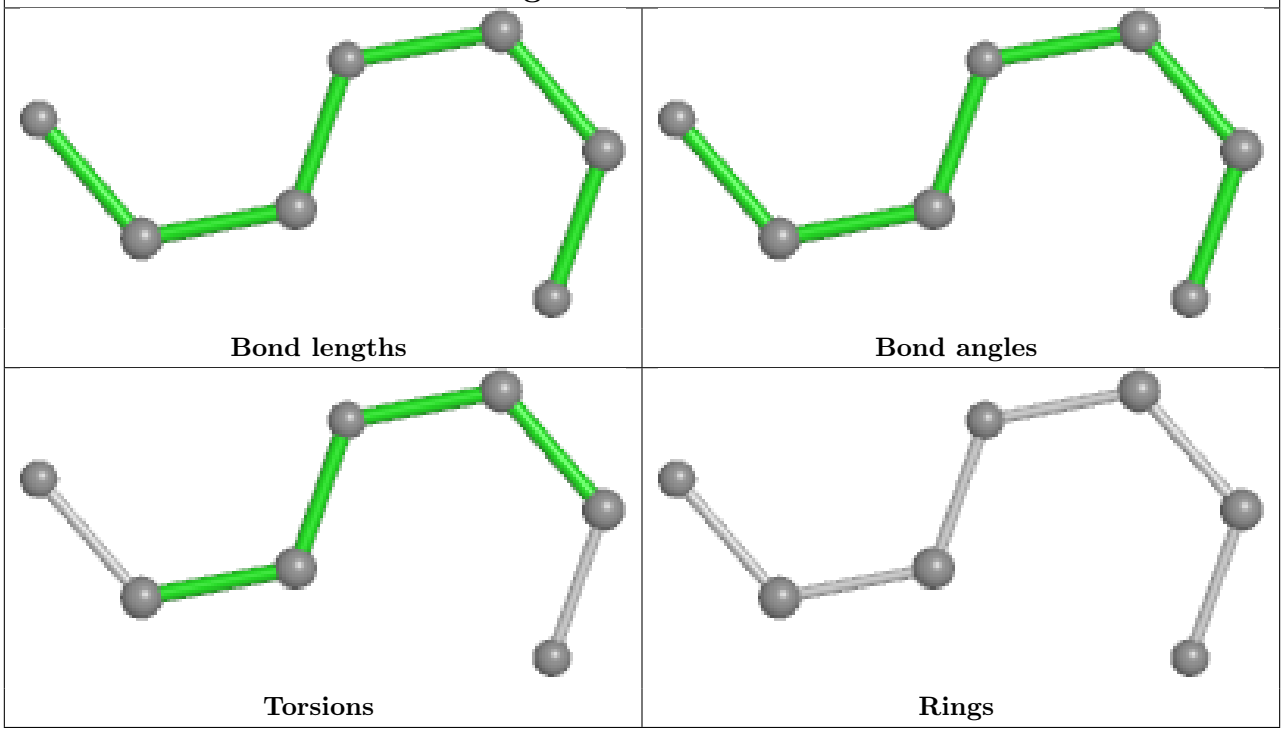
There are no ring outliers.

1 monomer is involved in 1 short contact:

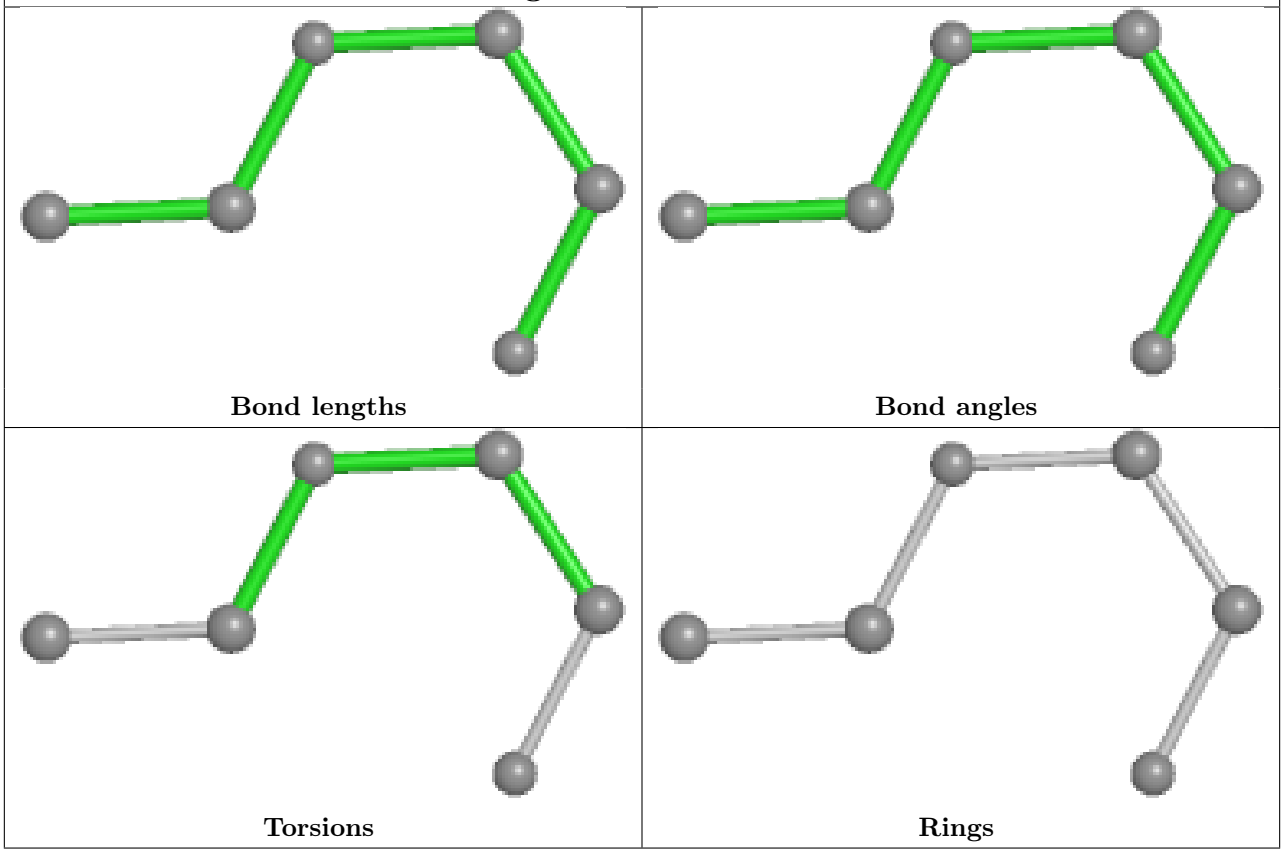
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	GOL	1	0

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 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.

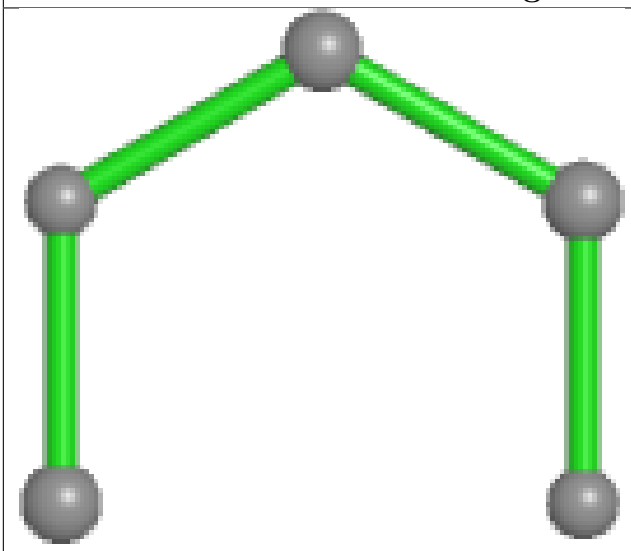
Ligand PEG D 501



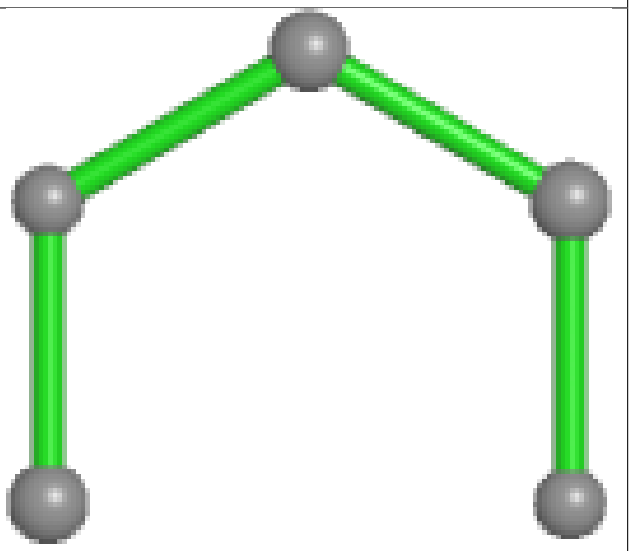
Ligand PEG B 501



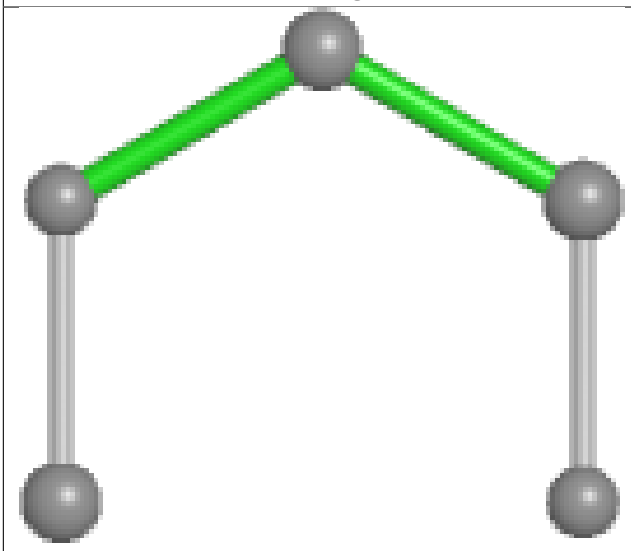
Ligand PEG C 503



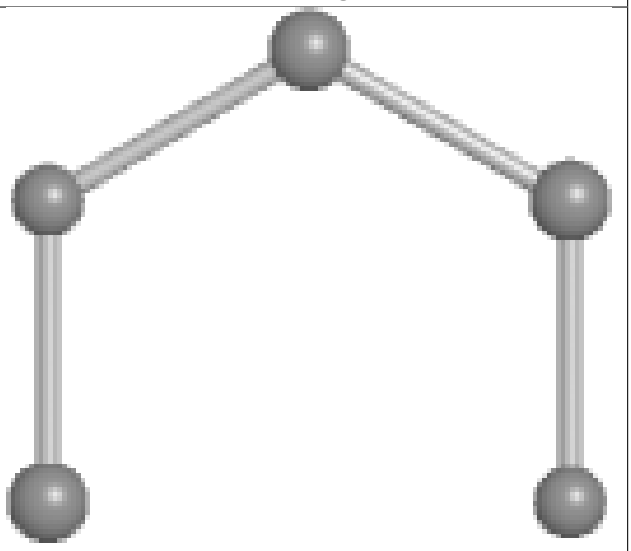
Bond lengths



Bond angles

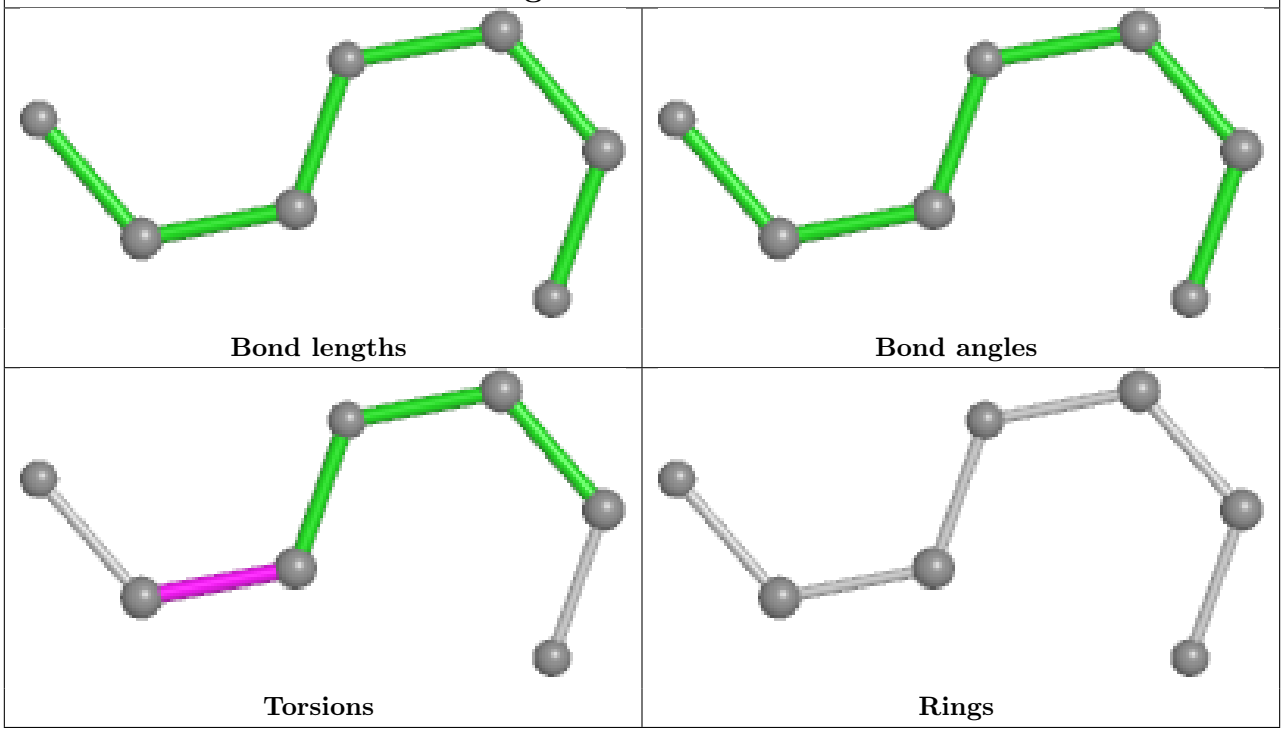


Torsions

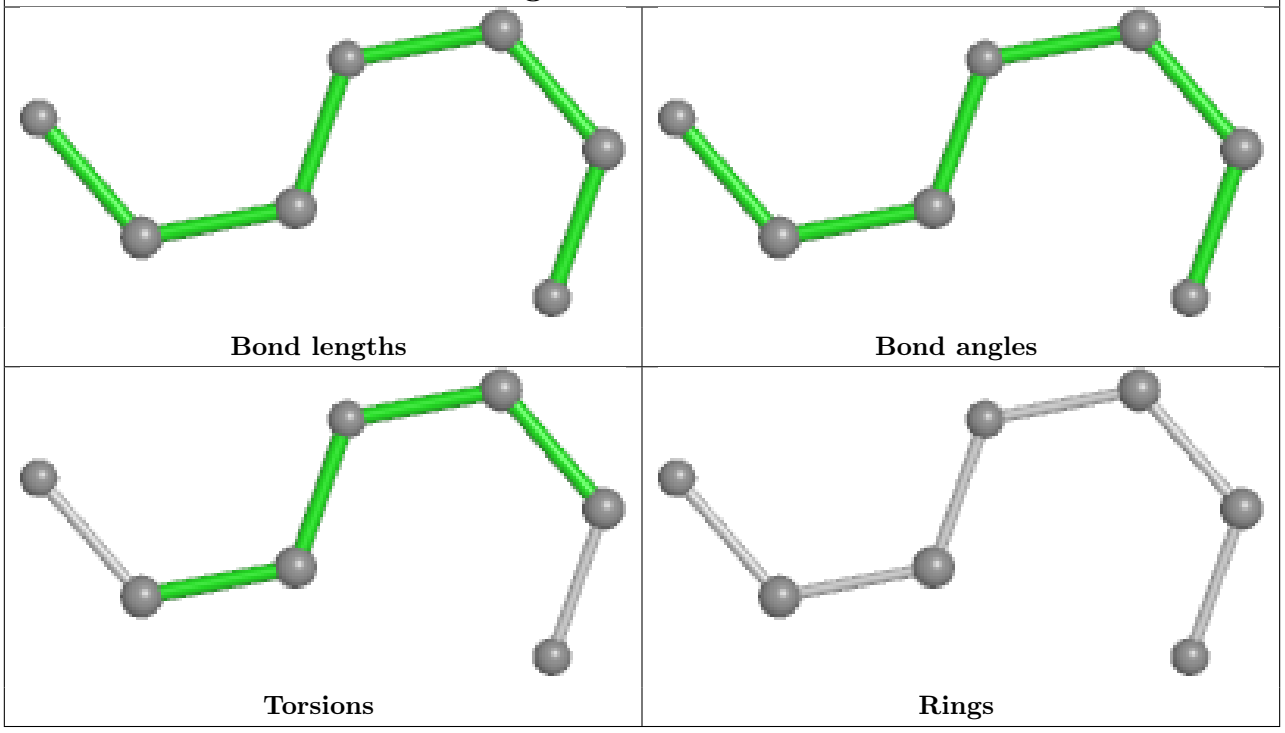


Rings

Ligand PEG B 502



Ligand PEG C 504



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, 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(Å^2)	Q<0.9
1	A	475/490 (96%)	0.51	43 (9%) 9 5	23, 44, 92, 100	0
1	B	476/490 (97%)	0.52	41 (8%) 10 5	21, 43, 90, 102	0
1	C	457/490 (93%)	0.48	37 (8%) 12 6	23, 44, 101, 112	0
1	D	462/490 (94%)	0.64	65 (14%) 2 1	24, 44, 109, 123	0
All	All	1870/1960 (95%)	0.54	186 (9%) 7 4	21, 44, 98, 123	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	428	VAL	6.9
1	D	473	LEU	6.5
1	D	443	GLU	6.4
1	D	469	GLU	6.1
1	B	53	THR	6.0
1	C	438	LEU	5.7
1	B	100	ASN	5.5
1	D	444	GLU	5.5
1	D	454	LEU	5.3
1	C	418	GLN	5.0
1	D	420	GLU	4.9
1	A	415	LEU	4.9
1	A	421	LYS	4.8
1	C	447	ARG	4.7
1	D	33	ILE	4.4
1	D	424	LYS	4.4
1	C	458	ARG	4.3
1	A	49	GLN	4.3
1	D	455	GLU	4.3
1	B	49	GLN	4.2
1	D	458	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	414	GLU	4.2
1	B	398	GLU	4.1
1	D	471	ILE	4.1
1	D	475	GLU	4.1
1	D	415	LEU	4.1
1	D	426	LEU	4.1
1	D	411	HIS	4.1
1	D	425	GLU	4.0
1	D	416	LEU	4.0
1	C	431	GLU	4.0
1	D	447	ARG	3.9
1	A	405	GLN	3.9
1	B	449	LYS	3.9
1	D	453	ARG	3.8
1	B	418	GLN	3.8
1	C	175	LYS	3.8
1	A	448	ARG	3.8
1	B	172	GLU	3.8
1	D	460	LYS	3.8
1	D	463	GLU	3.7
1	C	422	LYS	3.7
1	A	428	VAL	3.6
1	B	402	LYS	3.6
1	A	408	GLU	3.6
1	B	454	LEU	3.6
1	D	418	GLN	3.6
1	C	428	VAL	3.6
1	D	419	GLU	3.5
1	C	426	LEU	3.5
1	A	73	SER	3.5
1	B	45	GLU	3.5
1	D	448	ARG	3.5
1	D	474	LYS	3.4
1	B	452	ALA	3.4
1	C	416	LEU	3.4
1	D	466	LYS	3.4
1	A	407	ALA	3.3
1	C	412	ARG	3.3
1	D	429	GLU	3.3
1	D	446	LYS	3.3
1	D	427	LYS	3.2
1	C	421	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	476	GLU	3.2
1	C	451	GLU	3.2
1	D	422	LYS	3.2
1	D	414	GLU	3.1
1	C	45	GLU	3.1
1	B	405	GLN	3.1
1	C	52	ALA	3.1
1	B	403	LYS	3.1
1	D	442	LYS	3.1
1	B	465	LEU	3.1
1	C	415	LEU	3.1
1	C	429	GLU	3.0
1	A	441	GLN	3.0
1	D	461	GLU	3.0
1	D	421	LYS	3.0
1	A	53	THR	3.0
1	D	467	LYS	3.0
1	A	436	ALA	3.0
1	C	53	THR	2.9
1	A	416	LEU	2.9
1	B	54	GLY	2.9
1	D	171	TYR	2.9
1	A	439	LYS	2.9
1	B	399	LYS	2.9
1	A	5	GLY	2.9
1	D	438	LEU	2.9
1	A	423	LYS	2.9
1	A	471	ILE	2.8
1	B	420	GLU	2.8
1	D	412	ARG	2.8
1	B	421	LYS	2.8
1	A	477	ALA	2.8
1	C	239	LYS	2.8
1	D	401	LEU	2.8
1	B	409	GLU	2.8
1	A	237	THR	2.8
1	C	445	GLU	2.8
1	D	439	LYS	2.8
1	B	55	ASP	2.7
1	C	417	ARG	2.7
1	A	55	ASP	2.7
1	A	447	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	32	GLY	2.7
1	D	437	GLU	2.7
1	B	450	GLU	2.7
1	D	470	GLU	2.7
1	D	445	GLU	2.7
1	C	441	GLN	2.6
1	A	207	ASP	2.6
1	D	431	GLU	2.6
1	A	56	GLY	2.6
1	B	424	LYS	2.6
1	C	30	ASP	2.6
1	A	397	ARG	2.6
1	A	432	ARG	2.6
1	D	462	GLU	2.6
1	B	3	GLU	2.5
1	C	410	LYS	2.5
1	B	4	GLU	2.5
1	D	408	GLU	2.5
1	C	5	GLY	2.5
1	D	41	ASP	2.5
1	D	239	LYS	2.5
1	B	425	GLU	2.5
1	B	473	LEU	2.5
1	A	399	LYS	2.4
1	A	406	ARG	2.4
1	D	472	ARG	2.4
1	D	456	ALA	2.4
1	C	427	LYS	2.4
1	A	464	ARG	2.4
1	A	6	LYS	2.4
1	D	440	LYS	2.4
1	C	403	LYS	2.4
1	A	123	PRO	2.4
1	D	45	GLU	2.4
1	C	414	GLU	2.3
1	B	36	THR	2.3
1	C	444	GLU	2.3
1	C	411	HIS	2.3
1	A	418	GLN	2.3
1	A	100	ASN	2.3
1	D	211	SER	2.3
1	A	412	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	211	SER	2.3
1	D	430	GLU	2.2
1	D	295	LYS	2.2
1	B	419	GLU	2.2
1	B	430	GLU	2.2
1	B	448	ARG	2.2
1	C	459	ARG	2.2
1	D	173	ASN	2.2
1	B	416	LEU	2.2
1	B	441	GLN	2.2
1	A	452	ALA	2.2
1	B	334	PRO	2.2
1	C	454	LEU	2.2
1	C	405	GLN	2.2
1	D	176	TYR	2.2
1	B	207	ASP	2.1
1	C	440	LYS	2.1
1	D	175	LYS	2.1
1	B	461	GLU	2.1
1	A	54	GLY	2.1
1	A	403	LYS	2.1
1	D	49	GLN	2.1
1	D	29	LYS	2.1
1	A	396	LYS	2.1
1	C	32	GLY	2.1
1	A	173	ASN	2.1
1	D	138	GLU	2.1
1	D	410	LYS	2.1
1	B	445	GLU	2.0
1	A	459	ARG	2.0
1	A	450	GLU	2.0
1	B	407	ALA	2.0
1	A	453	ARG	2.0
1	B	272	ASN	2.0
1	C	400	GLU	2.0
1	B	237	THR	2.0
1	A	413	LYS	2.0
1	B	413	LYS	2.0
1	D	403	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 monosaccharides in this entry.

6.4 Ligands (i)

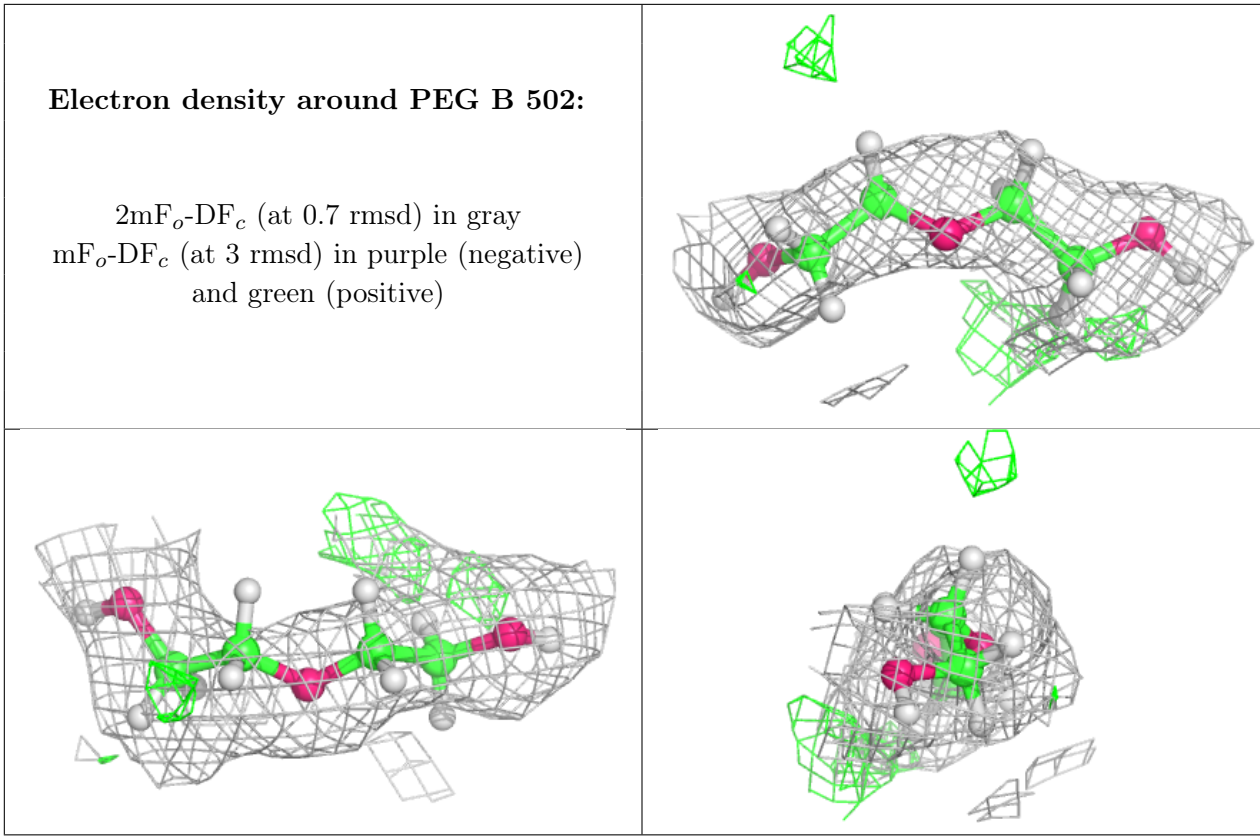
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PEG	B	502	7/7	0.65	0.29	49,59,63,63	0
2	PEG	B	501	6/7	0.71	0.36	40,47,54,54	0
3	PO4	C	501	5/5	0.75	0.21	55,64,68,84	0
4	GOL	C	502	6/6	0.77	0.25	36,46,49,51	0
2	PEG	C	503	5/7	0.82	0.31	33,50,56,56	0
2	PEG	C	504	7/7	0.82	0.23	39,47,54,55	0
2	PEG	D	501	7/7	0.87	0.21	32,44,50,57	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.

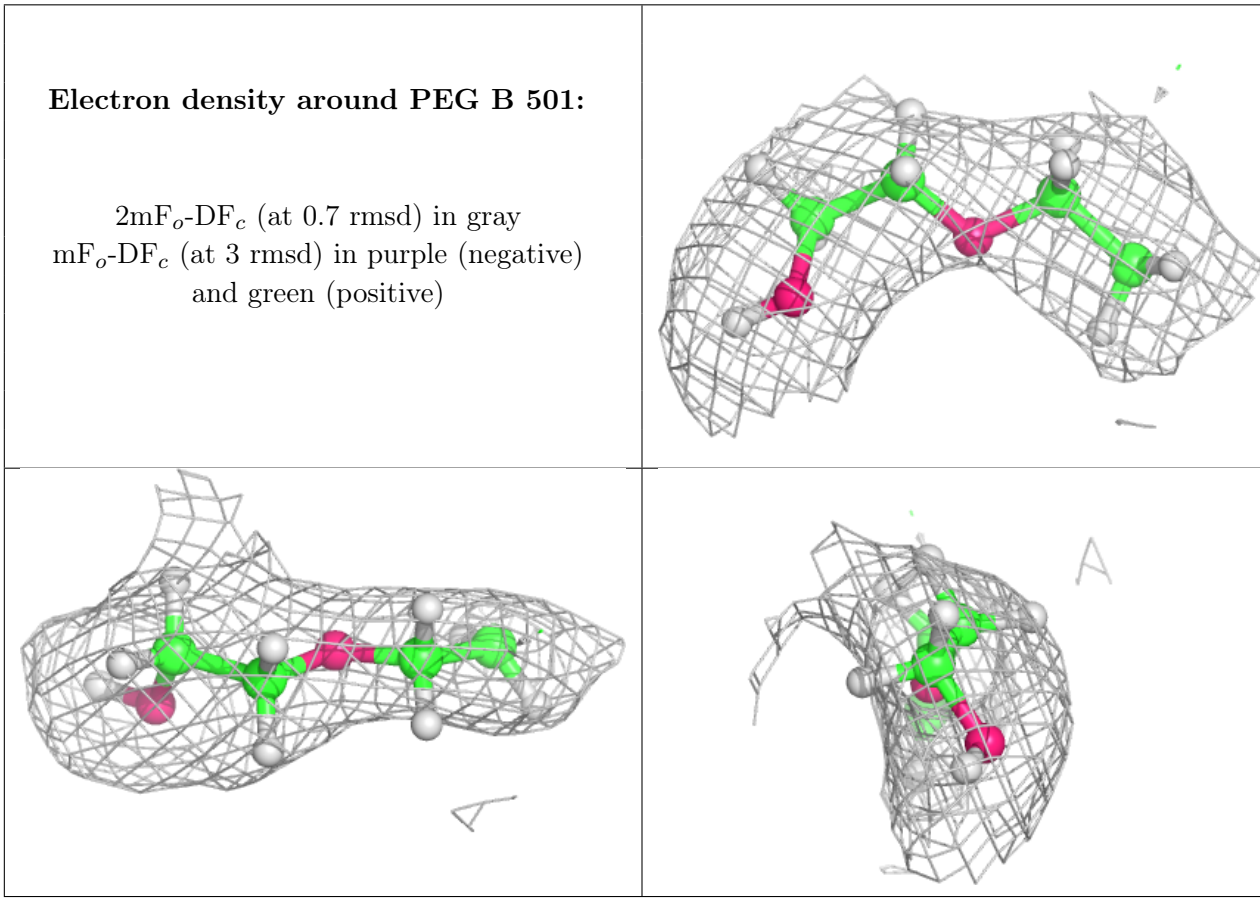
Electron density around PEG B 502:

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



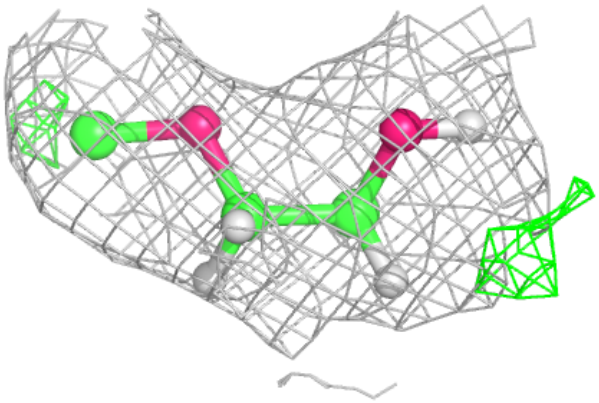
Electron density around PEG B 501:

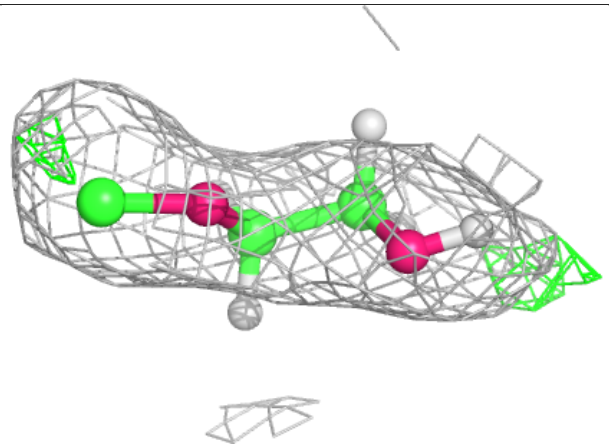
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

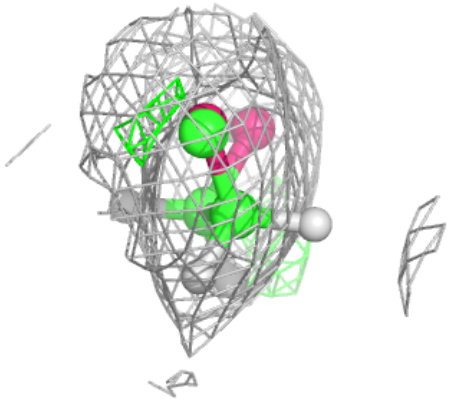


Electron density around PEG C 503:

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

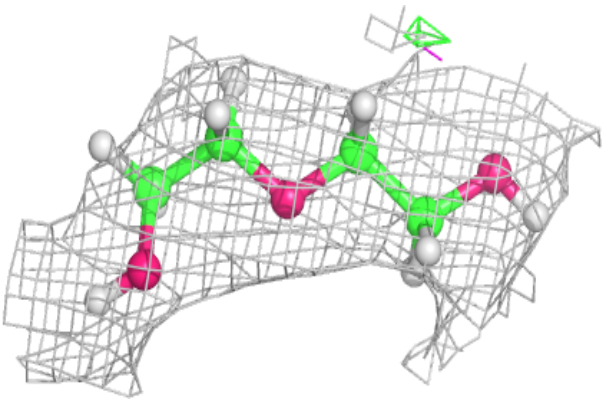


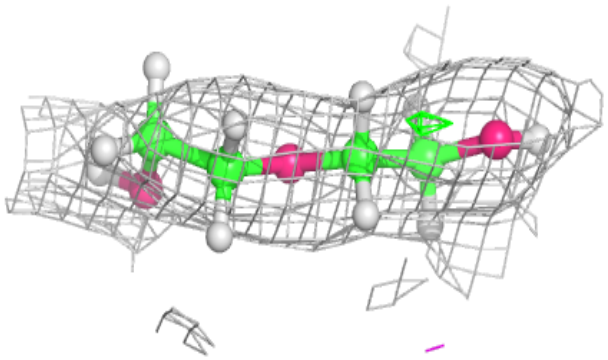


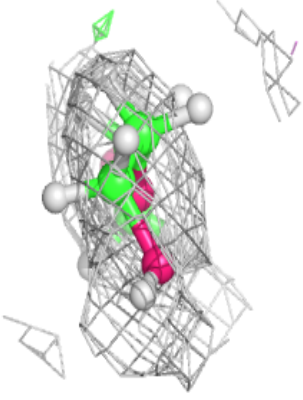


Electron density around PEG C 504:

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

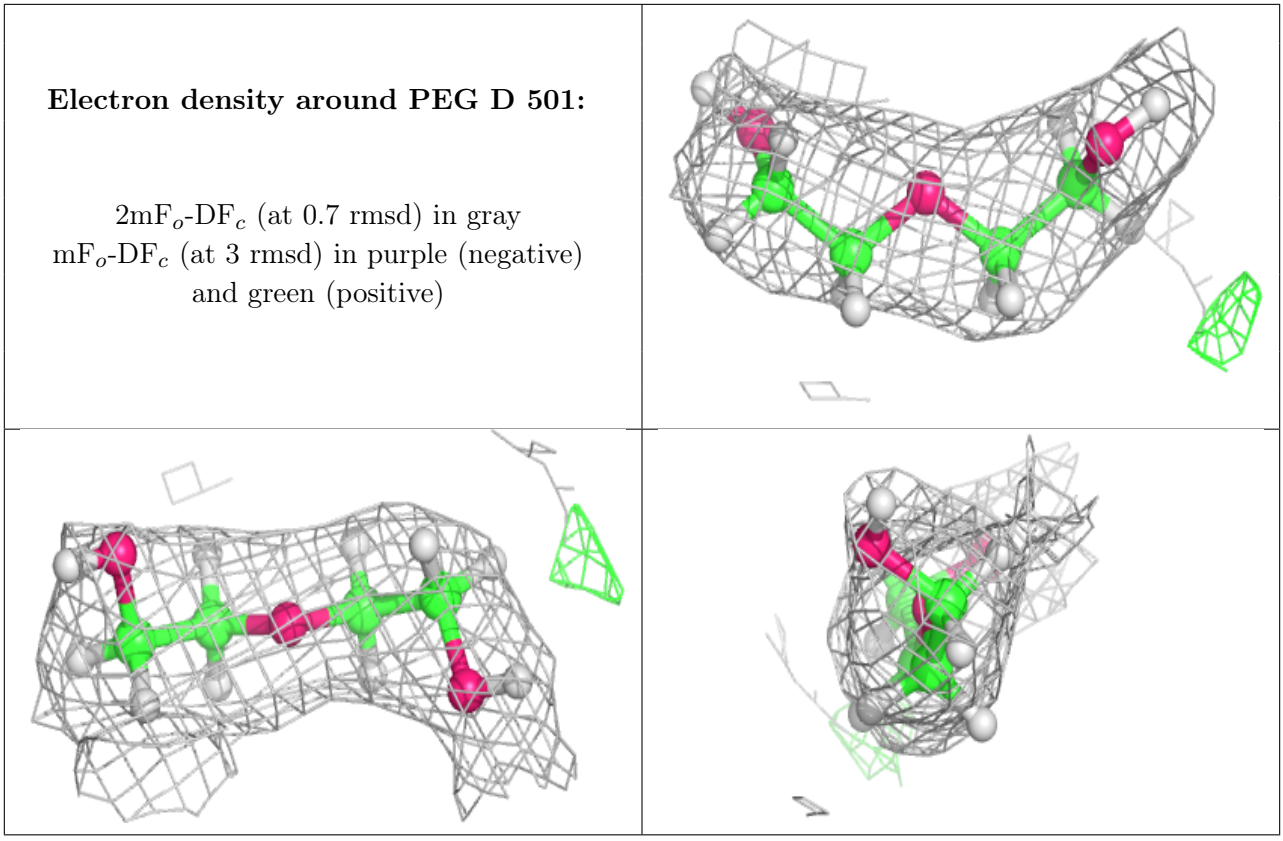






Electron density around PEG D 501:

$2mF_o$-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.