Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 10:51 AM EDT

PDB ID	:	6WKU
Title	:	Twelve Chloride Ions Drive Assembly of Human alpha345 Collagen IV NC1 domain
Authors	:	Boudko, S.P.; Hudson, B.G.
Deposited on	:	2020-04-17
Resolution	:	1.76 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:

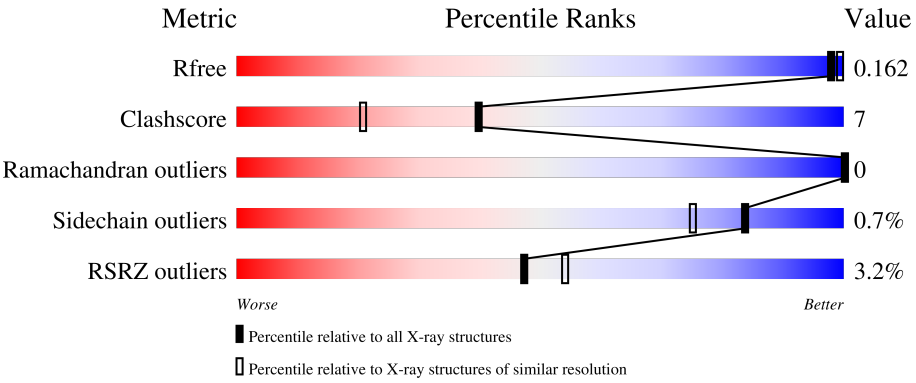
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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

Mol	Chain	Length	Quality of chain
1	A	695	3% 86% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PG4	A	728	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 6430 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 Collagen alpha-3(IV) chain,Collagen alpha-4(IV) chain,Collagen alpha-5(IV) chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	677	5389	3420	923	986	60	0	30	0

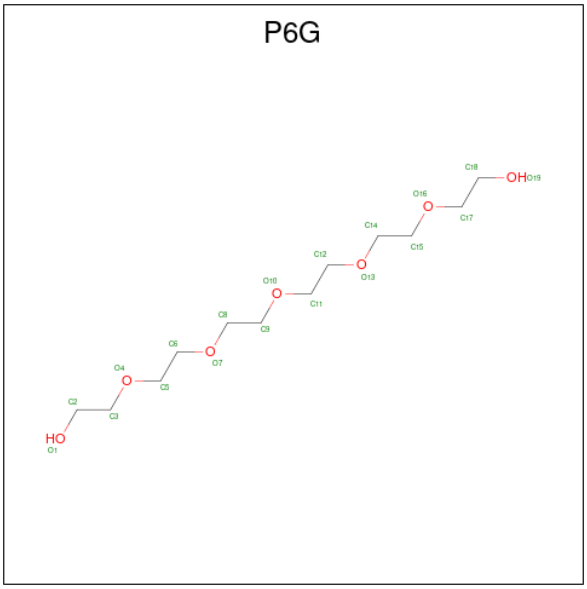
There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	ALA	-	expression tag	UNP Q01955
A	-15	PRO	-	expression tag	UNP Q01955
A	-14	LEU	-	expression tag	UNP Q01955
A	-13	ALA	-	expression tag	UNP Q01955
A	-12	ASP	-	expression tag	UNP Q01955
A	-11	TYR	-	expression tag	UNP Q01955
A	-10	LYS	-	expression tag	UNP Q01955
A	-9	ASP	-	expression tag	UNP Q01955
A	-8	ASP	-	expression tag	UNP Q01955
A	-7	ASP	-	expression tag	UNP Q01955
A	-6	ASP	-	expression tag	UNP Q01955
A	-5	LYS	-	expression tag	UNP Q01955
A	-4	LEU	-	expression tag	UNP Q01955
A	-3	ALA	-	expression tag	UNP Q01955
A	-2	GLY	-	expression tag	UNP Q01955
A	227	GLY	-	linker	UNP Q01955
A	228	THR	-	linker	UNP Q01955
A	452	ALA	-	linker	UNP P53420
A	453	PRO	-	linker	UNP P53420

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

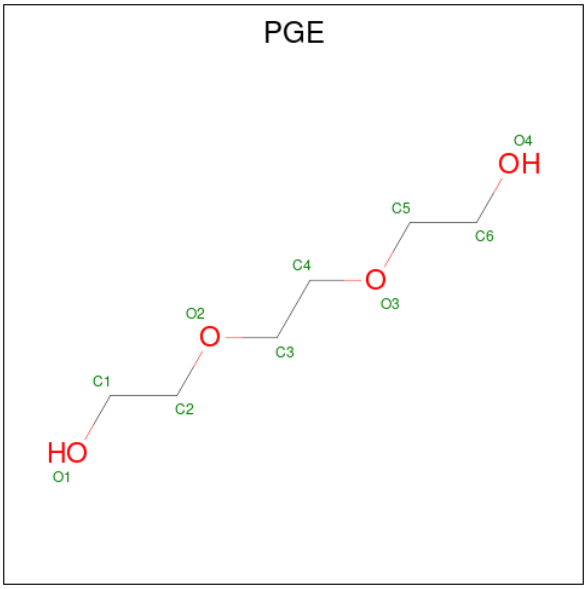
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total Cl 6 6	0	0

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



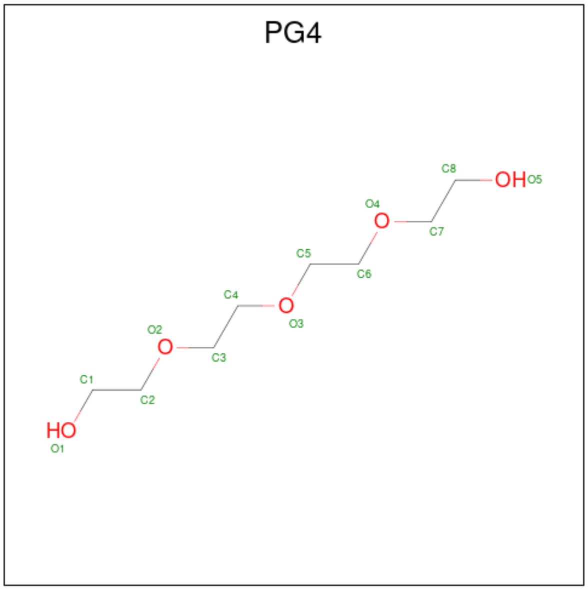
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 19 12 7	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



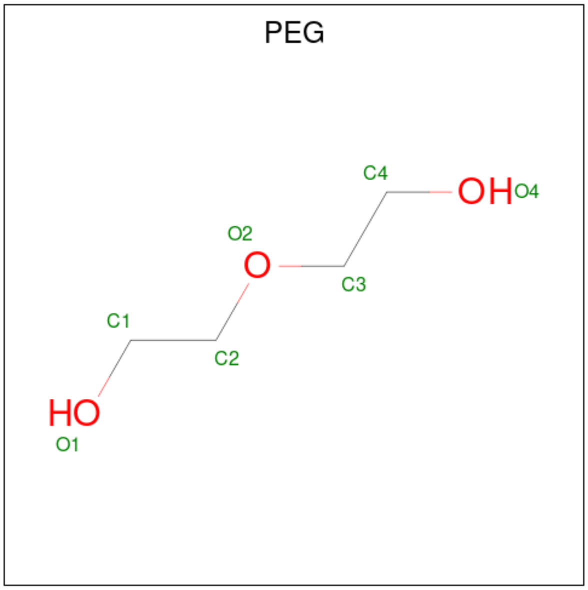
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0
4	A	1	Total C O 10 6 4	0	0
4	A	1	Total C O 10 6 4	0	0
4	A	1	Total C O 10 6 4	0	0
4	A	1	Total C O 10 6 4	0	0
4	A	1	Total C O 10 6 4	0	0
4	A	1	Total C O 10 6 4	0	0
4	A	1	Total C O 10 6 4	0	0
4	A	1	Total C O 10 6 4	0	0
4	A	1	Total C O 10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

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 8 5	0	0
5	A	1	Total C O 13 8 5	0	0
5	A	1	Total C O 13 8 5	0	0
5	A	1	Total C O 13 8 5	0	0
5	A	1	Total C O 13 8 5	0	0
5	A	1	Total C O 13 8 5	0	0
5	A	1	Total C O 13 8 5	0	0
5	A	1	Total C O 13 8 5	0	0
5	A	1	Total C O 13 8 5	0	0
5	A	1	Total C O 13 8 5	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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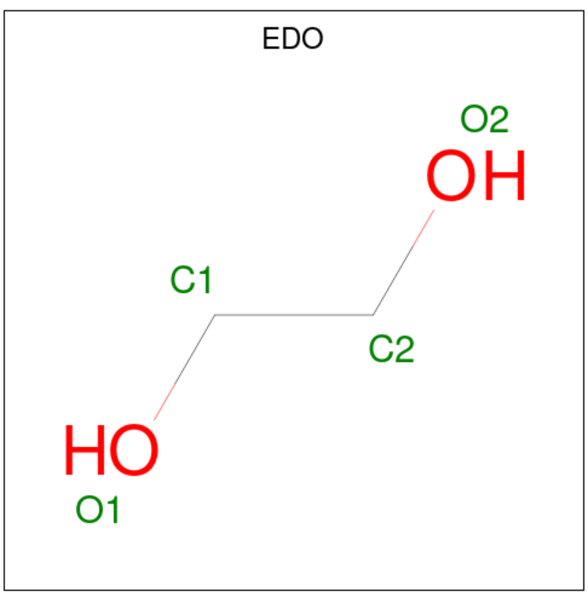
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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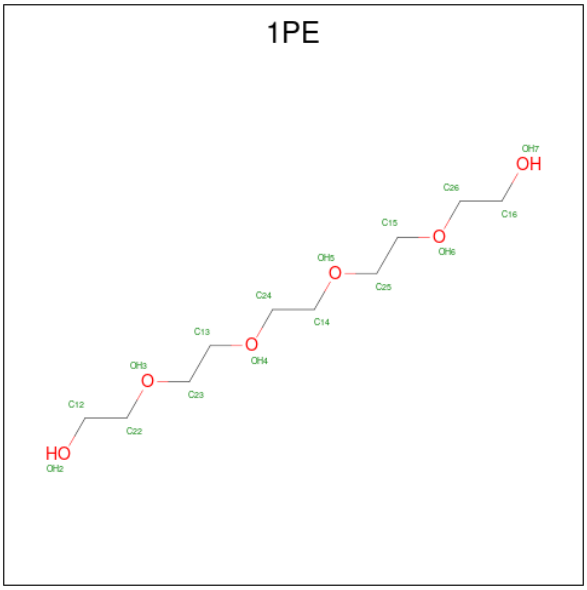
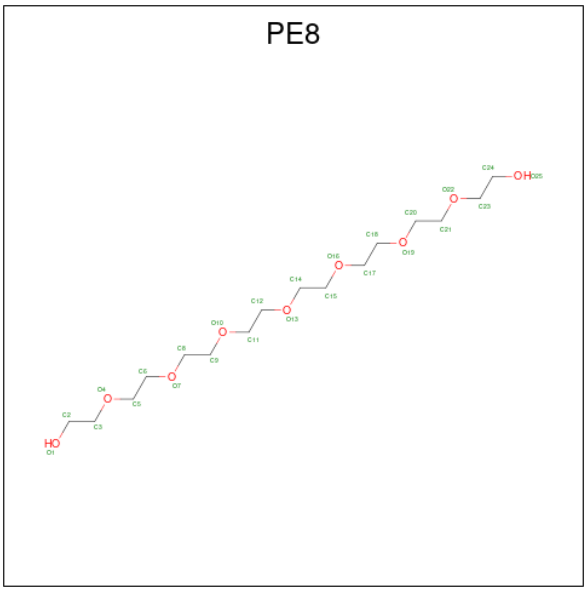
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0

- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 16 10 6	0	0

- Molecule 9 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula: $C_{16}H_{34}O_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 25 16 9	0	0

- Molecule 10 is water.

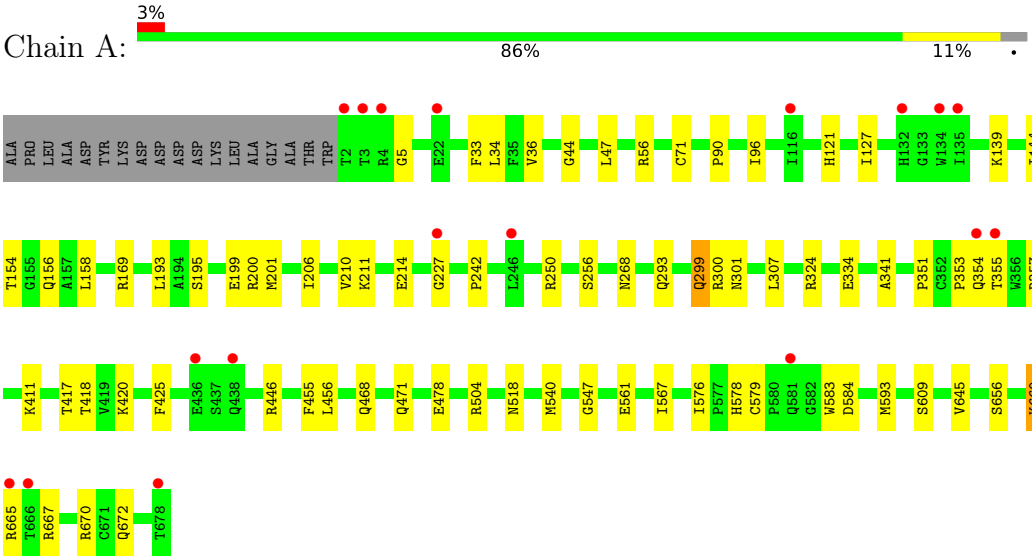
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	357	Total O 357 357	0	0

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: Collagen alpha-3(IV) chain,Collagen alpha-4(IV) chain,Collagen alpha-5(IV) chain

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	128.42Å 128.42Å 104.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.40 – 1.76 68.60 – 1.76	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.40-1.76) 96.4 (68.60-1.76)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.139 , 0.162 0.139 , 0.162	Depositor DCC
R_{free} test set	2000 reflections (2.30%)	wwPDB-VP
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 59.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	6430	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: CL, PGE, EDO, PEG, 1PE, PG4, P6G, PE8

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	0.35	0/5635	0.57	0/7656

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	5389	0	5247	75	0
2	A	6	0	0	0	0
3	A	19	0	26	2	0
4	A	200	0	280	20	0
5	A	130	0	180	14	0
6	A	168	0	240	14	0
7	A	120	0	180	6	0
8	A	16	0	22	2	0
9	A	25	0	34	8	0
10	A	357	0	0	5	0
All	All	6430	0	6209	90	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 7.

All (90) 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:456:LEU:H	4:A:715:PGE:H6	1.30	0.94
1:A:250:ARG:HE	4:A:724:PGE:H6	1.47	0.79
1:A:354[B]:GLN:H	5:A:728:PG4:H31	1.46	0.79
1:A:354[A]:GLN:H	5:A:728:PG4:H31	1.46	0.79
1:A:144[B]:ILE:HG22	1:A:158:LEU:HD21	1.65	0.76
1:A:584:ASP:HB3	9:A:771:PE8:H92	1.73	0.70
1:A:471:GLN:HG2	9:A:771:PE8:H31	1.74	0.70
1:A:324:ARG:HH12	6:A:761:PEG:H32	1.55	0.70
1:A:44:GLY:HA3	1:A:154:THR:HG21	1.76	0.67
1:A:121:HIS:HD2	4:A:768:PGE:H22	1.60	0.66
1:A:354[A]:GLN:HG2	5:A:728:PG4:H31	1.77	0.66
1:A:672:GLN:HE22	9:A:771:PE8:H172	1.63	0.62
1:A:382:SER:HB2	6:A:713:PEG:H31	1.81	0.62
1:A:200:ARG:HD2	4:A:710:PGE:H5	1.84	0.60
1:A:324:ARG:HH22	6:A:761:PEG:H22	1.66	0.60
1:A:578:HIS:HA	9:A:771:PE8:H171	1.83	0.59
4:A:709:PGE:H62	6:A:720:PEG:H42	1.85	0.59
1:A:456:LEU:N	4:A:715:PGE:H6	2.11	0.59
1:A:121:HIS:CD2	4:A:768:PGE:H22	2.40	0.56
1:A:408:PHE:H	1:A:411:LYS:NZ	2.04	0.56
1:A:408:PHE:H	1:A:411:LYS:HZ2	1.54	0.56
1:A:33:PHE:HZ	1:A:36:VAL:HG13	1.71	0.55
8:A:721:1PE:H242	6:A:789:PEG:H42	1.88	0.54
4:A:722:PGE:H22	10:A:824:HOH:O	2.07	0.54
1:A:299:GLN:HE21	1:A:299:GLN:HA	1.71	0.54
1:A:127:ILE:HD13	1:A:139:LYS:HD3	1.89	0.54
1:A:71:CYS:SG	1:A:664:LEU:HD22	2.48	0.53
1:A:211:LYS:O	1:A:214:GLU:HG2	2.08	0.53
1:A:195:SER:OG	6:A:723:PEG:H22	2.08	0.53
1:A:609:SER:HB2	4:A:736:PGE:H5	1.91	0.52
1:A:672:GLN:NE2	9:A:771:PE8:H172	2.23	0.52
1:A:34[B]:LEU:HD23	1:A:47:LEU:HD21	1.91	0.52
1:A:210:VAL:HB	1:A:214:GLU:HG3	1.92	0.52
1:A:36:VAL:HG11	1:A:593:MET:HE1	1.91	0.51
6:A:776:PEG:H42	4:A:777:PGE:H6	1.92	0.51
1:A:227[B]:GLY:HA2	5:A:751:PG4:H51	1.93	0.50
1:A:468:GLN:NE2	10:A:822:HOH:O	2.43	0.50
4:A:724:PGE:H1	4:A:730:PGE:H2	1.94	0.50
1:A:201:MET:CE	4:A:730:PGE:H3	2.42	0.50
1:A:199:GLU:HB2	4:A:710:PGE:H12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ALA:O	3:A:707:P6G:H122	2.12	0.49
1:A:656:SER:HB2	7:A:785:EDO:H21	1.93	0.49
1:A:670:ARG:HH22	5:A:712:PG4:H12	1.77	0.49
1:A:357:ARG:HA	7:A:767:EDO:H12	1.95	0.48
1:A:425:PHE:O	1:A:547:GLY:HA2	2.13	0.48
1:A:242:PRO:HB3	5:A:772:PG4:H21	1.95	0.48
1:A:579:CYS:H	9:A:771:PE8:H171	1.78	0.48
1:A:353:PRO:HB3	5:A:728:PG4:H52	1.94	0.48
5:A:756:PG4:H11	5:A:756:PG4:H31	1.54	0.48
4:A:730:PGE:H1	4:A:730:PGE:H32	1.75	0.48
1:A:5:GLY:HA2	1:A:583:TRP:CZ2	2.50	0.47
1:A:446:ARG:HH12	7:A:774:EDO:H22	1.79	0.47
7:A:725:EDO:H21	10:A:1000:HOH:O	2.14	0.46
1:A:660:LYS:NZ	10:A:829:HOH:O	2.49	0.46
1:A:518:ASN:HD22	6:A:787:PEG:H42	1.81	0.46
1:A:351:PRO:HA	6:A:757:PEG:H31	1.96	0.46
1:A:567:ILE:HG22	4:A:736:PGE:H2	1.98	0.46
1:A:561:GLU:OE1	5:A:728:PG4:H82	2.15	0.46
1:A:34[B]:LEU:CD2	1:A:47:LEU:HD21	2.46	0.45
1:A:201:MET:HE3	4:A:730:PGE:H3	1.98	0.45
1:A:300:ARG:HB3	1:A:301:ASN:H	1.68	0.45
1:A:540[B]:MET:SD	7:A:791:EDO:H11	2.57	0.45
1:A:146:PHE:O	1:A:153:GLY:HA3	2.17	0.44
1:A:455:PHE:CD1	4:A:715:PGE:H3	2.52	0.44
1:A:353:PRO:HA	5:A:728:PG4:H32	1.98	0.44
6:A:739:PEG:H11	6:A:739:PEG:H32	1.91	0.44
4:A:718:PGE:H52	4:A:718:PGE:H3	1.74	0.43
1:A:334:GLU:HG2	5:A:752:PG4:H12	2.00	0.43
1:A:670:ARG:NH2	5:A:712:PG4:H12	2.33	0.43
1:A:660:LYS:CE	1:A:660:LYS:H	2.30	0.43
4:A:715:PGE:H42	6:A:746:PEG:H22	2.00	0.43
6:A:776:PEG:H21	6:A:776:PEG:H41	1.74	0.43
1:A:576:ILE:HB	9:A:771:PE8:H212	2.00	0.43
1:A:256:SER:HB2	1:A:307:LEU:HB2	2.01	0.43
1:A:417[B]:THR:OG1	1:A:418:THR:N	2.51	0.43
1:A:146:PHE:HE2	1:A:156:GLN:HE21	1.66	0.43
1:A:665:ARG:H	1:A:665:ARG:HG3	1.69	0.43
1:A:478:GLU:HB2	7:A:747:EDO:H22	2.01	0.42
6:A:713:PEG:H42	6:A:746:PEG:H11	2.01	0.42
1:A:144[A]:ILE:HD11	1:A:193:LEU:HD23	2.02	0.42
1:A:169:ARG:HD3	8:A:721:1PE:H221	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLN:HG3	6:A:789:PEG:H31	2.01	0.42
1:A:504:ARG:HD2	5:A:727:PG4:H31	2.00	0.42
1:A:56:ARG:HD3	1:A:645:VAL:O	2.19	0.42
9:A:771:PE8:H32	9:A:771:PE8:H61	1.83	0.42
1:A:206:ILE:HB	4:A:711:PGE:H3	2.01	0.41
3:A:707:P6G:H22	5:A:728:PG4:H41	2.02	0.41
1:A:90:PRO:HD3	1:A:96:ILE:HD11	2.03	0.40
1:A:268[B]:ASN:ND2	10:A:837:HOH:O	2.53	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	707/695 (102%)	687 (97%)	20 (3%)	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	603/585 (103%)	599 (99%)	4 (1%)	84 75

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	GLN
1	A	420	LYS
1	A	660	LYS
1	A	667	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 93 ligands modelled in this entry, 6 are monoatomic - leaving 87 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PGE	A	709	-	9,9,9	0.51	0	8,8,8	0.18	0
7	EDO	A	747	-	3,3,3	0.47	0	2,2,2	0.32	0
5	PG4	A	716	-	12,12,12	0.53	0	11,11,11	0.18	0
7	EDO	A	760	-	3,3,3	0.47	0	2,2,2	0.34	0
6	PEG	A	758	-	6,6,6	0.49	0	5,5,5	0.23	0
6	PEG	A	714	-	6,6,6	0.49	0	5,5,5	0.28	0
4	PGE	A	768	-	9,9,9	0.50	0	8,8,8	0.33	0
6	PEG	A	763	-	6,6,6	0.47	0	5,5,5	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	PEG	A	773	-	6,6,6	0.48	0	5,5,5	0.28	0
5	PG4	A	753	-	12,12,12	0.52	0	11,11,11	0.22	0
7	EDO	A	778	-	3,3,3	0.47	0	2,2,2	0.30	0
7	EDO	A	717	-	3,3,3	0.47	0	2,2,2	0.31	0
6	PEG	A	734	-	6,6,6	0.48	0	5,5,5	0.29	0
6	PEG	A	776	-	6,6,6	0.48	0	5,5,5	0.24	0
7	EDO	A	786	-	3,3,3	0.46	0	2,2,2	0.39	0
6	PEG	A	787	-	6,6,6	0.49	0	5,5,5	0.28	0
6	PEG	A	732	-	6,6,6	0.49	0	5,5,5	0.25	0
6	PEG	A	723	-	6,6,6	0.48	0	5,5,5	0.19	0
6	PEG	A	720	-	6,6,6	0.48	0	5,5,5	0.30	0
6	PEG	A	739	-	6,6,6	0.48	0	5,5,5	0.27	0
7	EDO	A	792	-	3,3,3	0.47	0	2,2,2	0.34	0
7	EDO	A	767	-	3,3,3	0.47	0	2,2,2	0.36	0
4	PGE	A	748	-	9,9,9	0.51	0	8,8,8	0.29	0
6	PEG	A	740	-	6,6,6	0.49	0	5,5,5	0.27	0
4	PGE	A	711	-	9,9,9	0.49	0	8,8,8	0.58	0
7	EDO	A	762	-	3,3,3	0.50	0	2,2,2	0.44	0
7	EDO	A	780	-	3,3,3	0.47	0	2,2,2	0.27	0
7	EDO	A	769	-	3,3,3	0.47	0	2,2,2	0.35	0
4	PGE	A	777	-	9,9,9	0.50	0	8,8,8	0.31	0
8	1PE	A	721	-	15,15,15	0.53	0	14,14,14	0.27	0
6	PEG	A	746	-	6,6,6	0.49	0	5,5,5	0.26	0
6	PEG	A	713	-	6,6,6	0.49	0	5,5,5	0.20	0
7	EDO	A	791	-	3,3,3	0.47	0	2,2,2	0.38	0
4	PGE	A	733	-	9,9,9	0.51	0	8,8,8	0.25	0
5	PG4	A	751	-	12,12,12	0.53	0	11,11,11	0.24	0
4	PGE	A	736	-	9,9,9	0.49	0	8,8,8	0.28	0
7	EDO	A	750	-	3,3,3	0.47	0	2,2,2	0.39	0
6	PEG	A	745	-	6,6,6	0.50	0	5,5,5	0.31	0
7	EDO	A	785	-	3,3,3	0.48	0	2,2,2	0.22	0
4	PGE	A	738	-	9,9,9	0.52	0	8,8,8	0.26	0
7	EDO	A	726	-	3,3,3	0.47	0	2,2,2	0.32	0
6	PEG	A	761	-	6,6,6	0.50	0	5,5,5	0.23	0
4	PGE	A	729	-	9,9,9	0.52	0	8,8,8	0.32	0
4	PGE	A	754	-	9,9,9	0.52	0	8,8,8	0.27	0
6	PEG	A	790	-	6,6,6	0.48	0	5,5,5	0.25	0
7	EDO	A	744	-	3,3,3	0.48	0	2,2,2	0.26	0
6	PEG	A	759	-	6,6,6	0.49	0	5,5,5	0.27	0
7	EDO	A	783	-	3,3,3	0.48	0	2,2,2	0.33	0
5	PG4	A	752	-	12,12,12	0.52	0	11,11,11	0.28	0
7	EDO	A	731	-	3,3,3	0.47	0	2,2,2	0.38	0
7	EDO	A	749	-	3,3,3	0.46	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	EDO	A	764	-	3,3,3	0.48	0	2,2,2	0.30	0
3	P6G	A	707	-	18,18,18	0.53	0	17,17,17	0.34	0
7	EDO	A	793	-	3,3,3	0.47	0	2,2,2	0.36	0
7	EDO	A	784	-	3,3,3	0.47	0	2,2,2	0.34	0
7	EDO	A	775	-	3,3,3	0.47	0	2,2,2	0.30	0
4	PGE	A	710	-	9,9,9	0.51	0	8,8,8	0.27	0
7	EDO	A	770	-	3,3,3	0.48	0	2,2,2	0.27	0
7	EDO	A	782	-	3,3,3	0.48	0	2,2,2	0.29	0
4	PGE	A	724	-	9,9,9	0.51	0	8,8,8	0.17	0
6	PEG	A	757	-	6,6,6	0.49	0	5,5,5	0.26	0
6	PEG	A	788	-	6,6,6	0.48	0	5,5,5	0.23	0
7	EDO	A	774	-	3,3,3	0.47	0	2,2,2	0.30	0
7	EDO	A	725	-	3,3,3	0.46	0	2,2,2	0.29	0
6	PEG	A	735	-	6,6,6	0.48	0	5,5,5	0.26	0
4	PGE	A	741	-	9,9,9	0.51	0	8,8,8	0.23	0
7	EDO	A	719	-	3,3,3	0.47	0	2,2,2	0.33	0
4	PGE	A	708	-	9,9,9	0.50	0	8,8,8	0.25	0
5	PG4	A	765	-	12,12,12	0.52	0	11,11,11	0.28	0
6	PEG	A	781	-	6,6,6	0.48	0	5,5,5	0.20	0
7	EDO	A	766	-	3,3,3	0.47	0	2,2,2	0.30	0
4	PGE	A	715	-	9,9,9	0.49	0	8,8,8	0.34	0
4	PGE	A	742	-	9,9,9	0.50	0	8,8,8	0.27	0
5	PG4	A	756	-	12,12,12	0.52	0	11,11,11	0.27	0
5	PG4	A	727	-	12,12,12	0.53	0	11,11,11	0.25	0
5	PG4	A	728	-	12,12,12	0.52	0	11,11,11	0.44	0
6	PEG	A	737	-	6,6,6	0.48	0	5,5,5	0.18	0
9	PE8	A	771	-	24,24,24	0.54	0	23,23,23	0.27	0
4	PGE	A	755	-	9,9,9	0.51	0	8,8,8	0.26	0
4	PGE	A	730	-	9,9,9	0.51	0	8,8,8	0.40	0
7	EDO	A	743	-	3,3,3	0.47	0	2,2,2	0.30	0
4	PGE	A	722	-	9,9,9	0.54	0	8,8,8	0.49	0
5	PG4	A	712	-	12,12,12	0.52	0	11,11,11	0.26	0
5	PG4	A	772	-	12,12,12	0.53	0	11,11,11	0.20	0
6	PEG	A	789	-	6,6,6	0.48	0	5,5,5	0.26	0
4	PGE	A	718	-	9,9,9	0.51	0	8,8,8	0.28	0
7	EDO	A	779	-	3,3,3	0.45	0	2,2,2	0.31	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	PGE	A	709	-	-	1/7/7/7	-
7	EDO	A	747	-	-	0/1/1/1	-
5	PG4	A	716	-	-	5/10/10/10	-
7	EDO	A	760	-	-	0/1/1/1	-
6	PEG	A	758	-	-	1/4/4/4	-
6	PEG	A	714	-	-	1/4/4/4	-
4	PGE	A	768	-	-	2/7/7/7	-
6	PEG	A	763	-	-	2/4/4/4	-
6	PEG	A	773	-	-	1/4/4/4	-
5	PG4	A	753	-	-	4/10/10/10	-
7	EDO	A	778	-	-	0/1/1/1	-
7	EDO	A	717	-	-	0/1/1/1	-
6	PEG	A	734	-	-	0/4/4/4	-
6	PEG	A	776	-	-	1/4/4/4	-
7	EDO	A	786	-	-	1/1/1/1	-
6	PEG	A	787	-	-	2/4/4/4	-
6	PEG	A	732	-	-	0/4/4/4	-
6	PEG	A	723	-	-	2/4/4/4	-
6	PEG	A	720	-	-	2/4/4/4	-
6	PEG	A	739	-	-	4/4/4/4	-
7	EDO	A	792	-	-	0/1/1/1	-
7	EDO	A	767	-	-	1/1/1/1	-
4	PGE	A	748	-	-	4/7/7/7	-
6	PEG	A	740	-	-	2/4/4/4	-
4	PGE	A	711	-	-	3/7/7/7	-
7	EDO	A	762	-	-	0/1/1/1	-
7	EDO	A	780	-	-	0/1/1/1	-
7	EDO	A	769	-	-	1/1/1/1	-
4	PGE	A	777	-	-	2/7/7/7	-
8	1PE	A	721	-	-	8/13/13/13	-
6	PEG	A	746	-	-	0/4/4/4	-
6	PEG	A	713	-	-	1/4/4/4	-
7	EDO	A	791	-	-	0/1/1/1	-
4	PGE	A	733	-	-	4/7/7/7	-
5	PG4	A	751	-	-	5/10/10/10	-
4	PGE	A	736	-	-	2/7/7/7	-
7	EDO	A	750	-	-	0/1/1/1	-
6	PEG	A	745	-	-	1/4/4/4	-
7	EDO	A	785	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	A	738	-	-	2/7/7/7	-
7	EDO	A	726	-	-	0/1/1/1	-
6	PEG	A	761	-	-	3/4/4/4	-
4	PGE	A	729	-	-	4/7/7/7	-
4	PGE	A	754	-	-	1/7/7/7	-
6	PEG	A	790	-	-	2/4/4/4	-
7	EDO	A	744	-	-	1/1/1/1	-
6	PEG	A	759	-	-	2/4/4/4	-
7	EDO	A	783	-	-	1/1/1/1	-
5	PG4	A	752	-	-	5/10/10/10	-
7	EDO	A	731	-	-	0/1/1/1	-
7	EDO	A	749	-	-	1/1/1/1	-
7	EDO	A	764	-	-	1/1/1/1	-
3	P6G	A	707	-	-	4/16/16/16	-
7	EDO	A	793	-	-	0/1/1/1	-
7	EDO	A	784	-	-	0/1/1/1	-
7	EDO	A	775	-	-	0/1/1/1	-
4	PGE	A	710	-	-	5/7/7/7	-
7	EDO	A	770	-	-	1/1/1/1	-
7	EDO	A	782	-	-	0/1/1/1	-
4	PGE	A	724	-	-	4/7/7/7	-
6	PEG	A	757	-	-	2/4/4/4	-
6	PEG	A	788	-	-	3/4/4/4	-
7	EDO	A	774	-	-	0/1/1/1	-
7	EDO	A	725	-	-	1/1/1/1	-
6	PEG	A	735	-	-	0/4/4/4	-
4	PGE	A	741	-	-	1/7/7/7	-
7	EDO	A	719	-	-	0/1/1/1	-
4	PGE	A	708	-	-	1/7/7/7	-
5	PG4	A	765	-	-	4/10/10/10	-
6	PEG	A	781	-	-	2/4/4/4	-
7	EDO	A	766	-	-	1/1/1/1	-
4	PGE	A	715	-	-	4/7/7/7	-
4	PGE	A	742	-	-	3/7/7/7	-
5	PG4	A	756	-	-	5/10/10/10	-
5	PG4	A	727	-	-	3/10/10/10	-
5	PG4	A	728	-	-	6/10/10/10	-
6	PEG	A	737	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PE8	A	771	-	-	11/22/22/22	-
4	PGE	A	755	-	-	4/7/7/7	-
4	PGE	A	730	-	-	4/7/7/7	-
7	EDO	A	743	-	-	1/1/1/1	-
4	PGE	A	722	-	-	3/7/7/7	-
5	PG4	A	712	-	-	7/10/10/10	-
5	PG4	A	772	-	-	5/10/10/10	-
6	PEG	A	789	-	-	1/4/4/4	-
4	PGE	A	718	-	-	2/7/7/7	-
7	EDO	A	779	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (175) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	757	PEG	O1-C1-C2-O2
4	A	730	PGE	O2-C3-C4-O3
8	A	721	1PE	OH6-C15-C25-OH5
5	A	756	PG4	O3-C5-C6-O4
9	A	771	PE8	O7-C8-C9-O10
5	A	751	PG4	O3-C5-C6-O4
5	A	727	PG4	O4-C7-C8-O5
6	A	763	PEG	O1-C1-C2-O2
6	A	723	PEG	C4-C3-O2-C2
6	A	740	PEG	C1-C2-O2-C3
4	A	711	PGE	O2-C3-C4-O3
5	A	728	PG4	O2-C3-C4-O3
4	A	718	PGE	C3-C4-O3-C5
9	A	771	PE8	O10-C11-C12-O13
5	A	728	PG4	O3-C5-C6-O4
5	A	756	PG4	C1-C2-O2-C3
4	A	738	PGE	O2-C3-C4-O3
4	A	711	PGE	O3-C5-C6-O4
4	A	748	PGE	O3-C5-C6-O4
5	A	728	PG4	O4-C7-C8-O5
6	A	720	PEG	O1-C1-C2-O2
6	A	739	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
6	A	788	PEG	O2-C3-C4-O4
6	A	789	PEG	O1-C1-C2-O2
8	A	721	1PE	OH2-C12-C22-OH3
7	A	764	EDO	O1-C1-C2-O2
5	A	752	PG4	O3-C5-C6-O4
8	A	721	1PE	OH5-C14-C24-OH4
4	A	733	PGE	O2-C3-C4-O3
4	A	748	PGE	O2-C3-C4-O3
4	A	733	PGE	O1-C1-C2-O2
4	A	748	PGE	O1-C1-C2-O2
6	A	790	PEG	O2-C3-C4-O4
9	A	771	PE8	O4-C5-C6-O7
3	A	707	P6G	O7-C8-C9-O10
4	A	722	PGE	O2-C3-C4-O3
4	A	724	PGE	O2-C3-C4-O3
9	A	771	PE8	O13-C14-C15-O16
4	A	729	PGE	C4-C3-O2-C2
9	A	771	PE8	C9-C8-O7-C6
5	A	716	PG4	O3-C5-C6-O4
5	A	712	PG4	O1-C1-C2-O2
6	A	759	PEG	O1-C1-C2-O2
7	A	749	EDO	O1-C1-C2-O2
7	A	766	EDO	O1-C1-C2-O2
7	A	769	EDO	O1-C1-C2-O2
7	A	785	EDO	O1-C1-C2-O2
4	A	742	PGE	O2-C3-C4-O3
9	A	771	PE8	O16-C17-C18-O19
6	A	739	PEG	C1-C2-O2-C3
5	A	728	PG4	C3-C4-O3-C5
6	A	781	PEG	O1-C1-C2-O2
4	A	755	PGE	O3-C5-C6-O4
5	A	756	PG4	O1-C1-C2-O2
5	A	765	PG4	O4-C7-C8-O5
6	A	761	PEG	O2-C3-C4-O4
6	A	763	PEG	O2-C3-C4-O4
6	A	788	PEG	O1-C1-C2-O2
9	A	771	PE8	O1-C2-C3-O4
5	A	712	PG4	O2-C3-C4-O3
6	A	787	PEG	O2-C3-C4-O4
4	A	730	PGE	C1-C2-O2-C3
5	A	753	PG4	O2-C3-C4-O3
5	A	772	PG4	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
5	A	752	PG4	O2-C3-C4-O3
4	A	736	PGE	O1-C1-C2-O2
6	A	776	PEG	C4-C3-O2-C2
4	A	724	PGE	O1-C1-C2-O2
7	A	744	EDO	O1-C1-C2-O2
7	A	767	EDO	O1-C1-C2-O2
9	A	771	PE8	C6-C5-O4-C3
4	A	729	PGE	O2-C3-C4-O3
4	A	730	PGE	O3-C5-C6-O4
4	A	742	PGE	O1-C1-C2-O2
6	A	723	PEG	O1-C1-C2-O2
6	A	761	PEG	C1-C2-O2-C3
4	A	755	PGE	C6-C5-O3-C4
4	A	724	PGE	C3-C4-O3-C5
6	A	788	PEG	C1-C2-O2-C3
9	A	771	PE8	C20-C21-O22-C23
4	A	709	PGE	C1-C2-O2-C3
8	A	721	1PE	C16-C26-OH6-C15
4	A	730	PGE	C3-C4-O3-C5
4	A	733	PGE	C6-C5-O3-C4
4	A	755	PGE	C1-C2-O2-C3
5	A	765	PG4	C8-C7-O4-C6
5	A	712	PG4	C4-C3-O2-C2
5	A	728	PG4	C4-C3-O2-C2
4	A	710	PGE	C3-C4-O3-C5
9	A	771	PE8	C21-C20-O19-C18
3	A	707	P6G	C5-C6-O7-C8
4	A	710	PGE	C1-C2-O2-C3
3	A	707	P6G	C8-C9-O10-C11
4	A	754	PGE	C1-C2-O2-C3
5	A	751	PG4	C8-C7-O4-C6
6	A	761	PEG	C4-C3-O2-C2
5	A	752	PG4	C4-C3-O2-C2
4	A	710	PGE	O3-C5-C6-O4
6	A	739	PEG	O1-C1-C2-O2
9	A	771	PE8	O22-C23-C24-O25
5	A	716	PG4	C3-C4-O3-C5
4	A	715	PGE	C6-C5-O3-C4
6	A	720	PEG	C4-C3-O2-C2
3	A	707	P6G	C18-C17-O16-C15
5	A	752	PG4	C6-C5-O3-C4
5	A	772	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
7	A	725	EDO	O1-C1-C2-O2
4	A	748	PGE	C3-C4-O3-C5
4	A	768	PGE	C6-C5-O3-C4
5	A	728	PG4	C6-C5-O3-C4
6	A	714	PEG	C4-C3-O2-C2
8	A	721	1PE	C24-C14-OH5-C25
5	A	753	PG4	C8-C7-O4-C6
5	A	751	PG4	C3-C4-O3-C5
4	A	710	PGE	C4-C3-O2-C2
5	A	772	PG4	C3-C4-O3-C5
4	A	715	PGE	C1-C2-O2-C3
6	A	757	PEG	C1-C2-O2-C3
4	A	741	PGE	C1-C2-O2-C3
4	A	711	PGE	C1-C2-O2-C3
4	A	768	PGE	C3-C4-O3-C5
5	A	727	PG4	C3-C4-O3-C5
5	A	712	PG4	C8-C7-O4-C6
6	A	739	PEG	C4-C3-O2-C2
6	A	790	PEG	C4-C3-O2-C2
8	A	721	1PE	C13-C23-OH3-C22
5	A	727	PG4	O3-C5-C6-O4
6	A	787	PEG	C1-C2-O2-C3
4	A	718	PGE	O3-C5-C6-O4
5	A	712	PG4	O4-C7-C8-O5
7	A	770	EDO	O1-C1-C2-O2
4	A	729	PGE	C6-C5-O3-C4
5	A	751	PG4	C4-C3-O2-C2
5	A	772	PG4	O2-C3-C4-O3
4	A	777	PGE	C6-C5-O3-C4
4	A	733	PGE	C1-C2-O2-C3
4	A	722	PGE	C6-C5-O3-C4
4	A	715	PGE	O1-C1-C2-O2
4	A	736	PGE	O3-C5-C6-O4
6	A	773	PEG	O1-C1-C2-O2
5	A	716	PG4	C1-C2-O2-C3
4	A	715	PGE	O2-C3-C4-O3
6	A	781	PEG	C1-C2-O2-C3
8	A	721	1PE	C14-C24-OH4-C13
5	A	751	PG4	C5-C6-O4-C7
5	A	753	PG4	C6-C5-O3-C4
5	A	752	PG4	C5-C6-O4-C7
6	A	758	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
5	A	712	PG4	O3-C5-C6-O4
4	A	738	PGE	O3-C5-C6-O4
6	A	713	PEG	O1-C1-C2-O2
7	A	743	EDO	O1-C1-C2-O2
7	A	786	EDO	O1-C1-C2-O2
5	A	772	PG4	C1-C2-O2-C3
5	A	716	PG4	O4-C7-C8-O5
4	A	729	PGE	C3-C4-O3-C5
6	A	740	PEG	C4-C3-O2-C2
4	A	777	PGE	O2-C3-C4-O3
4	A	724	PGE	C1-C2-O2-C3
6	A	745	PEG	O1-C1-C2-O2
5	A	753	PG4	O3-C5-C6-O4
7	A	783	EDO	O1-C1-C2-O2
4	A	708	PGE	C1-C2-O2-C3
5	A	765	PG4	O3-C5-C6-O4
5	A	765	PG4	C5-C6-O4-C7
4	A	722	PGE	O1-C1-C2-O2
5	A	756	PG4	O4-C7-C8-O5
6	A	759	PEG	C1-C2-O2-C3
5	A	716	PG4	O2-C3-C4-O3
4	A	742	PGE	O3-C5-C6-O4
4	A	755	PGE	O2-C3-C4-O3
4	A	710	PGE	O2-C3-C4-O3
5	A	756	PG4	C3-C4-O3-C5
5	A	712	PG4	C5-C6-O4-C7
8	A	721	1PE	OH4-C13-C23-OH3

There are no ring outliers.

37 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	709	PGE	1	0
7	A	747	EDO	1	0
4	A	768	PGE	2	0
6	A	776	PEG	2	0
6	A	787	PEG	1	0
6	A	723	PEG	1	0
6	A	720	PEG	1	0
6	A	739	PEG	1	0
7	A	767	EDO	1	0
4	A	711	PGE	1	0

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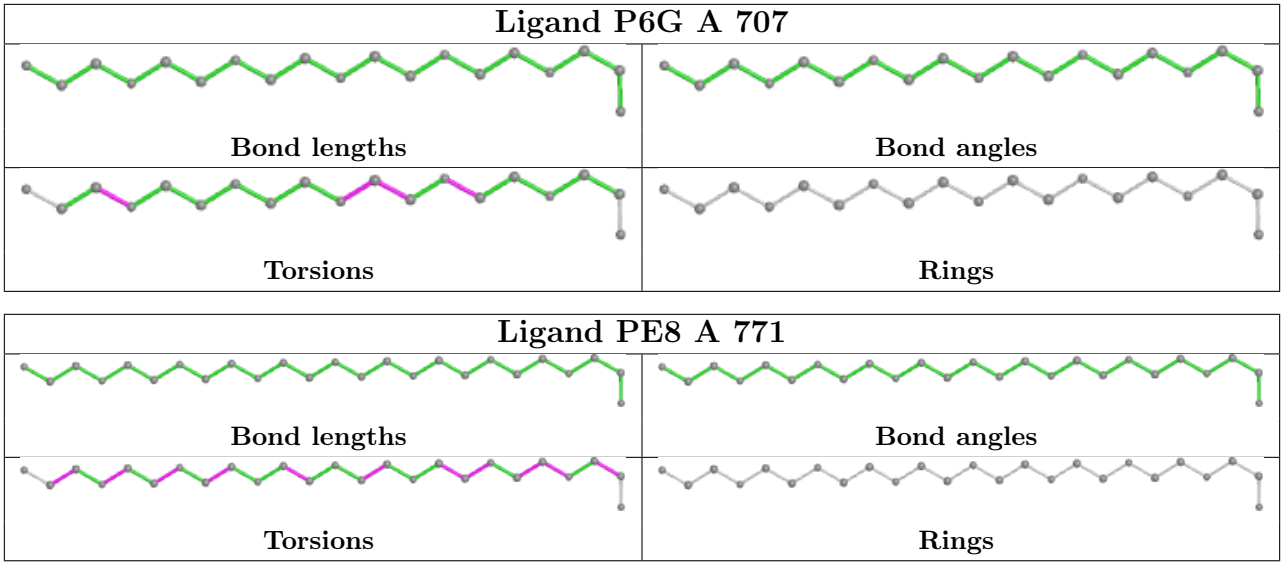
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	777	PGE	1	0
8	A	721	1PE	2	0
6	A	746	PEG	2	0
6	A	713	PEG	2	0
7	A	791	EDO	1	0
5	A	751	PG4	1	0
4	A	736	PGE	2	0
7	A	785	EDO	1	0
6	A	761	PEG	2	0
5	A	752	PG4	1	0
3	A	707	P6G	2	0
4	A	710	PGE	2	0
4	A	724	PGE	2	0
6	A	757	PEG	1	0
7	A	774	EDO	1	0
7	A	725	EDO	1	0
4	A	715	PGE	4	0
5	A	756	PG4	1	0
5	A	727	PG4	1	0
5	A	728	PG4	7	0
9	A	771	PE8	8	0
4	A	730	PGE	4	0
4	A	722	PGE	1	0
5	A	712	PG4	2	0
5	A	772	PG4	1	0
6	A	789	PEG	2	0
4	A	718	PGE	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.



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	677/695 (97%)	0.02	22 (3%) 47 54	15, 23, 43, 78	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	THR	6.9
1	A	355	THR	6.2
1	A	661	ALA	5.0
1	A	246	LEU	4.3
1	A	4	ARG	4.1
1	A	354[A]	GLN	4.1
1	A	3	THR	4.0
1	A	134	TRP	3.8
1	A	664	LEU	3.6
1	A	132	HIS	3.5
1	A	678	THR	3.2
1	A	665	ARG	2.9
1	A	227[A]	GLY	2.7
1	A	438	GLN	2.6
1	A	663	ASP	2.5
1	A	666	THR	2.3
1	A	146	PHE	2.2
1	A	22	GLU	2.2
1	A	135	ILE	2.2
1	A	436	GLU	2.2
1	A	116	ILE	2.1
1	A	581	GLN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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
7	EDO	A	770	4/4	0.37	0.30	87,88,90,91	0
6	PEG	A	758	7/7	0.50	0.40	74,79,84,85	0
6	PEG	A	723	7/7	0.55	0.23	58,69,71,74	0
5	PG4	A	772	13/13	0.57	0.33	65,88,92,94	0
6	PEG	A	788	7/7	0.60	0.25	68,71,73,74	0
6	PEG	A	789	7/7	0.60	0.17	75,77,80,80	0
6	PEG	A	713	7/7	0.60	0.24	50,57,65,68	0
6	PEG	A	787	7/7	0.61	0.23	76,77,77,79	0
7	EDO	A	775	4/4	0.61	0.29	79,80,80,81	0
7	EDO	A	780	4/4	0.62	0.31	60,67,70,72	0
7	EDO	A	744	4/4	0.63	0.23	65,66,70,74	0
7	EDO	A	766	4/4	0.65	0.23	73,74,75,75	0
4	PGE	A	718	10/10	0.68	0.24	59,63,76,77	0
6	PEG	A	773	7/7	0.69	0.26	60,68,75,75	0
6	PEG	A	740	7/7	0.69	0.20	64,74,80,81	0
6	PEG	A	714	7/7	0.69	0.29	77,78,82,83	0
5	PG4	A	728	13/13	0.71	0.30	51,87,97,98	0
4	PGE	A	742	10/10	0.71	0.20	63,68,70,70	0
6	PEG	A	732	7/7	0.72	0.20	59,67,69,70	0
4	PGE	A	729	10/10	0.72	0.32	72,80,83,84	0
4	PGE	A	724	10/10	0.73	0.35	59,65,78,81	0
7	EDO	A	764	4/4	0.73	0.16	66,68,69,72	0
4	PGE	A	755	10/10	0.73	0.30	33,65,75,76	0
5	PG4	A	753	13/13	0.74	0.33	77,86,98,98	0
6	PEG	A	761	7/7	0.74	0.18	70,72,74,77	0
7	EDO	A	786	4/4	0.75	0.23	69,69,74,78	0
6	PEG	A	735	7/7	0.76	0.28	70,73,84,85	0
9	PE8	A	771	25/25	0.76	0.27	50,73,81,83	0
4	PGE	A	754	10/10	0.77	0.26	28,74,81,82	0
6	PEG	A	745	7/7	0.77	0.31	58,70,81,84	0
7	EDO	A	792	4/4	0.78	0.18	74,74,75,77	0
5	PG4	A	756	13/13	0.78	0.23	51,68,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	A	731	4/4	0.79	0.15	67,67,69,71	0
4	PGE	A	738	10/10	0.79	0.18	72,76,78,79	0
5	PG4	A	751	13/13	0.79	0.39	68,73,78,78	0
6	PEG	A	757	7/7	0.79	0.29	68,75,77,79	0
7	EDO	A	717	4/4	0.79	0.18	71,71,74,74	0
7	EDO	A	791	4/4	0.80	0.18	75,76,79,79	0
7	EDO	A	784	4/4	0.80	0.14	68,68,70,71	0
4	PGE	A	730	10/10	0.80	0.15	66,73,73,75	0
6	PEG	A	746	7/7	0.81	0.26	66,72,75,75	0
7	EDO	A	749	4/4	0.81	0.15	56,57,58,63	0
5	PG4	A	765	13/13	0.81	0.28	67,69,73,74	0
5	PG4	A	727	13/13	0.82	0.20	46,55,67,68	0
7	EDO	A	782	4/4	0.82	0.23	52,54,56,57	0
5	PG4	A	712	13/13	0.82	0.20	49,68,74,75	0
5	PG4	A	716	13/13	0.82	0.21	47,62,69,72	0
6	PEG	A	781	7/7	0.82	0.20	47,64,65,67	0
6	PEG	A	739	7/7	0.82	0.31	73,76,86,89	0
7	EDO	A	778	4/4	0.82	0.22	70,71,73,75	0
4	PGE	A	708	10/10	0.83	0.18	37,41,44,50	0
4	PGE	A	715	10/10	0.83	0.21	29,52,59,59	0
3	P6G	A	707	19/19	0.83	0.20	28,47,72,73	0
7	EDO	A	785	4/4	0.83	0.15	48,51,52,52	0
7	EDO	A	767	4/4	0.84	0.28	61,71,78,82	0
6	PEG	A	737	7/7	0.84	0.27	42,45,49,50	0
6	PEG	A	763	7/7	0.85	0.20	29,55,67,68	0
5	PG4	A	752	13/13	0.85	0.32	37,63,73,74	0
6	PEG	A	759	7/7	0.85	0.31	61,68,72,76	0
8	1PE	A	721	16/16	0.85	0.15	26,62,72,72	0
4	PGE	A	777	10/10	0.85	0.15	39,48,52,55	0
7	EDO	A	774	4/4	0.86	0.32	61,64,71,72	0
4	PGE	A	733	10/10	0.87	0.19	41,49,56,63	0
7	EDO	A	793	4/4	0.87	0.24	62,66,67,70	0
6	PEG	A	776	7/7	0.88	0.14	39,46,47,49	0
4	PGE	A	736	10/10	0.88	0.20	48,59,65,65	0
4	PGE	A	711	10/10	0.88	0.14	38,42,59,66	0
7	EDO	A	726	4/4	0.88	0.10	59,60,62,62	0
7	EDO	A	783	4/4	0.89	0.17	66,67,68,71	0
7	EDO	A	750	4/4	0.89	0.12	66,67,68,69	0
7	EDO	A	725	4/4	0.89	0.10	51,54,55,58	0
4	PGE	A	768	10/10	0.90	0.15	29,42,59,66	0
6	PEG	A	790	7/7	0.90	0.16	41,60,74,77	0
7	EDO	A	769	4/4	0.90	0.14	63,66,67,70	0

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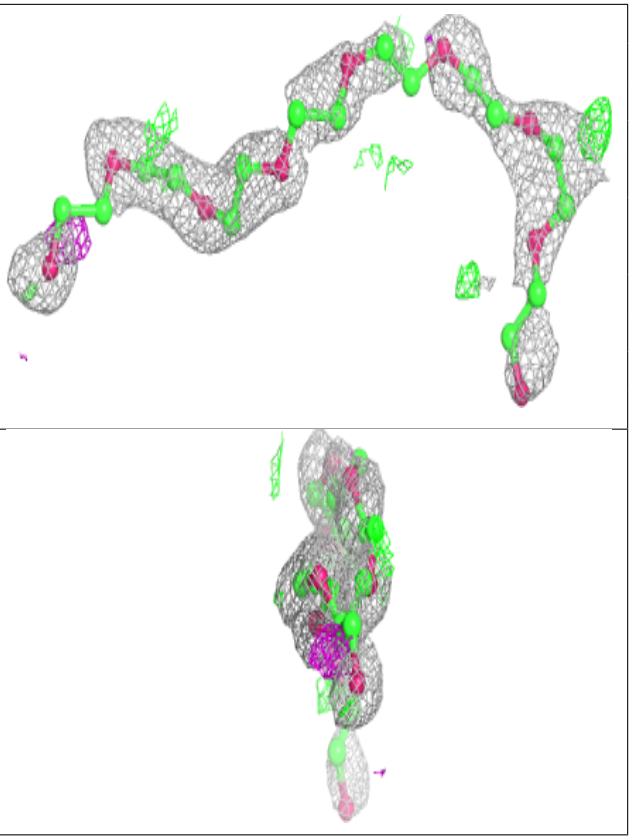
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PGE	A	710	10/10	0.90	0.15	44,52,54,60	0
7	EDO	A	760	4/4	0.90	0.32	74,74,74,77	0
7	EDO	A	743	4/4	0.90	0.19	59,60,64,65	0
6	PEG	A	734	7/7	0.91	0.10	31,32,41,53	0
7	EDO	A	719	4/4	0.92	0.10	50,55,58,63	0
4	PGE	A	722	10/10	0.92	0.12	26,35,50,58	0
6	PEG	A	720	7/7	0.92	0.16	54,55,61,65	0
4	PGE	A	741	10/10	0.92	0.20	36,49,60,61	0
7	EDO	A	779	4/4	0.93	0.24	42,57,68,77	0
7	EDO	A	762	4/4	0.93	0.23	41,44,52,55	0
7	EDO	A	747	4/4	0.93	0.25	30,33,44,46	0
4	PGE	A	748	10/10	0.93	0.16	41,53,65,69	0
4	PGE	A	709	10/10	0.96	0.08	25,30,39,41	0
2	CL	A	706	1/1	0.99	0.08	19,19,19,19	0
2	CL	A	705	1/1	0.99	0.11	19,19,19,19	0
2	CL	A	702	1/1	1.00	0.12	19,19,19,19	0
2	CL	A	703	1/1	1.00	0.09	19,19,19,19	0
2	CL	A	704	1/1	1.00	0.10	19,19,19,19	0
2	CL	A	701	1/1	1.00	0.08	19,19,19,19	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.

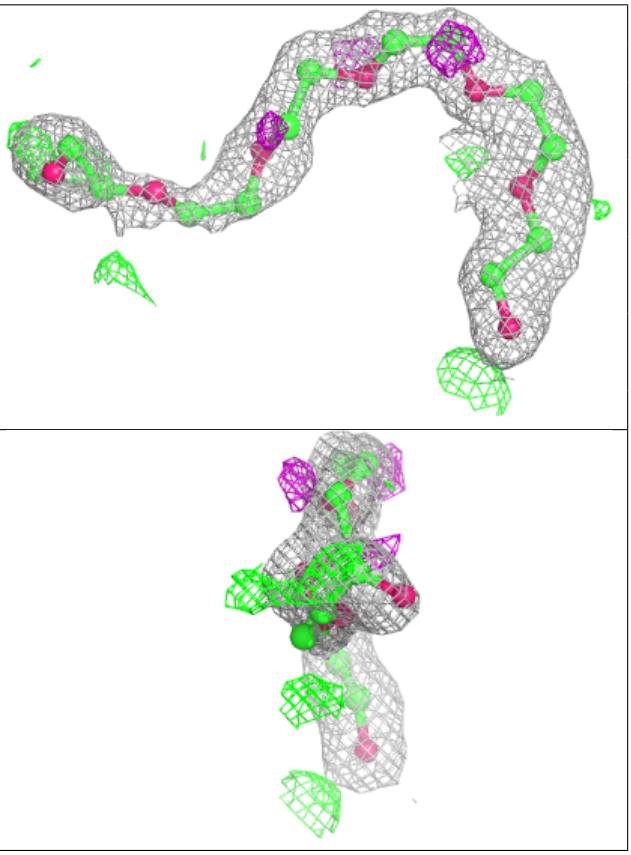
Electron density around PE8 A 771:

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



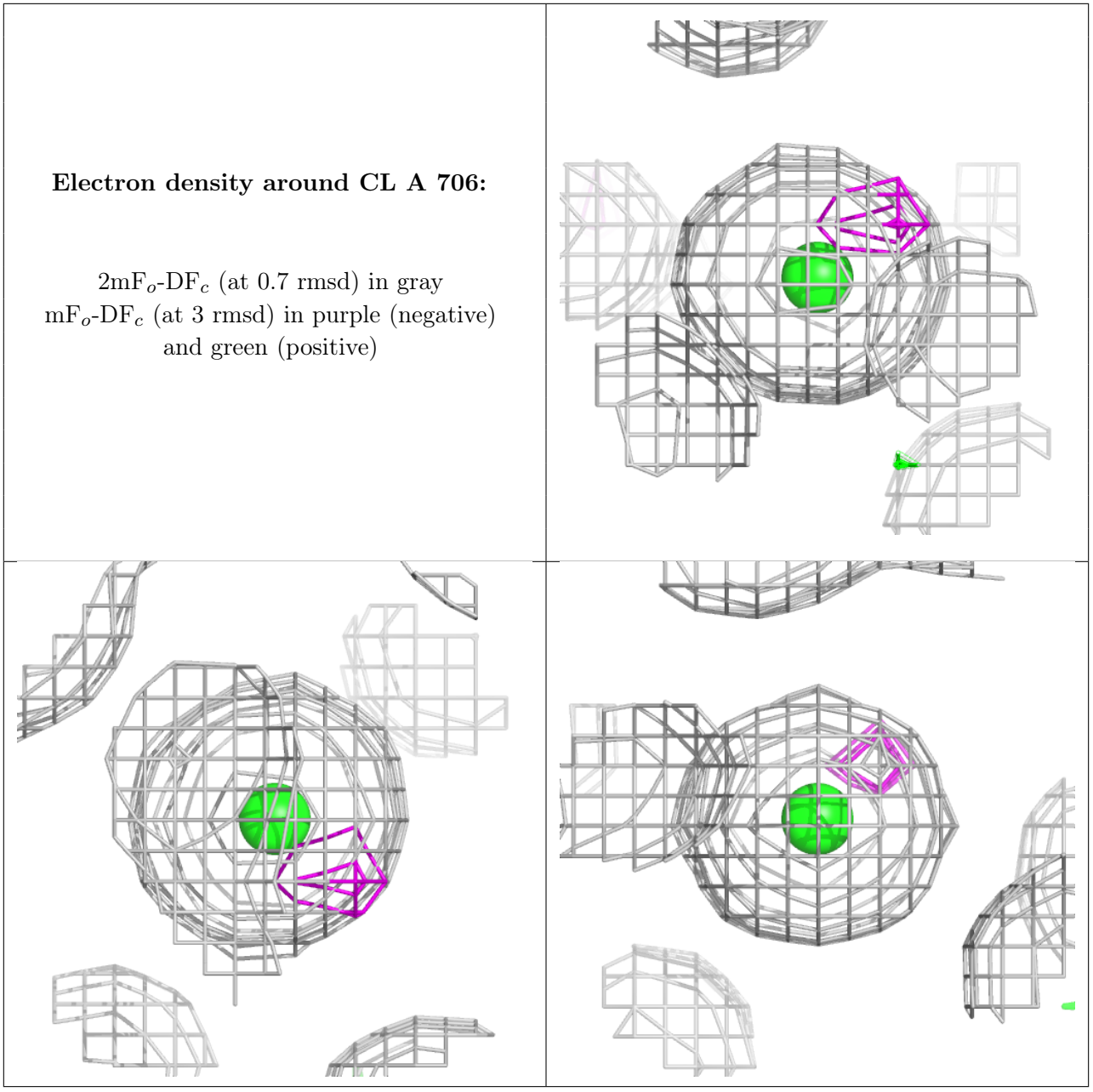
Electron density around P6G A 707:

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



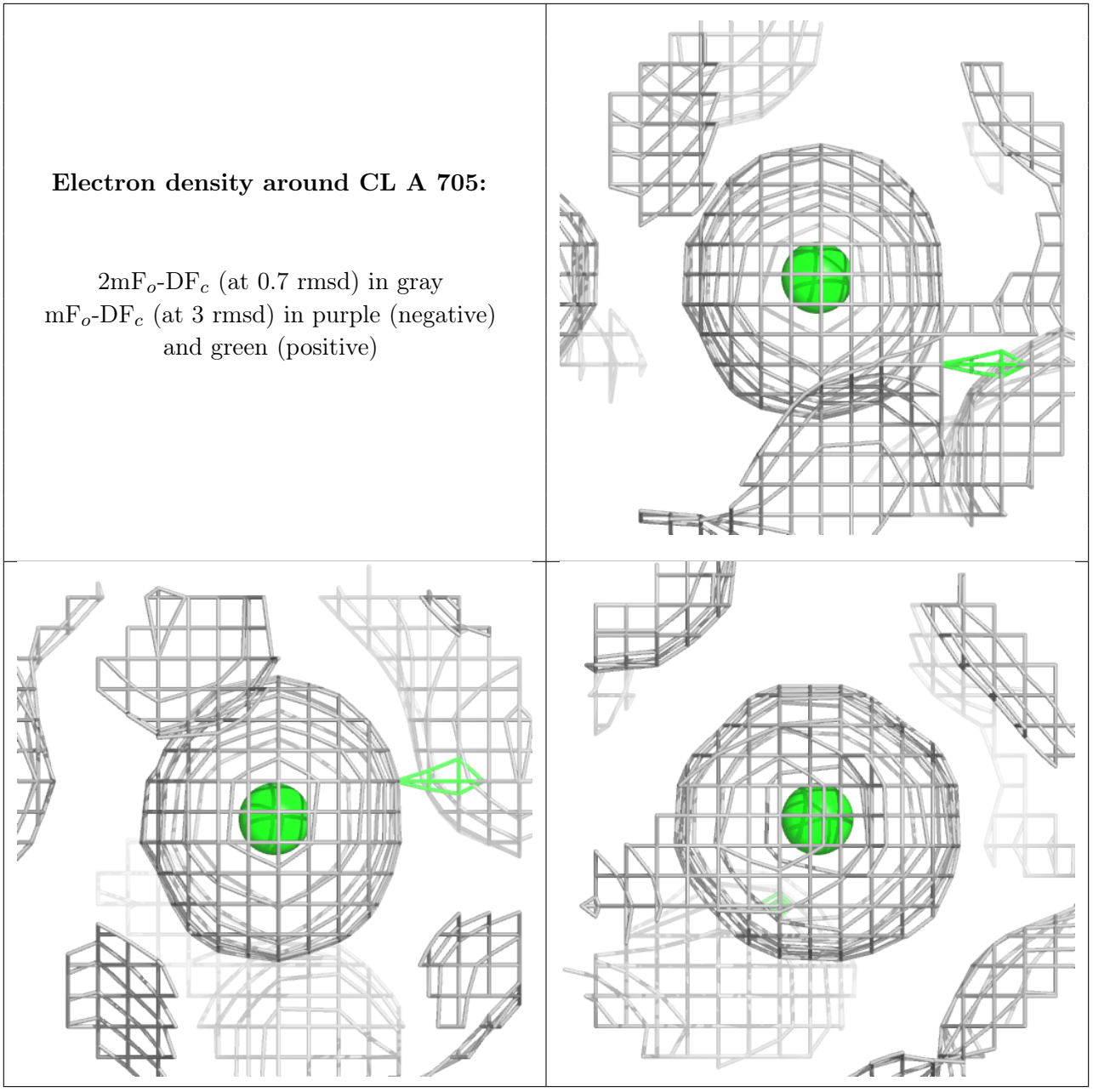
Electron density around CL A 706:

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



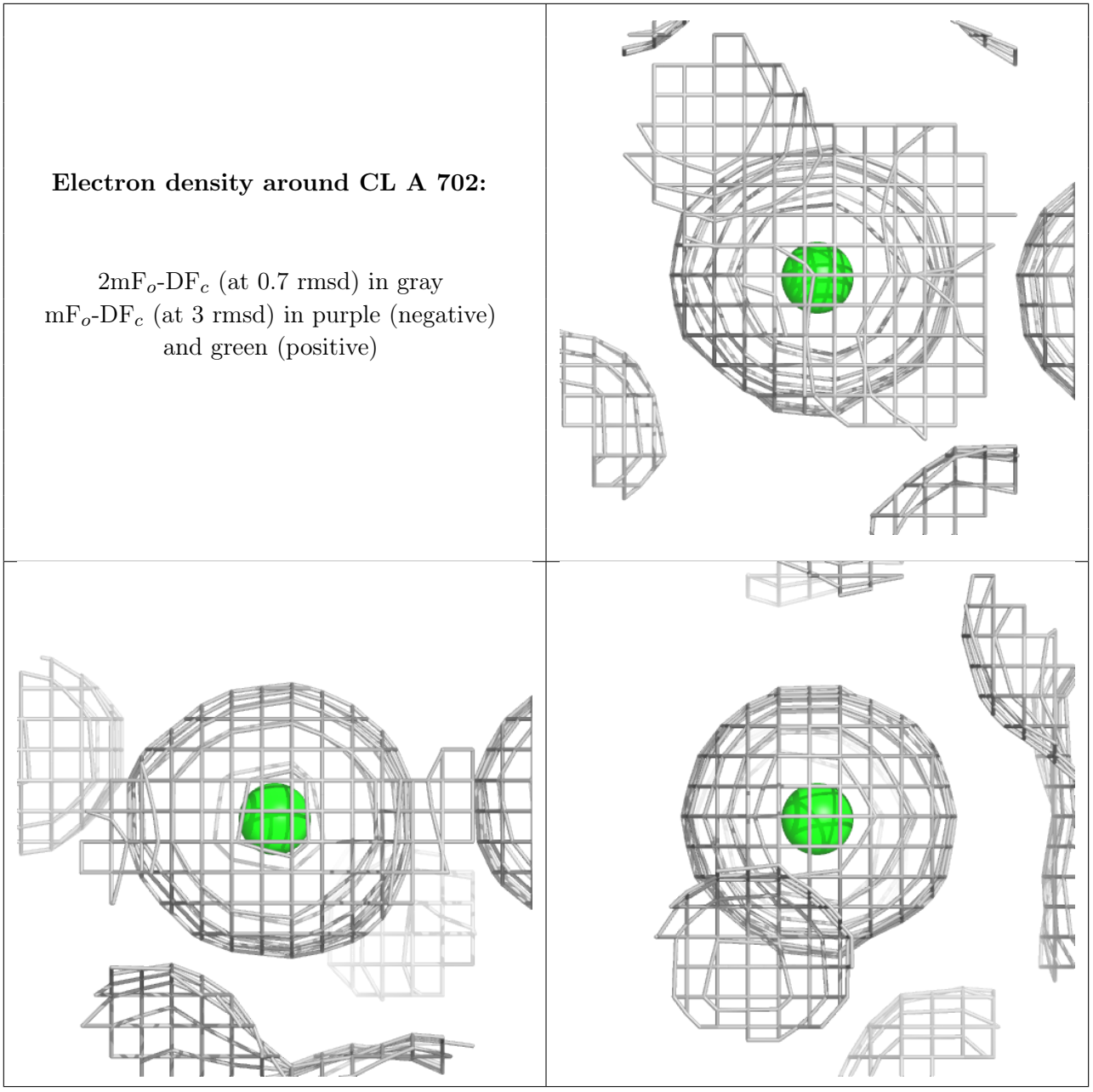
Electron density around CL A 705:

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



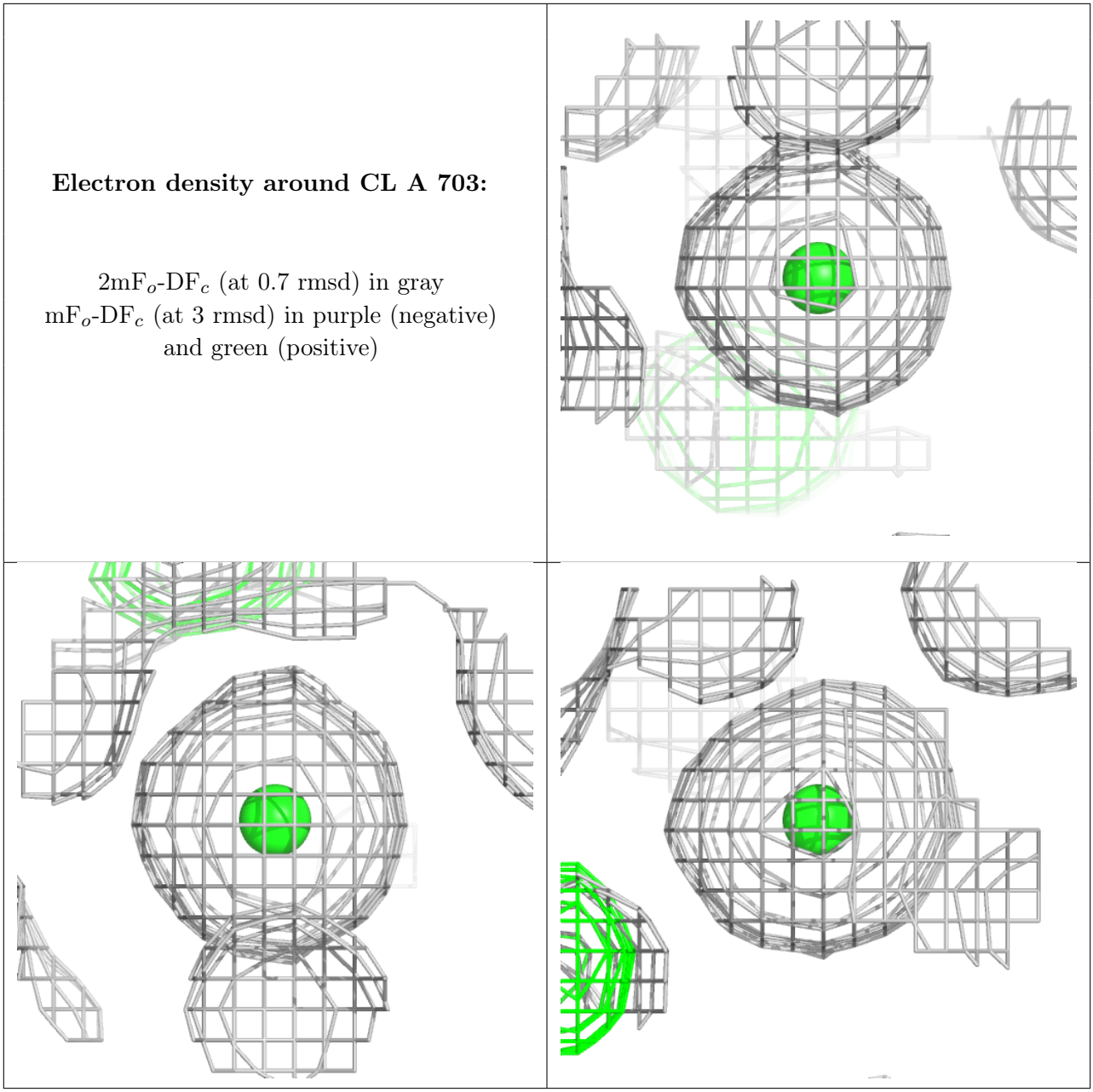
Electron density around CL A 702:

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



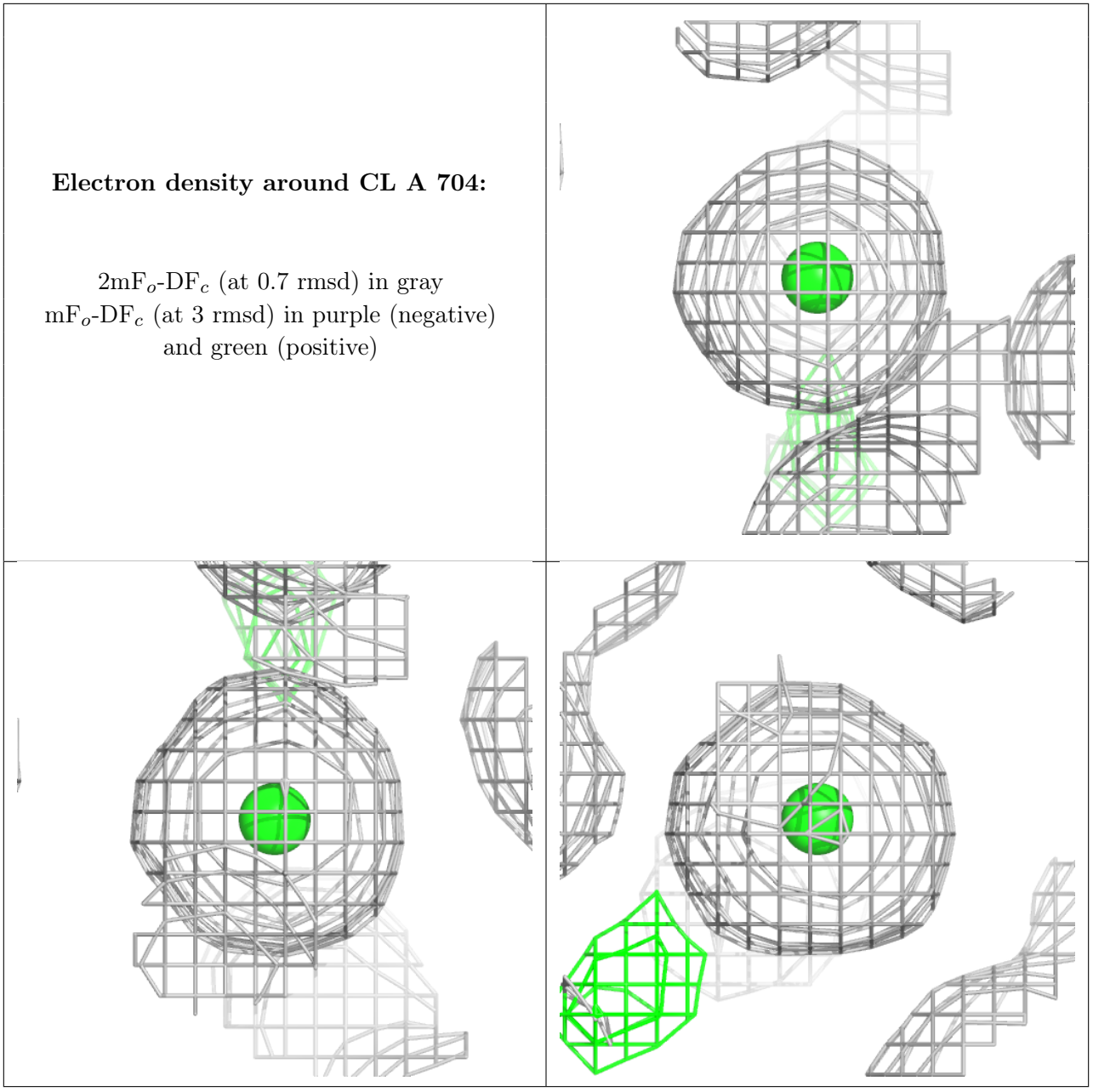
Electron density around CL A 703:

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



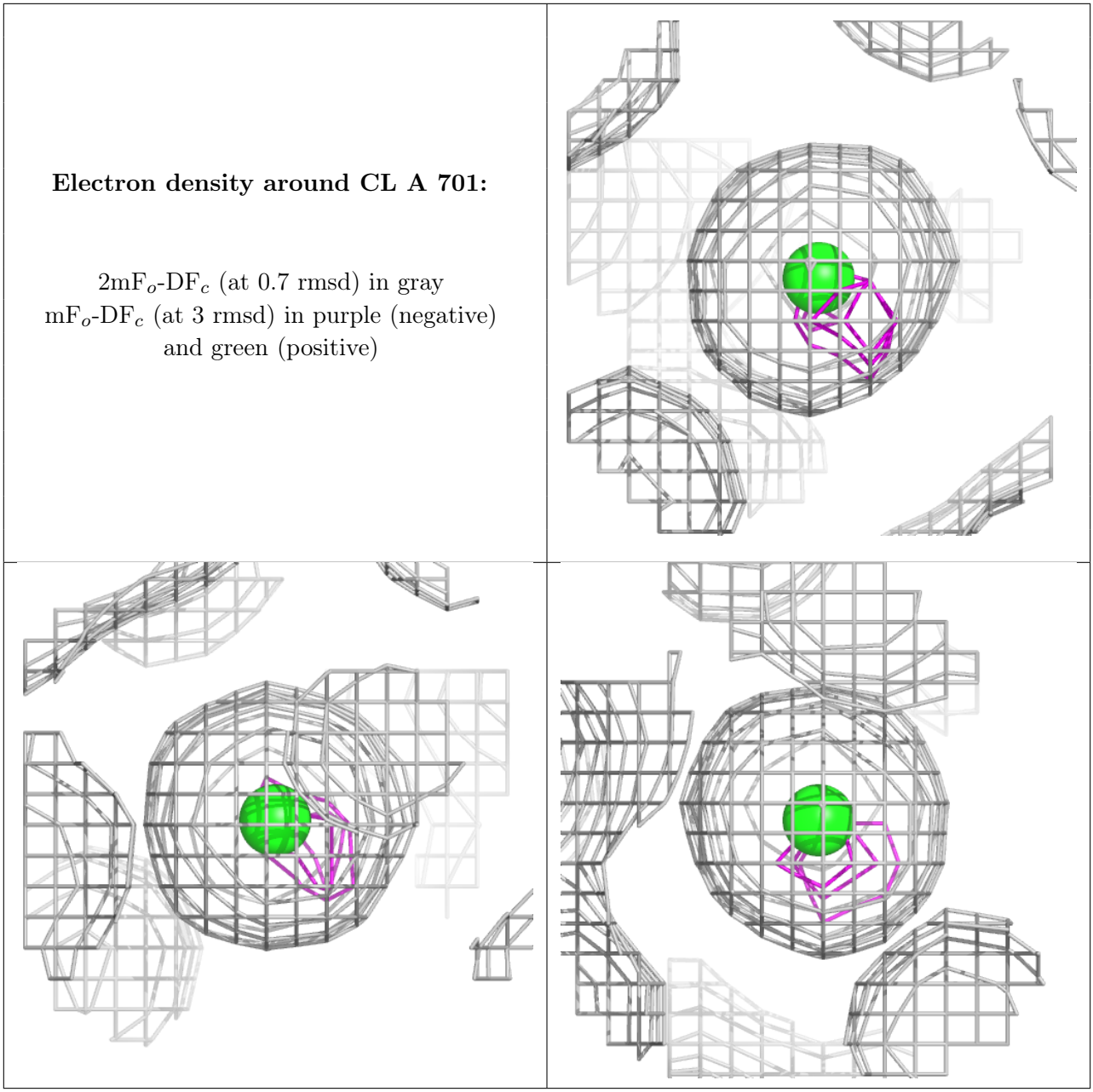
Electron density around CL A 704:

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



Electron density around CL A 701:

$2mF_o$-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.