



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:18 PM UTC

PDB ID : 8JT1 / pdb_00008jt1
Title : COLLAGENASE FROM GRIMONTIA (VIBRIO) HOLLISAE 1706B COM-
PLEXED WITH GLY-PRO-HYP-GLY-PRO-HYP
Authors : Ueshima, S.; Yaskawa, K.; Takita, T.; Mikami, B.
Deposited on : 2023-06-21
Resolution : 2.00 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

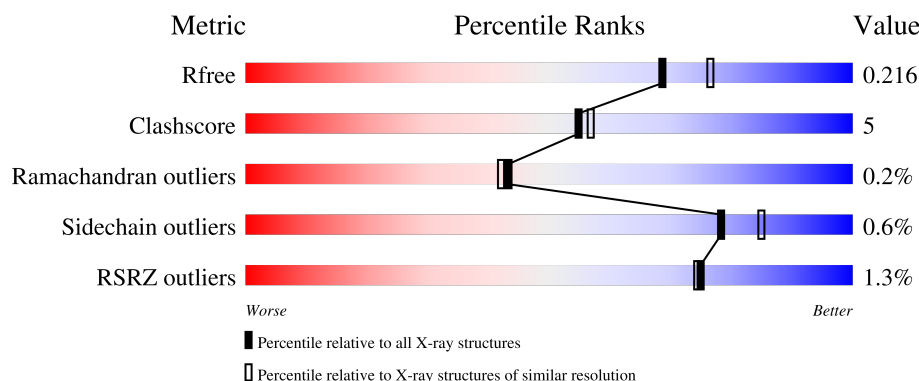
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	559	88% 8% 5%
1	B	559	87% 8% 5%
2	C	6	17% 33% 50% 17%
2	E	6	50% 50%
2	F	6	17% 17% 33% 50%

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Mol	Chain	Length	Quality of chain
2	G	6	
2	I	6	
2	J	6	

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	EDO	B	732	-	-	X	-
5	EDO	B	742	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 9660 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 Microbial collagenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	9	0
			4251	2692	713	827	19			
1	B	532	Total	C	N	O	S	0	7	0
			4246	2689	711	827	19			

- Molecule 2 is a protein called 6-mer peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			39	24	6	9			
2	E	6	Total	C	N	O	0	0	0
			39	24	6	9			
2	F	3	Total	C	N	O	0	0	0
			19	12	3	4			
2	G	6	Total	C	N	O	0	0	0
			39	24	6	9			
2	I	6	Total	C	N	O	0	0	0
			39	24	6	9			
2	J	3	Total	C	N	O	0	0	0
			19	12	3	4			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Ca 4 4	0	0
4	B	4	Total Ca 4 4	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

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

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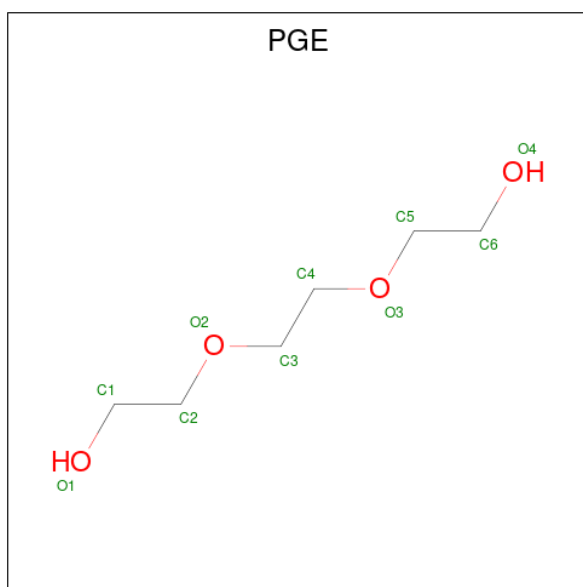
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total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

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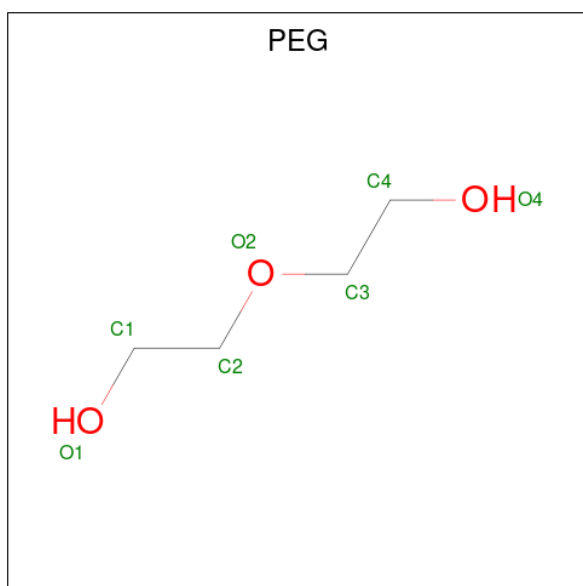
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total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

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$) (labeled as "Ligand of Interest" by depositor).



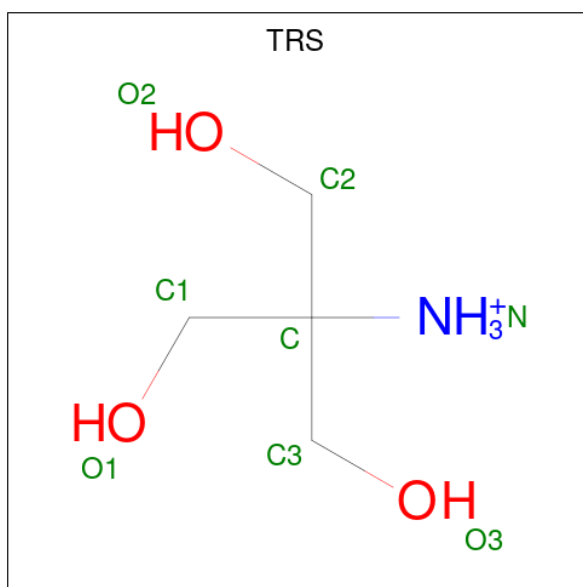
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$) (labeled as "Ligand of Interest" by depositor).



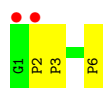
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	269	Total	O	0	2
			271	271		
9	B	288	Total	O	0	0
			288	288		
9	C	5	Total	O	0	0
			5	5		
9	E	7	Total	O	0	0
			7	7		
9	G	2	Total	O	0	0
			2	2		
9	I	4	Total	O	0	0
			4	4		
9	J	1	Total	O	0	0
			1	1		



- Molecule 2: 6-mer peptide



- Molecule 2: 6-mer peptide



- Molecule 2: 6-mer peptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	178.02Å 74.89Å 135.13Å 90.00° 126.02° 90.00°	Depositor
Resolution (Å)	37.44 – 2.00 37.44 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.44-2.00) 99.5 (37.44-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.176 , 0.214 0.182 , 0.216	Depositor DCC
R_{free} test set	4826 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9660	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, EDO, PGE, ZN, HYP, PEG, CA

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	0.28	0/4386	0.46	0/5977
1	B	0.29	0/4373	0.47	0/5960
2	C	0.22	0/22	0.55	0/28
2	E	0.30	0/22	0.42	0/28
2	F	0.24	0/11	0.51	0/14
2	G	0.28	0/22	0.42	0/28
2	I	0.26	0/22	0.55	0/28
2	J	0.34	0/11	0.37	0/14
All	All	0.28	0/8869	0.47	0/12077

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 [i](#)

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	4251	0	3947	35	0
1	B	4246	0	3925	42	0
2	C	39	0	36	4	0
2	E	39	0	36	1	0
2	F	19	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	39	0	36	2	0
2	I	39	0	36	0	0
2	J	19	0	16	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	176	0	264	21	0
5	B	180	0	270	26	0
6	A	10	0	14	0	0
7	B	7	0	10	2	0
8	B	8	0	12	0	0
9	A	271	0	0	3	0
9	B	288	0	0	3	0
9	C	5	0	0	2	0
9	E	7	0	0	0	0
9	G	2	0	0	0	0
9	I	4	0	0	0	0
9	J	1	0	0	0	0
All	All	9660	0	8618	85	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 (85) 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:554:THR:H	5:A:727:EDO:H21	1.35	0.91
1:B:251:ARG:HE	7:B:751:PEG:H22	1.33	0.91
1:B:544:THR:H	5:B:709:EDO:H11	1.45	0.82
1:B:462:GLY:H	5:B:732:EDO:H12	1.51	0.76
1:B:386:LYS:NZ	9:B:801:HOH:O	2.21	0.74
1:B:133:SER:HB2	5:B:723:EDO:H21	1.70	0.72
1:B:251:ARG:HH22	5:B:716:EDO:H22	1.56	0.70
1:B:265:GLN:HG2	5:B:735:EDO:H22	1.73	0.70
1:B:211:LYS:HD2	5:B:734:EDO:H11	1.72	0.69
1:A:311:ARG:HG2	5:A:739:EDO:H12	1.75	0.68
1:A:314:ARG:HG3	1:A:355:TYR:CD1	2.30	0.66
1:A:491:GLU:HB2	5:A:722:EDO:H12	1.77	0.65
1:B:590:ARG:HH11	5:B:742:EDO:H21	1.61	0.64
2:C:1:GLY:N	9:C:102:HOH:O	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2:PRO:O	9:C:101:HOH:O	2.16	0.63
1:B:462:GLY:H	5:B:732:EDO:C1	2.13	0.61
1:B:565:ARG:HE	5:B:736:EDO:HO1	1.50	0.60
1:A:492:HIS:HB2	5:A:722:EDO:H21	1.85	0.58
5:A:724:EDO:H11	5:A:726:EDO:H12	1.85	0.58
1:B:157:ASP:HB2	5:B:724:EDO:H21	1.88	0.56
5:A:723:EDO:H22	9:A:851:HOH:O	2.05	0.55
1:A:386:LYS:HD2	5:A:728:EDO:O2	2.06	0.55
1:A:315:TYR:CE2	5:A:739:EDO:H21	2.42	0.55
1:B:499:ASP:OD2	5:B:729:EDO:O2	2.25	0.53
1:A:314:ARG:HG3	1:A:355:TYR:CE1	2.43	0.52
1:B:269:GLN:HG2	5:B:714:EDO:H12	1.90	0.52
1:B:587:SER:HA	5:B:742:EDO:H22	1.91	0.51
1:A:230:LEU:HD13	1:A:277:GLN:HG3	1.92	0.51
1:A:412:HIS:O	5:A:741:EDO:H21	2.10	0.51
1:A:555:TYR:H	5:A:725:EDO:H12	1.75	0.51
1:A:381:CYS:SG	1:A:401[B]:CYS:HB2	2.51	0.51
1:B:590:ARG:HD2	5:B:742:EDO:H21	1.93	0.50
5:A:730:EDO:H11	9:A:1003:HOH:O	2.11	0.50
1:B:462:GLY:N	5:B:732:EDO:H12	2.25	0.49
1:A:200:ALA:HB3	5:A:713:EDO:H11	1.95	0.49
1:B:312:LEU:HD23	5:B:735:EDO:H12	1.94	0.49
1:B:591:GLN:HA	5:B:727:EDO:H22	1.95	0.48
1:B:593:ARG:HG2	1:B:593:ARG:HH11	1.78	0.48
1:B:508:PHE:CD1	2:G:2:PRO:HD3	2.49	0.48
1:B:381[B]:CYS:SG	1:B:387:ILE:HG13	2.54	0.48
1:A:429:GLN:OE1	5:A:710:EDO:H22	2.14	0.48
1:B:315:TYR:OH	5:B:735:EDO:H21	2.14	0.48
1:A:489:ASN:HA	5:A:722:EDO:O1	2.14	0.47
1:A:262:PHE:CE2	2:F:5:PRO:HB3	2.50	0.46
1:A:458:MET:HE2	1:A:458:MET:HB2	1.82	0.46
1:A:358:CYS:SG	1:A:364[B]:CYS:HB3	2.56	0.45
5:A:724:EDO:O2	2:C:2:PRO:HG3	2.17	0.45
1:A:429:GLN:O	1:A:471:PRO:HD2	2.15	0.45
1:A:146:THR:HG21	9:A:1027:HOH:O	2.16	0.45
1:A:200:ALA:HA	5:A:737:EDO:H21	1.99	0.45
1:A:574:MET:HE2	1:A:604:TRP:CE3	2.52	0.45
1:B:590:ARG:HH11	5:B:742:EDO:C2	2.30	0.45
1:A:574:MET:HE2	1:A:604:TRP:CD2	2.51	0.44
1:B:487:VAL:HB	1:B:490:LEU:HB2	2.00	0.44
1:A:469:ASN:O	1:A:470:ILE:HD13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:ILE:HD12	1:B:619:LEU:HG	1.99	0.44
1:A:388:ARG:HD3	5:A:728:EDO:H11	1.99	0.44
1:B:251:ARG:NE	7:B:751:PEG:H22	2.16	0.44
1:B:306:ALA:HB1	1:B:348:ALA:HB2	1.98	0.44
1:B:593:ARG:NH2	9:B:812:HOH:O	2.51	0.44
1:A:281:VAL:HG12	1:A:285[A]:GLN:OE1	2.18	0.44
1:B:460:LEU:HA	5:B:732:EDO:H11	2.00	0.44
5:A:744:EDO:H22	2:C:3:HYP:HG	2.00	0.43
1:A:517:TRP:CG	1:A:518:TRP:N	2.87	0.43
1:A:307:ARG:HH22	5:A:719:EDO:H11	1.82	0.43
1:B:287:PHE:CZ	1:B:293:LYS:HE2	2.54	0.43
1:A:544:THR:HA	1:A:566:TRP:CZ2	2.54	0.43
1:B:565:ARG:HG3	5:B:736:EDO:O2	2.19	0.43
1:A:171:TYR:HA	2:E:2:PRO:HG2	2.01	0.43
1:B:438:ASP:OD1	1:B:439:THR:N	2.52	0.43
1:B:275:GLY:HA3	5:B:718:EDO:H12	2.01	0.43
1:A:555:TYR:H	5:A:725:EDO:C1	2.32	0.42
1:B:508:PHE:CE1	2:G:2:PRO:HD3	2.55	0.42
1:B:429:GLN:O	1:B:471:PRO:HD2	2.19	0.41
2:J:4:GLY:HA2	2:J:5:PRO:HD3	1.90	0.41
1:A:496:HIS:O	5:A:724:EDO:H22	2.20	0.41
1:A:601:ILE:HG22	1:A:604:TRP:CZ3	2.56	0.41
1:A:580:ASP:OD1	1:A:580:ASP:N	2.54	0.41
1:B:248:TRP:CE2	5:B:743:EDO:H22	2.55	0.41
1:B:608:TYR:HD1	5:B:737:EDO:H11	1.86	0.41
1:B:262:PHE:CD2	5:B:746:EDO:H11	2.56	0.41
1:B:495:VAL:HG11	1:B:523:ALA:HA	2.03	0.41
1:A:281:VAL:O	1:A:285[A]:GLN:HG3	2.20	0.41
1:B:235:GLN:HG3	5:B:730:EDO:H22	2.03	0.41
1:B:323:LYS:NZ	9:B:803:HOH:O	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	539/559 (96%)	534 (99%)	4 (1%)	1 (0%)	43	42
1	B	537/559 (96%)	528 (98%)	8 (2%)	1 (0%)	43	42
2	C	3/6 (50%)	3 (100%)	0	0	100	100
2	E	3/6 (50%)	3 (100%)	0	0	100	100
2	F	1/6 (17%)	1 (100%)	0	0	100	100
2	G	3/6 (50%)	3 (100%)	0	0	100	100
2	I	3/6 (50%)	3 (100%)	0	0	100	100
2	J	1/6 (17%)	1 (100%)	0	0	100	100
All	All	1090/1154 (94%)	1076 (99%)	12 (1%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	529	VAL
1	B	529	VAL

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	437/442 (99%)	435 (100%)	2 (0%)	81	87
1	B	434/442 (98%)	430 (99%)	4 (1%)	70	78
2	C	2/2 (100%)	2 (100%)	0	100	100
2	E	2/2 (100%)	2 (100%)	0	100	100
2	F	1/2 (50%)	1 (100%)	0	100	100
2	G	2/2 (100%)	2 (100%)	0	100	100
2	I	2/2 (100%)	2 (100%)	0	100	100
2	J	1/2 (50%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	881/896 (98%)	875 (99%)	6 (1%)	78	82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	SER
1	A	319	THR
1	B	146	THR
1	B	316	THR
1	B	326[A]	GLU
1	B	326[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	135	ASN
1	A	142	GLN
1	A	394	GLN
1	A	591	GLN
1	A	606	ASN
1	B	214	ASN
1	B	243	GLN
1	B	419	ASN
1	B	606	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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	$\# Z > 2$
2	HYP	G	3	3,2	7,8,9	1.03	0	5,10,12	1.67	2 (40%)
2	HYP	I	3	2	7,8,9	0.88	0	5,10,12	1.46	1 (20%)
2	HYP	G	6	2	9,9,9	1.08	0	10,12,12	1.67	2 (20%)
2	HYP	E	3	2	7,8,9	1.01	0	5,10,12	1.62	2 (40%)
2	HYP	C	3	3,2	7,8,9	0.90	0	5,10,12	1.62	1 (20%)
2	HYP	F	6	2	7,8,9	0.95	0	5,10,12	2.30	2 (40%)
2	HYP	E	6	2	9,9,9	1.18	1 (11%)	10,12,12	1.38	2 (20%)
2	HYP	J	6	2	7,8,9	1.24	1 (14%)	5,10,12	2.83	3 (60%)
2	HYP	I	6	2	9,9,9	1.04	0	10,12,12	1.17	1 (10%)
2	HYP	C	6	2	9,9,9	1.30	1 (11%)	10,12,12	1.66	3 (30%)

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	HYP	G	3	3,2	-	0/0/11/13	0/1/1/1
2	HYP	I	3	2	-	0/0/11/13	0/1/1/1
2	HYP	G	6	2	-	0/4/13/13	0/1/1/1
2	HYP	E	3	2	-	0/0/11/13	0/1/1/1
2	HYP	C	3	3,2	-	0/0/11/13	0/1/1/1
2	HYP	F	6	2	-	0/0/11/13	0/1/1/1
2	HYP	E	6	2	-	0/4/13/13	0/1/1/1
2	HYP	J	6	2	-	0/0/11/13	0/1/1/1
2	HYP	I	6	2	-	3/4/13/13	0/1/1/1
2	HYP	C	6	2	-	0/4/13/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	6	HYP	CA-C	2.56	1.59	1.52
2	C	6	HYP	CA-C	2.29	1.58	1.52
2	J	6	HYP	CD-CG	2.05	1.58	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	6	HYP	O-C-CA	-4.14	114.12	124.77
2	F	6	HYP	CB-CG-CD	-3.62	99.13	103.16
2	J	6	HYP	CB-CG-CD	-3.23	99.56	103.16
2	G	6	HYP	O-C-CA	-2.77	113.32	122.26
2	E	6	HYP	CB-CG-CD	-2.67	100.18	103.16
2	C	6	HYP	O-C-CA	-2.52	114.14	122.26
2	E	3	HYP	CB-CG-CD	-2.36	100.52	103.16
2	C	6	HYP	CG-CB-CA	2.36	106.48	103.75
2	J	6	HYP	CG-CB-CA	-2.32	101.07	103.75
2	I	3	HYP	OD1-CG-CB	2.15	115.33	110.10
2	C	6	HYP	OD1-CG-CB	2.14	115.31	110.10
2	G	3	HYP	OD1-CG-CB	2.11	115.24	110.10
2	I	6	HYP	OD1-CG-CB	2.10	115.21	110.10
2	G	3	HYP	CG-CB-CA	2.07	106.15	103.75
2	F	6	HYP	O-C-CA	-2.07	119.44	124.77
2	E	6	HYP	OD1-CG-CB	2.07	115.12	110.10
2	C	3	HYP	OD1-CG-CB	2.06	115.11	110.10
2	E	3	HYP	OD1-CG-CB	2.04	115.05	110.10
2	G	6	HYP	CB-CG-CD	-2.03	100.90	103.16

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	6	HYP	O-C-CA-N
2	I	6	HYP	OXT-C-CA-N
2	I	6	HYP	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	HYP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 102 ligands modelled in this entry, 10 are monoatomic - leaving 92 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	$\# Z > 2$
5	EDO	B	716	-	3,3,3	0.44	0	2,2,2	0.44	0
5	EDO	B	722	-	3,3,3	0.46	0	2,2,2	0.33	0
5	EDO	B	743	-	3,3,3	0.46	0	2,2,2	0.38	0
5	EDO	B	728	-	3,3,3	0.47	0	2,2,2	0.51	0
5	EDO	A	715	-	3,3,3	0.38	0	2,2,2	0.55	0
5	EDO	B	710	-	3,3,3	0.50	0	2,2,2	0.25	0
5	EDO	B	709	-	3,3,3	0.40	0	2,2,2	0.57	0
5	EDO	A	734	-	3,3,3	0.54	0	2,2,2	0.24	0
5	EDO	A	725	-	3,3,3	0.42	0	2,2,2	0.35	0
5	EDO	A	722	-	3,3,3	0.29	0	2,2,2	0.63	0
5	EDO	B	730	-	3,3,3	0.37	0	2,2,2	0.70	0
5	EDO	B	715	-	3,3,3	0.47	0	2,2,2	0.39	0
5	EDO	B	750	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	B	717	-	3,3,3	0.48	0	2,2,2	0.16	0
5	EDO	B	742	-	3,3,3	0.35	0	2,2,2	0.67	0
5	EDO	B	714	-	3,3,3	0.61	0	2,2,2	0.11	0
5	EDO	B	749[A]	-	3,3,3	0.39	0	2,2,2	0.62	0
5	EDO	A	739	-	3,3,3	0.47	0	2,2,2	0.02	0
5	EDO	A	707	-	3,3,3	0.44	0	2,2,2	0.31	0
5	EDO	A	721	-	3,3,3	0.53	0	2,2,2	0.33	0
8	TRS	B	752	-	7,7,7	0.27	0	9,9,9	0.33	0
5	EDO	A	745	-	3,3,3	0.47	0	2,2,2	0.42	0
5	EDO	B	737	-	3,3,3	0.42	0	2,2,2	0.51	0
5	EDO	B	708	-	3,3,3	0.49	0	2,2,2	0.35	0
5	EDO	B	744	-	3,3,3	0.50	0	2,2,2	0.28	0
5	EDO	B	718	-	3,3,3	0.52	0	2,2,2	0.43	0
5	EDO	B	721	-	3,3,3	0.47	0	2,2,2	0.47	0
6	PGE	A	750	-	9,9,9	0.38	0	8,8,8	0.32	0
5	EDO	B	711	-	3,3,3	0.40	0	2,2,2	0.53	0
5	EDO	B	726	-	3,3,3	0.44	0	2,2,2	0.56	0
5	EDO	B	720	-	3,3,3	0.45	0	2,2,2	0.28	0
5	EDO	A	749	-	3,3,3	0.54	0	2,2,2	0.14	0
5	EDO	B	719	-	3,3,3	0.41	0	2,2,2	0.53	0
5	EDO	A	746	-	3,3,3	0.55	0	2,2,2	0.16	0
5	EDO	A	718	-	3,3,3	0.45	0	2,2,2	0.31	0
5	EDO	B	735	-	3,3,3	0.55	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	724	-	3,3,3	0.38	0	2,2,2	0.47	0
5	EDO	A	717	-	3,3,3	0.42	0	2,2,2	0.63	0
5	EDO	A	711	-	3,3,3	0.41	0	2,2,2	0.28	0
5	EDO	B	723	-	3,3,3	0.46	0	2,2,2	0.35	0
5	EDO	A	731	-	3,3,3	0.56	0	2,2,2	0.12	0
5	EDO	A	743	-	3,3,3	0.38	0	2,2,2	0.56	0
5	EDO	A	740	-	3,3,3	0.46	0	2,2,2	0.41	0
5	EDO	A	735	-	3,3,3	0.54	0	2,2,2	0.25	0
7	PEG	B	751	-	6,6,6	0.23	0	5,5,5	0.08	0
5	EDO	B	713	-	3,3,3	0.48	0	2,2,2	0.31	0
5	EDO	A	733	-	3,3,3	0.50	0	2,2,2	0.23	0
5	EDO	B	747	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	714	-	3,3,3	0.51	0	2,2,2	0.32	0
5	EDO	A	741	-	3,3,3	0.43	0	2,2,2	0.46	0
5	EDO	A	727	-	3,3,3	0.49	0	2,2,2	0.35	0
5	EDO	A	729	-	3,3,3	0.46	0	2,2,2	0.37	0
5	EDO	A	737	-	3,3,3	0.46	0	2,2,2	0.40	0
5	EDO	A	708	-	3,3,3	0.42	0	2,2,2	0.43	0
5	EDO	A	744	-	3,3,3	0.44	0	2,2,2	0.38	0
5	EDO	A	716	-	3,3,3	0.44	0	2,2,2	0.61	0
5	EDO	A	730	-	3,3,3	0.46	0	2,2,2	0.41	0
5	EDO	B	712	-	3,3,3	0.50	0	2,2,2	0.34	0
5	EDO	A	713	-	3,3,3	0.44	0	2,2,2	0.45	0
5	EDO	B	732	-	3,3,3	0.36	0	2,2,2	0.52	0
5	EDO	B	729	-	3,3,3	0.36	0	2,2,2	0.71	0
5	EDO	A	726	-	3,3,3	0.56	0	2,2,2	0.49	0
5	EDO	A	742	-	3,3,3	0.45	0	2,2,2	0.22	0
5	EDO	B	746	-	3,3,3	0.39	0	2,2,2	0.50	0
5	EDO	A	709	-	3,3,3	0.47	0	2,2,2	0.29	0
5	EDO	B	736	-	3,3,3	0.46	0	2,2,2	0.31	0
5	EDO	A	738	-	3,3,3	0.46	0	2,2,2	0.38	0
5	EDO	A	723	-	3,3,3	0.38	0	2,2,2	0.47	0
5	EDO	B	707	-	3,3,3	0.46	0	2,2,2	0.48	0
5	EDO	B	734	-	3,3,3	0.43	0	2,2,2	0.50	0
5	EDO	A	712	-	3,3,3	0.48	0	2,2,2	0.39	0
5	EDO	B	725	-	3,3,3	0.50	0	2,2,2	0.33	0
5	EDO	B	738	-	3,3,3	0.40	0	2,2,2	0.42	0
5	EDO	A	719	-	3,3,3	0.45	0	2,2,2	0.31	0
5	EDO	B	706	-	3,3,3	0.36	0	2,2,2	0.61	0
5	EDO	A	710	-	3,3,3	0.47	0	2,2,2	0.33	0
5	EDO	B	740	-	3,3,3	0.55	0	2,2,2	0.38	0
5	EDO	B	739	-	3,3,3	0.44	0	2,2,2	0.34	0
5	EDO	B	733	-	3,3,3	0.39	0	2,2,2	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	728	-	3,3,3	0.48	0	2,2,2	0.45	0
5	EDO	A	748	-	3,3,3	0.52	0	2,2,2	0.37	0
5	EDO	B	741	-	3,3,3	0.44	0	2,2,2	0.53	0
5	EDO	A	706	-	3,3,3	0.44	0	2,2,2	0.42	0
5	EDO	A	732	-	3,3,3	0.39	0	2,2,2	0.47	0
5	EDO	B	745	-	3,3,3	0.44	0	2,2,2	0.44	0
5	EDO	A	736	-	3,3,3	0.50	0	2,2,2	0.24	0
5	EDO	B	731	-	3,3,3	0.46	0	2,2,2	0.46	0
5	EDO	A	724	-	3,3,3	0.38	0	2,2,2	0.55	0
5	EDO	A	747	-	3,3,3	0.47	0	2,2,2	0.38	0
5	EDO	B	748	-	3,3,3	0.34	0	2,2,2	0.87	0
5	EDO	B	727	-	3,3,3	0.45	0	2,2,2	0.25	0
5	EDO	A	720	-	3,3,3	0.47	0	2,2,2	0.36	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
5	EDO	B	716	-	-	0/1/1/1	-
5	EDO	B	722	-	-	0/1/1/1	-
5	EDO	B	743	-	-	0/1/1/1	-
5	EDO	B	728	-	-	0/1/1/1	-
5	EDO	A	715	-	-	1/1/1/1	-
5	EDO	B	710	-	-	0/1/1/1	-
5	EDO	B	709	-	-	1/1/1/1	-
5	EDO	A	734	-	-	1/1/1/1	-
5	EDO	A	725	-	-	1/1/1/1	-
5	EDO	A	722	-	-	0/1/1/1	-
5	EDO	B	730	-	-	0/1/1/1	-
5	EDO	B	715	-	-	1/1/1/1	-
5	EDO	B	750	-	-	0/1/1/1	-
5	EDO	B	717	-	-	0/1/1/1	-
5	EDO	B	742	-	-	1/1/1/1	-
5	EDO	B	714	-	-	1/1/1/1	-
5	EDO	B	749[A]	-	-	1/1/1/1	-
5	EDO	A	739	-	-	1/1/1/1	-
5	EDO	A	707	-	-	0/1/1/1	-
5	EDO	A	721	-	-	0/1/1/1	-
8	TRS	B	752	-	-	6/9/9/9	-
5	EDO	A	745	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	737	-	-	0/1/1/1	-
5	EDO	B	708	-	-	0/1/1/1	-
5	EDO	B	744	-	-	1/1/1/1	-
5	EDO	B	718	-	-	1/1/1/1	-
5	EDO	B	721	-	-	0/1/1/1	-
6	PGE	A	750	-	-	3/7/7/7	-
5	EDO	B	711	-	-	1/1/1/1	-
5	EDO	B	726	-	-	0/1/1/1	-
5	EDO	B	720	-	-	1/1/1/1	-
5	EDO	A	749	-	-	1/1/1/1	-
5	EDO	B	719	-	-	0/1/1/1	-
5	EDO	A	746	-	-	1/1/1/1	-
5	EDO	A	718	-	-	0/1/1/1	-
5	EDO	B	735	-	-	1/1/1/1	-
5	EDO	B	724	-	-	1/1/1/1	-
5	EDO	A	717	-	-	0/1/1/1	-
5	EDO	A	711	-	-	0/1/1/1	-
5	EDO	B	723	-	-	1/1/1/1	-
5	EDO	A	731	-	-	1/1/1/1	-
5	EDO	A	743	-	-	1/1/1/1	-
5	EDO	A	740	-	-	0/1/1/1	-
5	EDO	A	735	-	-	1/1/1/1	-
7	PEG	B	751	-	-	3/4/4/4	-
5	EDO	B	713	-	-	0/1/1/1	-
5	EDO	A	733	-	-	0/1/1/1	-
5	EDO	B	747	-	-	0/1/1/1	-
5	EDO	A	714	-	-	0/1/1/1	-
5	EDO	A	741	-	-	1/1/1/1	-
5	EDO	A	727	-	-	0/1/1/1	-
5	EDO	A	729	-	-	0/1/1/1	-
5	EDO	A	737	-	-	1/1/1/1	-
5	EDO	A	708	-	-	0/1/1/1	-
5	EDO	A	744	-	-	0/1/1/1	-
5	EDO	A	716	-	-	0/1/1/1	-
5	EDO	A	730	-	-	0/1/1/1	-
5	EDO	B	712	-	-	0/1/1/1	-
5	EDO	A	713	-	-	1/1/1/1	-
5	EDO	B	732	-	-	0/1/1/1	-
5	EDO	B	729	-	-	1/1/1/1	-
5	EDO	A	726	-	-	1/1/1/1	-
5	EDO	A	742	-	-	1/1/1/1	-
5	EDO	B	746	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	709	-	-	1/1/1/1	-
5	EDO	B	736	-	-	0/1/1/1	-
5	EDO	A	738	-	-	1/1/1/1	-
5	EDO	A	723	-	-	1/1/1/1	-
5	EDO	B	707	-	-	0/1/1/1	-
5	EDO	B	734	-	-	1/1/1/1	-
5	EDO	A	712	-	-	0/1/1/1	-
5	EDO	B	725	-	-	0/1/1/1	-
5	EDO	B	738	-	-	1/1/1/1	-
5	EDO	A	719	-	-	1/1/1/1	-
5	EDO	B	706	-	-	0/1/1/1	-
5	EDO	A	710	-	-	1/1/1/1	-
5	EDO	B	740	-	-	1/1/1/1	-
5	EDO	B	739	-	-	0/1/1/1	-
5	EDO	B	733	-	-	1/1/1/1	-
5	EDO	A	728	-	-	1/1/1/1	-
5	EDO	A	748	-	-	1/1/1/1	-
5	EDO	B	741	-	-	0/1/1/1	-
5	EDO	A	706	-	-	0/1/1/1	-
5	EDO	A	732	-	-	0/1/1/1	-
5	EDO	B	745	-	-	1/1/1/1	-
5	EDO	A	736	-	-	0/1/1/1	-
5	EDO	B	731	-	-	0/1/1/1	-
5	EDO	A	724	-	-	0/1/1/1	-
5	EDO	A	747	-	-	1/1/1/1	-
5	EDO	B	748	-	-	1/1/1/1	-
5	EDO	B	727	-	-	0/1/1/1	-
5	EDO	A	720	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	752	TRS	C1-C-C2-O2
8	B	752	TRS	C3-C-C2-O2
7	B	751	PEG	O2-C3-C4-O4
5	A	710	EDO	O1-C1-C2-O2
5	A	735	EDO	O1-C1-C2-O2
5	A	742	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	745	EDO	O1-C1-C2-O2
5	A	748	EDO	O1-C1-C2-O2
5	B	711	EDO	O1-C1-C2-O2
5	B	724	EDO	O1-C1-C2-O2
6	A	750	PGE	C1-C2-O2-C3
6	A	750	PGE	O2-C3-C4-O3
5	A	709	EDO	O1-C1-C2-O2
5	A	731	EDO	O1-C1-C2-O2
5	A	734	EDO	O1-C1-C2-O2
5	A	738	EDO	O1-C1-C2-O2
5	B	735	EDO	O1-C1-C2-O2
5	B	738	EDO	O1-C1-C2-O2
7	B	751	PEG	C1-C2-O2-C3
8	B	752	TRS	N-C-C1-O1
8	B	752	TRS	N-C-C2-O2
5	A	713	EDO	O1-C1-C2-O2
5	B	723	EDO	O1-C1-C2-O2
5	B	715	EDO	O1-C1-C2-O2
6	A	750	PGE	C3-C4-O3-C5
8	B	752	TRS	C2-C-C1-O1
8	B	752	TRS	C3-C-C1-O1
5	B	745	EDO	O1-C1-C2-O2
7	B	751	PEG	C4-C3-O2-C2
5	A	726	EDO	O1-C1-C2-O2
5	B	729	EDO	O1-C1-C2-O2
5	B	733	EDO	O1-C1-C2-O2
5	A	749	EDO	O1-C1-C2-O2
5	A	719	EDO	O1-C1-C2-O2
5	A	743	EDO	O1-C1-C2-O2
5	A	747	EDO	O1-C1-C2-O2
5	B	709	EDO	O1-C1-C2-O2
5	B	714	EDO	O1-C1-C2-O2
5	B	744	EDO	O1-C1-C2-O2
5	B	749[A]	EDO	O1-C1-C2-O2
5	A	715	EDO	O1-C1-C2-O2
5	A	723	EDO	O1-C1-C2-O2
5	A	728	EDO	O1-C1-C2-O2
5	A	737	EDO	O1-C1-C2-O2
5	A	741	EDO	O1-C1-C2-O2
5	B	718	EDO	O1-C1-C2-O2
5	B	734	EDO	O1-C1-C2-O2
5	B	740	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	742	EDO	O1-C1-C2-O2
5	B	748	EDO	O1-C1-C2-O2
5	A	720	EDO	O1-C1-C2-O2
5	B	720	EDO	O1-C1-C2-O2
5	A	725	EDO	O1-C1-C2-O2
5	A	739	EDO	O1-C1-C2-O2
5	A	746	EDO	O1-C1-C2-O2

There are no ring outliers.

33 monomers are involved in 49 short contacts:

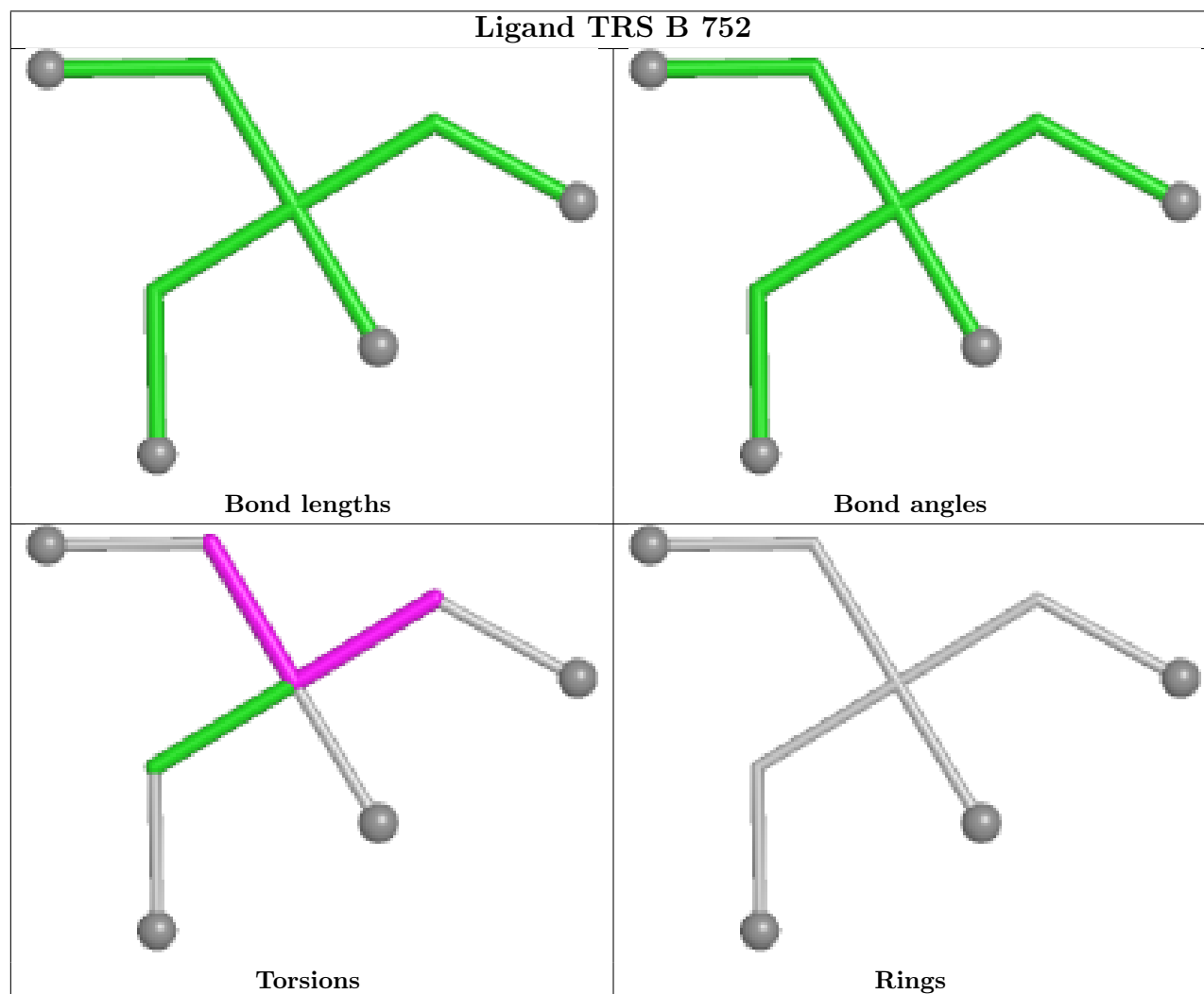
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	716	EDO	1	0
5	B	743	EDO	1	0
5	B	709	EDO	1	0
5	A	725	EDO	2	0
5	A	722	EDO	3	0
5	B	730	EDO	1	0
5	B	742	EDO	4	0
5	B	714	EDO	1	0
5	A	739	EDO	2	0
5	B	737	EDO	1	0
5	B	718	EDO	1	0
5	B	735	EDO	3	0
5	B	724	EDO	1	0
5	B	723	EDO	1	0
7	B	751	PEG	2	0
5	A	741	EDO	1	0
5	A	727	EDO	1	0
5	A	737	EDO	1	0
5	A	744	EDO	1	0
5	A	730	EDO	1	0
5	A	713	EDO	1	0
5	B	732	EDO	4	0
5	B	729	EDO	1	0
5	A	726	EDO	1	0
5	B	746	EDO	1	0
5	B	736	EDO	2	0
5	A	723	EDO	1	0
5	B	734	EDO	1	0
5	A	719	EDO	1	0
5	A	710	EDO	1	0

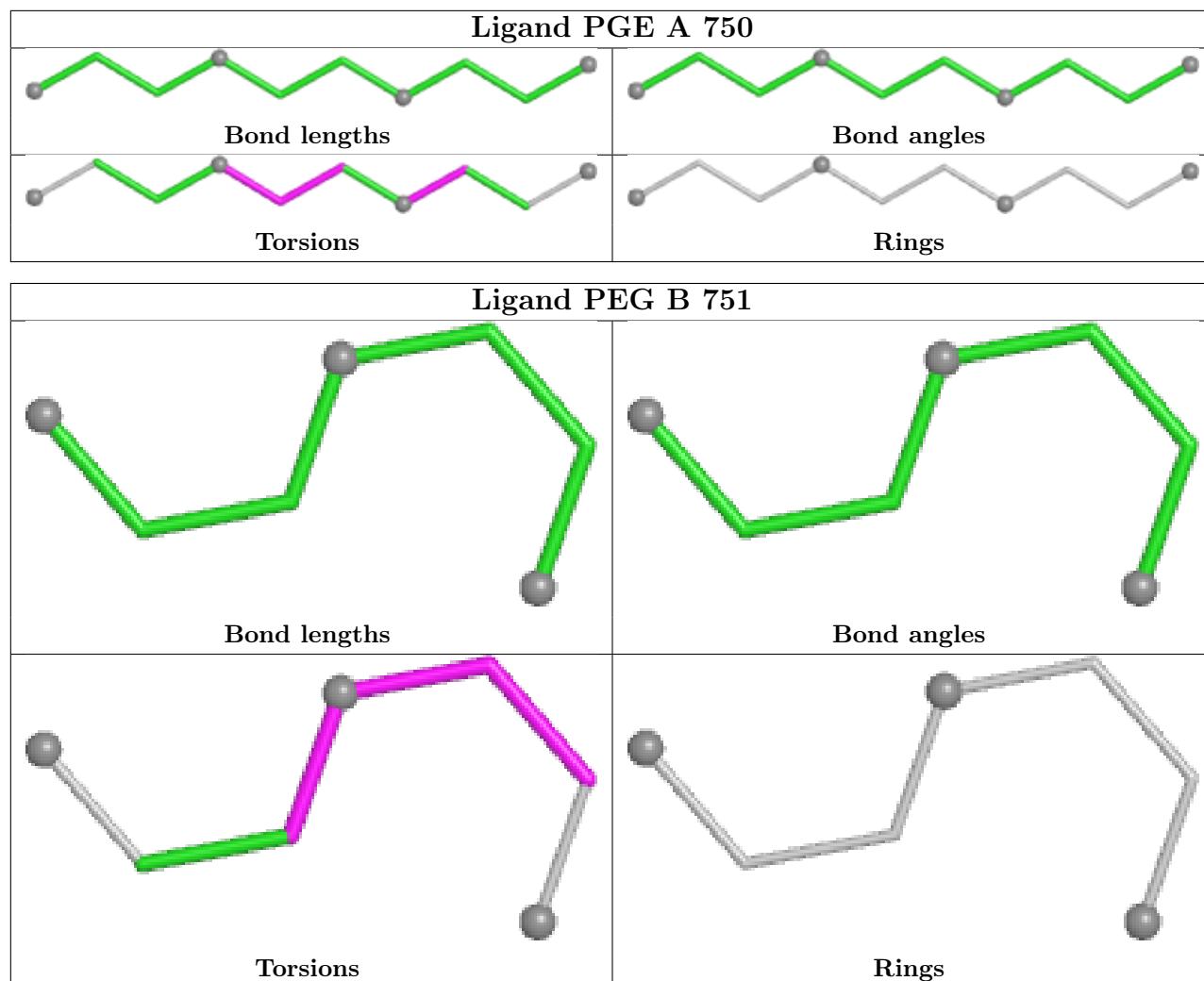
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	728	EDO	2	0
5	A	724	EDO	3	0
5	B	727	EDO	1	0

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 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	532/559 (95%)	-0.19	8 (1%) 72 71	15, 31, 55, 86	9 (1%)
1	B	532/559 (95%)	-0.31	1 (0%) 91 90	13, 29, 48, 77	7 (1%)
2	C	4/6 (66%)	1.01	1 (25%) 2 1	27, 28, 29, 30	4 (100%)
2	E	4/6 (66%)	0.36	0 100 100	36, 38, 42, 48	0
2	F	2/6 (33%)	1.79	1 (50%) 0 1	36, 36, 36, 43	2 (100%)
2	G	4/6 (66%)	1.46	2 (50%) 0 1	25, 26, 29, 30	4 (100%)
2	I	4/6 (66%)	-0.18	0 100 100	34, 36, 39, 40	0
2	J	2/6 (33%)	2.50	1 (50%) 0 1	53, 53, 53, 56	0
All	All	1084/1154 (93%)	-0.23	14 (1%) 75 74	13, 30, 51, 86	26 (2%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	CYS	3.4
2	J	4	GLY	3.2
1	A	100	THR	3.0
2	G	2	PRO	3.0
1	A	135	ASN	2.4
1	A	130	ALA	2.3
2	C	2	PRO	2.3
1	A	94	LEU	2.3
2	G	1	GLY	2.2
1	A	99	THR	2.2
1	A	127	VAL	2.1
2	F	5	PRO	2.0
1	A	622	GLY	2.0
1	A	354	TYR	2.0

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

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
2	HYP	J	6	8/9	0.83	0.11	35,40,49,49	0
2	HYP	F	6	8/9	0.84	0.13	33,37,47,47	8
2	HYP	G	6	9/9	0.85	0.13	34,37,41,42	9
2	HYP	G	3	8/9	0.86	0.13	34,37,40,42	8
2	HYP	C	6	9/9	0.87	0.13	35,38,41,42	9
2	HYP	I	6	9/9	0.88	0.10	34,35,45,55	0
2	HYP	C	3	8/9	0.91	0.10	35,38,43,45	8
2	HYP	E	6	9/9	0.91	0.09	36,42,48,61	0
2	HYP	I	3	8/9	0.95	0.08	27,34,37,44	0
2	HYP	E	3	8/9	0.95	0.07	31,34,35,40	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	A	730	4/4	0.64	0.20	48,50,51,57	0
5	EDO	A	746	4/4	0.69	0.17	52,55,56,61	0
5	EDO	B	721	4/4	0.72	0.17	52,55,55,61	0
5	EDO	B	709	4/4	0.73	0.16	37,51,55,67	0
5	EDO	A	735	4/4	0.74	0.19	43,46,47,47	0
5	EDO	B	712	4/4	0.74	0.17	47,52,53,53	0
5	EDO	A	720	4/4	0.74	0.17	46,48,50,53	0
5	EDO	A	736	4/4	0.75	0.21	54,58,60,61	0
5	EDO	B	722	4/4	0.75	0.14	65,66,69,72	0
5	EDO	B	726	4/4	0.76	0.15	51,51,54,64	0
8	TRS	B	752	8/8	0.76	0.14	54,56,64,65	0
5	EDO	A	745	4/4	0.79	0.15	45,52,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	716	4/4	0.79	0.15	49,49,49,55	0
5	EDO	B	719	4/4	0.80	0.15	39,48,52,66	0
5	EDO	B	714	4/4	0.81	0.16	46,50,50,55	0
5	EDO	A	728	4/4	0.81	0.22	42,46,46,48	0
5	EDO	B	718	4/4	0.81	0.17	36,48,50,52	0
5	EDO	B	744	4/4	0.81	0.20	39,60,60,64	0
5	EDO	B	749[A]	4/4	0.81	0.16	26,33,36,39	4
5	EDO	A	715	4/4	0.81	0.13	44,45,46,50	0
5	EDO	B	729	4/4	0.82	0.18	38,39,44,47	0
5	EDO	B	736	4/4	0.82	0.15	49,50,52,53	0
7	PEG	B	751	7/7	0.82	0.15	30,47,52,54	0
5	EDO	B	740	4/4	0.82	0.15	46,47,48,57	0
5	EDO	B	747	4/4	0.83	0.13	56,57,58,65	0
5	EDO	B	730	4/4	0.83	0.13	44,45,45,46	0
5	EDO	B	743	4/4	0.83	0.13	53,55,57,62	0
5	EDO	B	707	4/4	0.83	0.15	33,39,45,52	0
5	EDO	B	725	4/4	0.84	0.13	37,48,52,62	0
5	EDO	A	733	4/4	0.84	0.16	48,52,56,56	0
5	EDO	B	723	4/4	0.84	0.16	46,47,50,54	0
5	EDO	A	721	4/4	0.85	0.14	45,49,50,54	0
5	EDO	A	747	4/4	0.85	0.12	36,44,52,56	0
6	PGE	A	750	10/10	0.85	0.17	38,48,56,59	0
5	EDO	A	744	4/4	0.85	0.13	54,54,56,64	0
5	EDO	A	727	4/4	0.85	0.13	27,39,49,49	0
5	EDO	B	733	4/4	0.86	0.16	35,36,39,44	0
5	EDO	A	748	4/4	0.86	0.14	40,46,47,58	0
5	EDO	A	749	4/4	0.87	0.13	34,48,53,62	0
5	EDO	B	737	4/4	0.87	0.15	38,42,44,45	0
5	EDO	B	735	4/4	0.88	0.21	24,31,41,44	0
5	EDO	A	718	4/4	0.88	0.10	46,47,48,51	0
5	EDO	B	748	4/4	0.88	0.12	38,41,47,59	0
5	EDO	A	726	4/4	0.88	0.24	31,41,43,44	0
5	EDO	B	750	4/4	0.88	0.12	42,44,50,56	0
5	EDO	B	710	4/4	0.88	0.19	31,37,44,46	0
5	EDO	B	742	4/4	0.88	0.13	31,38,48,60	0
5	EDO	A	738	4/4	0.88	0.11	39,42,46,56	0
5	EDO	B	746	4/4	0.89	0.12	32,52,55,57	0
5	EDO	B	731	4/4	0.89	0.11	43,48,50,60	0
5	EDO	B	739	4/4	0.89	0.14	48,49,50,57	0
5	EDO	A	737	4/4	0.89	0.15	39,43,44,47	0
5	EDO	A	712	4/4	0.90	0.14	35,50,53,58	0
5	EDO	A	731	4/4	0.90	0.12	33,39,43,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	739	4/4	0.90	0.21	36,40,41,57	0
5	EDO	B	720	4/4	0.90	0.14	45,54,58,61	0
5	EDO	A	732	4/4	0.90	0.12	36,41,42,45	0
5	EDO	A	714	4/4	0.90	0.11	43,44,45,59	0
5	EDO	A	709	4/4	0.90	0.13	32,37,39,50	0
5	EDO	B	713	4/4	0.90	0.10	36,40,41,46	0
5	EDO	A	729	4/4	0.90	0.14	30,35,36,38	0
5	EDO	B	727	4/4	0.90	0.11	42,44,49,53	0
5	EDO	A	725	4/4	0.91	0.14	39,46,47,52	0
5	EDO	B	717	4/4	0.91	0.13	41,41,43,46	0
5	EDO	A	719	4/4	0.91	0.12	35,42,52,54	0
5	EDO	B	745	4/4	0.91	0.10	35,41,44,63	0
5	EDO	A	716	4/4	0.91	0.11	37,39,41,42	0
5	EDO	A	734	4/4	0.91	0.11	39,40,44,52	0
5	EDO	B	734	4/4	0.91	0.18	32,36,38,50	0
5	EDO	B	711	4/4	0.91	0.13	32,35,36,38	0
5	EDO	A	713	4/4	0.91	0.13	29,41,45,46	0
5	EDO	A	722	4/4	0.91	0.24	34,36,37,43	0
5	EDO	A	723	4/4	0.91	0.12	34,34,36,49	0
5	EDO	B	715	4/4	0.91	0.11	38,42,50,51	0
5	EDO	A	740	4/4	0.92	0.10	38,39,46,47	0
5	EDO	B	738	4/4	0.92	0.11	40,42,45,46	0
5	EDO	A	743	4/4	0.92	0.11	37,38,44,51	0
5	EDO	B	732	4/4	0.92	0.12	24,31,36,39	0
5	EDO	A	710	4/4	0.92	0.15	37,43,44,46	0
5	EDO	B	706	4/4	0.92	0.12	24,35,39,47	0
5	EDO	A	708	4/4	0.92	0.11	40,53,54,57	0
5	EDO	A	707	4/4	0.92	0.13	47,48,51,54	0
4	CA	B	705	1/1	0.93	0.13	62,62,62,62	0
5	EDO	A	711	4/4	0.93	0.11	37,41,44,51	0
5	EDO	B	728	4/4	0.93	0.09	29,32,34,40	0
5	EDO	A	742	4/4	0.94	0.13	29,37,40,52	0
5	EDO	B	724	4/4	0.94	0.09	33,38,41,45	0
4	CA	A	705	1/1	0.94	0.39	29,29,29,29	0
5	EDO	A	724	4/4	0.94	0.09	30,38,45,49	0
5	EDO	A	741	4/4	0.94	0.10	36,42,48,52	0
5	EDO	A	706	4/4	0.95	0.09	29,33,37,51	0
5	EDO	A	717	4/4	0.95	0.08	30,38,38,52	0
5	EDO	B	741	4/4	0.95	0.08	38,39,40,51	0
5	EDO	B	708	4/4	0.96	0.06	30,39,47,47	0
4	CA	A	704	1/1	0.98	0.03	35,35,35,35	0
3	ZN	B	701	1/1	0.99	0.03	38,38,38,38	1

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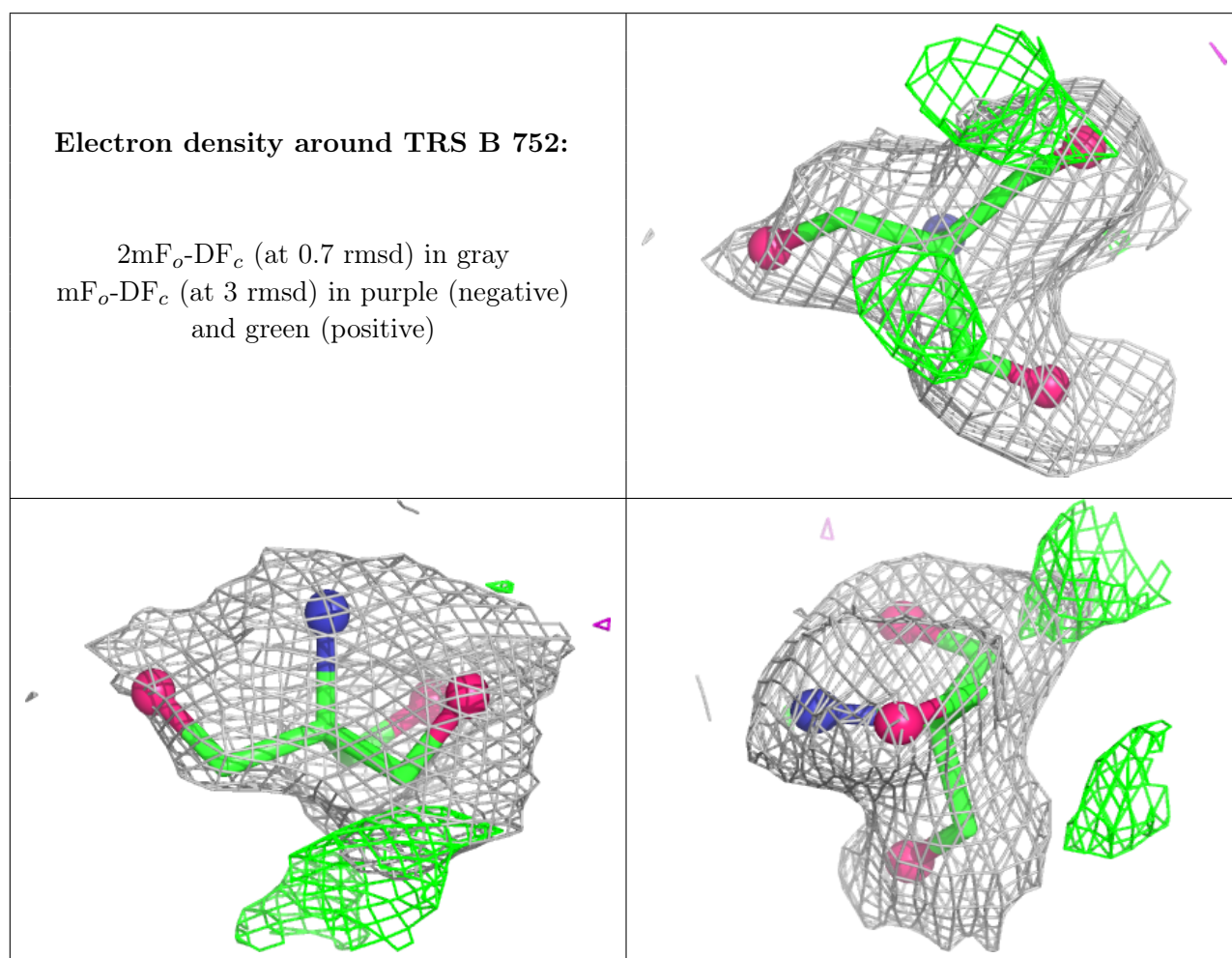
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	B	703	1/1	0.99	0.02	30,30,30,30	0
4	CA	B	704	1/1	0.99	0.03	33,33,33,33	0
4	CA	A	702	1/1	0.99	0.03	21,21,21,21	0
4	CA	A	703	1/1	0.99	0.03	32,32,32,32	0
3	ZN	A	701	1/1	0.99	0.02	40,40,40,40	1
4	CA	B	702	1/1	1.00	0.02	23,23,23,23	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.

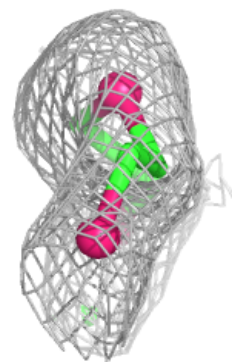
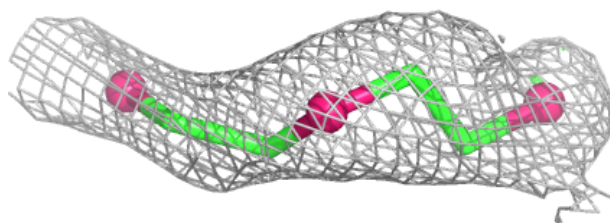
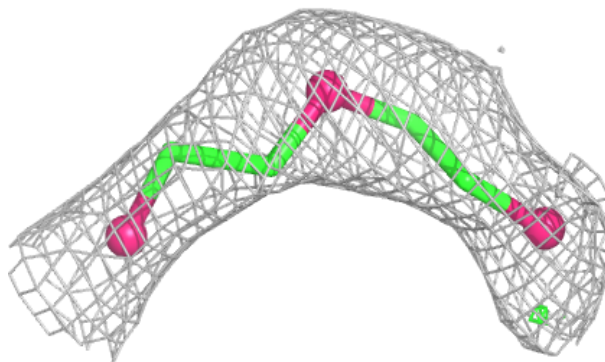
Electron density around TRS B 752:

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

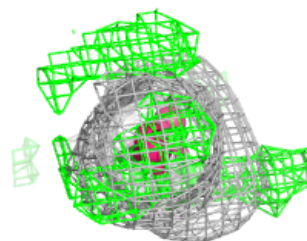
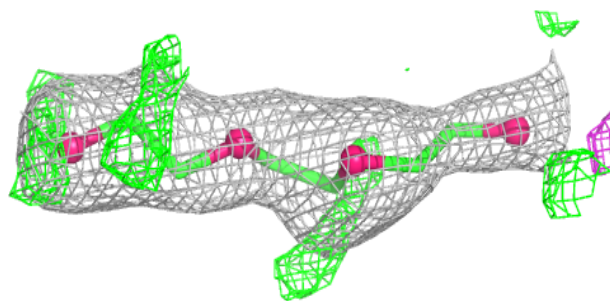
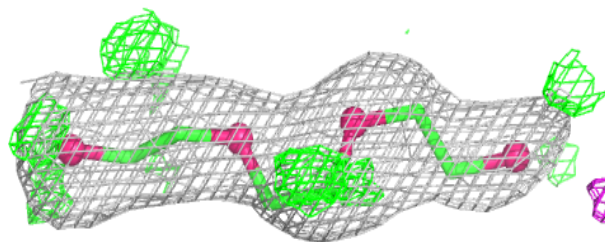


Electron density around PEG B 751:

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

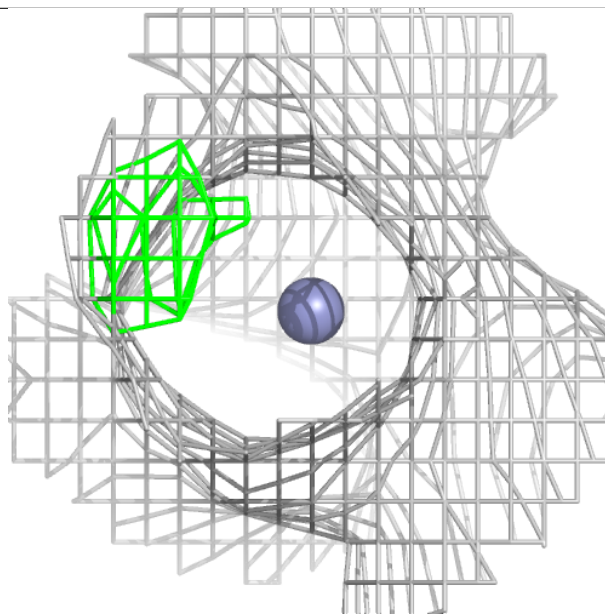
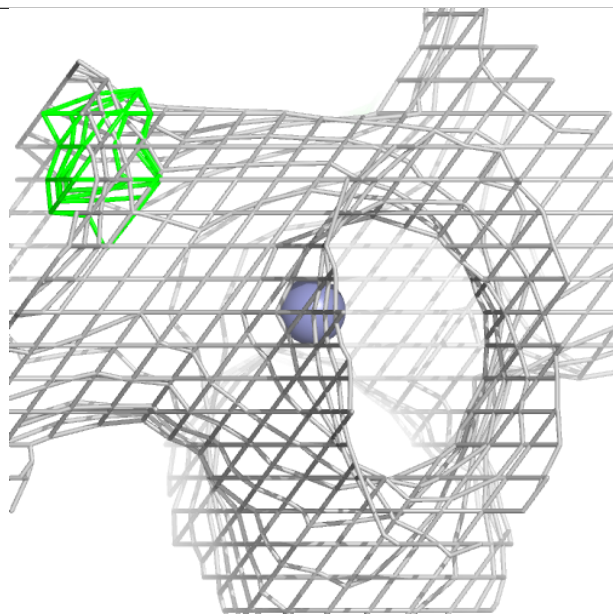
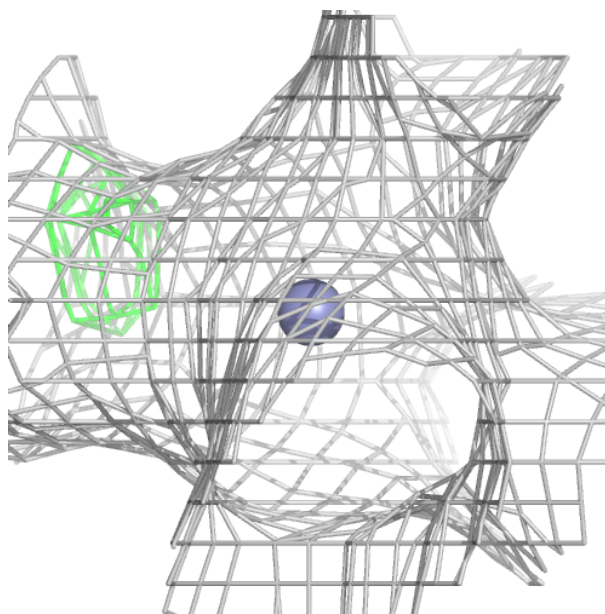
**Electron density around PGE A 750:**

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



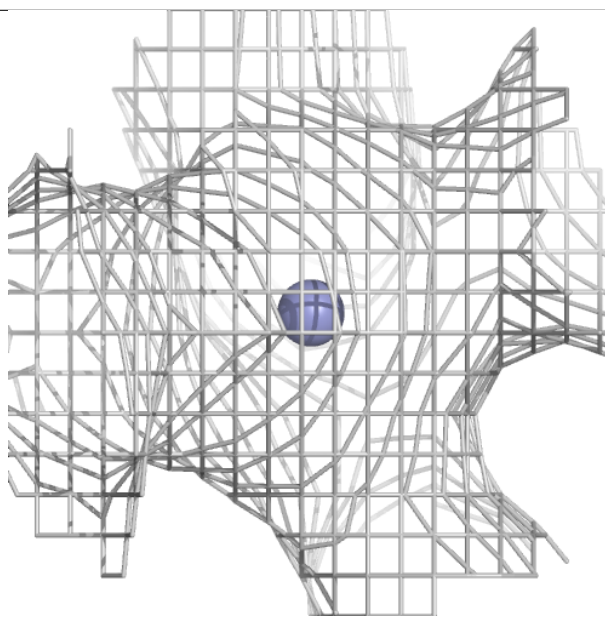
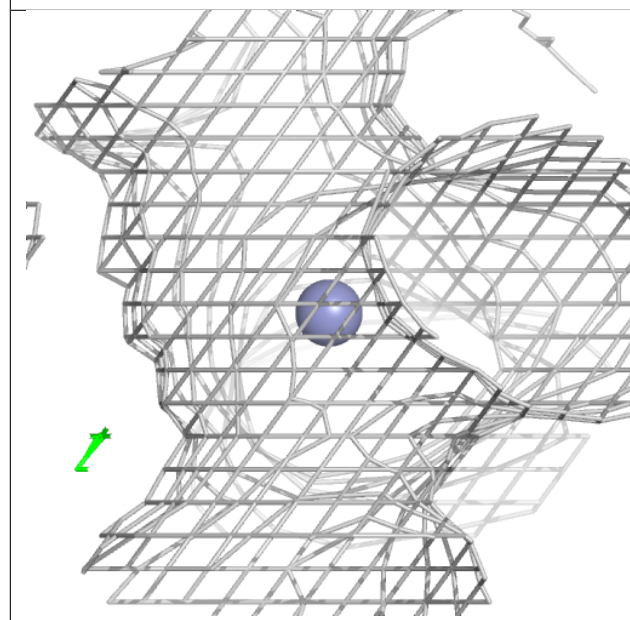
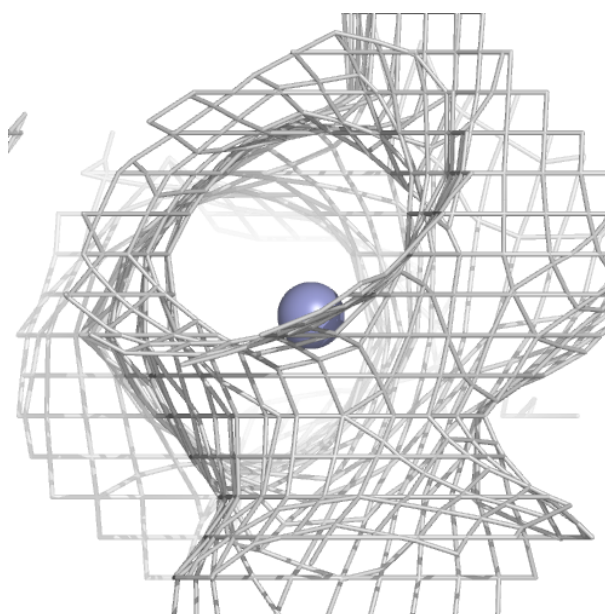
Electron density around ZN B 701:

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



Electron density around ZN 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 ⓘ

There are no such residues in this entry.