



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 06:06 PM EDT

PDB ID : 8DW7 / pdb_00008dw7
Title : DNA glycosylase MutY variant N146S in complex with DNA containing the transition state analog 1N paired with d(8-oxo-G)
Authors : Demir, M.; Russelburg, L.P.; Horvath, M.P.; David, S.S.
Deposited on : 2022-07-31
Resolution : 1.96 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

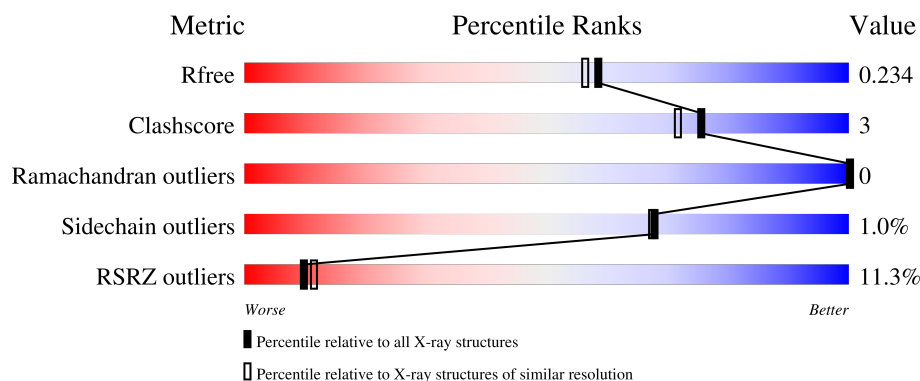
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	365	12% 90% 7%
1	D	365	12% 86% 9%
2	B	11	91% 9%
2	E	11	82% 18%
3	C	11	100%

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Mol	Chain	Length	Quality of chain
3	F	11	 82% 9% 9%

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
7	TRS	B	101	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12035 atoms, of which 5606 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 Adenine DNA glycosylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	352	Total	C	H	N	O	S	0	0	0
			5202	1734	2532	454	472	10			
1	D	349	Total	C	H	N	O	S	0	0	0
			5248	1739	2566	456	478	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	SER	ASN	engineered mutation	UNP P83847
D	146	SER	ASN	engineered mutation	UNP P83847

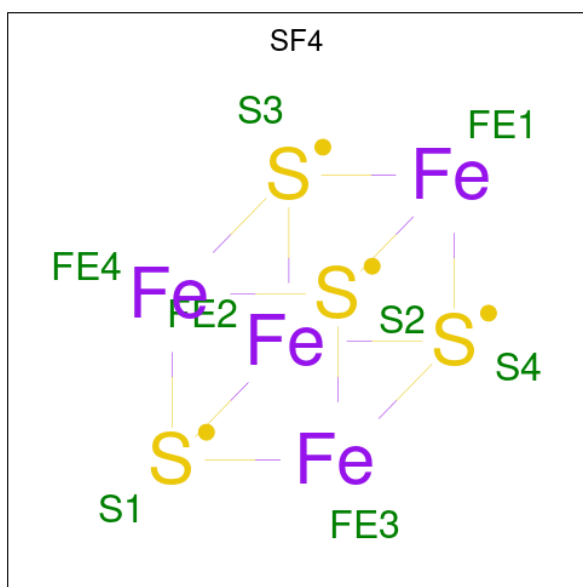
- Molecule 2 is a DNA chain called DNA (5'-D(*AP*AP*GP*AP*CP*(8OG)P*TP*GP*GP*AP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	11	Total	C	H	N	O	P	0	0	0
			352	108	124	48	62	10			
2	E	11	Total	C	H	N	O	P	0	0	0
			352	108	124	48	62	10			

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*TP*CP*CP*AP*(NRI)P*GP*TP*CP*T)-3').

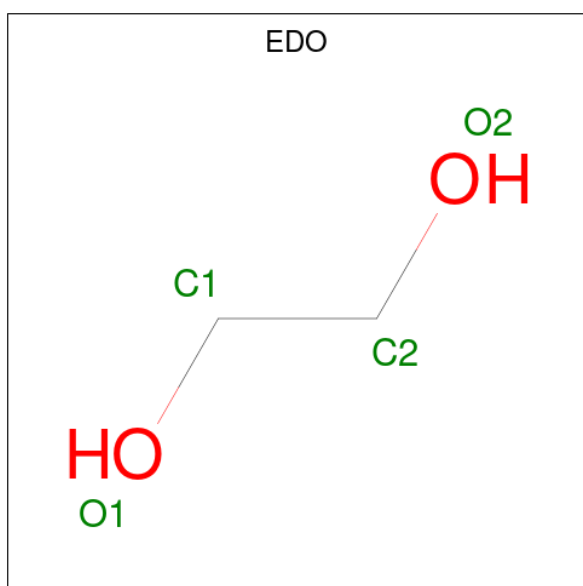
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	11	Total	C	H	N	O	P	0	0	1
			305	92	111	31	61	10			
3	F	11	Total	C	H	N	O	P	0	0	1
			307	92	113	31	61	10			

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

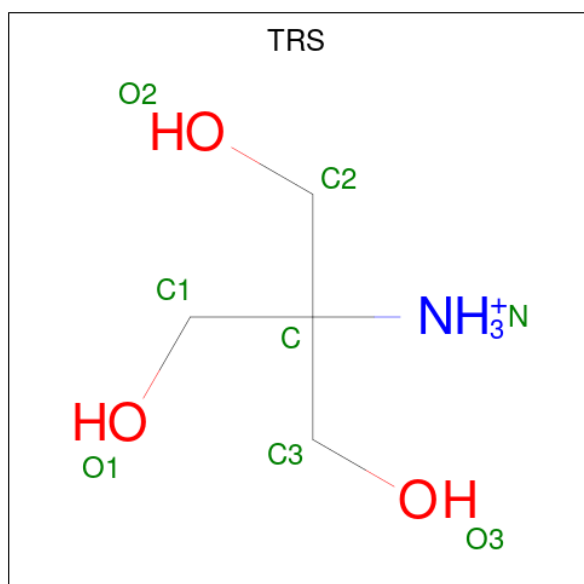


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0
6	D	1	Total Ca 1 1	0	0

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C H N O 20 4 12 1 3	0	0
7	E	1	Total C H N O 20 4 12 1 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	57	Total O 57 57	0	0
8	B	12	Total O 12 12	0	0
8	C	22	Total O 22 22	0	0
8	D	57	Total O 58 58	0	1

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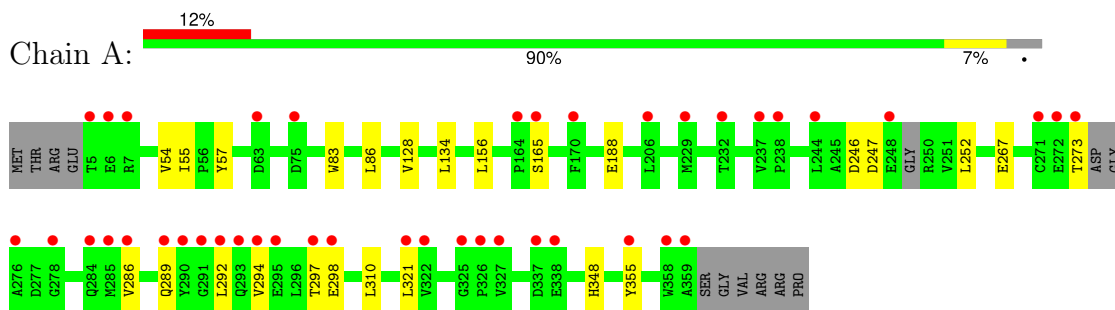
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	17	Total	O	0	0
			17	17		
8	F	25	Total	O	0	0
			25	25		

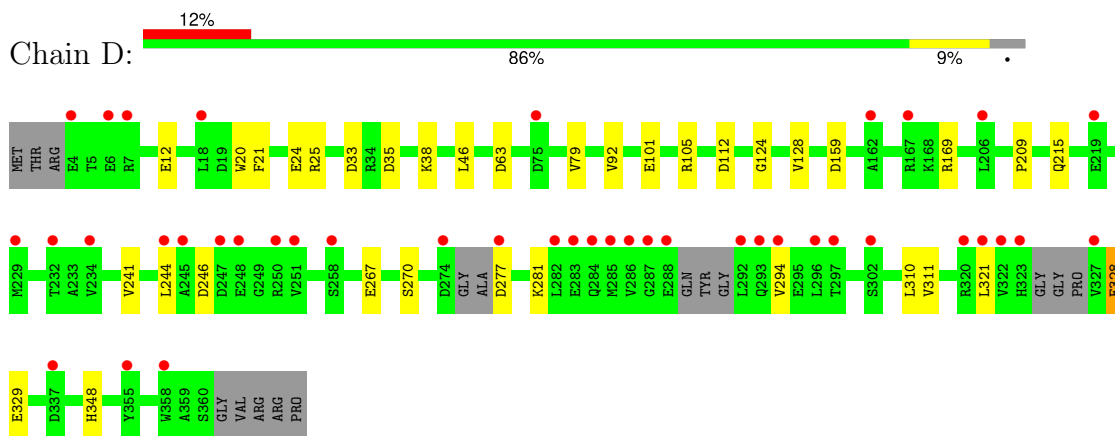
3 Residue-property plots [i](#)

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.

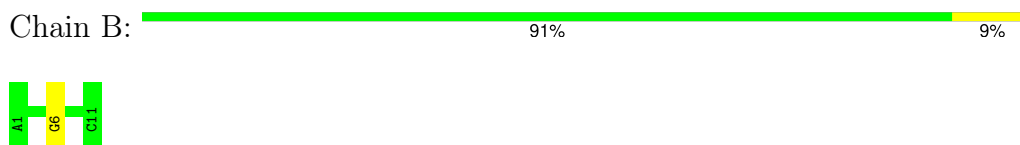
- Molecule 1: Adenine DNA glycosylase



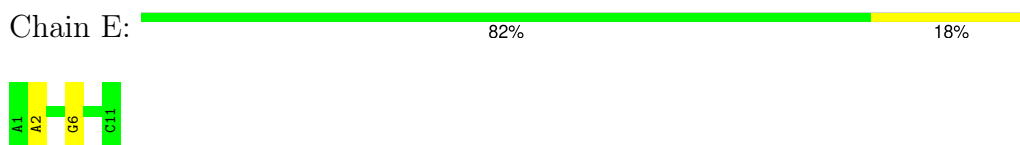
- Molecule 1: Adenine DNA glycosylase



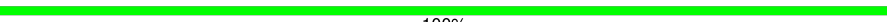
- Molecule 2: DNA (5'-D(*AP*AP*GP*AP*CP*(8OG)P*TP*GP*GP*AP*C)-3')



- Molecule 2: DNA (5'-D(*AP*AP*GP*AP*CP*(8OG)P*TP*GP*GP*AP*C)-3')



- Molecule 3: DNA (5'-D(P*GP*TP*CP*CP*AP*(NRI)P*GP*TP*CP*T)-3')

Chain C:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: DNA (5'-D(P*GP*TP*CP*CP*AP*(NRI)P*GP*TP*CP*T)-3')

Chain F:  82% 9% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.89Å 137.21Å 74.16Å 90.00° 101.00° 90.00°	Depositor
Resolution (Å)	72.80 – 1.96 72.80 – 1.96	Depositor EDS
% Data completeness (in resolution range)	94.1 (72.80-1.96) 93.9 (72.80-1.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.203 , 0.234 0.203 , 0.234	Depositor DCC
R_{free} test set	1636 reflections (2.16%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12035	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.77% 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: CA, SF4, NRI, TRS, EDO, SOG

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	0.90	1/2740 (0.0%)	0.71	0/3747
1	D	0.95	0/2750	0.70	0/3753
2	B	1.16	0/230	1.13	0/351
2	E	1.42	0/230	1.26	0/351
3	C	1.25	0/202	1.18	0/308
3	F	1.40	0/202	1.24	0/308
All	All	0.99	1/6354 (0.0%)	0.80	0/8818

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	VAL	N-CA	-5.03	1.40	1.46

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	2670	2532	2532	14	1
1	D	2682	2566	2566	20	1
2	B	228	124	124	0	0
2	E	228	124	124	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	194	111	110	0	0
3	F	194	113	109	2	0
4	A	8	0	0	0	0
4	D	8	0	0	0	0
5	A	4	6	6	0	0
5	D	4	6	6	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	B	8	12	12	0	0
7	E	8	12	12	0	0
8	A	57	0	0	0	0
8	B	12	0	0	0	0
8	C	22	0	0	0	0
8	D	58	0	0	1	0
8	E	17	0	0	1	0
8	F	25	0	0	1	0
All	All	6429	5606	5601	36	1

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 (36) 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)
2:E:2:DA:OP2	8:E:201:HOH:O	1.87	0.92
1:A:286:VAL:HG11	1:A:294:VAL:HG21	1.71	0.71
1:D:244:LEU:HD13	1:D:294:VAL:HG11	1.81	0.63
1:D:310:LEU:C	1:D:310:LEU:HD12	2.25	0.61
1:D:101:GLU:OE2	1:D:105:ARG:NE	2.28	0.59
1:D:246:ASP:HB3	1:D:321:LEU:HD11	1.84	0.57
1:A:297:THR:HG22	1:A:298:GLU:N	2.21	0.55
1:D:215:GLN:NE2	8:D:501:HOH:O	2.22	0.54
1:D:328:GLU:HG2	1:D:329:GLU:O	2.09	0.53
1:A:267:GLU:HB2	1:A:348:HIS:CE1	2.44	0.52
1:D:310:LEU:HD12	1:D:311:VAL:N	2.25	0.51
1:D:35:ASP:OD2	1:D:38:LYS:HG3	2.11	0.50
1:A:310:LEU:C	1:A:310:LEU:HD12	2.38	0.49
3:F:13:DG:OP2	8:F:101:HOH:O	2.20	0.48
1:A:57:TYR:CG	1:A:86:LEU:HD13	2.49	0.48
1:D:277:ASP:O	1:D:281:LYS:HG3	2.14	0.47
1:D:33:ASP:C	1:D:33:ASP:OD1	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:VAL:HG22	1:D:270:SER:HB3	1.98	0.46
1:D:20:TRP:CG	1:D:209:PRO:HG3	2.51	0.45
1:D:21:PHE:O	1:D:25:ARG:HB2	2.17	0.45
1:A:297:THR:HG22	1:A:298:GLU:H	1.81	0.44
1:D:321:LEU:HD12	1:D:321:LEU:C	2.43	0.44
1:A:246:ASP:OD1	1:A:247:ASP:N	2.51	0.43
1:A:57:TYR:CD2	1:A:86:LEU:HD13	2.54	0.43
1:A:355:TYR:CD1	1:A:355:TYR:C	2.97	0.42
1:D:46:LEU:O	3:F:18:NRI:H3'	2.19	0.42
1:A:289:GLN:CB	1:A:292:LEU:HD12	2.50	0.42
1:D:159:ASP:OD2	1:D:169:ARG:NH2	2.44	0.42
1:A:54:VAL:O	1:A:55:ILE:C	2.63	0.42
1:A:252:LEU:HD22	1:A:321:LEU:HD21	2.02	0.42
1:D:20:TRP:NE1	1:D:24:GLU:HG3	2.34	0.41
1:D:124:GLY:O	1:D:128:VAL:HG23	2.20	0.41
1:A:134:LEU:HD21	1:A:188:GLU:HG3	2.01	0.41
1:D:79:VAL:CG1	1:D:92:VAL:HG22	2.51	0.41
1:D:267:GLU:HB2	1:D:348:HIS:CE1	2.56	0.41
1:A:83:TRP:CE2	1:A:86:LEU:HD23	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:SER:OG	1:D:112:ASP:OD2[2_655]	2.02	0.18

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	346/365 (95%)	338 (98%)	8 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	341/365 (93%)	333 (98%)	8 (2%)	0	100	100
All	All	687/730 (94%)	671 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/312 (82%)	255 (99%)	2 (1%)	73	74
1	D	264/312 (85%)	261 (99%)	3 (1%)	65	64
All	All	521/624 (84%)	516 (99%)	5 (1%)	68	67

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

Mol	Chain	Res	Type
1	A	156	LEU
1	A	273	THR
1	D	12	GLU
1	D	63	ASP
1	D	328	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	172	GLN
1	A	323	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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$
3	NRI	C	18	3	7,11,12	0.85	0	3,14,17	0.74	0
2	8OG	B	6	2	22,25,26	0.74	1 (4%)	26,37,40	1.39	4 (15%)
3	NRI	F	18	3	7,11,12	0.66	0	3,14,17	1.25	1 (33%)
2	8OG	E	6	2	22,25,26	0.89	1 (4%)	26,37,40	1.41	3 (11%)

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
3	NRI	C	18	3	-	0/3/15/16	0/1/1/1
2	8OG	B	6	2	-	1/7/21/22	0/3/3/3
3	NRI	F	18	3	-	0/3/15/16	0/1/1/1
2	8OG	E	6	2	-	1/7/21/22	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	8OG	C8-N9	-2.72	1.35	1.40
2	E	6	8OG	C5-C4	2.47	1.40	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	6	8OG	N7-C8-N9	4.41	111.52	106.61
2	B	6	8OG	N7-C8-N9	3.80	110.83	106.61
2	B	6	8OG	C5-N7-C8	-3.59	104.52	109.47
2	E	6	8OG	C5-N7-C8	-3.35	104.86	109.47
2	B	6	8OG	C4-C5-N7	2.94	111.44	106.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	6	8OG	C4-C5-N7	2.93	111.42	106.06
2	B	6	8OG	C1'-N9-C4	-2.39	122.67	126.88
3	F	18	NRI	O3'-C3'-C2'	-2.11	105.98	110.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	6	8OG	C4'-C5'-O5'-P
2	E	6	8OG	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	18	NRI	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	D	402	-	3,3,3	0.60	0	2,2,2	0.30	0
7	TRS	E	101	-	7,7,7	1.59	1 (14%)	9,9,9	1.40	1 (11%)
5	EDO	A	402	-	3,3,3	0.85	0	2,2,2	0.21	0
4	SF4	D	401	1	0,12,12	-	-	-	-	-
7	TRS	B	101	-	7,7,7	1.70	1 (14%)	9,9,9	2.09	4 (44%)
4	SF4	A	401	1	0,12,12	-	-	-	-	-

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	D	402	-	-	0/1/1/1	-
7	TRS	E	101	-	-	3/9/9/9	-
5	EDO	A	402	-	-	0/1/1/1	-
4	SF4	D	401	1	-	-	0/6/5/5
7	TRS	B	101	-	-	5/9/9/9	-
4	SF4	A	401	1	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	101	TRS	C3-C	-3.86	1.42	1.53
7	E	101	TRS	C1-C	-3.08	1.44	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	101	TRS	C2-C-N	-3.48	99.29	108.17
7	B	101	TRS	O3-C3-C	2.83	118.76	110.88
7	B	101	TRS	C3-C-C2	2.80	118.12	110.66
7	B	101	TRS	C1-C-N	-2.47	101.86	108.17
7	E	101	TRS	C2-C-C1	2.14	116.34	110.66

There are no chirality outliers.

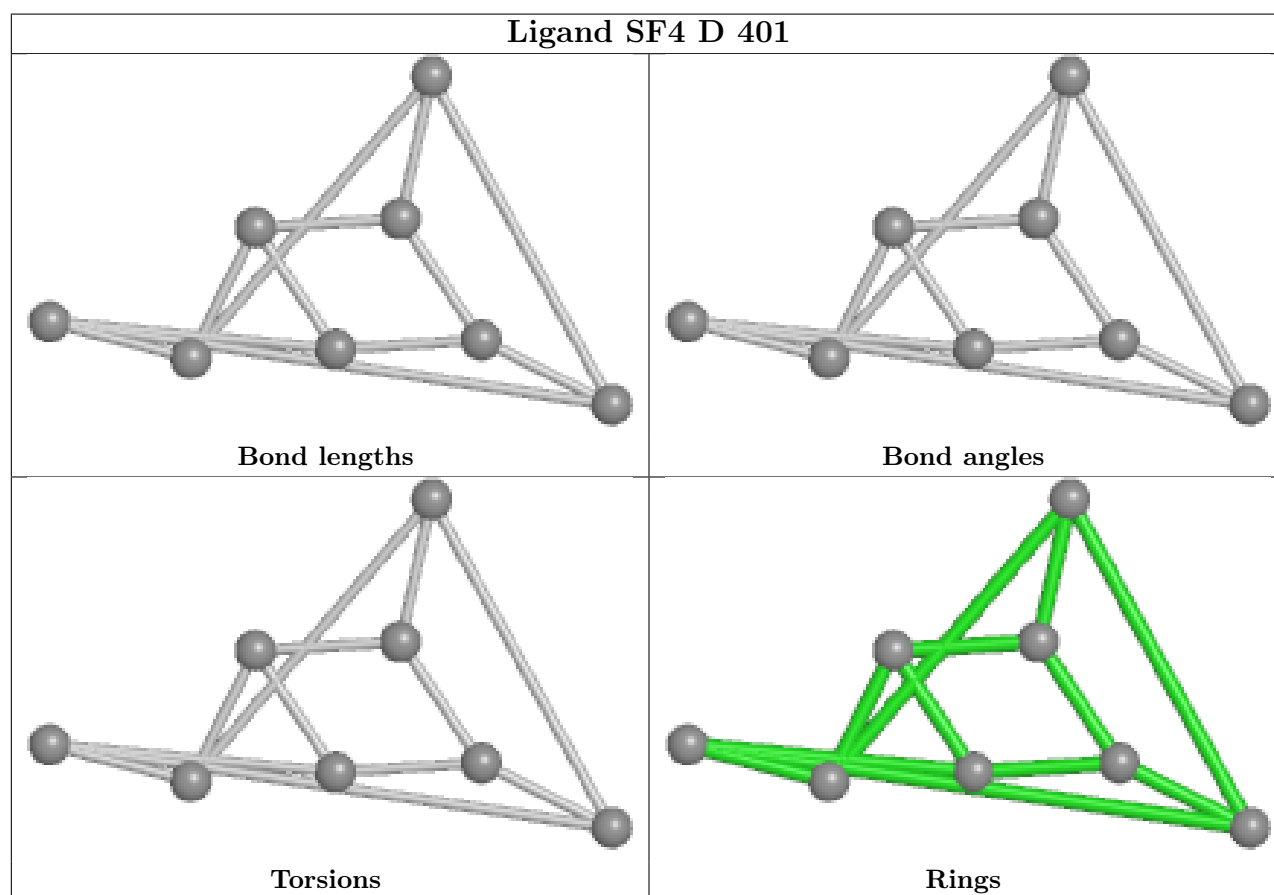
All (8) torsion outliers are listed below:

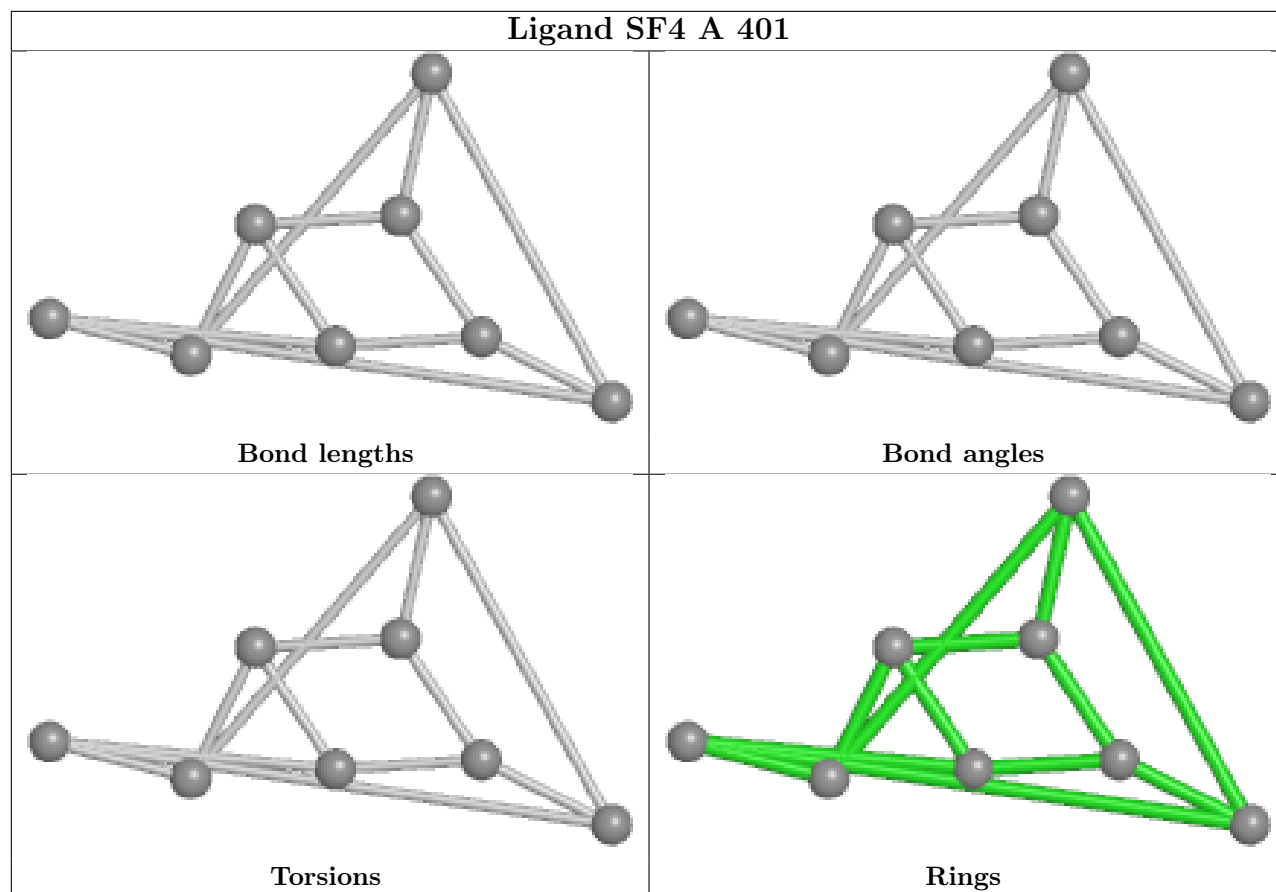
Mol	Chain	Res	Type	Atoms
7	E	101	TRS	C2-C-C1-O1
7	E	101	TRS	C3-C-C1-O1
7	E	101	TRS	N-C-C1-O1
7	B	101	TRS	N-C-C1-O1
7	B	101	TRS	N-C-C3-O3
7	B	101	TRS	C2-C-C3-O3
7	B	101	TRS	C1-C-C3-O3
7	B	101	TRS	C3-C-C1-O1

There are no ring outliers.

No monomer is involved in short contacts.

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	352/365 (96%)	0.94	42 (11%)	9	10	35, 55, 101, 122	0
1	D	349/365 (95%)	0.86	42 (12%)	9	10	33, 55, 101, 134	0
2	B	10/11 (90%)	-0.17	0	100	100	42, 44, 61, 62	0
2	E	10/11 (90%)	-0.38	0	100	100	38, 43, 56, 57	0
3	C	10/11 (90%)	-0.51	0	100	100	36, 45, 49, 74	0
3	F	10/11 (90%)	-0.50	0	100	100	35, 43, 50, 85	0
All	All	741/774 (95%)	0.83	84 (11%)	10	11	33, 54, 101, 134	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	321	LEU	7.2
1	D	322	VAL	6.2
1	A	359	ALA	5.6
1	D	247	ASP	5.3
1	D	286	VAL	4.7
1	A	248	GLU	4.4
1	D	277	ASP	4.3
1	D	293	GLN	4.2
1	A	293	GLN	4.1
1	A	286	VAL	4.0
1	D	323	HIS	3.9
1	D	296	LEU	3.9
1	D	288	GLU	3.9
1	A	325	GLY	3.8
1	A	289	GLN	3.7
1	D	292	LEU	3.7
1	A	291	GLY	3.7
1	A	290	TYR	3.6
1	A	337	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	7	ARG	3.5
1	D	321	LEU	3.4
1	A	5	THR	3.4
1	A	272	GLU	3.3
1	D	248	GLU	3.3
1	D	244	LEU	3.3
1	D	4	GLU	3.1
1	A	295	GLU	3.1
1	A	298	GLU	3.1
1	D	245	ALA	3.1
1	D	285	MET	3.0
1	D	274	ASP	3.0
1	D	287	GLY	3.0
1	A	276	ALA	3.0
1	D	327	VAL	3.0
1	A	285	MET	3.0
1	A	322	VAL	2.9
1	D	251	VAL	2.9
1	A	75	ASP	2.9
1	D	6	GLU	2.9
1	D	283	GLU	2.9
1	A	164	PRO	2.8
1	D	206	LEU	2.8
1	D	337	ASP	2.8
1	A	284	GLN	2.8
1	D	282	LEU	2.7
1	A	278	GLY	2.6
1	D	297	THR	2.6
1	D	229	MET	2.6
1	D	258	SER	2.6
1	A	273	THR	2.6
1	A	292	LEU	2.5
1	D	75	ASP	2.5
1	D	284	GLN	2.5
1	A	6	GLU	2.5
1	D	294	VAL	2.5
1	A	206	LEU	2.5
1	A	358	TRP	2.5
1	A	271	CYS	2.4
1	A	294	VAL	2.4
1	D	7	ARG	2.3
1	A	229	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	18	LEU	2.3
1	D	167	ARG	2.3
1	D	320	ARG	2.3
1	A	237	VAL	2.3
1	A	297	THR	2.3
1	D	219	GLU	2.3
1	D	234	VAL	2.3
1	D	358	TRP	2.2
1	A	327	VAL	2.2
1	A	63	ASP	2.2
1	A	326	PRO	2.2
1	A	238	PRO	2.2
1	D	250	ARG	2.2
1	A	244	LEU	2.1
1	A	338	GLU	2.1
1	A	355	TYR	2.1
1	A	165	SER	2.1
1	D	232	THR	2.1
1	D	355	TYR	2.1
1	D	302	SER	2.1
1	A	232	THR	2.0
1	D	162	ALA	2.0
1	A	170	PHE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	8OG	E	6	23/24	0.97	0.06	32,36,40,40	0
2	8OG	B	6	23/24	0.98	0.06	35,40,42,43	0
3	NRI	C	18	11/12	0.98	0.06	35,40,44,45	0
3	NRI	F	18	11/12	0.98	0.07	35,38,40,44	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

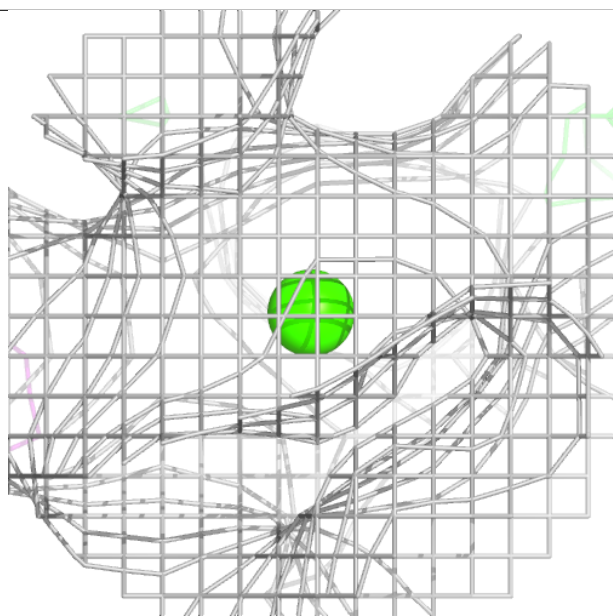
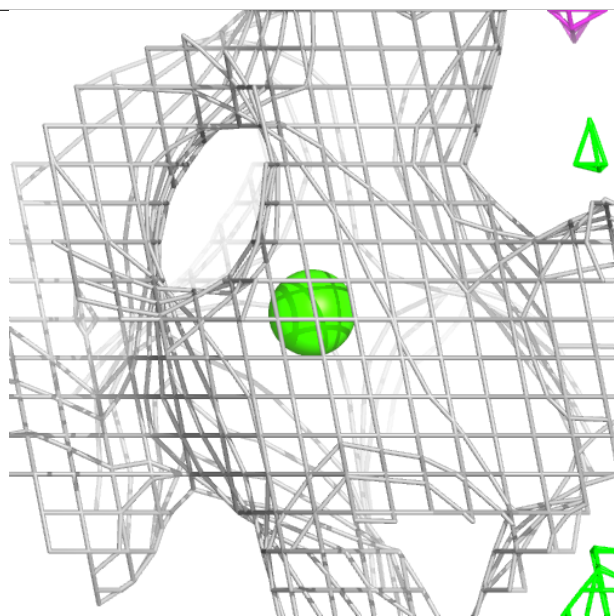
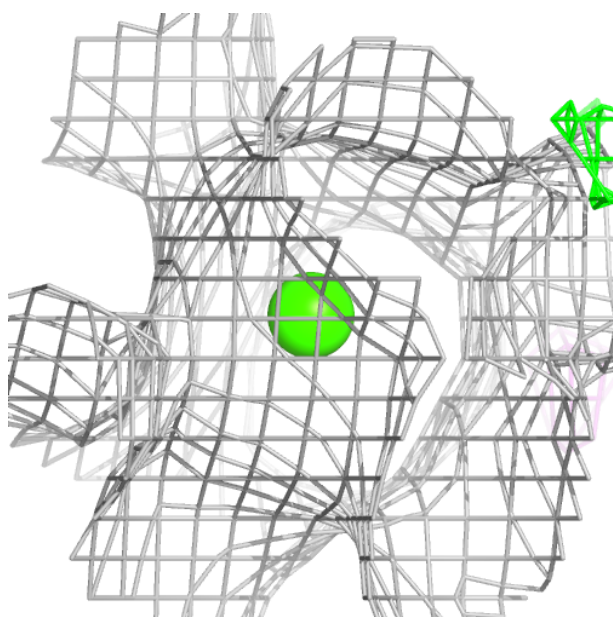
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	402	4/4	0.73	0.19	58,64,65,65	10
7	TRS	E	101	8/8	0.75	0.20	36,44,63,63	20
7	TRS	B	101	8/8	0.79	0.15	37,45,59,59	20
5	EDO	D	402	4/4	0.79	0.19	68,75,76,76	10
6	CA	A	403	1/1	0.99	0.03	40,40,40,40	0
6	CA	D	403	1/1	0.99	0.03	38,38,38,38	0
4	SF4	A	401	8/8	0.99	0.04	49,52,56,57	0
4	SF4	D	401	8/8	0.99	0.04	44,48,51,52	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.

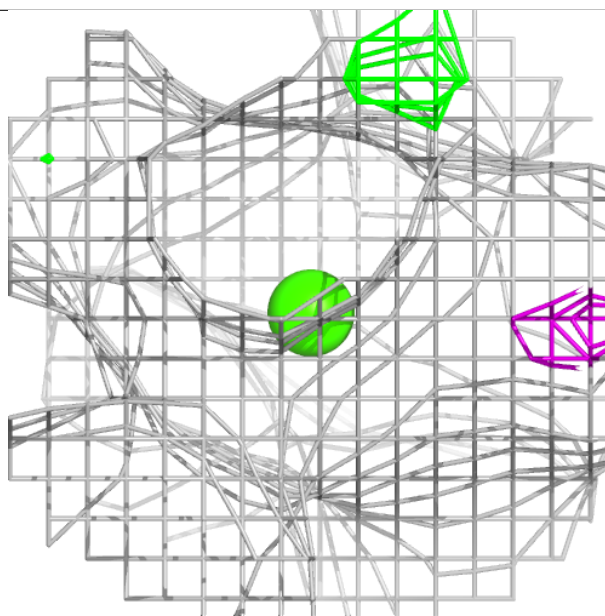
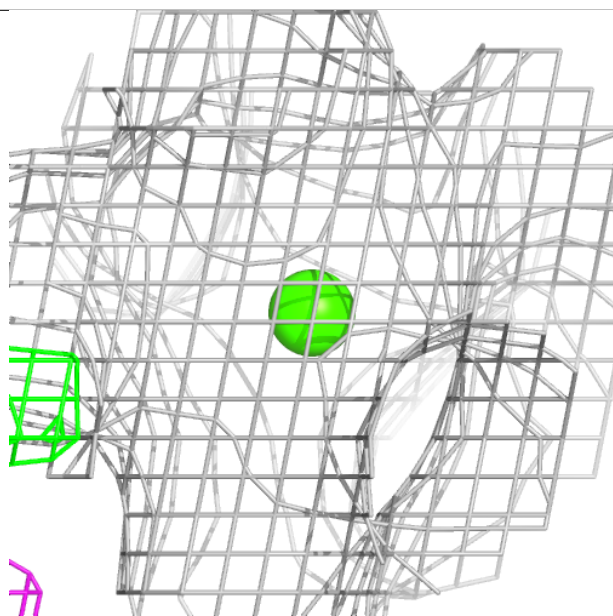
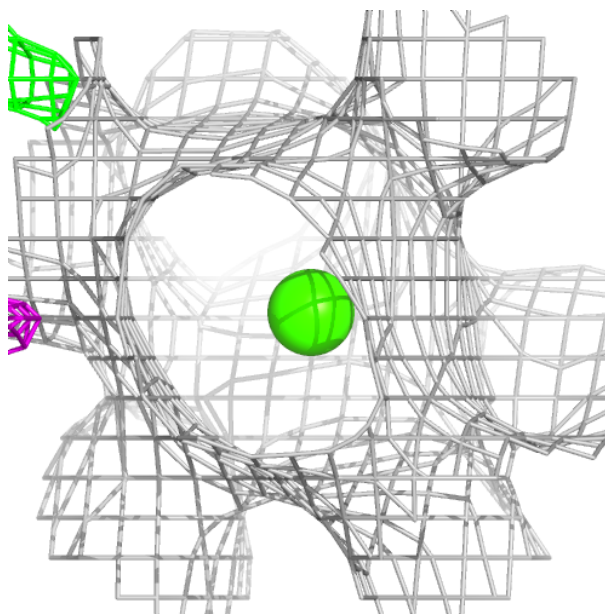
Electron density around CA A 403:

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



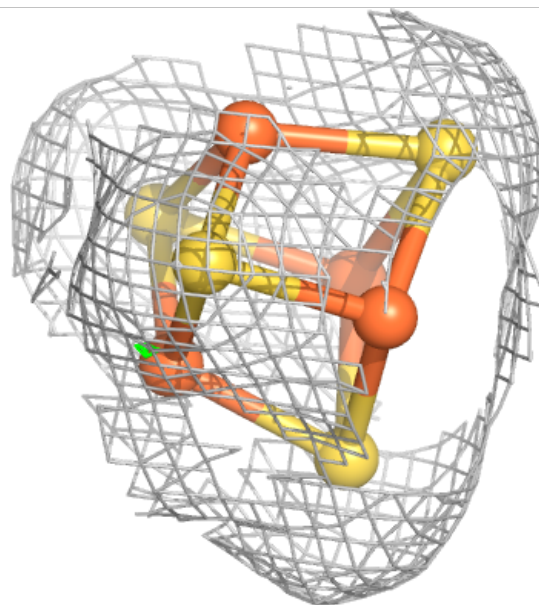
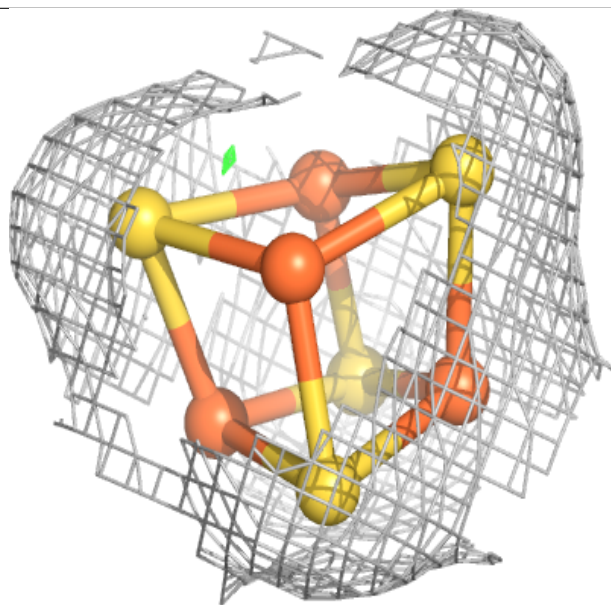
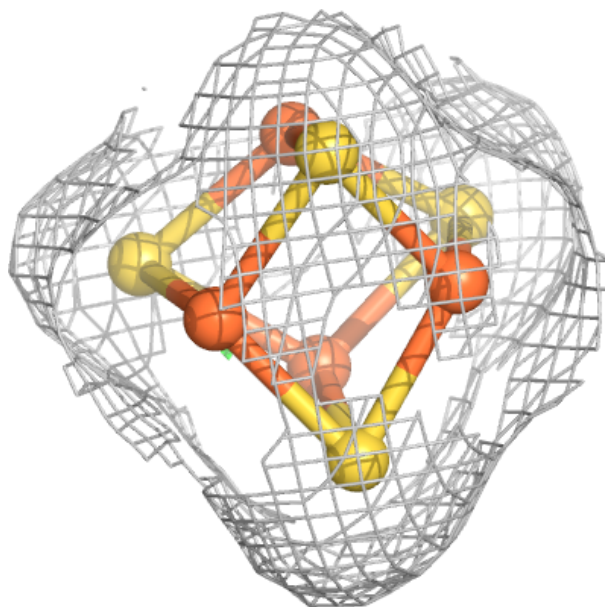
Electron density around CA D 403:

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



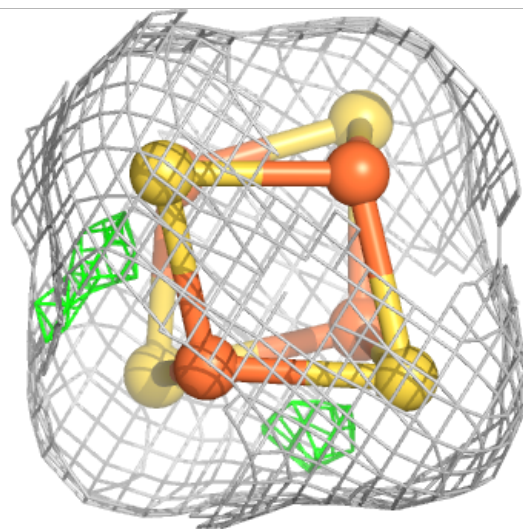
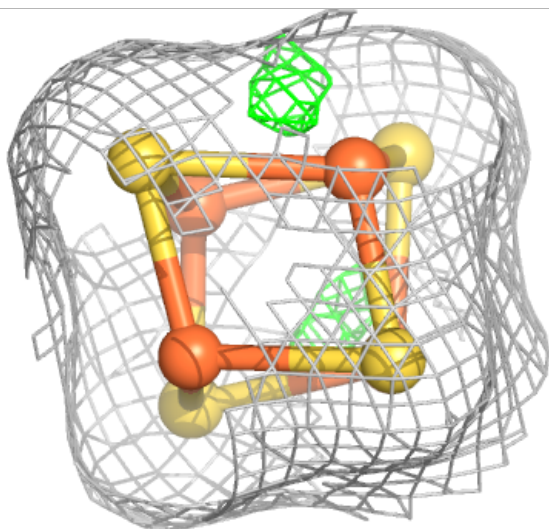
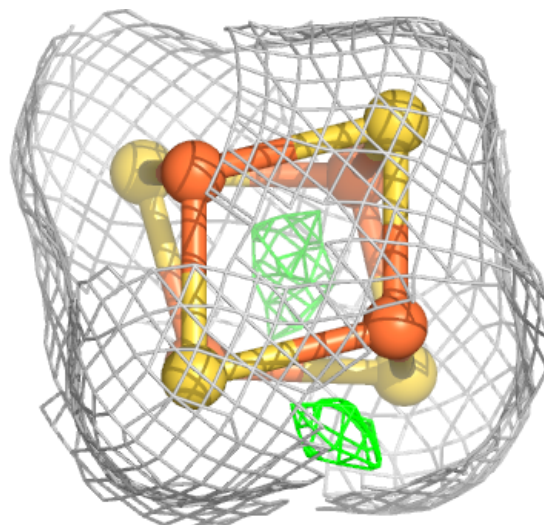
Electron density around SF4 A 401:

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



Electron density around SF4 D 401:

$2mF_o-DF_c$ (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.