



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:44 AM UTC

PDB ID : 6HM2 / pdb_00006hm2
Title : Structure in P1 form of the PBP AgtB in complex with agropinic acid from A.tumefaciens R10
Authors : Morera, S.; Marty, L.; Vigouroux, A.
Deposited on : 2018-09-12
Resolution : 1.74 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

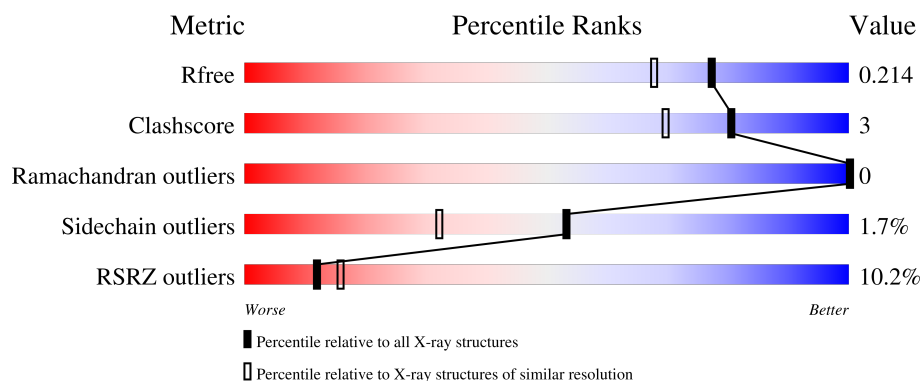
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	341	
1	B	341	
1	C	341	
1	D	341	
1	E	341	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13234 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 Agropine permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2426	1556	400	462	8			
1	B	317	Total	C	N	O	S	0	0	0
			2435	1561	402	464	8			
1	C	314	Total	C	N	O	S	0	0	0
			2410	1547	396	459	8			
1	D	314	Total	C	N	O	S	0	0	0
			2410	1547	396	459	8			
1	E	312	Total	C	N	O	S	0	0	0
			2394	1537	394	457	6			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	initiating methionine	UNP W8FRA6
A	9	GLY	-	expression tag	UNP W8FRA6
A	10	SER	-	expression tag	UNP W8FRA6
A	11	SER	-	expression tag	UNP W8FRA6
A	12	HIS	-	expression tag	UNP W8FRA6
A	13	HIS	-	expression tag	UNP W8FRA6
A	14	HIS	-	expression tag	UNP W8FRA6
A	15	HIS	-	expression tag	UNP W8FRA6
A	16	HIS	-	expression tag	UNP W8FRA6
A	17	HIS	-	expression tag	UNP W8FRA6
A	18	SER	-	expression tag	UNP W8FRA6
A	19	SER	-	expression tag	UNP W8FRA6
A	20	GLY	-	expression tag	UNP W8FRA6
A	21	LEU	-	expression tag	UNP W8FRA6
A	22	VAL	-	expression tag	UNP W8FRA6
A	23	PRO	-	expression tag	UNP W8FRA6
A	24	ARG	-	expression tag	UNP W8FRA6
A	25	GLY	-	expression tag	UNP W8FRA6
A	26	SER	-	expression tag	UNP W8FRA6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	27	HIS	-	expression tag	UNP W8FRA6
A	28	MET	-	expression tag	UNP W8FRA6
A	29	MET	-	expression tag	UNP W8FRA6
A	343	HIS	-	expression tag	UNP W8FRA6
A	344	HIS	-	expression tag	UNP W8FRA6
A	345	HIS	-	expression tag	UNP W8FRA6
A	346	HIS	-	expression tag	UNP W8FRA6
A	347	HIS	-	expression tag	UNP W8FRA6
A	348	HIS	-	expression tag	UNP W8FRA6
B	8	MET	-	initiating methionine	UNP W8FRA6
B	9	GLY	-	expression tag	UNP W8FRA6
B	10	SER	-	expression tag	UNP W8FRA6
B	11	SER	-	expression tag	UNP W8FRA6
B	12	HIS	-	expression tag	UNP W8FRA6
B	13	HIS	-	expression tag	UNP W8FRA6
B	14	HIS	-	expression tag	UNP W8FRA6
B	15	HIS	-	expression tag	UNP W8FRA6
B	16	HIS	-	expression tag	UNP W8FRA6
B	17	HIS	-	expression tag	UNP W8FRA6
B	18	SER	-	expression tag	UNP W8FRA6
B	19	SER	-	expression tag	UNP W8FRA6
B	20	GLY	-	expression tag	UNP W8FRA6
B	21	LEU	-	expression tag	UNP W8FRA6
B	22	VAL	-	expression tag	UNP W8FRA6
B	23	PRO	-	expression tag	UNP W8FRA6
B	24	ARG	-	expression tag	UNP W8FRA6
B	25	GLY	-	expression tag	UNP W8FRA6
B	26	SER	-	expression tag	UNP W8FRA6
B	27	HIS	-	expression tag	UNP W8FRA6
B	28	MET	-	expression tag	UNP W8FRA6
B	29	MET	-	expression tag	UNP W8FRA6
B	343	HIS	-	expression tag	UNP W8FRA6
B	344	HIS	-	expression tag	UNP W8FRA6
B	345	HIS	-	expression tag	UNP W8FRA6
B	346	HIS	-	expression tag	UNP W8FRA6
B	347	HIS	-	expression tag	UNP W8FRA6
B	348	HIS	-	expression tag	UNP W8FRA6
C	8	MET	-	initiating methionine	UNP W8FRA6
C	9	GLY	-	expression tag	UNP W8FRA6
C	10	SER	-	expression tag	UNP W8FRA6
C	11	SER	-	expression tag	UNP W8FRA6
C	12	HIS	-	expression tag	UNP W8FRA6

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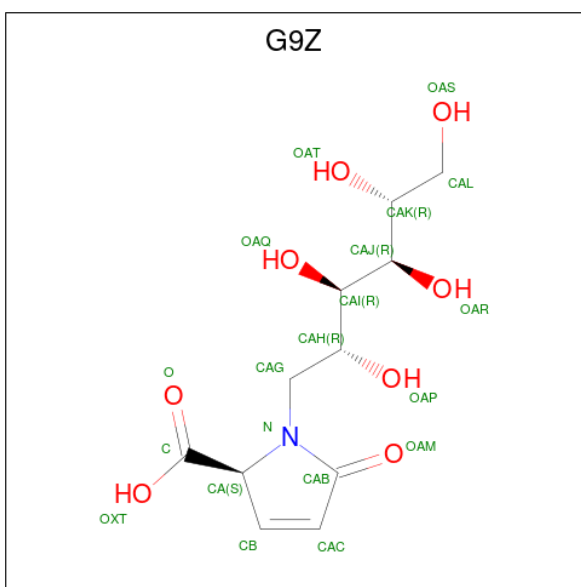
Chain	Residue	Modelled	Actual	Comment	Reference
C	13	HIS	-	expression tag	UNP W8FRA6
C	14	HIS	-	expression tag	UNP W8FRA6
C	15	HIS	-	expression tag	UNP W8FRA6
C	16	HIS	-	expression tag	UNP W8FRA6
C	17	HIS	-	expression tag	UNP W8FRA6
C	18	SER	-	expression tag	UNP W8FRA6
C	19	SER	-	expression tag	UNP W8FRA6
C	20	GLY	-	expression tag	UNP W8FRA6
C	21	LEU	-	expression tag	UNP W8FRA6
C	22	VAL	-	expression tag	UNP W8FRA6
C	23	PRO	-	expression tag	UNP W8FRA6
C	24	ARG	-	expression tag	UNP W8FRA6
C	25	GLY	-	expression tag	UNP W8FRA6
C	26	SER	-	expression tag	UNP W8FRA6
C	27	HIS	-	expression tag	UNP W8FRA6
C	28	MET	-	expression tag	UNP W8FRA6
C	29	MET	-	expression tag	UNP W8FRA6
C	343	HIS	-	expression tag	UNP W8FRA6
C	344	HIS	-	expression tag	UNP W8FRA6
C	345	HIS	-	expression tag	UNP W8FRA6
C	346	HIS	-	expression tag	UNP W8FRA6
C	347	HIS	-	expression tag	UNP W8FRA6
C	348	HIS	-	expression tag	UNP W8FRA6
D	8	MET	-	initiating methionine	UNP W8FRA6
D	9	GLY	-	expression tag	UNP W8FRA6
D	10	SER	-	expression tag	UNP W8FRA6
D	11	SER	-	expression tag	UNP W8FRA6
D	12	HIS	-	expression tag	UNP W8FRA6
D	13	HIS	-	expression tag	UNP W8FRA6
D	14	HIS	-	expression tag	UNP W8FRA6
D	15	HIS	-	expression tag	UNP W8FRA6
D	16	HIS	-	expression tag	UNP W8FRA6
D	17	HIS	-	expression tag	UNP W8FRA6
D	18	SER	-	expression tag	UNP W8FRA6
D	19	SER	-	expression tag	UNP W8FRA6
D	20	GLY	-	expression tag	UNP W8FRA6
D	21	LEU	-	expression tag	UNP W8FRA6
D	22	VAL	-	expression tag	UNP W8FRA6
D	23	PRO	-	expression tag	UNP W8FRA6
D	24	ARG	-	expression tag	UNP W8FRA6
D	25	GLY	-	expression tag	UNP W8FRA6
D	26	SER	-	expression tag	UNP W8FRA6

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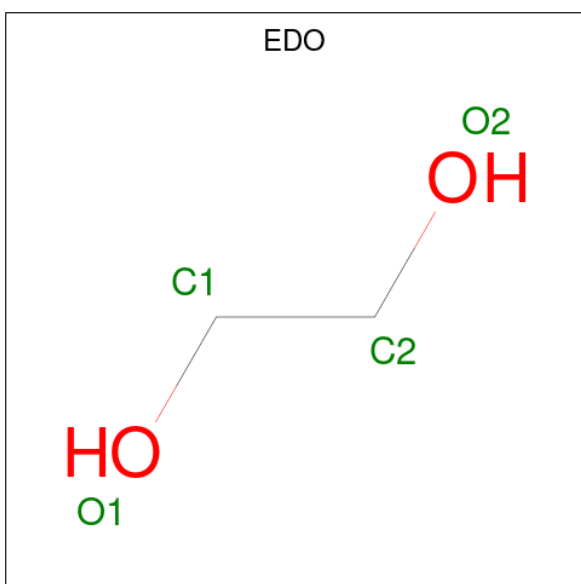
Chain	Residue	Modelled	Actual	Comment	Reference
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D	28	MET	-	expression tag	UNP W8FRA6
D	29	MET	-	expression tag	UNP W8FRA6
D	343	HIS	-	expression tag	UNP W8FRA6
D	344	HIS	-	expression tag	UNP W8FRA6
D	345	HIS	-	expression tag	UNP W8FRA6
D	346	HIS	-	expression tag	UNP W8FRA6
D	347	HIS	-	expression tag	UNP W8FRA6
D	348	HIS	-	expression tag	UNP W8FRA6
E	8	MET	-	initiating methionine	UNP W8FRA6
E	9	GLY	-	expression tag	UNP W8FRA6
E	10	SER	-	expression tag	UNP W8FRA6
E	11	SER	-	expression tag	UNP W8FRA6
E	12	HIS	-	expression tag	UNP W8FRA6
E	13	HIS	-	expression tag	UNP W8FRA6
E	14	HIS	-	expression tag	UNP W8FRA6
E	15	HIS	-	expression tag	UNP W8FRA6
E	16	HIS	-	expression tag	UNP W8FRA6
E	17	HIS	-	expression tag	UNP W8FRA6
E	18	SER	-	expression tag	UNP W8FRA6
E	19	SER	-	expression tag	UNP W8FRA6
E	20	GLY	-	expression tag	UNP W8FRA6
E	21	LEU	-	expression tag	UNP W8FRA6
E	22	VAL	-	expression tag	UNP W8FRA6
E	23	PRO	-	expression tag	UNP W8FRA6
E	24	ARG	-	expression tag	UNP W8FRA6
E	25	GLY	-	expression tag	UNP W8FRA6
E	26	SER	-	expression tag	UNP W8FRA6
E	27	HIS	-	expression tag	UNP W8FRA6
E	28	MET	-	expression tag	UNP W8FRA6
E	29	MET	-	expression tag	UNP W8FRA6
E	343	HIS	-	expression tag	UNP W8FRA6
E	344	HIS	-	expression tag	UNP W8FRA6
E	345	HIS	-	expression tag	UNP W8FRA6
E	346	HIS	-	expression tag	UNP W8FRA6
E	347	HIS	-	expression tag	UNP W8FRA6
E	348	HIS	-	expression tag	UNP W8FRA6

- Molecule 2 is agropinic acid (CCD ID: G9Z) (formula: C₁₁H₁₇NO₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 20	C 11	N 1	O 8	0	0
2	B	1	Total 20	C 11	N 1	O 8	0	0
2	C	1	Total 20	C 11	N 1	O 8	0	0
2	D	1	Total 20	C 11	N 1	O 8	0	0
2	E	1	Total 20	C 11	N 1	O 8	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0

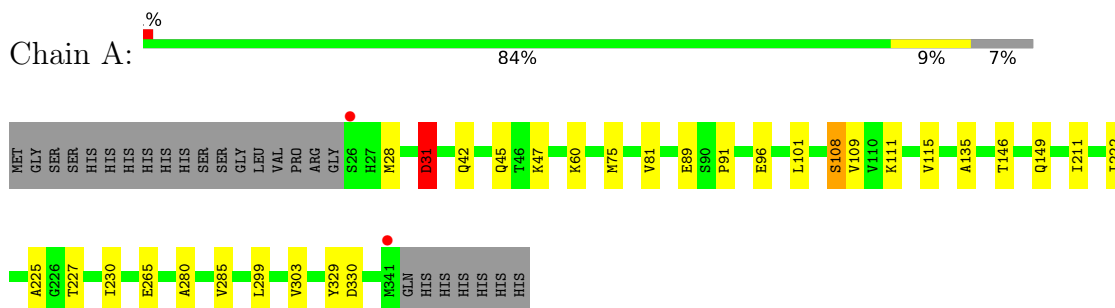
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	263	Total O 263 263	0	0
5	B	250	Total O 250 250	0	0
5	C	229	Total O 229 229	0	0
5	D	256	Total O 256 256	0	0
5	E	21	Total O 21 21	0	0

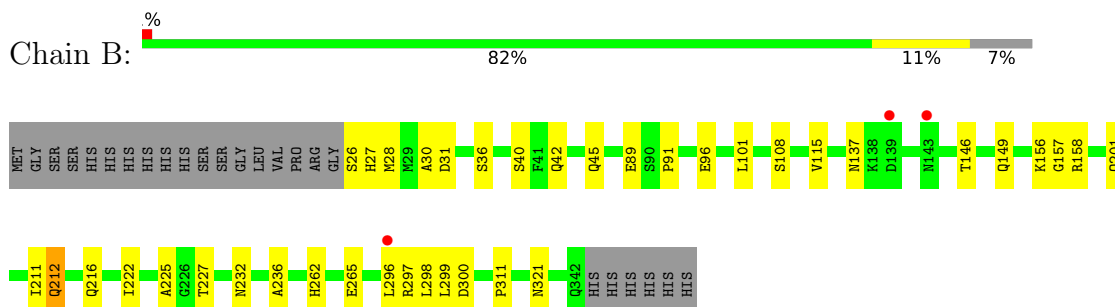
3 Residue-property plots [i](#)

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.

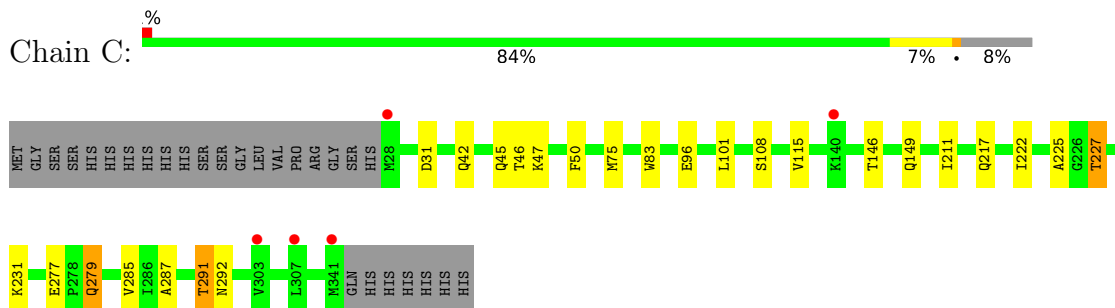
- Molecule 1: Agropine permease



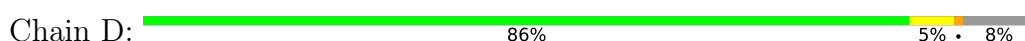
- Molecule 1: Agropine permease

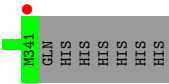
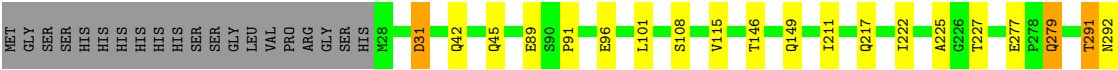


- Molecule 1: Agropine permease

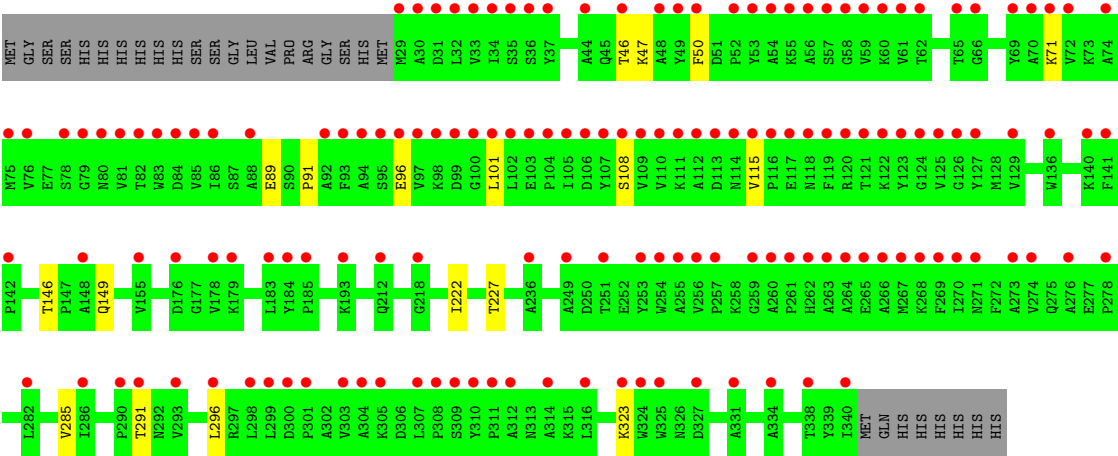
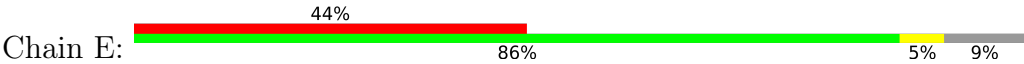


- Molecule 1: Agropine permease





● Molecule 1: Agropine permease



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	40.57Å 86.31Å 106.52Å 71.14° 81.00° 76.32°	Depositor
Resolution (Å)	49.73 – 1.74 49.73 – 1.74	Depositor EDS
% Data completeness (in resolution range)	95.9 (49.73-1.74) 95.6 (49.73-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.74Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.174 , 0.201 0.186 , 0.214	Depositor DCC
R_{free} test set	6483 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.083 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13234	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, EDO, G9Z

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	0.80	0/2488	1.04	3/3388 (0.1%)
1	B	0.84	0/2497	1.06	5/3400 (0.1%)
1	C	0.82	0/2471	1.06	5/3365 (0.1%)
1	D	0.84	0/2471	1.06	5/3365 (0.1%)
1	E	0.68	0/2455	1.10	3/3345 (0.1%)
All	All	0.80	0/12382	1.06	21/16863 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	31	ASP	CA-CB-CG	6.82	119.42	112.60
1	B	108	SER	N-CA-C	-6.43	105.25	113.23
1	D	291	THR	N-CA-C	-6.05	106.05	113.50
1	D	108	SER	N-CA-C	-6.05	105.90	113.28
1	E	108	SER	N-CA-C	-5.99	105.81	113.23
1	A	31	ASP	CA-CB-CG	5.89	118.49	112.60
1	B	31	ASP	CA-CB-CG	5.87	118.47	112.60
1	C	108	SER	N-CA-C	-5.86	106.13	113.28
1	C	291	THR	N-CA-C	-5.79	106.38	113.50
1	A	108	SER	N-CA-C	-5.77	106.08	113.23
1	B	300	ASP	N-CA-C	-5.42	101.67	109.48
1	E	291	THR	N-CA-C	-5.38	106.88	113.50
1	A	115	VAL	N-CA-C	-5.36	101.77	107.77
1	B	115	VAL	N-CA-C	-5.33	101.80	107.77
1	B	212	GLN	CB-CG-CD	5.32	121.65	112.60
1	C	115	VAL	N-CA-C	-5.21	101.94	107.77
1	C	31	ASP	CA-CB-CG	5.11	117.71	112.60
1	D	277	GLU	CB-CG-CD	5.07	121.21	112.60
1	D	115	VAL	N-CA-C	-5.04	102.13	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	115	VAL	N-CA-C	-5.01	102.16	107.77
1	C	277	GLU	CB-CG-CD	5.01	121.11	112.60

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	2426	0	2373	15	0
1	B	2435	0	2381	23	0
1	C	2410	0	2361	14	0
1	D	2410	0	2361	7	0
1	E	2394	0	2343	6	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
2	C	20	0	0	0	0
2	D	20	0	0	0	0
2	E	20	0	0	0	0
3	A	8	0	12	2	0
3	B	8	0	12	2	0
3	C	8	0	12	0	0
3	D	12	0	18	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	263	0	0	0	0
5	B	250	0	0	0	0
5	C	229	0	0	0	0
5	D	256	0	0	0	0
5	E	21	0	0	0	0
All	All	13234	0	11873	62	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (62) 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:C:227:THR:HG22	1:C:231:LYS:HE2	1.44	0.99
1:C:231:LYS:HE3	1:C:287:ALA:CB	2.12	0.79
1:B:156:LYS:HA	1:B:201:GLN:HE22	1.49	0.77
1:D:279:GLN:HE22	1:D:291:THR:H	1.34	0.74
1:C:279:GLN:HE22	1:C:291:THR:H	1.36	0.72
1:A:146:THR:H	1:A:149:GLN:HE21	1.41	0.69
1:B:146:THR:H	1:B:149:GLN:HE21	1.40	0.69
1:C:146:THR:H	1:C:149:GLN:HE21	1.40	0.67
1:D:146:THR:H	1:D:149:GLN:HE21	1.43	0.66
1:D:42:GLN:HA	1:D:45:GLN:HE21	1.64	0.62
1:A:28:MET:SD	1:A:265:GLU:HG3	2.39	0.62
1:C:231:LYS:HE3	1:C:287:ALA:HB1	1.80	0.62
1:E:146:THR:H	1:E:149:GLN:HE21	1.44	0.62
1:C:42:GLN:HA	1:C:45:GLN:HE21	1.66	0.61
1:B:26:SER:HB3	1:B:27:HIS:HA	1.85	0.58
1:A:329:TYR:HB3	3:A:403:EDO:H12	1.86	0.58
1:A:42:GLN:HA	1:A:45:GLN:HE21	1.70	0.56
1:A:47:LYS:HD3	1:A:285:VAL:HG11	1.86	0.56
1:E:47:LYS:HD3	1:E:285:VAL:HG11	1.86	0.56
1:B:212:GLN:HE21	1:B:216:GLN:NE2	2.04	0.56
1:C:227:THR:HG22	1:C:231:LYS:CE	2.29	0.55
1:B:296:LEU:HA	1:B:299:LEU:HD12	1.88	0.54
1:D:279:GLN:NE2	1:D:292:ASN:H	2.05	0.54
1:C:279:GLN:NE2	1:C:292:ASN:H	2.06	0.54
1:A:31:ASP:HB3	1:A:60:LYS:HG2	1.89	0.53
1:B:42:GLN:HA	1:B:45:GLN:HE21	1.73	0.53
1:B:26:SER:CB	1:B:27:HIS:HA	2.39	0.52
1:B:216:GLN:HE21	1:B:236:ALA:HB3	1.76	0.49
1:C:231:LYS:HE3	1:C:287:ALA:HB3	1.90	0.49
1:A:109:VAL:HG22	1:B:297:ARG:NH1	2.28	0.48
1:D:89:GLU:HG3	1:D:91:PRO:HD2	1.96	0.48
1:B:28:MET:HE3	1:B:30:ALA:O	2.14	0.47
1:B:311:PRO:HB3	3:B:402:EDO:H12	1.96	0.47
1:B:89:GLU:HG3	1:B:91:PRO:HD2	1.96	0.47
1:A:89:GLU:HG3	1:A:91:PRO:HD2	1.97	0.46
1:B:40:SER:HB2	1:B:232:ASN:HD22	1.80	0.46
1:E:89:GLU:HG3	1:E:91:PRO:HD2	1.97	0.46
1:B:158:ARG:NH1	1:E:71:LYS:HG2	2.30	0.46
1:A:330:ASP:CG	3:A:403:EDO:H11	2.40	0.46
1:B:216:GLN:NE2	1:B:236:ALA:HB3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:GLU:HA	1:D:101:LEU:HD12	1.97	0.45
1:B:36:SER:CB	1:B:45:GLN:HE22	2.28	0.45
1:B:321:ASN:HB2	3:B:403:EDO:H11	1.98	0.45
1:D:211:ILE:HG21	1:D:225:ALA:HB2	1.99	0.45
1:E:46:THR:HA	1:E:50:PHE:HB2	1.98	0.45
1:C:96:GLU:HA	1:C:101:LEU:HD12	2.00	0.43
1:A:211:ILE:HG21	1:A:225:ALA:HB2	2.00	0.43
1:B:28:MET:HE1	1:B:262:HIS:CD2	2.54	0.43
1:E:96:GLU:HA	1:E:101:LEU:HD12	1.99	0.43
1:B:157:GLY:H	1:B:201:GLN:NE2	2.16	0.42
1:A:75:MET:HG2	1:A:81:VAL:HA	2.01	0.42
1:A:135:ALA:HB2	1:A:230:ILE:HD13	2.02	0.42
1:C:47:LYS:HD3	1:C:285:VAL:HG11	2.02	0.42
1:C:46:THR:HA	1:C:50:PHE:HB2	2.02	0.41
1:A:108:SER:HB2	1:B:298:LEU:HD11	2.03	0.41
1:B:96:GLU:HA	1:B:101:LEU:HD12	2.01	0.41
1:C:211:ILE:HG21	1:C:225:ALA:HB2	2.02	0.41
1:B:211:ILE:HG21	1:B:225:ALA:HB2	2.03	0.41
1:C:75:MET:HE1	1:C:83:TRP:CE2	2.56	0.41
1:A:96:GLU:HA	1:A:101:LEU:HD12	2.01	0.41
1:B:28:MET:SD	1:B:265:GLU:HG3	2.60	0.41
1:A:280:ALA:O	1:A:299:LEU:HD21	2.22	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	314/341 (92%)	309 (98%)	5 (2%)	0	100	100
1	B	315/341 (92%)	309 (98%)	6 (2%)	0	100	100
1	C	312/341 (92%)	307 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	312/341 (92%)	306 (98%)	6 (2%)	0	100	100
1	E	310/341 (91%)	304 (98%)	6 (2%)	0	100	100
All	All	1563/1705 (92%)	1535 (98%)	28 (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	248/270 (92%)	243 (98%)	5 (2%)	48	26
1	B	249/270 (92%)	246 (99%)	3 (1%)	63	47
1	C	246/270 (91%)	242 (98%)	4 (2%)	55	35
1	D	246/270 (91%)	241 (98%)	5 (2%)	48	26
1	E	244/270 (90%)	240 (98%)	4 (2%)	55	35
All	All	1233/1350 (91%)	1212 (98%)	21 (2%)	53	32

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASP
1	A	111	LYS
1	A	222	ILE
1	A	227	THR
1	A	303	VAL
1	B	137	ASN
1	B	222	ILE
1	B	227	THR
1	C	217	GLN
1	C	222	ILE
1	C	227	THR
1	C	279	GLN
1	D	31	ASP

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Mol	Chain	Res	Type
1	D	217	GLN
1	D	222	ILE
1	D	227	THR
1	D	279	GLN
1	E	222	ILE
1	E	227	THR
1	E	296	LEU
1	E	323	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	149	GLN
1	A	212	GLN
1	A	326	ASN
1	A	328	ASN
1	B	45	GLN
1	B	149	GLN
1	B	201	GLN
1	B	212	GLN
1	B	216	GLN
1	B	217	GLN
1	B	232	ASN
1	B	262	HIS
1	B	275	GLN
1	B	326	ASN
1	B	328	ASN
1	C	45	GLN
1	C	80	ASN
1	C	133	ASN
1	C	149	GLN
1	C	212	GLN
1	C	279	GLN
1	C	328	ASN
1	D	45	GLN
1	D	133	ASN
1	D	149	GLN
1	D	212	GLN
1	D	279	GLN
1	D	328	ASN
1	E	149	GLN

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Mol	Chain	Res	Type
1	E	212	GLN
1	E	328	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\# Z > 2$
3	EDO	B	402	-	3,3,3	0.59	0	2,2,2	0.10	0
3	EDO	C	402	-	3,3,3	0.74	0	2,2,2	0.20	0
2	G9Z	E	401	-	19,20,20	2.88	4 (21%)	19,28,28	3.23	4 (21%)
3	EDO	D	402	-	3,3,3	0.44	0	2,2,2	0.43	0
2	G9Z	C	401	4	19,20,20	2.85	3 (15%)	19,28,28	2.76	3 (15%)
3	EDO	A	403	-	3,3,3	0.44	0	2,2,2	0.28	0
3	EDO	D	404	-	3,3,3	0.52	0	2,2,2	0.20	0
3	EDO	C	403	-	3,3,3	0.61	0	2,2,2	0.16	0
2	G9Z	B	401	4	19,20,20	2.25	3 (15%)	19,28,28	2.91	3 (15%)
3	EDO	D	403	-	3,3,3	0.49	0	2,2,2	0.32	0
3	EDO	B	403	-	3,3,3	0.63	0	2,2,2	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	G9Z	D	401	4	19,20,20	2.73	4 (21%)	19,28,28	3.15	3 (15%)
2	G9Z	A	401	4	19,20,20	2.75	3 (15%)	19,28,28	2.28	3 (15%)
3	EDO	A	402	-	3,3,3	0.50	0	2,2,2	0.29	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
3	EDO	B	402	-	-	1/1/1/1	-
3	EDO	C	402	-	-	0/1/1/1	-
2	G9Z	E	401	-	-	3/22/35/35	0/1/1/1
3	EDO	D	402	-	-	0/1/1/1	-
2	G9Z	C	401	4	-	2/22/35/35	0/1/1/1
3	EDO	A	403	-	-	0/1/1/1	-
3	EDO	D	404	-	-	1/1/1/1	-
3	EDO	C	403	-	-	0/1/1/1	-
2	G9Z	B	401	4	-	2/22/35/35	0/1/1/1
3	EDO	D	403	-	-	0/1/1/1	-
3	EDO	B	403	-	-	1/1/1/1	-
2	G9Z	D	401	4	-	2/22/35/35	0/1/1/1
2	G9Z	A	401	4	-	3/22/35/35	0/1/1/1
3	EDO	A	402	-	-	1/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	G9Z	CAC-CB	10.25	1.55	1.33
2	D	401	G9Z	CAC-CB	9.14	1.53	1.33
2	E	401	G9Z	CAC-CB	8.93	1.52	1.33
2	A	401	G9Z	CAC-CB	8.57	1.51	1.33
2	B	401	G9Z	CAC-CB	6.71	1.47	1.33
2	E	401	G9Z	CA-C	-5.58	1.43	1.53
2	A	401	G9Z	CAC-CAB	-5.01	1.39	1.48
2	E	401	G9Z	CAC-CAB	-4.88	1.39	1.48
2	D	401	G9Z	CA-C	-4.74	1.44	1.53
2	A	401	G9Z	CA-C	-4.64	1.44	1.53
2	B	401	G9Z	CA-C	-4.37	1.45	1.53
2	D	401	G9Z	CAC-CAB	-4.28	1.40	1.48
2	B	401	G9Z	CAC-CAB	-3.97	1.41	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	G9Z	CA-C	-3.83	1.46	1.53
2	C	401	G9Z	CAC-CAB	-3.48	1.42	1.48
2	E	401	G9Z	CAG-N	2.55	1.51	1.47
2	D	401	G9Z	CAJ-CAI	2.17	1.57	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	G9Z	CAC-CAB-N	12.38	113.78	106.77
2	D	401	G9Z	CAC-CAB-N	11.56	113.31	106.77
2	B	401	G9Z	CAC-CAB-N	10.80	112.88	106.77
2	C	401	G9Z	CAC-CAB-N	9.97	112.41	106.77
2	A	401	G9Z	CAC-CAB-N	8.46	111.56	106.77
2	D	401	G9Z	CB-CAC-CAB	-5.68	106.03	110.09
2	C	401	G9Z	CB-CAC-CAB	-5.12	106.43	110.09
2	E	401	G9Z	CB-CAC-CAB	-4.35	106.98	110.09
2	B	401	G9Z	CB-CAC-CAB	-4.25	107.06	110.09
2	E	401	G9Z	OAM-CAB-CAC	-3.38	122.32	128.52
2	A	401	G9Z	OAM-CAB-CAC	-3.31	122.44	128.52
2	D	401	G9Z	OAM-CAB-CAC	-3.28	122.50	128.52
2	B	401	G9Z	OAM-CAB-CAC	-3.13	122.78	128.52
2	C	401	G9Z	OAM-CAB-CAC	-2.82	123.35	128.52
2	E	401	G9Z	CA-N-CAB	-2.68	109.89	113.46
2	A	401	G9Z	CA-N-CAB	-2.32	110.37	113.46

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	G9Z	CAG-CAH-CAI-CAJ
2	B	401	G9Z	CAG-CAH-CAI-CAJ
2	C	401	G9Z	CAG-CAH-CAI-CAJ
2	D	401	G9Z	CAG-CAH-CAI-CAJ
2	E	401	G9Z	CAG-CAH-CAI-CAJ
3	A	402	EDO	O1-C1-C2-O2
2	E	401	G9Z	OAP-CAH-CAI-CAJ
2	A	401	G9Z	OAP-CAH-CAI-CAJ
2	B	401	G9Z	OAP-CAH-CAI-CAJ
2	D	401	G9Z	OAP-CAH-CAI-CAJ
3	D	404	EDO	O1-C1-C2-O2
2	C	401	G9Z	OAP-CAH-CAI-CAJ
3	B	403	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	E	401	G9Z	OAP-CAH-CAI-OAQ
2	A	401	G9Z	OAP-CAH-CAI-OAQ
3	B	402	EDO	O1-C1-C2-O2

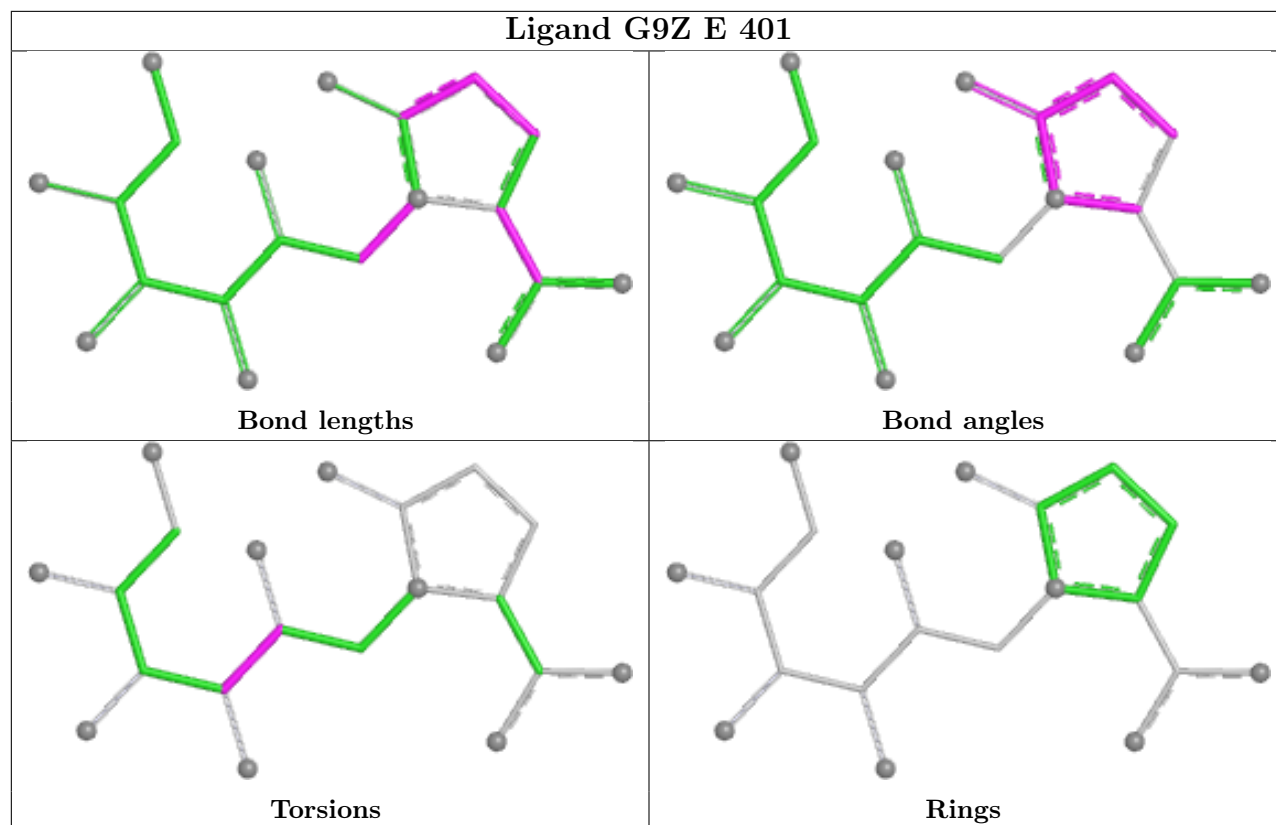
There are no ring outliers.

3 monomers are involved in 4 short contacts:

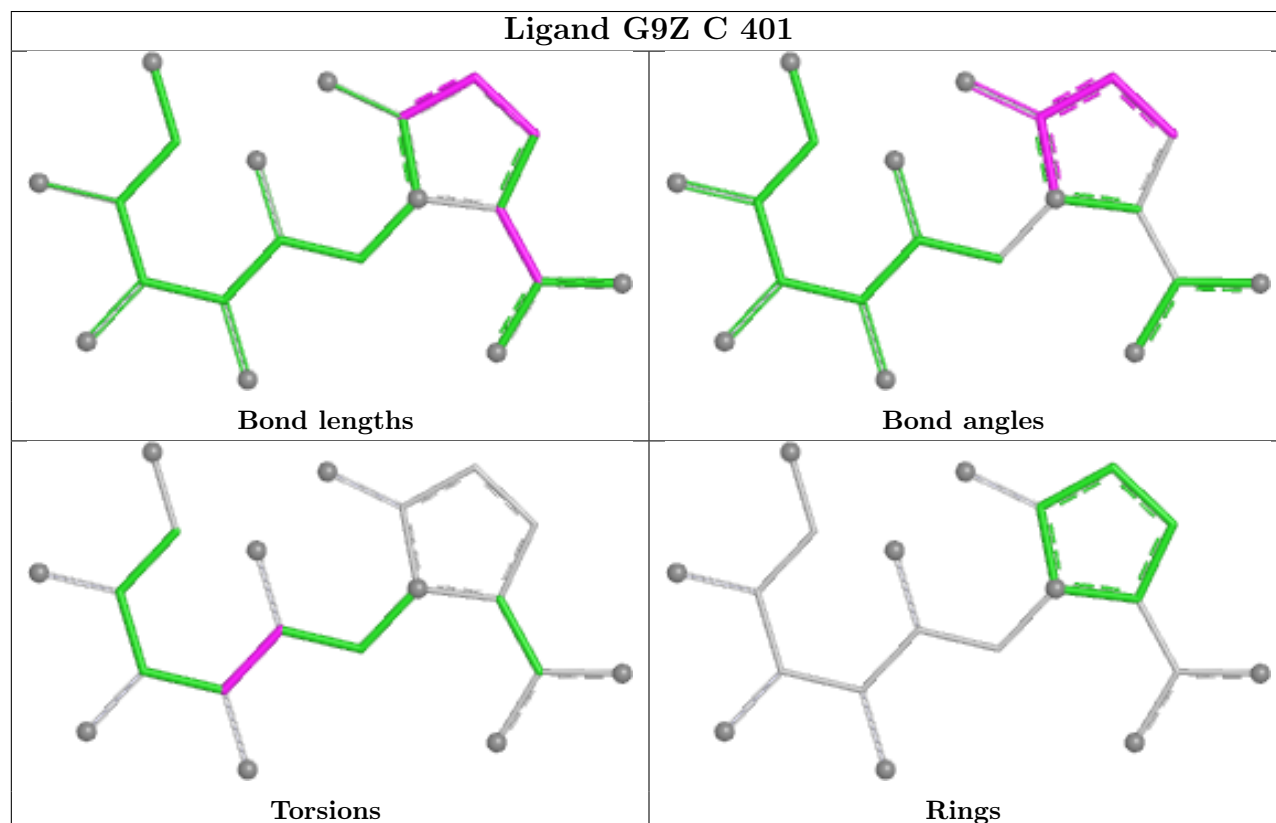
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	EDO	1	0
3	A	403	EDO	2	0
3	B	403	EDO	1	0

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.

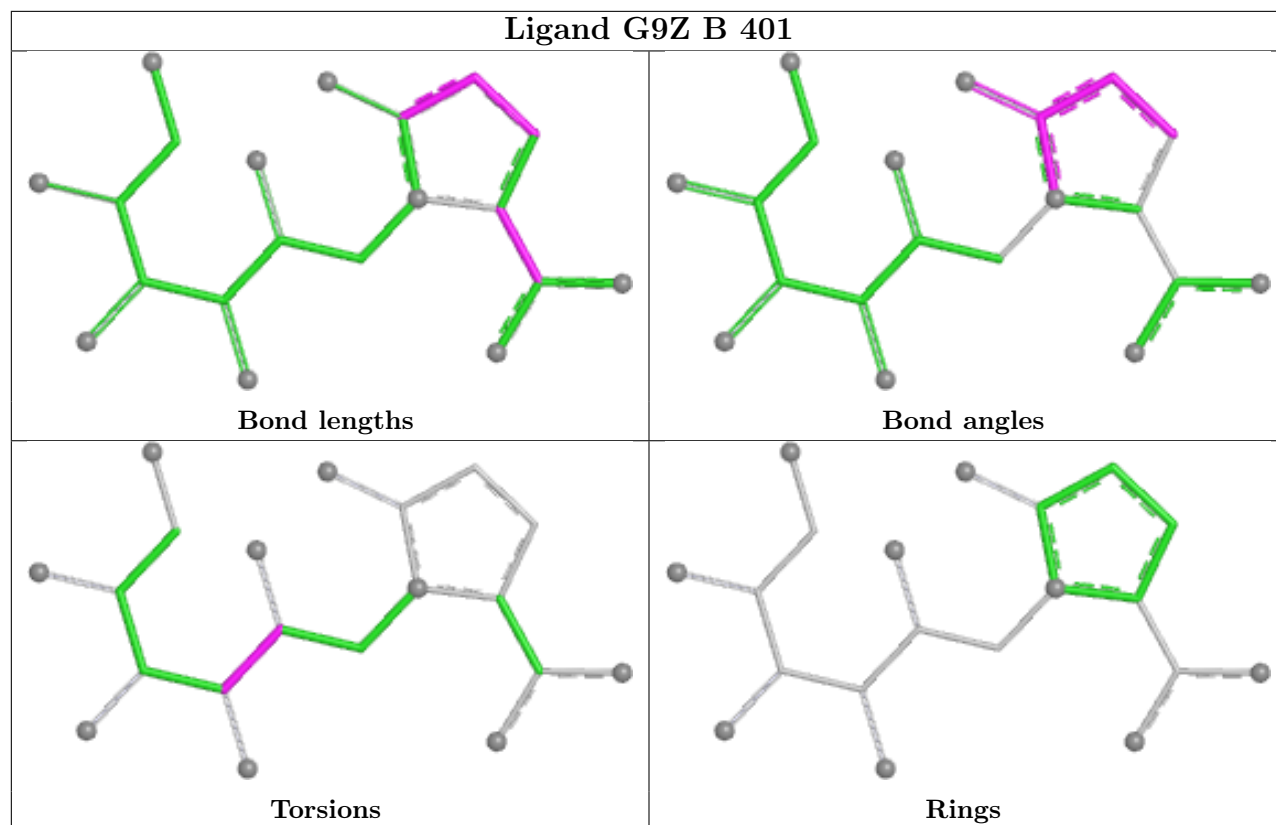
Ligand G9Z E 401



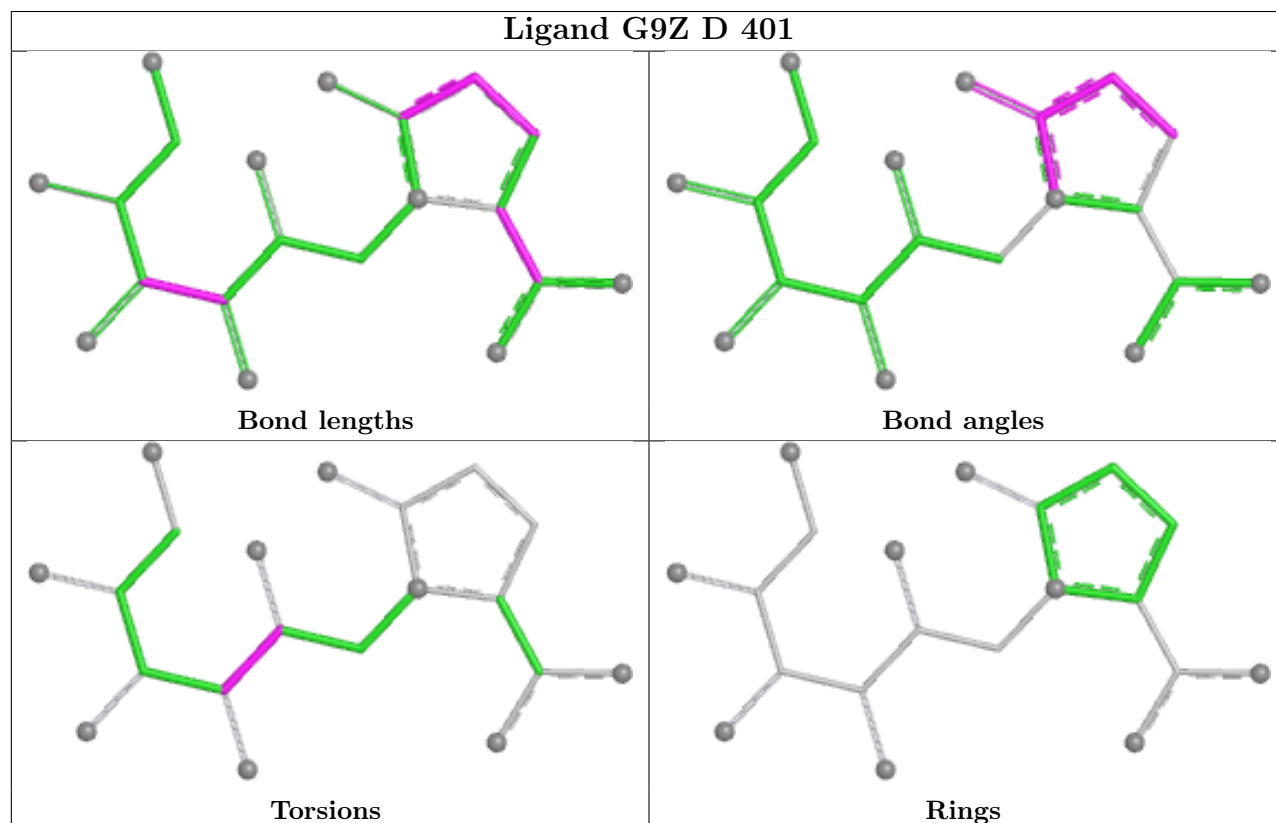
Ligand G9Z C 401

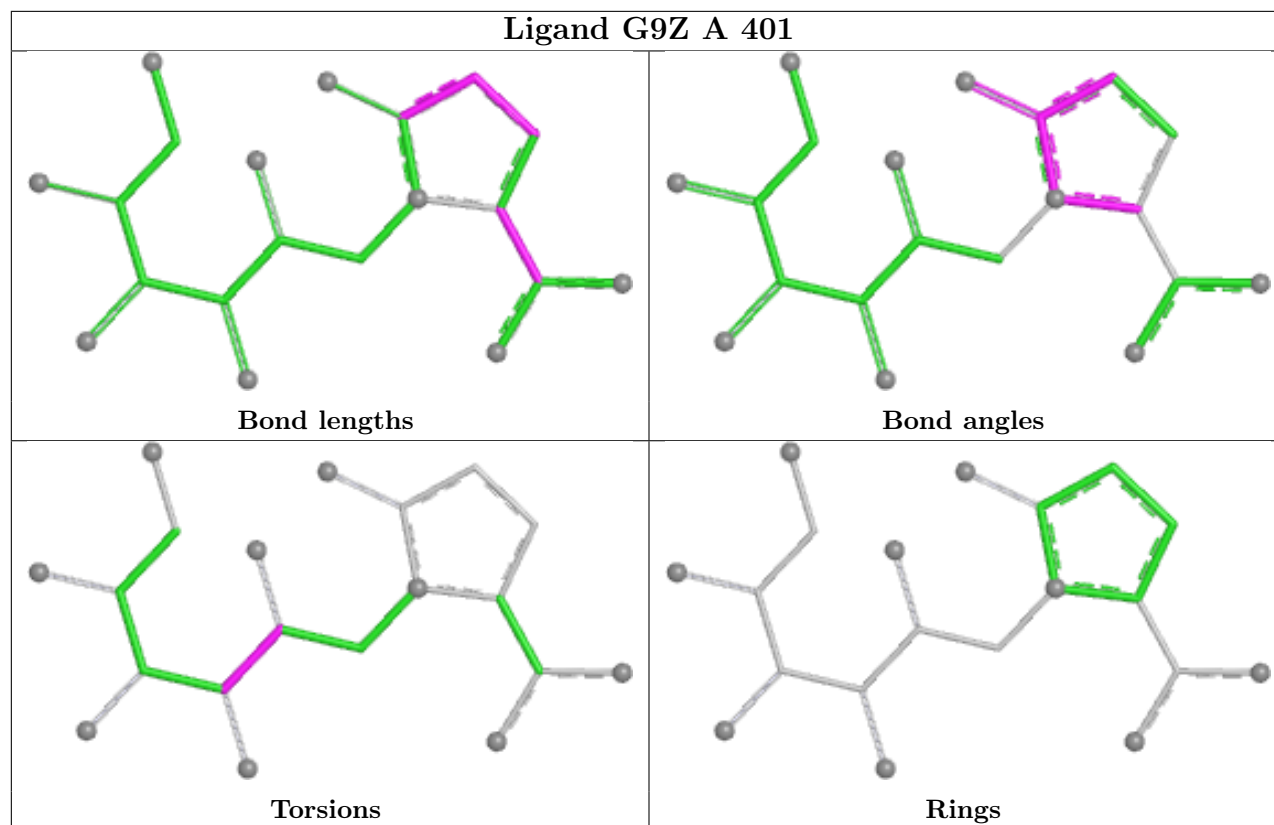


Ligand G9Z B 401



Ligand G9Z D 401





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	316/341 (92%)	-0.08	2 (0%) 85 90	13, 22, 39, 56	3 (0%)
1	B	317/341 (92%)	-0.06	3 (0%) 81 87	12, 22, 40, 69	3 (0%)
1	C	314/341 (92%)	-0.09	5 (1%) 70 77	14, 22, 39, 67	4 (1%)
1	D	314/341 (92%)	-0.16	1 (0%) 90 93	14, 21, 37, 70	4 (1%)
1	E	312/341 (91%)	2.12	150 (48%) 0 1	30, 78, 183, 214	3 (0%)
All	All	1573/1705 (92%)	0.34	161 (10%) 12 16	12, 24, 117, 214	17 (1%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	125	VAL	6.1
1	E	30	ALA	6.0
1	E	110	VAL	5.9
1	E	264	ALA	5.8
1	E	56	ALA	5.6
1	E	109	VAL	5.4
1	E	97	VAL	5.4
1	E	102	LEU	5.4
1	E	115	VAL	5.3
1	E	119	PHE	5.0
1	E	256	VAL	4.8
1	E	107	TYR	4.8
1	E	101	LEU	4.8
1	E	108	SER	4.6
1	E	116	PRO	4.6
1	E	83	TRP	4.5
1	E	76	VAL	4.5
1	E	54	ALA	4.3
1	E	266	ALA	4.3
1	E	59	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	85	VAL	4.3
1	E	261	PRO	4.3
1	E	32	LEU	4.3
1	E	263	ALA	4.2
1	E	104	PRO	4.2
1	E	114	ASN	4.2
1	E	311	PRO	4.1
1	E	33	VAL	4.1
1	E	86	ILE	4.1
1	E	74	ALA	4.1
1	E	331	ALA	4.0
1	E	93	PHE	4.0
1	E	61	VAL	4.0
1	E	58	GLY	3.9
1	E	112	ALA	3.9
1	E	274	VAL	3.9
1	E	269	PHE	3.8
1	E	273	ALA	3.8
1	E	310	TYR	3.8
1	E	105	ILE	3.7
1	E	29	MET	3.7
1	E	123	TYR	3.7
1	E	100	GLY	3.7
1	E	50	PHE	3.7
1	E	255	ALA	3.6
1	E	298	LEU	3.6
1	E	72	VAL	3.5
1	E	303	VAL	3.4
1	E	257	PRO	3.4
1	E	49	TYR	3.4
1	E	34	ILE	3.4
1	E	70	ALA	3.3
1	E	92	ALA	3.3
1	E	254	TRP	3.3
1	E	270	ILE	3.3
1	E	126	GLY	3.3
1	E	113	ASP	3.3
1	E	212	GLN	3.2
1	E	99	ASP	3.2
1	E	62	THR	3.2
1	E	276	ALA	3.2
1	E	52	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	183	LEU	3.1
1	E	71	LYS	3.1
1	E	98	LYS	3.1
1	E	299	LEU	3.0
1	E	48	ALA	3.0
1	E	121	THR	3.0
1	E	106	ASP	3.0
1	E	316	LEU	3.0
1	E	111	LYS	2.9
1	E	66	GLY	2.9
1	E	325	TRP	2.9
1	E	268	LYS	2.9
1	E	312	ALA	2.9
1	E	309	SER	2.9
1	E	301	PRO	2.8
1	E	65	THR	2.8
1	E	57	SER	2.8
1	E	53	TYR	2.8
1	E	142	PRO	2.7
1	E	253	TYR	2.7
1	E	46	THR	2.7
1	E	262	HIS	2.7
1	C	140	LYS	2.7
1	E	122	LYS	2.7
1	E	79	GLY	2.7
1	E	118	ASN	2.7
1	C	341	MET	2.7
1	E	314	ALA	2.7
1	E	31	ASP	2.7
1	E	75	MET	2.7
1	E	267	MET	2.7
1	E	304	ALA	2.7
1	A	26	SER	2.6
1	E	340	ILE	2.6
1	E	265	GLU	2.6
1	E	80	ASN	2.6
1	E	184	TYR	2.6
1	E	185	PRO	2.6
1	E	82	THR	2.6
1	E	81	VAL	2.6
1	E	293	VAL	2.6
1	E	60	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	139	ASP	2.5
1	C	303	VAL	2.5
1	E	129	VAL	2.5
1	E	338	THR	2.5
1	E	94	ALA	2.5
1	E	334	ALA	2.5
1	E	78	SER	2.5
1	C	307	LEU	2.4
1	E	69	TYR	2.4
1	B	143	ASN	2.4
1	E	103	GLU	2.4
1	E	127	TYR	2.4
1	E	327	ASP	2.4
1	E	193	LYS	2.4
1	E	305	LYS	2.4
1	E	95	SER	2.4
1	E	88	ALA	2.4
1	E	236	ALA	2.4
1	E	84	ASP	2.3
1	E	296	LEU	2.3
1	E	290	PRO	2.3
1	E	120	ARG	2.3
1	C	28	MET	2.3
1	E	117	GLU	2.3
1	A	341	MET	2.3
1	E	260	ALA	2.2
1	E	36	SER	2.2
1	E	37	TYR	2.2
1	E	291	THR	2.2
1	E	271	ASN	2.2
1	E	148	ALA	2.2
1	E	55	LYS	2.2
1	E	140	LYS	2.2
1	E	282	LEU	2.2
1	E	308	PRO	2.2
1	E	178	VAL	2.2
1	E	323	LYS	2.2
1	E	249	ALA	2.2
1	B	296	LEU	2.2
1	E	307	LEU	2.2
1	E	278	PRO	2.2
1	E	300	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	155	VAL	2.1
1	E	44	ALA	2.1
1	E	124	GLY	2.1
1	E	259	GLY	2.1
1	E	324	TRP	2.1
1	E	141	PHE	2.1
1	E	96	GLU	2.1
1	E	286	ILE	2.1
1	E	176	ASP	2.1
1	E	251	THR	2.1
1	E	136	TRP	2.1
1	D	341	MET	2.0
1	E	218	GLY	2.0
1	E	35	SER	2.0
1	E	179	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	403	4/4	0.66	0.20	52,52,52,55	0
3	EDO	C	402	4/4	0.78	0.14	40,43,45,47	0
3	EDO	B	403	4/4	0.79	0.14	46,48,48,48	0
3	EDO	C	403	4/4	0.82	0.13	48,50,52,53	0
3	EDO	D	404	4/4	0.85	0.14	37,41,44,44	0
3	EDO	B	402	4/4	0.86	0.20	38,39,40,41	0
3	EDO	D	402	4/4	0.87	0.11	42,45,45,47	0
3	EDO	A	402	4/4	0.88	0.12	34,38,41,44	0

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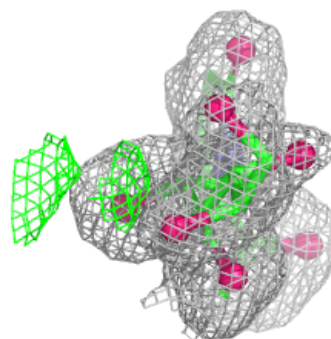
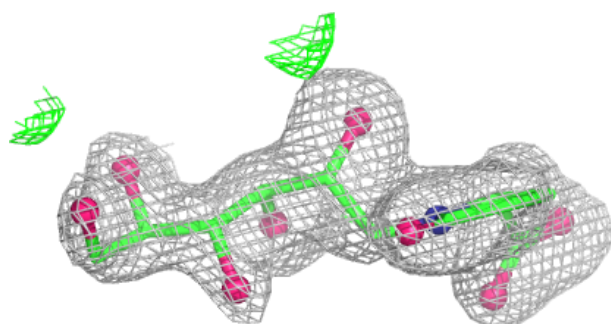
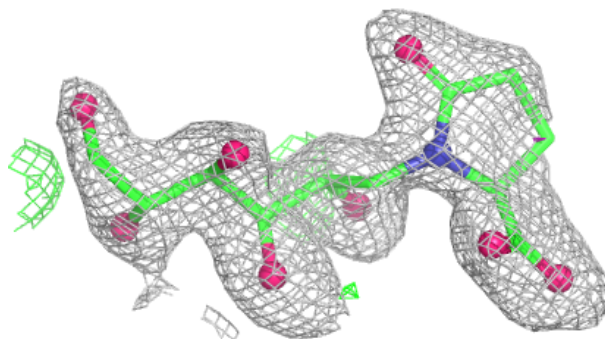
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	G9Z	E	401	20/20	0.89	0.10	36,42,47,50	0
3	EDO	D	403	4/4	0.92	0.10	36,41,45,48	0
2	G9Z	C	401	20/20	0.96	0.05	10,17,19,21	0
2	G9Z	A	401	20/20	0.97	0.04	12,15,19,20	0
2	G9Z	D	401	20/20	0.97	0.04	13,17,18,19	0
2	G9Z	B	401	20/20	0.98	0.04	11,16,20,21	0
4	NA	A	404	1/1	0.98	0.10	25,25,25,25	0
4	NA	D	405	1/1	0.98	0.08	23,23,23,23	0
4	NA	C	404	1/1	0.99	0.06	24,24,24,24	0
4	NA	B	404	1/1	0.99	0.03	24,24,24,24	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.

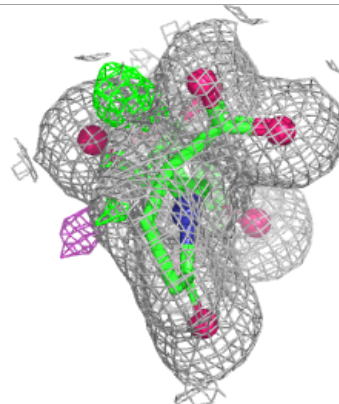
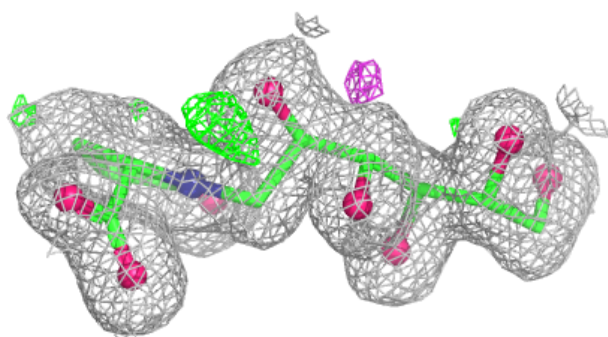
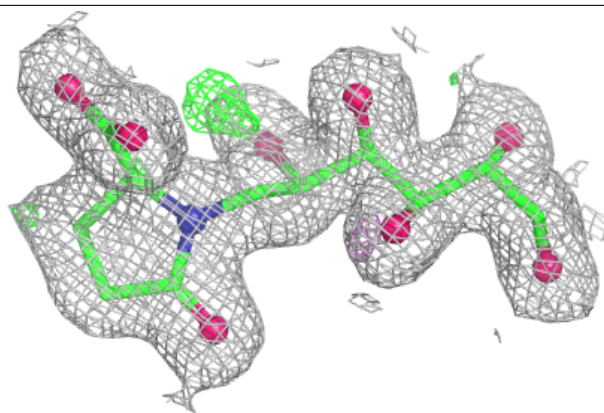
Electron density around G9Z E 401:

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

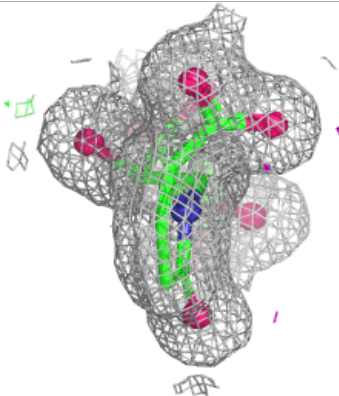
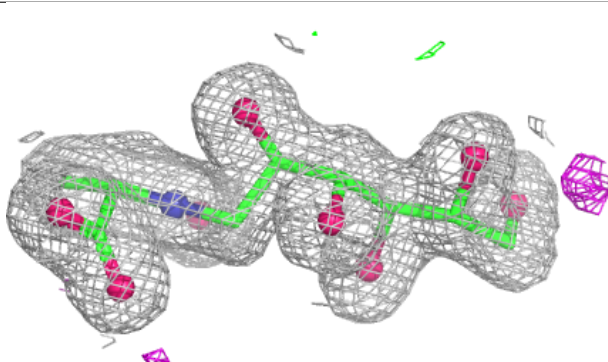
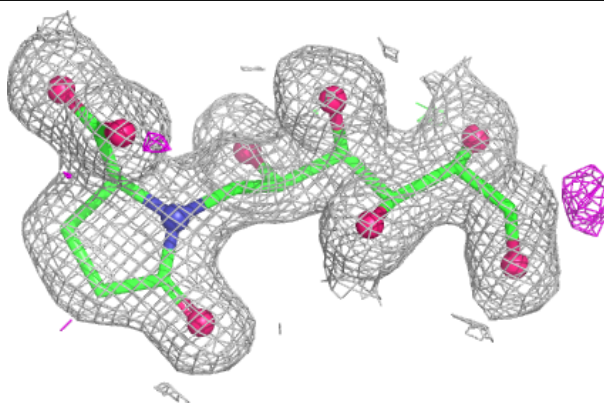


Electron density around G9Z C 401:

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

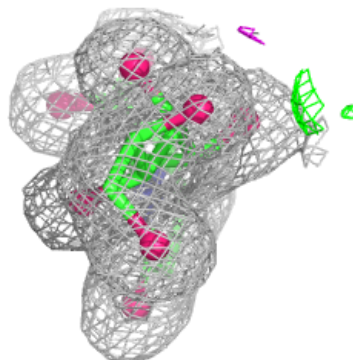
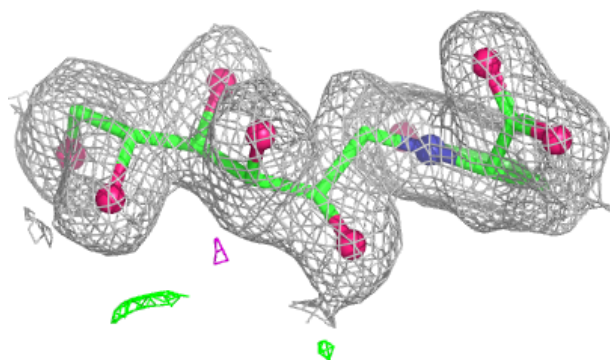
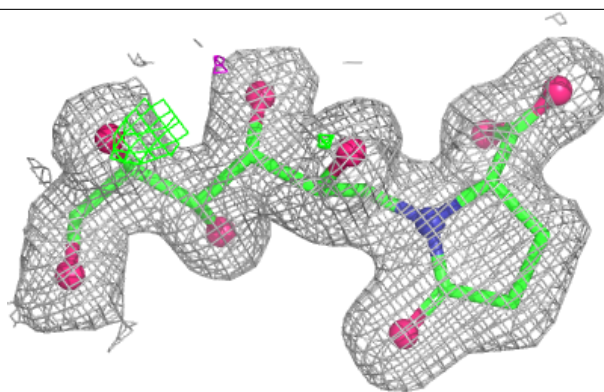
**Electron density around G9Z A 401:**

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

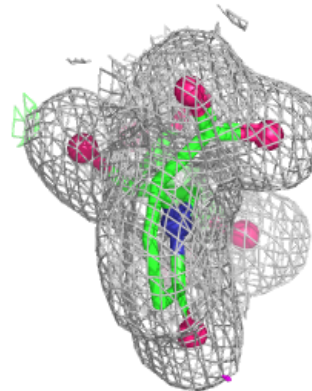
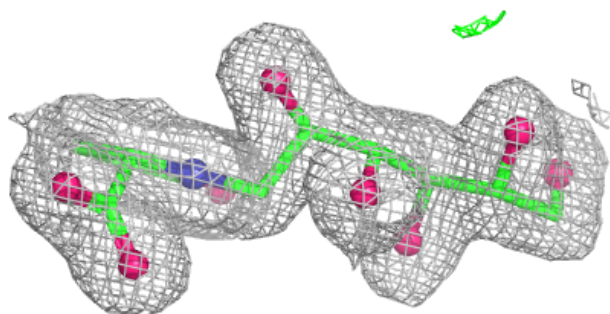
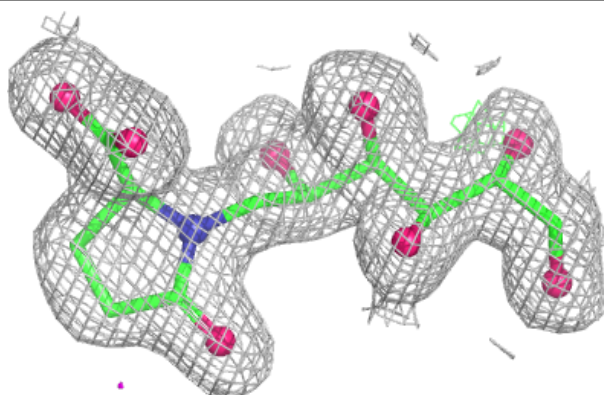


Electron density around G9Z D 401:

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

**Electron density around G9Z B 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.