



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:58 PM UTC

PDB ID : 9HZ1 / pdb_00009hz1
Title : Crystal structure of AlfB
Authors : Marina, A.; Gallego del Sol, F.
Deposited on : 2025-01-12
Resolution : 2.40 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

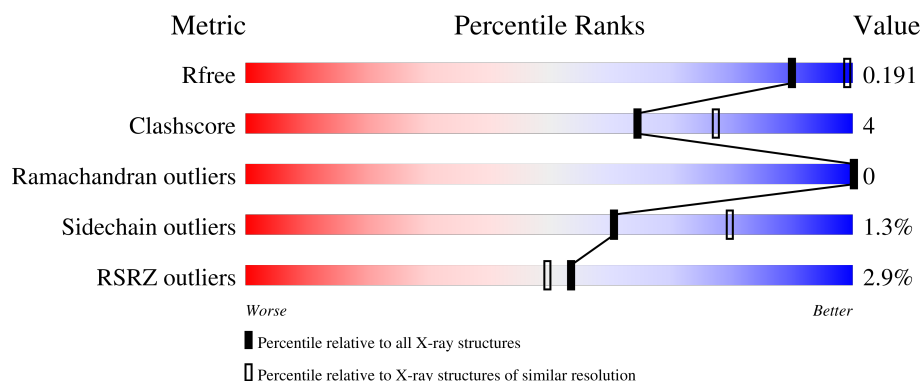
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	414	4% 87% 11% ..
1	B	414	3% 88% 11% .
1	C	414	2% 87% 10% ..
1	D	414	2% 88% 10% ..
1	E	414	3% 87% 10% ..

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Mol	Chain	Length	Quality of chain
1	F	414	

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
2	JFZ	A	1001	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20883 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 Alpha-L-fucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3292	2119	559	603	11			
1	B	411	Total	C	N	O	S	0	1	0
			3293	2119	559	604	11			
1	C	407	Total	C	N	O	S	0	0	0
			3263	2100	554	599	10			
1	D	407	Total	C	N	O	S	0	0	0
			3263	2100	554	599	10			
1	E	406	Total	C	N	O	S	0	0	0
			3254	2095	552	597	10			
1	F	407	Total	C	N	O	S	0	0	0
			3263	2100	554	599	10			

There are 18 discrepancies between the modelled and reference sequences:

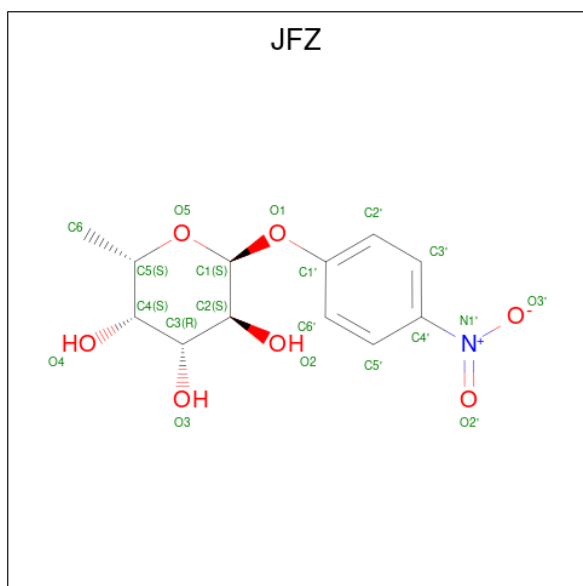
Chain	Residue	Modelled	Actual	Comment	Reference
A	196	SER	ASN	conflict	UNP A0A806EKD1
A	261	MET	VAL	conflict	UNP A0A806EKD1
A	346	LYS	ASN	conflict	UNP A0A806EKD1
B	196	SER	ASN	conflict	UNP A0A806EKD1
B	261	MET	VAL	conflict	UNP A0A806EKD1
B	346	LYS	ASN	conflict	UNP A0A806EKD1
C	196	SER	ASN	conflict	UNP A0A806EKD1
C	261	MET	VAL	conflict	UNP A0A806EKD1
C	346	LYS	ASN	conflict	UNP A0A806EKD1
D	196	SER	ASN	conflict	UNP A0A806EKD1
D	261	MET	VAL	conflict	UNP A0A806EKD1
D	346	LYS	ASN	conflict	UNP A0A806EKD1
E	196	SER	ASN	conflict	UNP A0A806EKD1
E	261	MET	VAL	conflict	UNP A0A806EKD1
E	346	LYS	ASN	conflict	UNP A0A806EKD1
F	196	SER	ASN	conflict	UNP A0A806EKD1
F	261	MET	VAL	conflict	UNP A0A806EKD1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	346	LYS	ASN	conflict	UNP A0A806EKD1

- Molecule 2 is 4-nitrophenyl 6-deoxy- α -L-galactopyranoside (CCD ID: JFZ) (formula: $C_{12}H_{15}NO_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	12	1	7		
2	B	1	Total	C	N	O	0	0
			20	12	1	7		
2	C	1	Total	C	N	O	0	0
			20	12	1	7		
2	D	1	Total	C	N	O	0	0
			20	12	1	7		
2	E	1	Total	C	N	O	0	0
			20	12	1	7		
2	F	1	Total	C	N	O	0	0
			20	12	1	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	210	Total	O	0	0
			210	210		
3	B	195	Total	O	0	0
			195	195		

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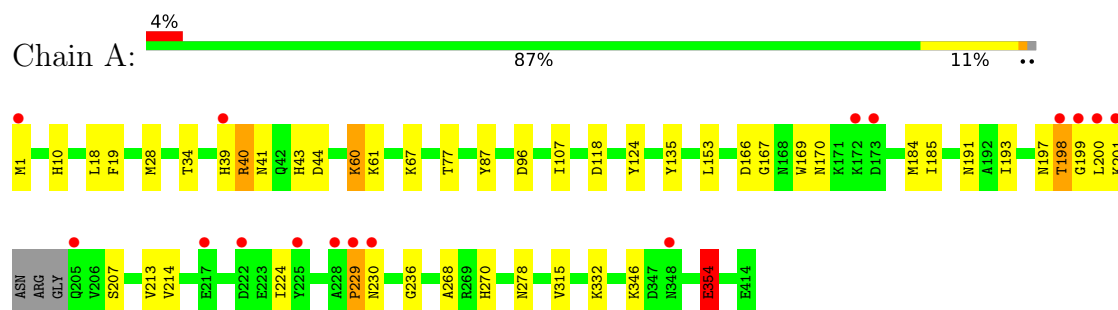
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	186	Total 186	O 186	0	0
3	D	228	Total 228	O 228	0	0
3	E	149	Total 149	O 149	0	0
3	F	167	Total 167	O 167	0	0

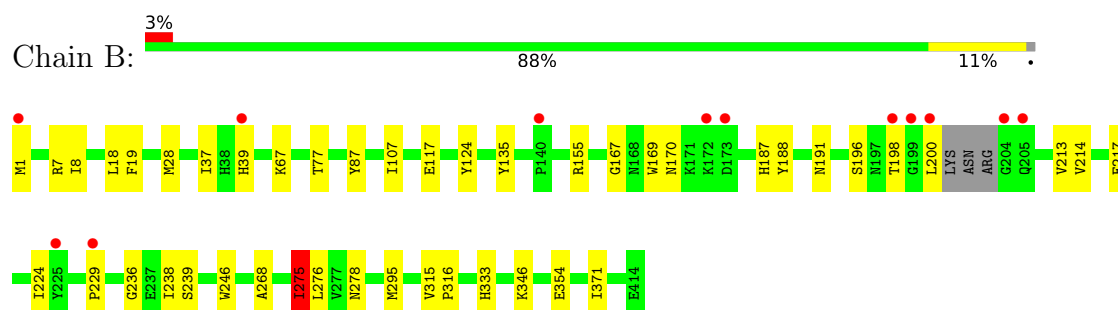
3 Residue-property plots [i](#)

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.

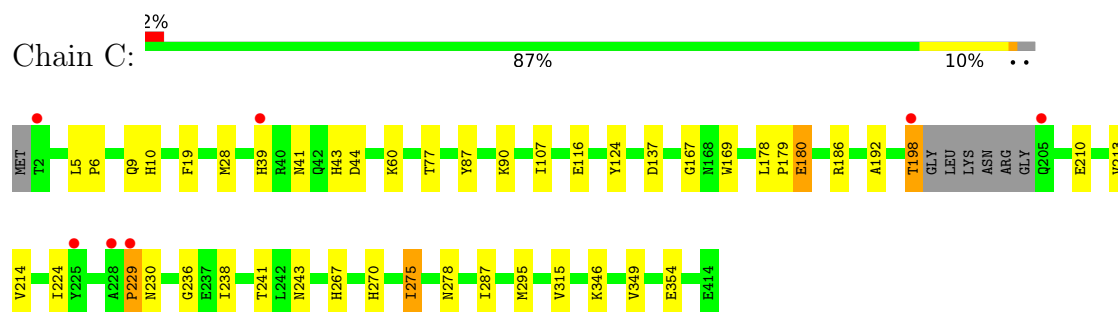
- Molecule 1: Alpha-L-fucosidase



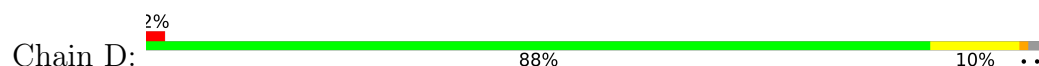
- Molecule 1: Alpha-L-fucosidase

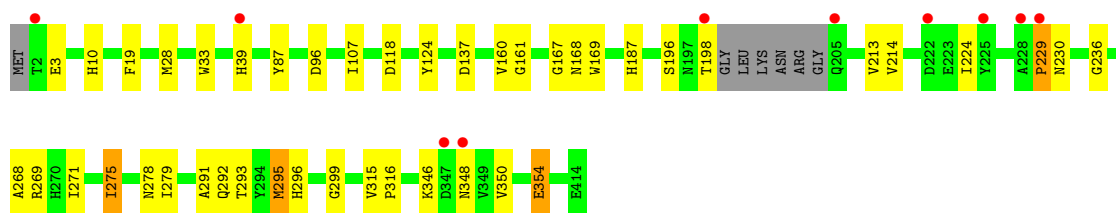


- Molecule 1: Alpha-L-fucosidase

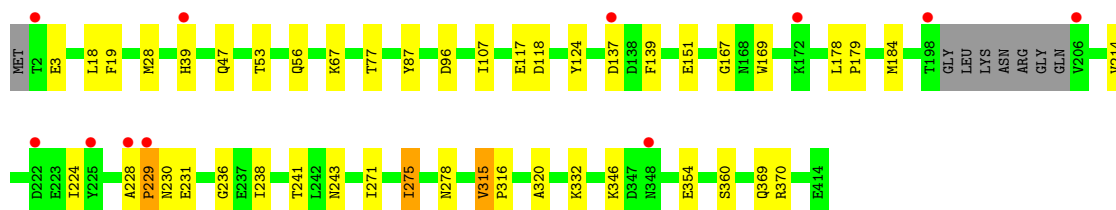
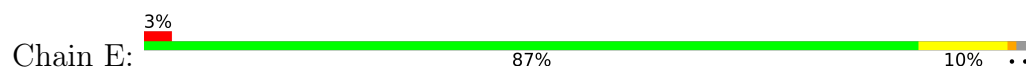


- Molecule 1: Alpha-L-fucosidase

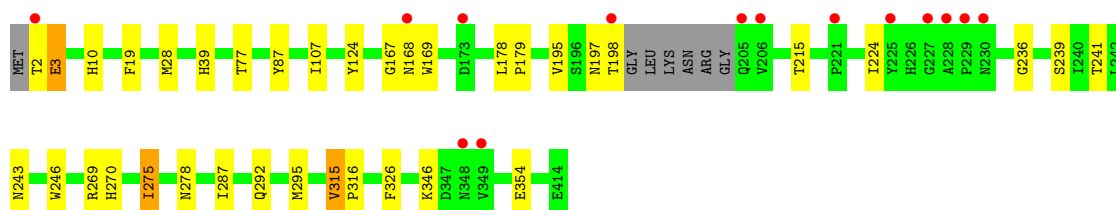
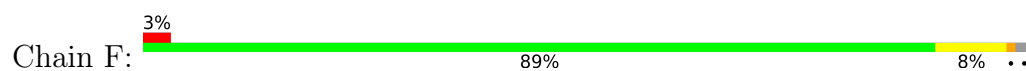




● Molecule 1: Alpha-L-fucosidase



● Molecule 1: Alpha-L-fucosidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	167.83Å 309.99Å 175.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.67 – 2.40 48.67 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.67-2.40) 100.0 (48.67-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.164 , 0.190 0.166 , 0.191	Depositor DCC
R_{free} test set	8664 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.9	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	20883	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 2.41% 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: JFZ

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	0.93	7/3389 (0.2%)	1.14	11/4619 (0.2%)
1	B	0.92	8/3393 (0.2%)	1.12	8/4625 (0.2%)
1	C	0.81	4/3360 (0.1%)	1.10	6/4582 (0.1%)
1	D	0.89	14/3360 (0.4%)	1.10	8/4582 (0.2%)
1	E	0.82	4/3351 (0.1%)	1.08	10/4570 (0.2%)
1	F	0.74	2/3360 (0.1%)	1.10	4/4582 (0.1%)
All	All	0.86	39/20213 (0.2%)	1.11	47/27560 (0.2%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	213	VAL	C-O	-7.32	1.16	1.24
1	D	213	VAL	C-O	-7.07	1.16	1.24
1	D	268	ALA	C-O	-6.53	1.16	1.24
1	F	275	ILE	C-O	-6.37	1.17	1.24
1	B	371	ILE	C-O	-6.37	1.17	1.24
1	C	270	HIS	C-O	-6.01	1.17	1.24
1	D	271	ILE	C-O	-5.84	1.17	1.24
1	E	271	ILE	C-O	-5.83	1.17	1.24
1	D	299	GLY	C-O	-5.82	1.16	1.23
1	B	275	ILE	C-O	-5.79	1.18	1.24
1	A	213	VAL	C-O	-5.78	1.18	1.24
1	A	185	ILE	C-O	-5.73	1.17	1.24
1	D	269	ARG	C-O	-5.67	1.17	1.24
1	B	213	VAL	C-O	-5.59	1.18	1.24
1	E	214	VAL	C-O	-5.58	1.18	1.24
1	D	275	ILE	C-O	-5.57	1.18	1.24
1	D	214	VAL	C-O	-5.57	1.18	1.24
1	A	268	ALA	C-O	-5.54	1.17	1.24
1	D	196	SER	C-O	-5.52	1.17	1.24
1	E	139	PHE	C-O	-5.48	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	295	MET	C-O	-5.44	1.17	1.24
1	A	153	LEU	C-O	-5.41	1.17	1.24
1	B	276	LEU	C-O	-5.36	1.17	1.24
1	B	8	ILE	C-O	-5.34	1.17	1.24
1	D	161	GLY	C-O	-5.32	1.17	1.23
1	C	214	VAL	C-O	-5.31	1.18	1.24
1	D	293	THR	C-O	-5.27	1.18	1.24
1	D	296	HIS	C-O	-5.26	1.18	1.24
1	B	7	ARG	C-O	-5.25	1.18	1.24
1	D	292	GLN	C-O	-5.23	1.18	1.24
1	B	268	ALA	C-O	-5.19	1.18	1.24
1	A	270	HIS	C-O	-5.14	1.18	1.24
1	D	160	VAL	C-O	-5.13	1.18	1.24
1	C	267	HIS	C-O	-5.11	1.18	1.24
1	B	196	SER	C-O	-5.06	1.18	1.24
1	A	184	MET	C-O	-5.04	1.18	1.24
1	E	369	GLN	C-O	-5.02	1.18	1.24
1	A	193	ILE	C-O	-5.01	1.18	1.24
1	F	195	VAL	C-O	-5.00	1.18	1.24

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	GLU	N-CA-C	12.33	124.72	111.28
1	F	3	GLU	CB-CA-C	7.95	120.08	108.87
1	D	3	GLU	CB-CA-C	7.82	119.89	108.87
1	B	188	TYR	N-CA-C	7.38	120.39	111.82
1	E	3	GLU	CB-CA-C	7.21	119.03	108.87
1	E	137	ASP	N-CA-C	7.09	119.09	111.36
1	B	333	HIS	N-CA-C	7.01	119.72	109.07
1	F	215	THR	CA-CB-OG1	-6.87	99.29	109.60
1	D	118	ASP	CA-CB-CG	6.62	119.22	112.60
1	B	28	MET	CG-SD-CE	-6.42	86.79	100.90
1	F	3	GLU	N-CA-CB	-6.06	102.11	110.29
1	C	137	ASP	CB-CA-C	5.93	120.08	109.29
1	E	3	GLU	N-CA-CB	-5.77	102.51	110.29
1	A	229	PRO	CB-CA-C	5.71	118.80	111.21
1	C	90	LYS	CB-CG-CD	5.70	124.41	111.30
1	D	229	PRO	CB-CA-C	5.64	118.71	111.21
1	C	229	PRO	CB-CA-C	5.56	118.61	111.21
1	F	315	VAL	N-CA-CB	-5.54	103.45	111.21
1	A	67	LYS	CB-CG-CD	5.52	123.99	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	GLU	N-CA-CB	5.45	118.32	110.20
1	A	315	VAL	N-CA-CB	-5.42	103.62	111.21
1	A	191	ASN	N-CA-C	5.42	119.90	113.28
1	B	37	ILE	N-CA-C	5.41	117.81	111.05
1	A	40	ARG	CG-CD-NE	-5.41	100.11	112.00
1	D	137	ASP	CB-CA-C	5.39	119.03	109.65
1	E	315	VAL	N-CA-CB	-5.37	103.69	111.21
1	B	155	ARG	N-CA-C	5.36	120.69	113.72
1	A	96	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	332	LYS	CB-CG-CD	5.34	123.58	111.30
1	E	229	PRO	CB-CA-C	5.32	118.29	111.21
1	A	60	LYS	CA-CB-CG	5.28	124.65	114.10
1	C	315	VAL	N-CA-CB	-5.25	103.86	111.21
1	B	187	HIS	CB-CA-C	5.21	118.98	110.96
1	D	354	GLU	N-CA-CB	5.21	118.31	110.30
1	E	118	ASP	CB-CA-C	5.17	119.08	111.73
1	A	118	ASP	CB-CA-C	5.17	119.07	111.73
1	E	369	GLN	N-CA-C	5.17	116.72	111.14
1	E	96	ASP	CA-CB-CG	5.14	117.74	112.60
1	E	18	LEU	N-CA-CB	-5.14	102.05	110.43
1	D	3	GLU	N-CA-CB	-5.13	103.36	110.29
1	B	18	LEU	N-CA-CB	-5.11	102.09	110.43
1	D	96	ASP	CA-CB-CG	5.10	117.70	112.60
1	D	187	HIS	CB-CA-C	5.09	118.88	110.88
1	A	18	LEU	N-CA-CB	-5.08	102.16	110.43
1	E	53	THR	CA-CB-OG1	-5.05	102.02	109.60
1	B	295	MET	CG-SD-CE	-5.05	89.79	100.90
1	C	180	GLU	CB-CG-CD	5.04	121.18	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	3292	0	3175	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3293	0	3173	21	0
1	C	3263	0	3136	34	0
1	D	3263	0	3136	28	0
1	E	3254	0	3128	26	0
1	F	3263	0	3136	27	0
2	A	20	0	0	8	0
2	B	20	0	0	2	0
2	C	20	0	0	0	0
2	D	20	0	0	0	0
2	E	20	0	0	0	0
2	F	20	0	0	3	0
3	A	210	0	0	1	0
3	B	195	0	0	0	0
3	C	186	0	0	2	0
3	D	228	0	0	1	0
3	E	149	0	0	1	0
3	F	167	0	0	2	0
All	All	20883	0	18884	149	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 4.

All (149) 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:169:TRP:CZ2	2:A:1001:JFZ:C5'	2.21	1.24
1:C:39:HIS:HB2	1:D:346:LYS:NZ	1.58	1.17
1:C:346:LYS:NZ	1:D:39:HIS:HB2	1.63	1.13
1:C:346:LYS:HZ3	1:D:39:HIS:HB2	1.11	1.12
1:D:168:ASN:HB2	1:D:198:THR:HG21	1.38	1.03
1:C:39:HIS:HB2	1:D:346:LYS:HZ2	1.19	1.01
1:C:186:ARG:HD2	1:C:210:GLU:OE1	1.69	0.92
1:E:346:LYS:NZ	1:F:39:HIS:HB2	1.87	0.88
1:E:151:GLU:HG3	1:E:184:MET:HE1	1.56	0.85
1:A:169:TRP:CE2	2:A:1001:JFZ:C5'	2.59	0.85
1:A:169:TRP:CH2	2:A:1001:JFZ:C5'	2.62	0.83
1:F:197:ASN:HD21	2:F:1001:JFZ:C6'	1.91	0.83
1:E:39:HIS:HB2	1:F:346:LYS:NZ	1.94	0.82
1:A:169:TRP:CZ2	2:A:1001:JFZ:C6'	2.63	0.82
1:C:41:ASN:HD22	1:C:44:ASP:H	1.27	0.80
1:F:168:ASN:HB2	1:F:198:THR:HG21	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:HIS:HB2	1:D:346:LYS:HZ1	1.42	0.79
1:A:41:ASN:HD22	1:A:44:ASP:H	1.29	0.79
1:E:346:LYS:HZ3	1:F:39:HIS:HB2	1.48	0.79
1:C:39:HIS:CB	1:D:346:LYS:NZ	2.42	0.78
1:A:34:THR:OG1	1:A:40:ARG:NH1	2.16	0.76
1:F:197:ASN:ND2	2:F:1001:JFZ:C6'	2.48	0.76
1:A:169:TRP:CZ3	2:A:1001:JFZ:O2'	2.38	0.76
1:A:169:TRP:CE3	2:A:1001:JFZ:O2'	2.39	0.74
1:D:279:ILE:HD11	1:D:295:MET:CE	2.19	0.72
1:E:39:HIS:HB2	1:F:346:LYS:HZ3	1.54	0.71
1:F:292:GLN:HG2	3:F:1258:HOH:O	1.92	0.69
1:B:169:TRP:CZ2	2:B:1001:JFZ:C3'	2.76	0.69
1:F:287:ILE:HG21	1:F:295:MET:HE1	1.75	0.67
1:F:167:GLY:HA2	1:F:169:TRP:CE2	2.32	0.65
1:A:167:GLY:HA2	1:A:169:TRP:CE2	2.31	0.65
1:A:41:ASN:ND2	1:A:44:ASP:H	1.94	0.65
1:C:167:GLY:HA2	1:C:169:TRP:CE2	2.31	0.65
1:D:87:TYR:HB3	1:D:107:ILE:HG12	1.77	0.65
1:C:224:ILE:HD13	1:C:236:GLY:HA3	1.79	0.65
1:A:224:ILE:HD13	1:A:236:GLY:HA3	1.78	0.64
1:D:167:GLY:HA2	1:D:169:TRP:CE2	2.32	0.64
1:B:224:ILE:HD13	1:B:236:GLY:HA3	1.79	0.64
1:D:279:ILE:HD11	1:D:295:MET:HE2	1.78	0.64
1:B:167:GLY:HA2	1:B:169:TRP:CE2	2.32	0.64
1:E:224:ILE:HD13	1:E:236:GLY:HA3	1.80	0.64
1:E:167:GLY:HA2	1:E:169:TRP:CE2	2.32	0.63
1:D:224:ILE:HD13	1:D:236:GLY:HA3	1.81	0.63
1:A:39:HIS:HB2	1:B:346:LYS:NZ	2.13	0.62
1:F:224:ILE:HD13	1:F:236:GLY:HA3	1.81	0.62
1:D:10:HIS:HB2	3:D:1294:HOH:O	1.98	0.62
1:B:169:TRP:HB3	1:B:198:THR:HG21	1.82	0.61
1:B:87:TYR:HB3	1:B:107:ILE:HG12	1.81	0.61
1:E:151:GLU:CG	1:E:184:MET:HE1	2.28	0.60
1:C:87:TYR:HB3	1:C:107:ILE:HG12	1.83	0.59
1:F:87:TYR:HB3	1:F:107:ILE:HG12	1.85	0.59
1:A:201:LYS:HD3	1:A:207:SER:HA	1.84	0.59
1:E:39:HIS:HB2	1:F:346:LYS:HZ1	1.66	0.59
1:C:41:ASN:ND2	1:C:44:ASP:H	1.97	0.59
1:A:87:TYR:HB3	1:A:107:ILE:HG12	1.84	0.58
1:C:39:HIS:CB	1:D:346:LYS:HZ2	2.07	0.58
1:E:87:TYR:HB3	1:E:107:ILE:HG12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASP:OD1	1:A:197:ASN:ND2	2.35	0.56
1:C:39:HIS:CG	1:D:346:LYS:NZ	2.74	0.56
1:C:186:ARG:NH2	1:C:192:ALA:O	2.38	0.56
1:C:346:LYS:HZ1	1:D:39:HIS:HB2	1.65	0.56
1:A:200:LEU:HG	1:A:214:VAL:HG11	1.87	0.56
1:C:10:HIS:HB2	3:C:1262:HOH:O	2.07	0.54
1:B:67:LYS:HD2	1:B:117:GLU:OE1	2.08	0.54
1:A:1:MET:HG2	1:A:230:ASN:ND2	2.23	0.54
1:D:291:ALA:O	1:D:295:MET:HG2	2.08	0.54
1:A:10:HIS:HB2	3:A:1292:HOH:O	2.07	0.53
1:B:238:ILE:HG13	1:B:275:ILE:HD12	1.90	0.53
1:A:169:TRP:HB3	1:A:198:THR:HG21	1.90	0.53
1:C:39:HIS:CB	1:D:346:LYS:HZ1	2.11	0.52
1:E:67:LYS:HD2	1:E:117:GLU:OE1	2.10	0.52
1:C:169:TRP:HB3	1:C:198:THR:HG21	1.93	0.51
1:E:238:ILE:HG13	1:E:275:ILE:HD12	1.92	0.51
1:F:10:HIS:HB2	3:F:1253:HOH:O	2.09	0.51
1:C:287:ILE:HG21	1:C:295:MET:HE1	1.93	0.50
1:E:228:ALA:HB3	1:E:231:GLU:OE1	2.12	0.50
1:E:346:LYS:HZ1	1:F:39:HIS:HB2	1.73	0.49
1:B:1:MET:HB3	1:B:229:PRO:O	2.14	0.48
1:D:168:ASN:HB2	1:D:198:THR:CG2	2.27	0.48
1:A:39:HIS:HB2	1:B:346:LYS:HZ3	1.77	0.48
1:C:238:ILE:HG13	1:C:275:ILE:HD12	1.95	0.47
1:E:47:GLN:NE2	3:E:1101:HOH:O	2.28	0.47
1:B:200:LEU:HD13	1:B:214:VAL:HG11	1.96	0.47
1:D:279:ILE:CD1	1:D:295:MET:HE2	2.43	0.47
1:F:197:ASN:ND2	2:F:1001:JFZ:C5'	2.79	0.46
1:D:19:PHE:HB3	1:D:278:ASN:HA	1.98	0.45
1:C:346:LYS:NZ	1:D:39:HIS:CB	2.56	0.45
1:A:346:LYS:NZ	1:B:39:HIS:CG	2.85	0.45
1:B:169:TRP:CZ2	2:B:1001:JFZ:C2'	2.99	0.45
1:A:61:LYS:HE3	1:A:61:LYS:HB3	1.51	0.45
1:A:77:THR:HA	1:A:124:TYR:HB3	1.99	0.45
1:E:229:PRO:O	1:E:230:ASN:HB2	2.16	0.45
1:A:354:GLU:CD	1:A:354:GLU:H	2.24	0.45
1:D:291:ALA:O	1:D:295:MET:CG	2.64	0.45
1:F:270:HIS:HB2	1:F:326:PHE:CE1	2.52	0.45
1:A:19:PHE:HB3	1:A:278:ASN:HA	1.99	0.44
1:E:19:PHE:HB3	1:E:278:ASN:HA	1.99	0.44
1:F:19:PHE:HB3	1:F:278:ASN:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:MET:HE2	1:E:184:MET:HB2	1.76	0.44
1:C:229:PRO:O	1:C:230:ASN:HB2	2.18	0.44
1:A:199:GLY:O	1:A:207:SER:N	2.49	0.44
1:A:229:PRO:O	1:A:230:ASN:HB2	2.17	0.44
1:F:124:TYR:C	1:F:124:TYR:CD1	2.96	0.43
1:F:77:THR:HA	1:F:124:TYR:HB3	2.00	0.43
1:B:124:TYR:C	1:B:124:TYR:CD1	2.96	0.43
1:C:124:TYR:C	1:C:124:TYR:CD1	2.96	0.43
1:F:287:ILE:HG21	1:F:295:MET:CE	2.46	0.43
1:B:19:PHE:HB3	1:B:278:ASN:HA	1.99	0.43
1:C:349:VAL:HG21	1:D:33:TRP:CZ3	2.53	0.43
1:B:239:SER:HB3	1:B:246:TRP:HH2	1.84	0.43
1:C:41:ASN:HD22	1:C:44:ASP:N	2.07	0.43
1:A:135:TYR:OH	1:A:170:ASN:ND2	2.49	0.43
1:C:77:THR:HA	1:C:124:TYR:HB3	2.01	0.43
1:D:229:PRO:O	1:D:230:ASN:HB2	2.19	0.43
1:A:124:TYR:CD1	1:A:124:TYR:C	2.96	0.42
1:C:19:PHE:HB3	1:C:278:ASN:HA	2.00	0.42
1:E:124:TYR:C	1:E:124:TYR:CD1	2.96	0.42
1:A:39:HIS:HB2	1:B:346:LYS:HZ2	1.82	0.42
1:C:5:LEU:O	1:C:6:PRO:C	2.59	0.42
1:A:167:GLY:HA2	1:A:169:TRP:NE1	2.34	0.42
1:D:315:VAL:HG22	1:D:316:PRO:HD2	2.01	0.42
1:D:124:TYR:CD1	1:D:124:TYR:C	2.98	0.42
1:F:315:VAL:HG22	1:F:316:PRO:HD2	2.01	0.42
1:B:87:TYR:HB3	1:B:107:ILE:CG1	2.50	0.42
1:E:332:LYS:HE3	1:E:332:LYS:HB2	1.90	0.42
1:B:77:THR:HA	1:B:124:TYR:HB3	2.01	0.41
1:A:169:TRP:HZ2	2:A:1001:JFZ:C6'	2.30	0.41
1:B:315:VAL:HG22	1:B:316:PRO:HD2	2.02	0.41
1:E:315:VAL:HG22	1:E:316:PRO:HD2	2.01	0.41
1:E:87:TYR:HB3	1:E:107:ILE:CG1	2.50	0.41
1:F:239:SER:HB3	1:F:246:TRP:HH2	1.85	0.41
1:D:348:ASN:HD22	1:D:348:ASN:HA	1.61	0.41
1:A:41:ASN:HD21	1:A:43:HIS:HB3	1.86	0.41
1:A:87:TYR:HB3	1:A:107:ILE:CG1	2.50	0.41
1:F:269:ARG:HA	1:F:269:ARG:HD2	1.79	0.41
1:C:178:LEU:N	1:C:179:PRO:CD	2.84	0.41
1:E:320:ALA:HB2	1:E:360:SER:HB2	2.03	0.41
1:F:241:THR:HG23	1:F:243:ASN:O	2.21	0.41
1:C:198:THR:HA	3:C:1164:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:THR:HG23	1:C:243:ASN:O	2.21	0.40
1:F:178:LEU:N	1:F:179:PRO:CD	2.84	0.40
1:C:41:ASN:HD21	1:C:43:HIS:HB3	1.85	0.40
1:E:178:LEU:N	1:E:179:PRO:CD	2.84	0.40
1:B:135:TYR:OH	1:B:170:ASN:ND2	2.46	0.40
1:C:60:LYS:HE2	1:C:116:GLU:OE2	2.22	0.40
1:E:241:THR:HG23	1:E:243:ASN:O	2.21	0.40
2:A:1001:JFZ:C6'	2:A:1001:JFZ:O2	2.70	0.40
1:E:77:THR:HA	1:E:124:TYR:HB3	2.03	0.40
1:F:2:THR:HG22	1:F:3:GLU:H	1.87	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	407/414 (98%)	398 (98%)	9 (2%)	0	100	100
1	B	408/414 (99%)	396 (97%)	12 (3%)	0	100	100
1	C	403/414 (97%)	392 (97%)	11 (3%)	0	100	100
1	D	403/414 (97%)	394 (98%)	9 (2%)	0	100	100
1	E	402/414 (97%)	393 (98%)	9 (2%)	0	100	100
1	F	403/414 (97%)	393 (98%)	10 (2%)	0	100	100
All	All	2426/2484 (98%)	2366 (98%)	60 (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	344/346 (99%)	340 (99%)	4 (1%)	63	81
1	B	344/346 (99%)	340 (99%)	4 (1%)	63	81
1	C	341/346 (99%)	335 (98%)	6 (2%)	51	73
1	D	341/346 (99%)	337 (99%)	4 (1%)	63	81
1	E	340/346 (98%)	335 (98%)	5 (2%)	57	77
1	F	341/346 (99%)	338 (99%)	3 (1%)	70	85
All	All	2051/2076 (99%)	2025 (99%)	26 (1%)	61	80

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	MET
1	A	60	LYS
1	A	198	THR
1	A	354	GLU
1	B	191	ASN
1	B	217	GLU
1	B	275	ILE
1	B	354	GLU
1	C	9	GLN
1	C	28	MET
1	C	180	GLU
1	C	198	THR
1	C	275	ILE
1	C	354	GLU
1	D	28	MET
1	D	275	ILE
1	D	350	VAL
1	D	354	GLU
1	E	28	MET
1	E	56	GLN
1	E	275	ILE
1	E	354	GLU

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Mol	Chain	Res	Type
1	E	370	ARG
1	F	28	MET
1	F	275	ILE
1	F	354	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	168	ASN
1	A	170	ASN
1	A	230	ASN
1	A	292	GLN
1	A	410	GLN
1	B	9	GLN
1	B	10	HIS
1	B	39	HIS
1	B	43	HIS
1	B	170	ASN
1	B	177	HIS
1	B	410	GLN
1	C	9	GLN
1	C	10	HIS
1	C	41	ASN
1	C	42	GLN
1	C	168	ASN
1	C	170	ASN
1	C	177	HIS
1	C	191	ASN
1	C	230	ASN
1	C	296	HIS
1	C	410	GLN
1	D	9	GLN
1	D	42	GLN
1	D	168	ASN
1	D	348	ASN
1	D	410	GLN
1	E	9	GLN
1	E	168	ASN
1	E	292	GLN
1	E	296	HIS
1	E	366	GLN

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Mol	Chain	Res	Type
1	E	410	GLN
1	F	9	GLN
1	F	42	GLN
1	F	168	ASN
1	F	292	GLN
1	F	410	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	JFZ	C	1001	-	21,21,21	0.50	0	28,30,30	0.69	0
2	JFZ	E	1001	-	21,21,21	0.64	0	28,30,30	0.75	0
2	JFZ	B	1001	-	21,21,21	0.49	0	28,30,30	0.51	0
2	JFZ	D	1001	-	21,21,21	0.49	0	28,30,30	0.70	0
2	JFZ	A	1001	-	21,21,21	0.49	0	28,30,30	0.67	0
2	JFZ	F	1001	-	21,21,21	0.50	0	28,30,30	0.71	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
2	JFZ	C	1001	-	-	2/6/28/28	0/2/2/2
2	JFZ	E	1001	-	-	0/6/28/28	0/2/2/2
2	JFZ	B	1001	-	-	2/6/28/28	0/2/2/2
2	JFZ	D	1001	-	-	2/6/28/28	0/2/2/2
2	JFZ	A	1001	-	-	2/6/28/28	0/2/2/2
2	JFZ	F	1001	-	-	0/6/28/28	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	JFZ	C2-C1-O1-C1'
2	A	1001	JFZ	O5-C1-O1-C1'
2	B	1001	JFZ	C2-C1-O1-C1'
2	B	1001	JFZ	O5-C1-O1-C1'
2	C	1001	JFZ	O5-C1-O1-C1'
2	D	1001	JFZ	O5-C1-O1-C1'
2	C	1001	JFZ	C2-C1-O1-C1'
2	D	1001	JFZ	C2-C1-O1-C1'

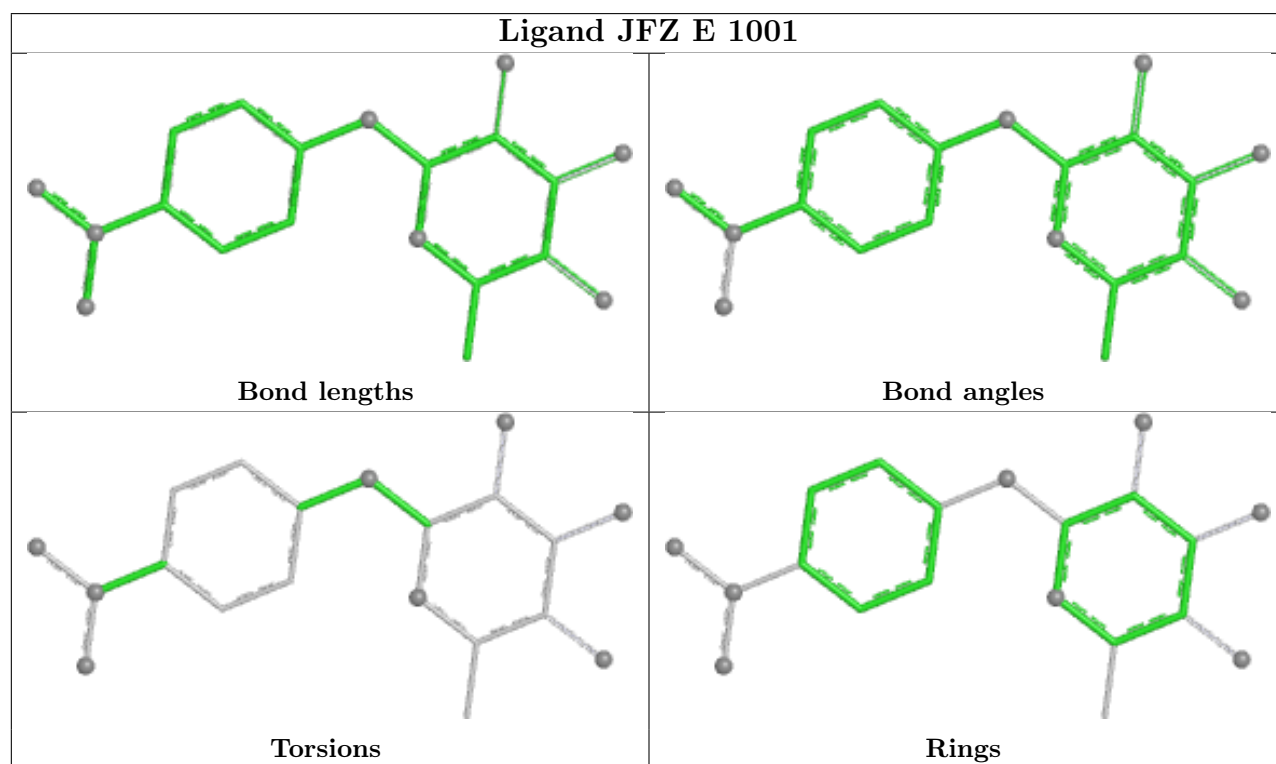
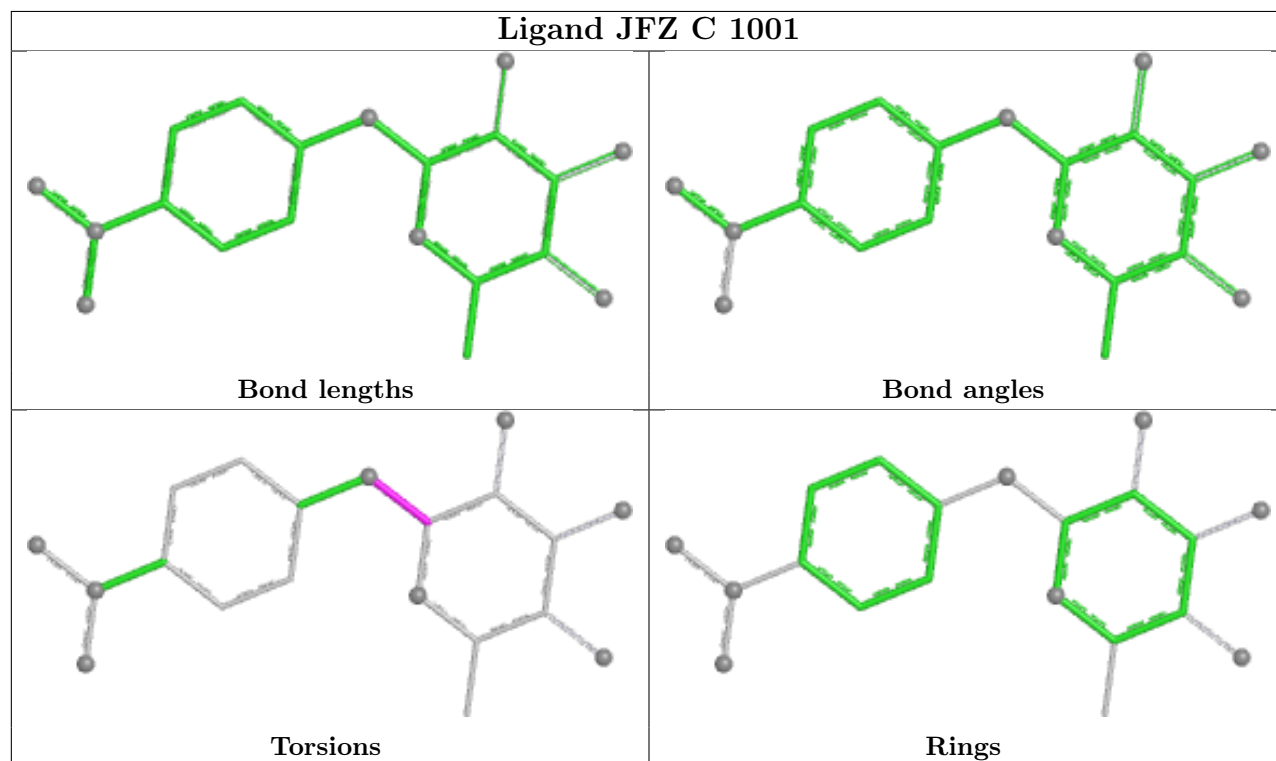
There are no ring outliers.

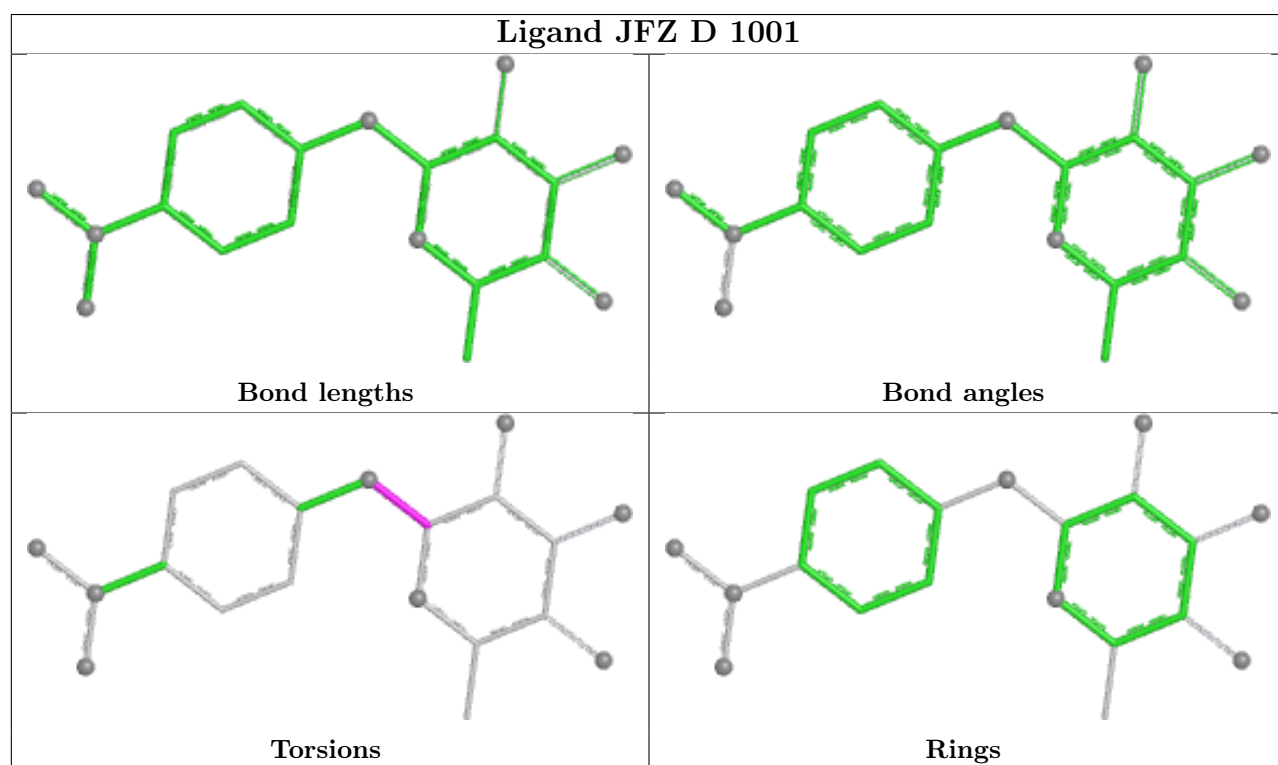
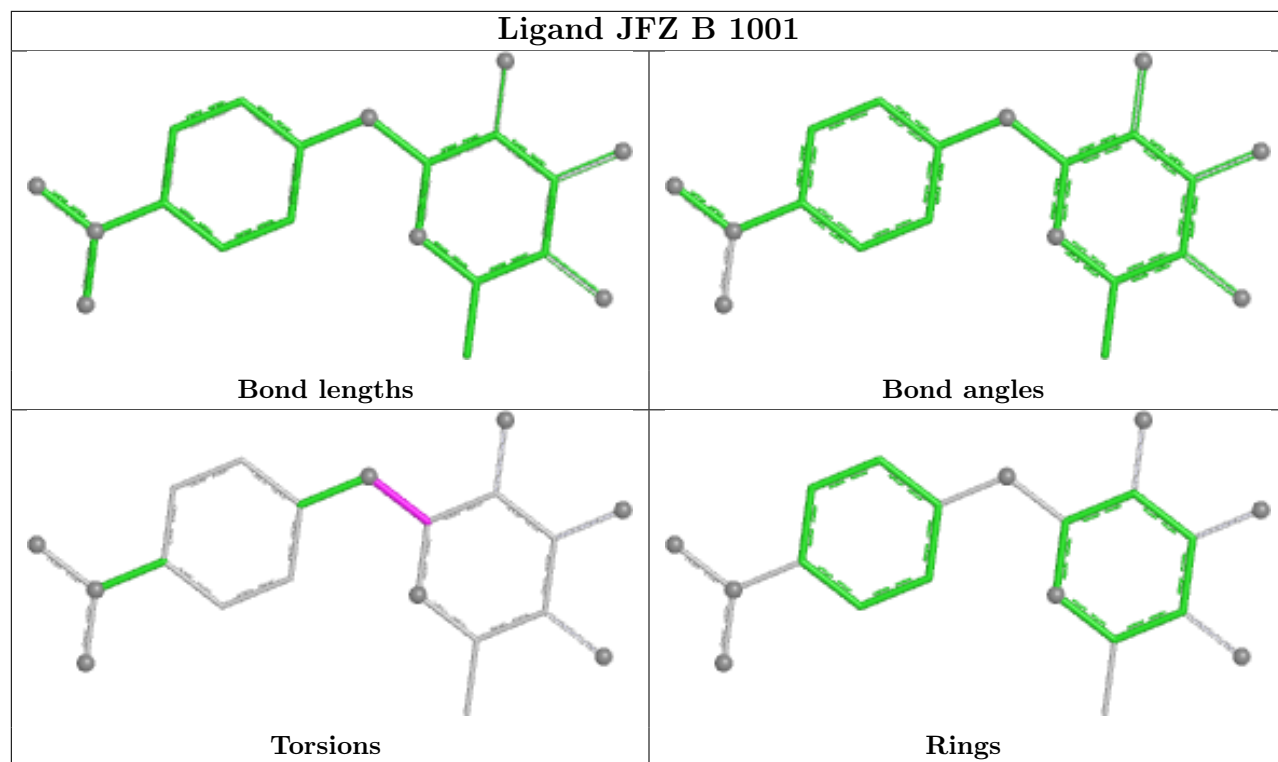
3 monomers are involved in 13 short contacts:

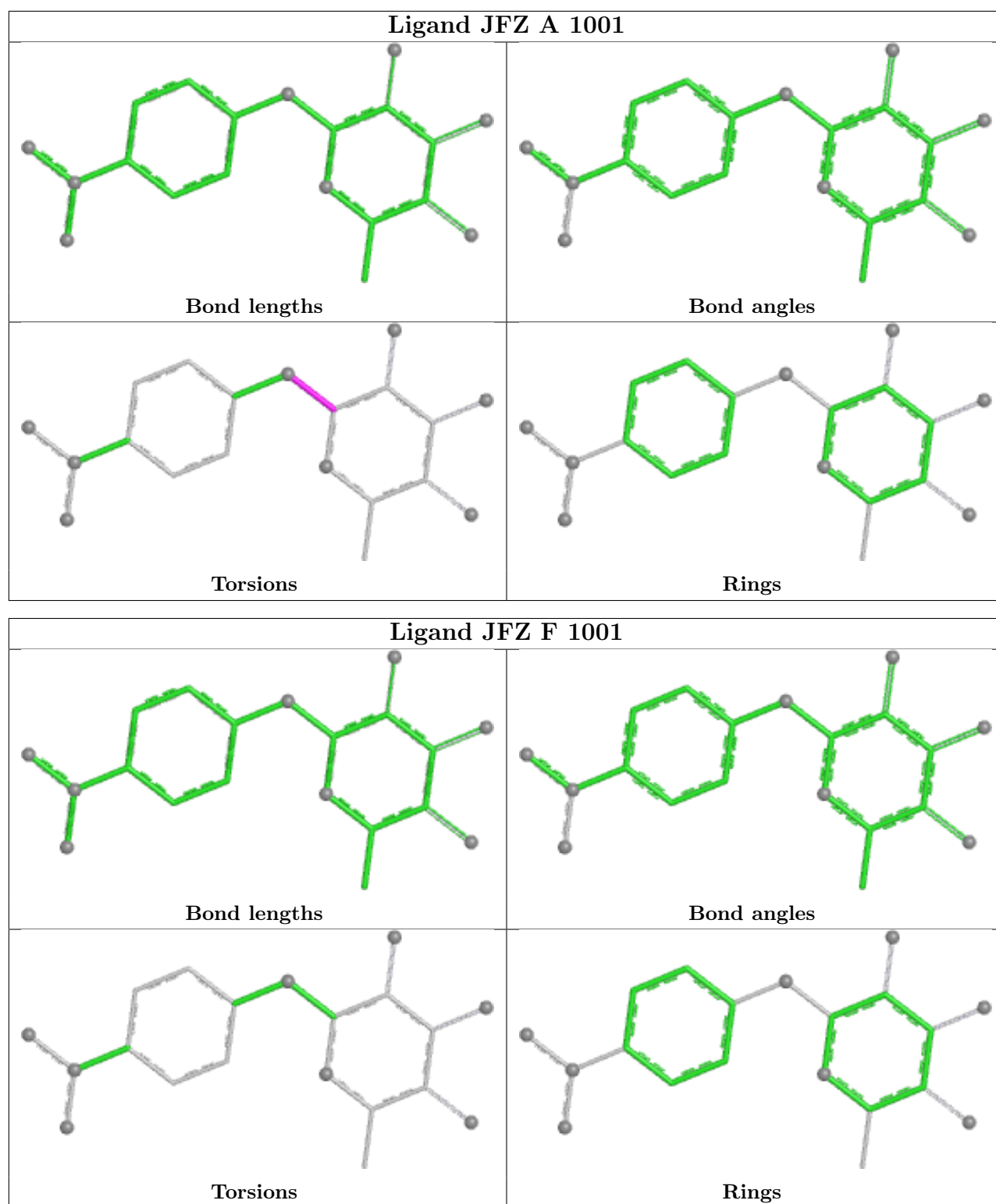
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	JFZ	2	0
2	A	1001	JFZ	8	0
2	F	1001	JFZ	3	0

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 ⓘ

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	411/414 (99%)	-0.63	16 (3%)	43 39	16, 26, 66, 104	0
1	B	411/414 (99%)	-0.59	12 (2%)	53 50	16, 26, 66, 109	1 (0%)
1	C	407/414 (98%)	-0.63	7 (1%)	69 65	18, 30, 64, 107	0
1	D	407/414 (98%)	-0.75	10 (2%)	58 54	17, 24, 63, 113	0
1	E	406/414 (98%)	-0.49	11 (2%)	56 52	18, 32, 68, 118	0
1	F	407/414 (98%)	-0.54	14 (3%)	48 44	19, 29, 69, 143	0
All	All	2449/2484 (98%)	-0.60	70 (2%)	53 50	16, 28, 66, 143	1 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	229	PRO	6.7
1	C	225	TYR	6.5
1	B	200	LEU	5.5
1	F	225	TYR	5.5
1	B	204	GLY	5.5
1	E	225	TYR	5.4
1	A	225	TYR	5.1
1	E	198	THR	4.9
1	D	225	TYR	4.8
1	E	229	PRO	4.7
1	F	205	GLN	4.5
1	D	198	THR	4.5
1	D	229	PRO	4.4
1	C	229	PRO	4.3
1	F	228	ALA	4.3
1	D	228	ALA	4.3
1	A	201	LYS	4.3
1	F	198	THR	4.2
1	C	198	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	199	GLY	4.0
1	B	39	HIS	3.8
1	A	1	MET	3.8
1	A	198	THR	3.7
1	A	200	LEU	3.7
1	B	198	THR	3.7
1	F	2	THR	3.7
1	A	205	GLN	3.4
1	A	172	LYS	3.3
1	F	230	ASN	3.2
1	E	206	VAL	3.2
1	A	228	ALA	3.1
1	C	228	ALA	3.1
1	D	348	ASN	3.1
1	B	1	MET	3.1
1	A	229	PRO	3.0
1	D	205	GLN	2.9
1	C	205	GLN	2.9
1	A	348	ASN	2.9
1	B	172	LYS	2.9
1	F	173	ASP	2.8
1	B	199	GLY	2.8
1	D	2	THR	2.8
1	B	225	TYR	2.7
1	C	39	HIS	2.7
1	D	39	HIS	2.7
1	E	39	HIS	2.6
1	E	2	THR	2.6
1	A	173	ASP	2.5
1	B	229	PRO	2.5
1	E	228	ALA	2.5
1	D	347	ASP	2.4
1	B	140	PRO	2.3
1	F	349	VAL	2.3
1	A	222	ASP	2.2
1	E	137	ASP	2.2
1	A	217	GLU	2.2
1	F	348	ASN	2.2
1	D	222	ASP	2.2
1	E	222	ASP	2.2
1	E	172	LYS	2.2
1	A	39	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	348	ASN	2.1
1	F	227	GLY	2.1
1	B	205	GLN	2.1
1	B	173	ASP	2.1
1	F	206	VAL	2.1
1	A	230	ASN	2.1
1	C	2	THR	2.1
1	F	221	PRO	2.0
1	F	168	ASN	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](#)

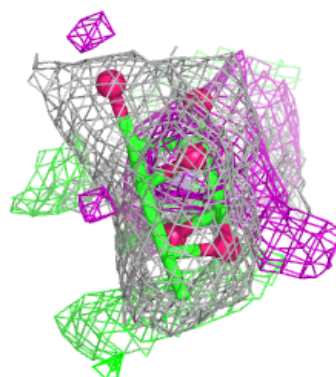
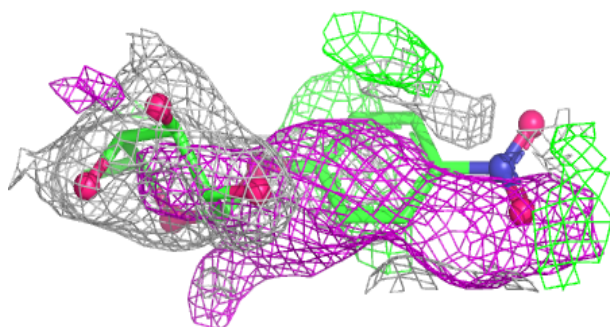
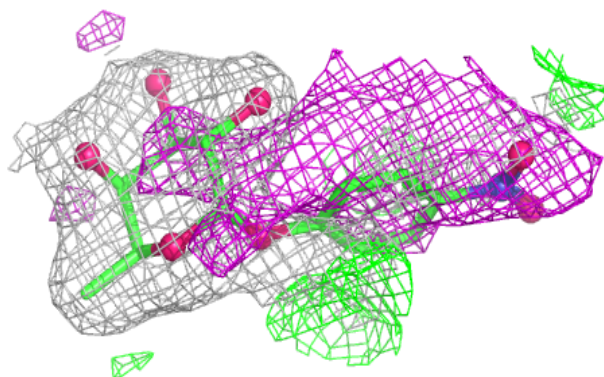
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	JFZ	A	1001	20/20	0.79	0.26	32,64,140,140	0
2	JFZ	B	1001	20/20	0.81	0.24	29,61,156,161	0
2	JFZ	C	1001	20/20	0.84	0.19	31,46,126,131	0
2	JFZ	F	1001	20/20	0.87	0.17	33,62,115,118	0
2	JFZ	D	1001	20/20	0.89	0.17	28,52,121,130	0
2	JFZ	E	1001	20/20	0.91	0.17	37,62,130,132	0

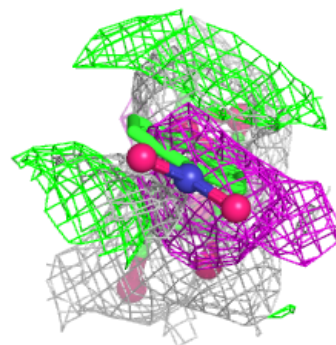
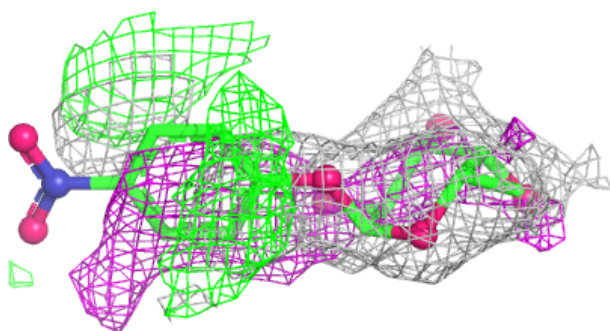
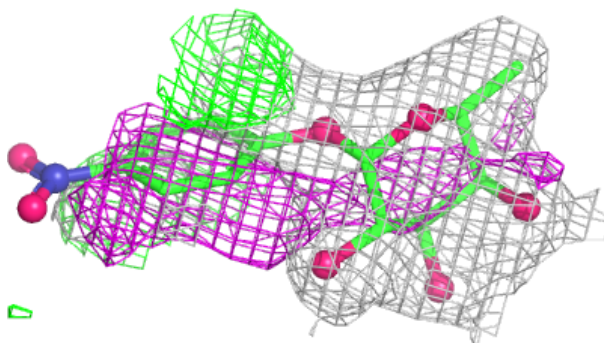
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around JFZ A 1001:

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

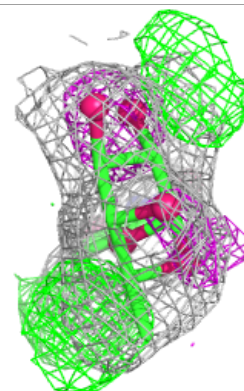
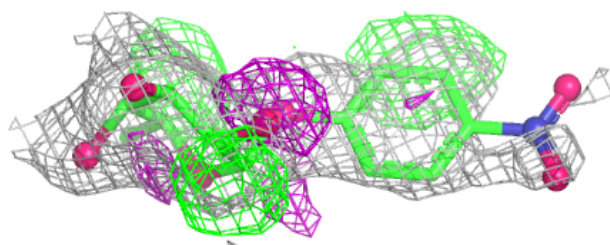
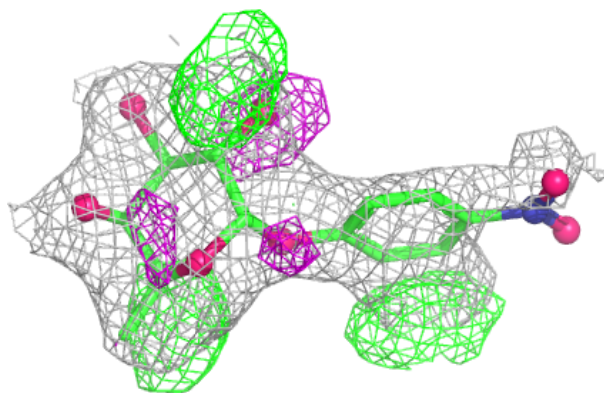
**Electron density around JFZ B 1001:**

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

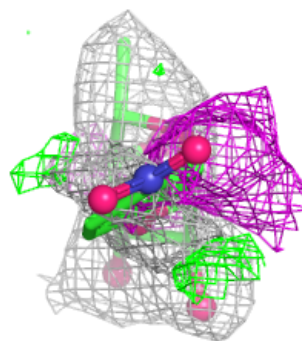
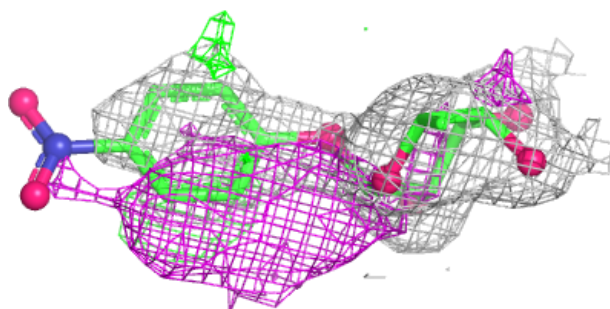
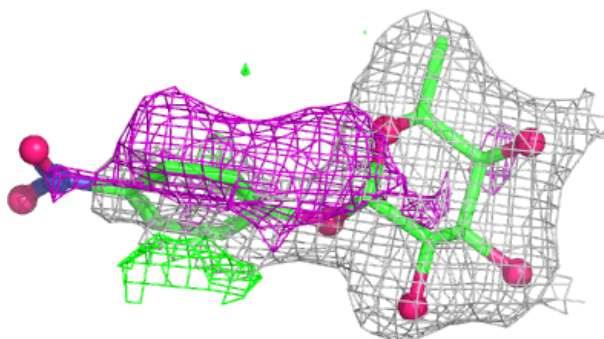


Electron density around JFZ C 1001:

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

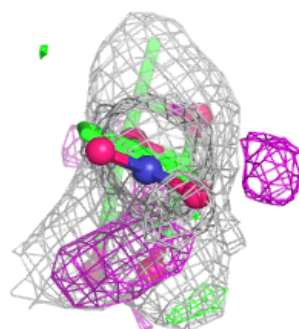
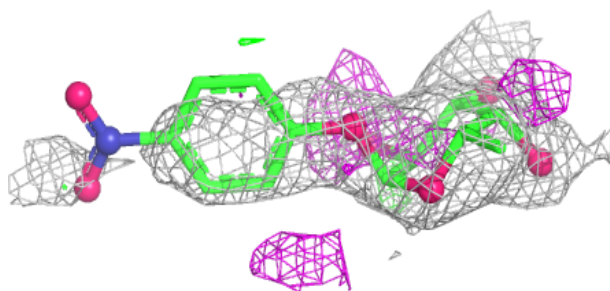
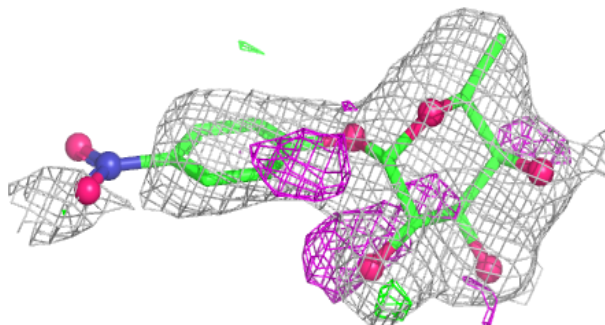
**Electron density around JFZ F 1001:**

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

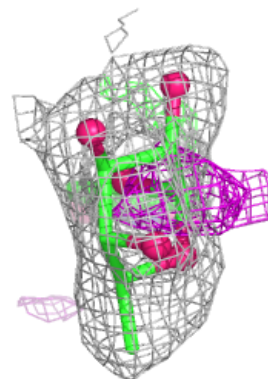
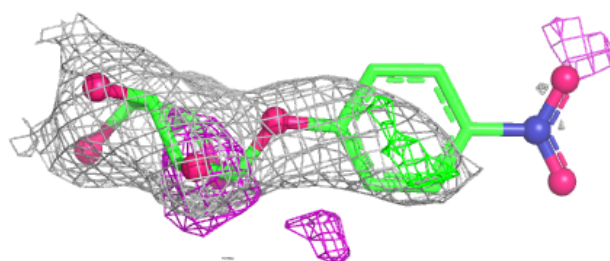
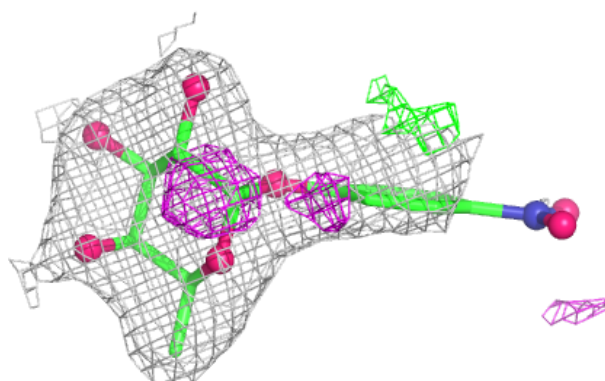


Electron density around JFZ D 1001:

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

**Electron density around JFZ E 1001:**

$2mF_o-DF_c$ (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.