



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2025 – 02:14 PM JST

PDB ID : 9J3V / pdb\_00009j3v  
Title : Fe2+/Fe2+ PolF-L-isoleucine complex  
Authors : Zhang, Z.Y.; Chen, W.Q.; Wang, B.J.; Qu, Y.; Gong, R.; Liu, J.  
Deposited on : 2024-08-08  
Resolution : 2.60 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](mailto: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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

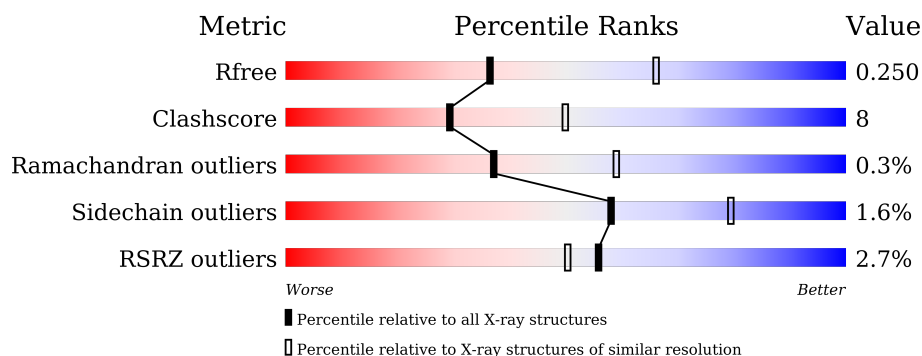
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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  $\geq 3$ , 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	275	<div> <div>86%</div> <div>10%</div> <div>..</div> </div>
1	B	275	<div>4%</div> <div>77%</div> <div>19%</div> <div>..</div>
1	C	275	<div>3%</div> <div>77%</div> <div>16%</div> <div>• 5%</div>
1	D	275	<div>3%</div> <div>75%</div> <div>20%</div> <div>• 5%</div>
1	E	275	<div>2%</div> <div>80%</div> <div>17%</div> <div>•</div>
1	F	275	<div>4%</div> <div>69%</div> <div>23%</div> <div>8%</div>

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
3	ILE	F	303	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11904 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 Putative molybdopterin oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			1996	1258	357	375	6			
1	B	269	Total	C	N	O	S	0	0	0
			1961	1237	348	371	5			
1	C	261	Total	C	N	O	S	0	0	0
			1910	1208	330	366	6			
1	D	262	Total	C	N	O	S	0	0	0
			1947	1223	354	365	5			
1	E	267	Total	C	N	O	S	0	0	0
			1963	1241	345	371	6			
1	F	252	Total	C	N	O	S	0	0	0
			1789	1127	316	340	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	VAL	MET	conflict	UNP C1IC29
B	21	VAL	MET	conflict	UNP C1IC29
C	21	VAL	MET	conflict	UNP C1IC29
D	21	VAL	MET	conflict	UNP C1IC29
E	21	VAL	MET	conflict	UNP C1IC29
F	21	VAL	MET	conflict	UNP C1IC29

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

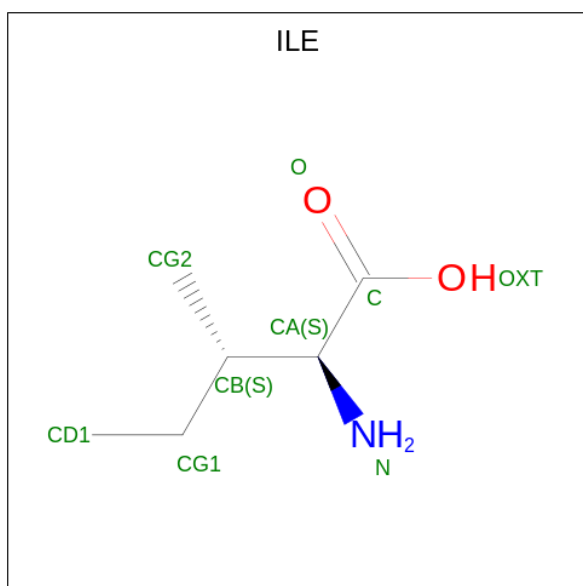
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		
2	C	2	Total	Fe	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Fe	0	0
			2	2		
2	E	2	Total	Fe	0	0
			2	2		
2	F	2	Total	Fe	0	0
			2	2		

- Molecule 3 is ISOLEUCINE (CCD ID: ILE) (formula:  $C_6H_{13}NO_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		
3	B	1	Total	C	N	O	0	0
			9	6	1	2		
3	C	1	Total	C	N	O	0	0
			9	6	1	2		
3	D	1	Total	C	N	O	0	0
			9	6	1	2		
3	F	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total	O	0	0
			46	46		

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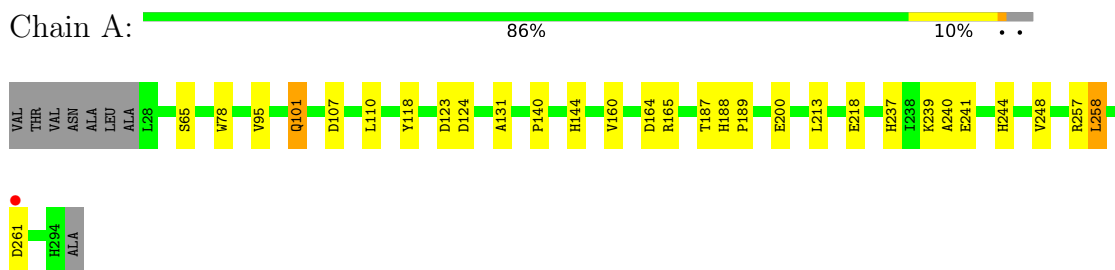
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	36	Total 36	O 36	0	0
4	C	52	Total 52	O 52	0	0
4	D	66	Total 66	O 66	0	0
4	E	53	Total 53	O 53	0	0
4	F	28	Total 28	O 28	0	0

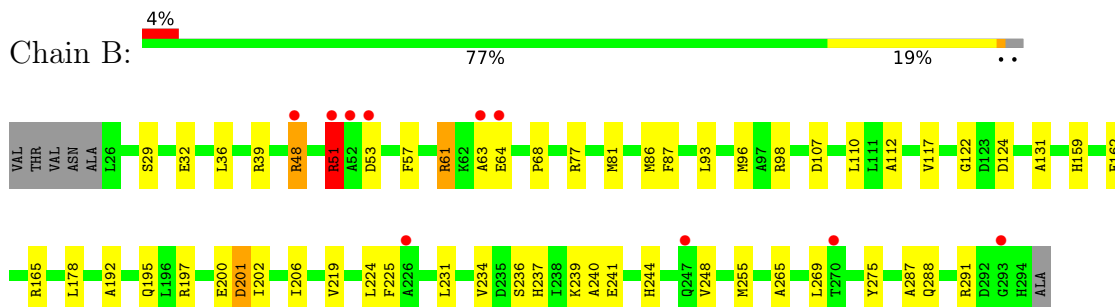
### 3 Residue-property plots

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.

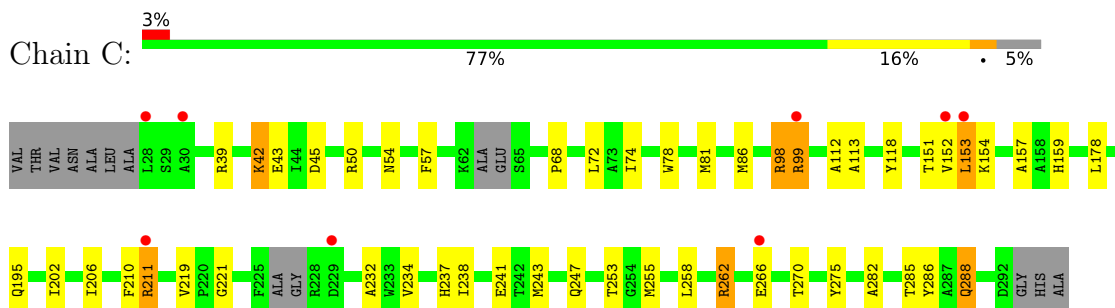
- Molecule 1: Putative molybdopterin oxidoreductase



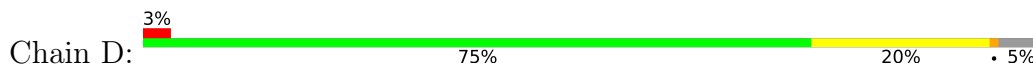
- Molecule 1: Putative molybdopterin oxidoreductase

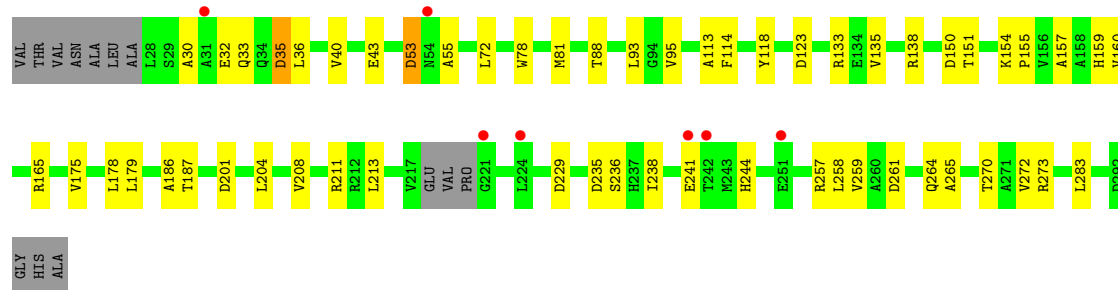


- Molecule 1: Putative molybdopterin oxidoreductase

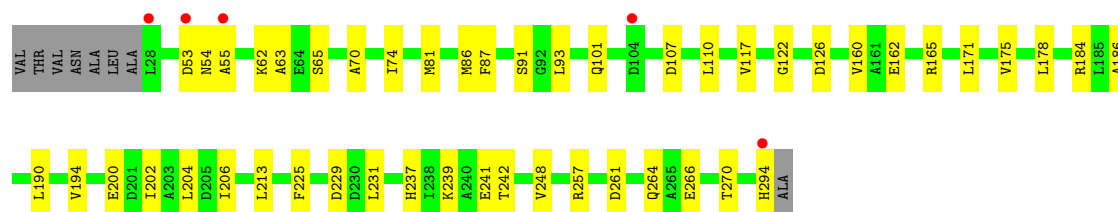
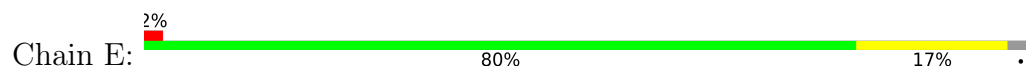


- Molecule 1: Putative molybdopterin oxidoreductase

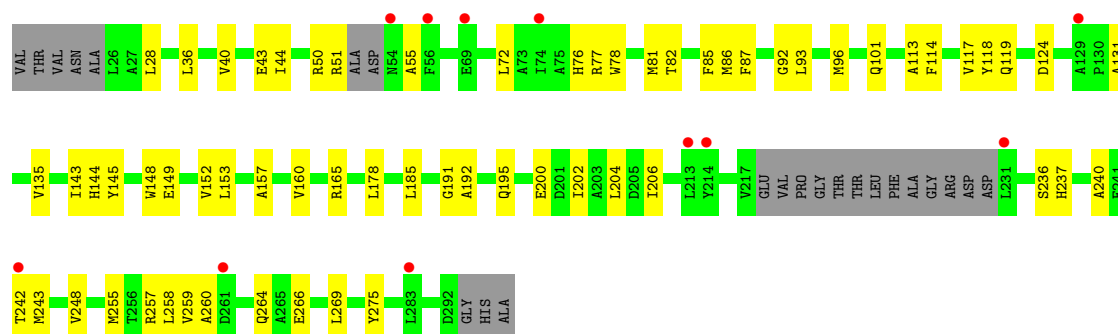




• Molecule 1: Putative molybdopterin oxidoreductase



• Molecule 1: Putative molybdopterin oxidoreductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.85Å 120.88Å 89.22Å 90.00° 91.51° 90.00°	Depositor
Resolution (Å)	24.74 – 2.60 24.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.74-2.60) 99.8 (24.74-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.60Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.228 , 0.248 0.231 , 0.250	Depositor DCC
$R_{free}$ test set	5552 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.3	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.035 for h,-k,-l 0.010 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11904	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FE2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.35	0/2038	0.62	1/2781 (0.0%)
1	B	0.40	0/2003	0.67	1/2743 (0.0%)
1	C	0.31	0/1949	0.70	5/2666 (0.2%)
1	D	0.32	0/1986	0.55	0/2710
1	E	0.37	0/2005	0.59	0/2743
1	F	0.25	0/1823	0.50	1/2499 (0.0%)
All	All	0.34	0/11804	0.61	8/16142 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	C	0	2
All	All	0	5

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	262	ARG	N-CA-C	-7.18	103.49	112.90
1	B	224	LEU	N-CA-C	6.79	118.37	110.97
1	C	99	ARG	N-CA-C	-5.63	105.22	111.36
1	C	98	ARG	CA-C-N	-5.55	112.41	120.29
1	C	98	ARG	C-N-CA	-5.55	112.41	120.29
1	A	258	LEU	N-CA-C	-5.22	106.69	113.16
1	C	288	GLN	CA-CB-CG	-5.14	103.81	114.10
1	F	266	GLU	CA-CB-CG	-5.03	104.04	114.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	48	ARG	Sidechain
1	B	51	ARG	Sidechain
1	B	61	ARG	Sidechain
1	C	211	ARG	Sidechain
1	C	262	ARG	Sidechain

## 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	1996	0	1902	19	0
1	B	1961	0	1820	38	0
1	C	1910	0	1772	35	0
1	D	1947	0	1836	37	0
1	E	1963	0	1848	30	0
1	F	1789	0	1628	42	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	9	0	10	2	0
3	B	9	0	10	0	0
3	C	9	0	10	2	0
3	D	9	0	10	2	0
3	F	9	0	10	7	0
4	A	46	0	0	2	0
4	B	36	0	0	4	0
4	C	52	0	0	4	0
4	D	66	0	0	2	0
4	E	53	0	0	2	0
4	F	28	0	0	0	0
All	All	11904	0	10856	191	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 8.

All (191) 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:D:43:GLU:OE2	1:D:273:ARG:NH1	2.20	0.74
1:F:86:MET:HE1	1:F:143:ILE:HG23	1.71	0.72
1:E:107:ASP:HB3	1:E:110:LEU:HD12	1.72	0.72
1:B:197:ARG:NH1	4:B:402:HOH:O	2.23	0.71
1:E:160:VAL:O	1:E:165:ARG:NE	2.23	0.71
1:D:123:ASP:OD2	1:D:244:HIS:NE2	2.23	0.70
1:B:39:ARG:HB3	1:B:269:LEU:HD11	1.77	0.67
1:C:74:ILE:HD11	1:C:286:TYR:HA	1.77	0.66
1:B:77:ARG:O	1:B:81:MET:HG3	1.96	0.66
1:C:237:HIS:O	1:C:241:GLU:HG2	1.98	0.64
1:E:184:ARG:NH2	4:E:401:HOH:O	2.30	0.64
1:E:261:ASP:HB3	1:E:264:GLN:H	1.62	0.64
1:D:261:ASP:HB2	1:D:264:GLN:HB2	1.79	0.63
1:B:96:MET:HE2	1:B:192:ALA:HB3	1.82	0.61
1:C:81:MET:HG2	1:C:178:LEU:HD23	1.84	0.59
1:F:82:THR:HG22	3:F:303:ILE:HD12	1.85	0.59
1:F:144:HIS:ND1	3:F:303:ILE:OXT	2.36	0.58
1:F:204:LEU:HD22	1:F:242:THR:HG22	1.85	0.58
1:F:77:ARG:O	1:F:81:MET:HG3	2.03	0.58
1:C:45:ASP:OD1	1:C:50:ARG:NE	2.34	0.58
3:A:303:ILE:N	4:A:402:HOH:O	2.35	0.58
1:A:160:VAL:HG13	1:A:164:ASP:HB2	1.86	0.58
1:A:118:TYR:OH	1:B:122:GLY:HA3	2.04	0.57
1:C:152:VAL:HG12	1:C:153:LEU:H	1.67	0.57
1:C:234:VAL:O	1:C:238:ILE:HG12	2.04	0.57
1:E:239:LYS:NZ	4:E:403:HOH:O	2.37	0.57
1:A:237:HIS:O	1:A:241:GLU:HG2	2.05	0.56
1:C:112:ALA:HB1	1:C:253:THR:HG22	1.88	0.56
1:F:145:TYR:O	1:F:149:GLU:HG3	2.05	0.56
1:C:266:GLU:O	1:C:270:THR:HG23	2.06	0.56
1:B:202:ILE:HD12	1:B:206:ILE:HD11	1.87	0.56
1:D:257:ARG:NE	1:D:257:ARG:HA	2.21	0.55
1:C:151:THR:HG21	4:C:401:HOH:O	2.06	0.55
1:D:93:LEU:HD21	1:D:118:TYR:HD2	1.72	0.55
1:F:81:MET:HE3	1:F:178:LEU:HD23	1.87	0.55
1:B:29:SER:OG	1:B:32:GLU:HG3	2.07	0.55
1:C:78:TRP:CZ2	3:C:303:ILE:HB	2.42	0.55
1:C:152:VAL:O	1:C:154:LYS:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:ILE:O	1:F:206:ILE:HG13	2.07	0.55
1:B:201:ASP:N	4:B:401:HOH:O	2.39	0.54
1:A:123:ASP:OD2	1:A:244:HIS:NE2	2.34	0.54
1:D:211:ARG:NH1	1:D:235:ASP:OD1	2.40	0.54
1:C:288:GLN:O	1:C:288:GLN:HG3	2.07	0.53
1:D:113:ALA:HB3	1:D:258:LEU:HG	1.90	0.53
1:F:36:LEU:O	1:F:40:VAL:HG23	2.09	0.53
1:E:81:MET:HE3	1:E:178:LEU:HD23	1.91	0.52
1:D:151:THR:HG21	4:D:401:HOH:O	2.09	0.52
1:E:122:GLY:HA3	1:F:118:TYR:OH	2.10	0.52
1:C:118:TYR:O	1:D:118:TYR:OH	2.27	0.52
1:A:78:TRP:HZ2	3:A:303:ILE:HB	1.76	0.52
1:B:288:GLN:OE1	1:B:291:ARG:NH2	2.44	0.51
1:E:237:HIS:O	1:E:241:GLU:HG2	2.09	0.51
1:D:36:LEU:O	1:D:40:VAL:HG23	2.10	0.51
1:B:239:LYS:NZ	1:C:221:GLY:O	2.21	0.51
1:F:96:MET:HE3	1:F:192:ALA:HB3	1.92	0.51
1:F:200:GLU:HB2	1:F:248:VAL:HG21	1.91	0.51
1:B:162:GLU:HA	1:B:165:ARG:HE	1.76	0.51
1:A:200:GLU:HB2	1:A:248:VAL:HG21	1.92	0.50
1:F:86:MET:HG3	1:F:124:ASP:HB3	1.93	0.50
1:D:257:ARG:HA	1:D:257:ARG:CZ	2.42	0.50
1:B:107:ASP:HB3	1:B:110:LEU:HD23	1.93	0.50
1:A:160:VAL:HG12	1:A:165:ARG:HG3	1.94	0.50
1:C:78:TRP:HZ2	3:C:303:ILE:HB	1.77	0.50
1:C:54:ASN:HB3	1:C:57:PHE:CD2	2.47	0.50
1:B:96:MET:SD	4:B:429:HOH:O	2.60	0.49
1:D:135:VAL:HG21	1:D:236:SER:HB3	1.94	0.49
1:E:200:GLU:HB2	1:E:248:VAL:HG21	1.93	0.49
1:F:260:ALA:H	1:F:264:GLN:NE2	2.10	0.49
1:B:93:LEU:HD12	1:B:117:VAL:HG12	1.95	0.49
1:C:39:ARG:HA	1:C:42:LYS:HE3	1.94	0.49
1:D:154:LYS:HB2	1:D:155:PRO:HD3	1.95	0.49
1:A:65:SER:HB2	1:A:218:GLU:HG2	1.94	0.48
1:E:225:PHE:HB3	1:E:231:LEU:HD21	1.95	0.48
1:C:74:ILE:CD1	1:C:286:TYR:HA	2.42	0.48
1:E:204:LEU:HD22	1:E:242:THR:HG22	1.95	0.48
1:C:211:ARG:HB2	1:C:234:VAL:HG11	1.95	0.48
1:E:87:PHE:HB3	1:F:101:GLN:HB2	1.94	0.48
1:B:86:MET:HG3	1:B:124:ASP:HB3	1.94	0.48
1:C:232:ALA:N	4:C:401:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:PRO:HG3	1:B:219:VAL:HG22	1.95	0.48
1:F:78:TRP:CZ2	3:F:303:ILE:HB	2.48	0.48
1:F:131:ALA:HB3	1:F:240:ALA:HB2	1.96	0.48
1:A:239:LYS:HG2	1:F:243:MET:HG3	1.95	0.47
1:F:78:TRP:HZ2	3:F:303:ILE:HB	1.79	0.47
1:B:225:PHE:CG	1:B:231:LEU:HD21	2.49	0.47
1:D:30:ALA:C	1:D:32:GLU:H	2.21	0.47
1:F:28:LEU:HD11	1:F:259:VAL:HG12	1.96	0.47
4:A:403:HOH:O	1:B:98:ARG:NH1	2.45	0.47
1:B:159:HIS:ND1	1:B:219:VAL:HG11	2.30	0.47
1:B:200:GLU:HB2	1:B:248:VAL:HG21	1.96	0.47
1:D:33:GLN:H	1:D:33:GLN:CD	2.22	0.47
1:D:95:VAL:HG21	1:D:187:THR:HA	1.97	0.47
1:D:133:ARG:HH22	1:E:229:ASP:CG	2.23	0.47
1:E:160:VAL:HG12	1:E:165:ARG:HG2	1.96	0.47
1:F:135:VAL:HG21	1:F:236:SER:HB3	1.97	0.47
1:C:43:GLU:HA	1:C:43:GLU:OE1	2.14	0.47
1:F:40:VAL:O	1:F:44:ILE:HD12	2.15	0.47
1:C:243:MET:O	1:C:247:GLN:HG3	2.15	0.46
1:B:248:VAL:HB	1:B:255:MET:HG2	1.98	0.46
1:C:282:ALA:O	1:C:285:THR:OG1	2.28	0.46
1:D:270:THR:HG22	1:D:273:ARG:HH21	1.81	0.46
1:D:175:VAL:O	1:D:179:LEU:HG	2.16	0.46
1:B:39:ARG:CB	1:B:269:LEU:HD11	2.46	0.46
1:D:40:VAL:HG13	1:D:272:VAL:HG11	1.97	0.46
1:E:86:MET:HE2	1:E:86:MET:HB3	1.88	0.46
1:E:110:LEU:HD23	1:E:257:ARG:O	2.16	0.46
1:B:86:MET:HE2	1:B:86:MET:HB3	1.79	0.45
1:E:62:LYS:O	1:E:63:ALA:C	2.59	0.45
1:E:266:GLU:O	1:E:270:THR:HG23	2.16	0.45
1:D:78:TRP:CZ2	3:D:303:ILE:HB	2.51	0.45
1:E:162:GLU:HA	1:E:165:ARG:HG3	1.97	0.45
1:B:237:HIS:O	1:B:241:GLU:HG2	2.17	0.45
1:F:185:LEU:HD22	1:F:191:GLY:HA2	1.99	0.45
1:B:197:ARG:O	4:B:401:HOH:O	2.21	0.45
1:D:72:LEU:HD22	1:D:157:ALA:HA	1.99	0.45
1:E:261:ASP:HB2	1:E:264:GLN:HG3	1.99	0.45
1:F:76:HIS:CE1	1:F:153:LEU:HD11	2.51	0.45
1:F:50:ARG:O	1:F:51:ARG:HG2	2.17	0.45
1:F:195:GLN:HA	1:F:275:TYR:CE1	2.52	0.44
1:A:140:PRO:HG3	1:B:112:ALA:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ASP:HA	1:D:154:LYS:HD2	2.00	0.44
1:A:101:GLN:HG2	1:B:87:PHE:HB2	2.00	0.44
1:B:287:ALA:O	1:B:291:ARG:HG3	2.16	0.44
1:F:113:ALA:HB3	1:F:258:LEU:HG	1.99	0.44
1:F:237:HIS:NE2	3:F:303:ILE:OXT	2.49	0.44
1:B:131:ALA:HB3	1:B:240:ALA:HB2	2.00	0.44
1:D:81:MET:HG2	1:D:178:LEU:HD23	2.00	0.44
1:F:117:VAL:HG22	1:F:255:MET:SD	2.58	0.44
1:B:63:ALA:O	1:B:64:GLU:C	2.61	0.44
1:D:88:THR:HG22	1:D:186:ALA:HB2	2.00	0.44
1:F:269:LEU:HD23	1:F:269:LEU:HA	1.76	0.43
1:A:107:ASP:HB3	1:A:110:LEU:HD13	1.99	0.43
1:D:259:VAL:HG11	1:D:265:ALA:HA	2.00	0.43
1:E:294:HIS:O	1:E:294:HIS:ND1	2.51	0.43
1:F:28:LEU:HD12	1:F:259:VAL:O	2.18	0.43
1:B:81:MET:HE3	1:B:178:LEU:HD23	2.00	0.43
1:B:225:PHE:HB3	1:B:231:LEU:HD21	2.00	0.43
1:E:202:ILE:HD12	1:E:206:ILE:HD11	2.00	0.43
1:F:257:ARG:NE	1:F:257:ARG:HA	2.34	0.43
1:A:257:ARG:NE	1:A:257:ARG:HA	2.34	0.43
1:A:95:VAL:HG21	1:A:187:THR:HA	2.00	0.43
1:E:91:SER:OG	1:E:186:ALA:O	2.31	0.43
1:B:57:PHE:O	1:B:61:ARG:HG3	2.19	0.42
1:D:160:VAL:HG12	1:D:165:ARG:HG3	2.01	0.42
1:D:204:LEU:O	1:D:208:VAL:HG23	2.19	0.42
1:D:229:ASP:OD2	1:D:229:ASP:N	2.36	0.42
1:F:160:VAL:HG12	1:F:165:ARG:HG2	2.01	0.42
1:D:159:HIS:N	1:D:159:HIS:CD2	2.86	0.42
1:F:72:LEU:HD22	1:F:157:ALA:HA	2.02	0.42
1:C:159:HIS:CE1	1:C:219:VAL:HG11	2.54	0.42
1:D:78:TRP:HZ2	3:D:303:ILE:HB	1.83	0.42
1:E:93:LEU:HD12	1:E:117:VAL:HG12	2.02	0.42
1:E:171:LEU:HD22	1:E:175:VAL:HG11	2.00	0.42
1:F:92:GLY:O	1:F:96:MET:HG3	2.20	0.42
1:D:93:LEU:HD21	1:D:118:TYR:CD2	2.52	0.42
1:A:200:GLU:HG3	1:A:248:VAL:HG11	2.01	0.42
1:C:202:ILE:O	1:C:206:ILE:HD12	2.20	0.42
1:E:190:LEU:O	1:E:194:VAL:HG23	2.19	0.42
1:D:204:LEU:HD23	1:D:241:GLU:HB2	2.01	0.42
1:B:51:ARG:O	1:B:61:ARG:NH1	2.53	0.41
1:E:126:ASP:OD2	1:F:119:GLN:NE2	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:LEU:HD12	1:B:234:VAL:HG21	2.01	0.41
1:C:153:LEU:O	1:C:157:ALA:N	2.49	0.41
1:F:85:PHE:CD2	3:F:303:ILE:HD11	2.56	0.41
1:B:195:GLN:HA	1:B:275:TYR:CE2	2.55	0.41
1:C:72:LEU:HD12	1:C:153:LEU:HD12	2.02	0.41
1:D:138:ARG:HB2	4:D:447:HOH:O	2.20	0.41
1:D:35:ASP:O	1:D:36:LEU:C	2.64	0.41
1:E:101:GLN:HB2	1:F:87:PHE:HB3	2.03	0.41
1:C:86:MET:HE2	1:C:86:MET:HB3	1.87	0.41
1:F:124:ASP:OD1	3:F:303:ILE:OXT	2.39	0.41
1:B:36:LEU:HD13	1:B:265:ALA:HB1	2.02	0.41
1:C:68:PRO:HB2	4:C:407:HOH:O	2.20	0.41
1:D:93:LEU:HD12	1:D:114:PHE:CE1	2.55	0.41
1:F:148:TRP:CE3	1:F:152:VAL:HG21	2.56	0.41
1:A:188:HIS:CD2	1:A:189:PRO:HD2	2.56	0.41
1:B:236:SER:O	1:B:239:LYS:HB2	2.21	0.40
1:C:98:ARG:O	1:C:99:ARG:C	2.62	0.40
1:C:151:THR:HG23	4:C:413:HOH:O	2.22	0.40
1:D:283:LEU:HD23	1:D:283:LEU:HA	1.92	0.40
1:E:70:ALA:O	1:E:74:ILE:HG13	2.20	0.40
1:F:43:GLU:HG3	1:F:269:LEU:HD22	2.02	0.40
1:A:131:ALA:HB3	1:A:240:ALA:HB2	2.02	0.40
1:C:210:PHE:HD1	1:C:210:PHE:HA	1.81	0.40
1:C:255:MET:HA	1:C:255:MET:HE2	2.03	0.40
1:A:65:SER:HB2	1:A:218:GLU:CG	2.52	0.40
1:A:124:ASP:HA	1:A:144:HIS:CE1	2.57	0.40
1:C:113:ALA:HB3	1:C:258:LEU:HG	2.02	0.40
1:C:195:GLN:HA	1:C:275:TYR:CE2	2.56	0.40
1:E:53:ASP:O	1:E:54:ASN:C	2.64	0.40
1:F:93:LEU:HD12	1:F:114:PHE:CE1	2.56	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	265/275 (96%)	257 (97%)	8 (3%)	0	100	100
1	B	267/275 (97%)	254 (95%)	13 (5%)	0	100	100
1	C	255/275 (93%)	248 (97%)	6 (2%)	1 (0%)	30	52
1	D	258/275 (94%)	248 (96%)	8 (3%)	2 (1%)	16	34
1	E	265/275 (96%)	256 (97%)	8 (3%)	1 (0%)	30	52
1	F	246/275 (90%)	241 (98%)	4 (2%)	1 (0%)	30	52
All	All	1556/1650 (94%)	1504 (97%)	47 (3%)	5 (0%)	37	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	153	LEU
1	D	53	ASP
1	D	55	ALA
1	E	55	ALA
1	F	55	ALA

### 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	187/207 (90%)	183 (98%)	4 (2%)	48	73
1	B	176/207 (85%)	171 (97%)	5 (3%)	38	65
1	C	175/207 (84%)	174 (99%)	1 (1%)	84	94
1	D	178/207 (86%)	173 (97%)	5 (3%)	38	65
1	E	181/207 (87%)	179 (99%)	2 (1%)	70	86
1	F	154/207 (74%)	154 (100%)	0	100	100
All	All	1051/1242 (85%)	1034 (98%)	17 (2%)	58	79

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	213	LEU
1	A	258	LEU
1	A	261	ASP
1	B	48	ARG
1	B	51	ARG
1	B	53	ASP
1	B	201	ASP
1	B	244	HIS
1	C	42	LYS
1	D	35	ASP
1	D	53	ASP
1	D	201	ASP
1	D	213	LEU
1	D	238	ILE
1	E	65	SER
1	E	213	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
1	A	278	HIS
1	A	294	HIS
1	B	54	ASN
1	B	119	GLN
1	B	278	HIS
1	C	108	HIS
1	C	195	GLN
1	C	247	GLN
1	D	119	GLN
1	D	159	HIS
1	E	33	GLN
1	E	54	ASN
1	E	76	HIS
1	E	108	HIS
1	E	159	HIS
1	E	278	HIS
1	F	108	HIS
1	F	195	GLN

### 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 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 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	ILE	A	303	2	7,8,8	0.84	0	7,10,10	0.55	0
3	ILE	D	303	2	7,8,8	0.82	0	7,10,10	0.61	0
3	ILE	F	303	2	7,8,8	0.77	0	7,10,10	0.66	0
3	ILE	C	303	2	7,8,8	0.81	0	7,10,10	0.68	0
3	ILE	B	303	2	7,8,8	0.75	0	7,10,10	0.67	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	ILE	A	303	2	-	2/10/10/10	-
3	ILE	D	303	2	-	2/10/10/10	-
3	ILE	F	303	2	-	2/10/10/10	-
3	ILE	C	303	2	-	2/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ILE	B	303	2	-	2/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

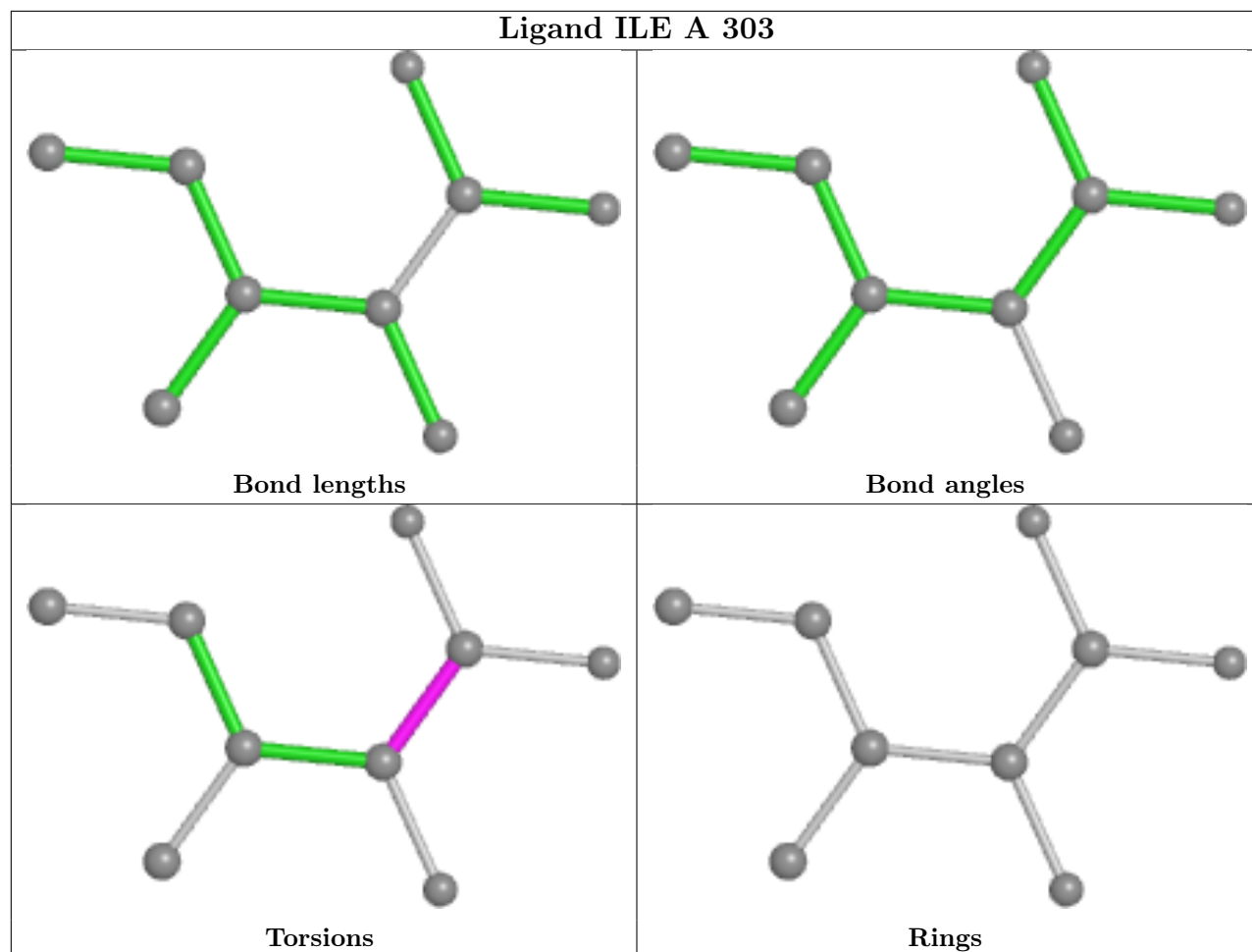
Mol	Chain	Res	Type	Atoms
3	B	303	ILE	O-C-CA-CB
3	C	303	ILE	O-C-CA-CB
3	F	303	ILE	O-C-CA-CB
3	A	303	ILE	OXT-C-CA-CB
3	B	303	ILE	OXT-C-CA-CB
3	C	303	ILE	OXT-C-CA-CB
3	D	303	ILE	O-C-CA-CB
3	D	303	ILE	OXT-C-CA-CB
3	F	303	ILE	OXT-C-CA-CB
3	A	303	ILE	O-C-CA-CB

There are no ring outliers.

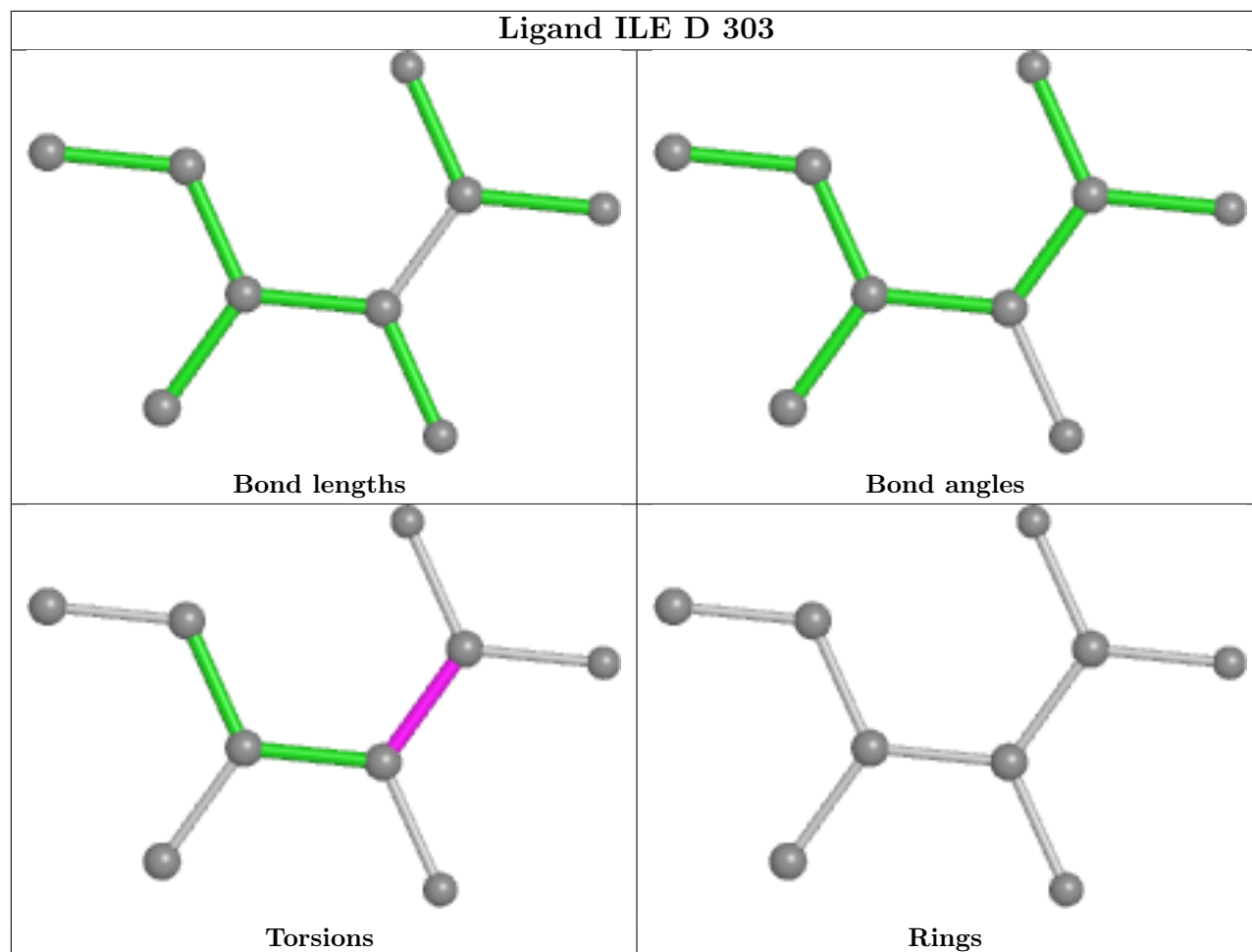
4 monomers are involved in 13 short contacts:

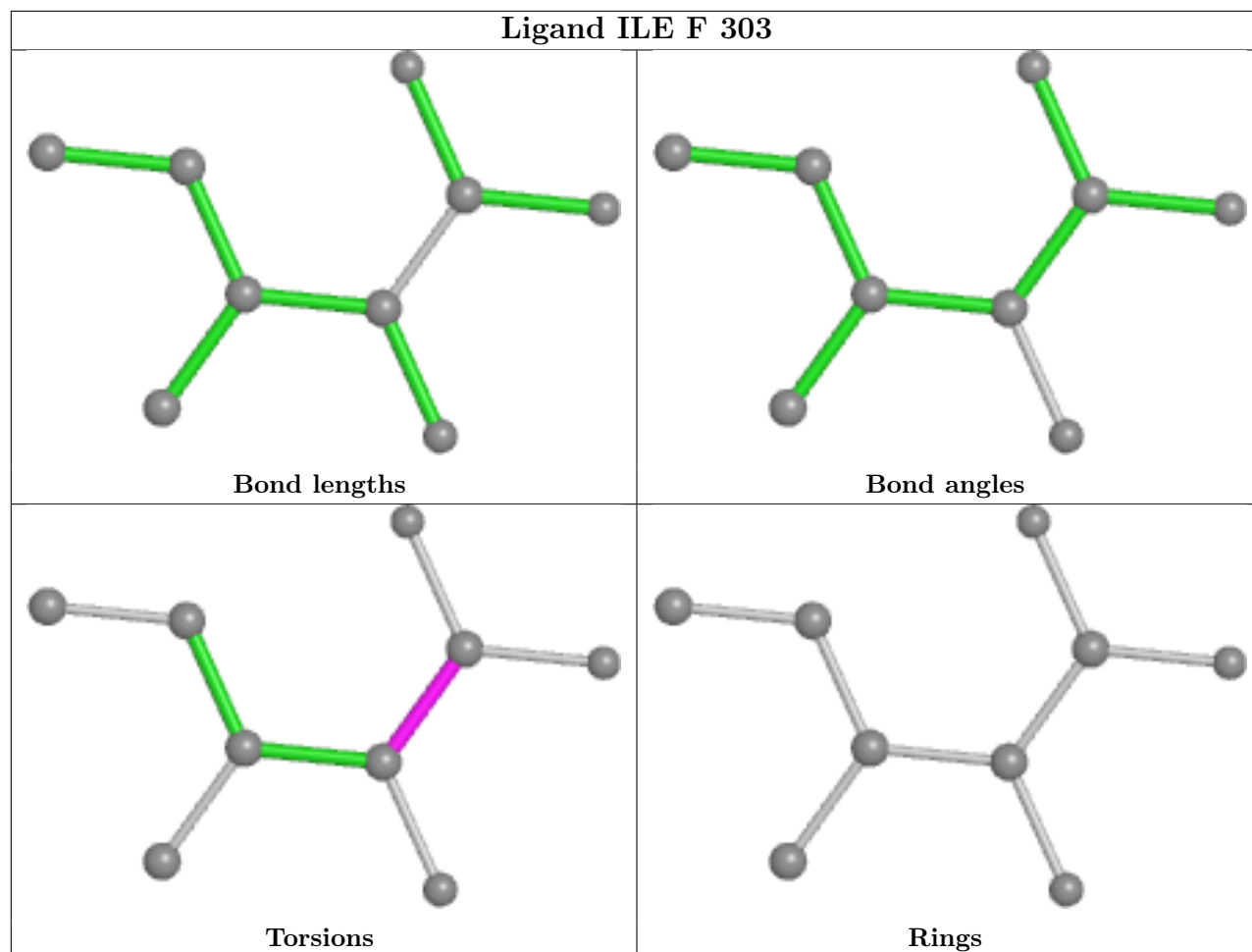
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	ILE	2	0
3	D	303	ILE	2	0
3	F	303	ILE	7	0
3	C	303	ILE	2	0

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.

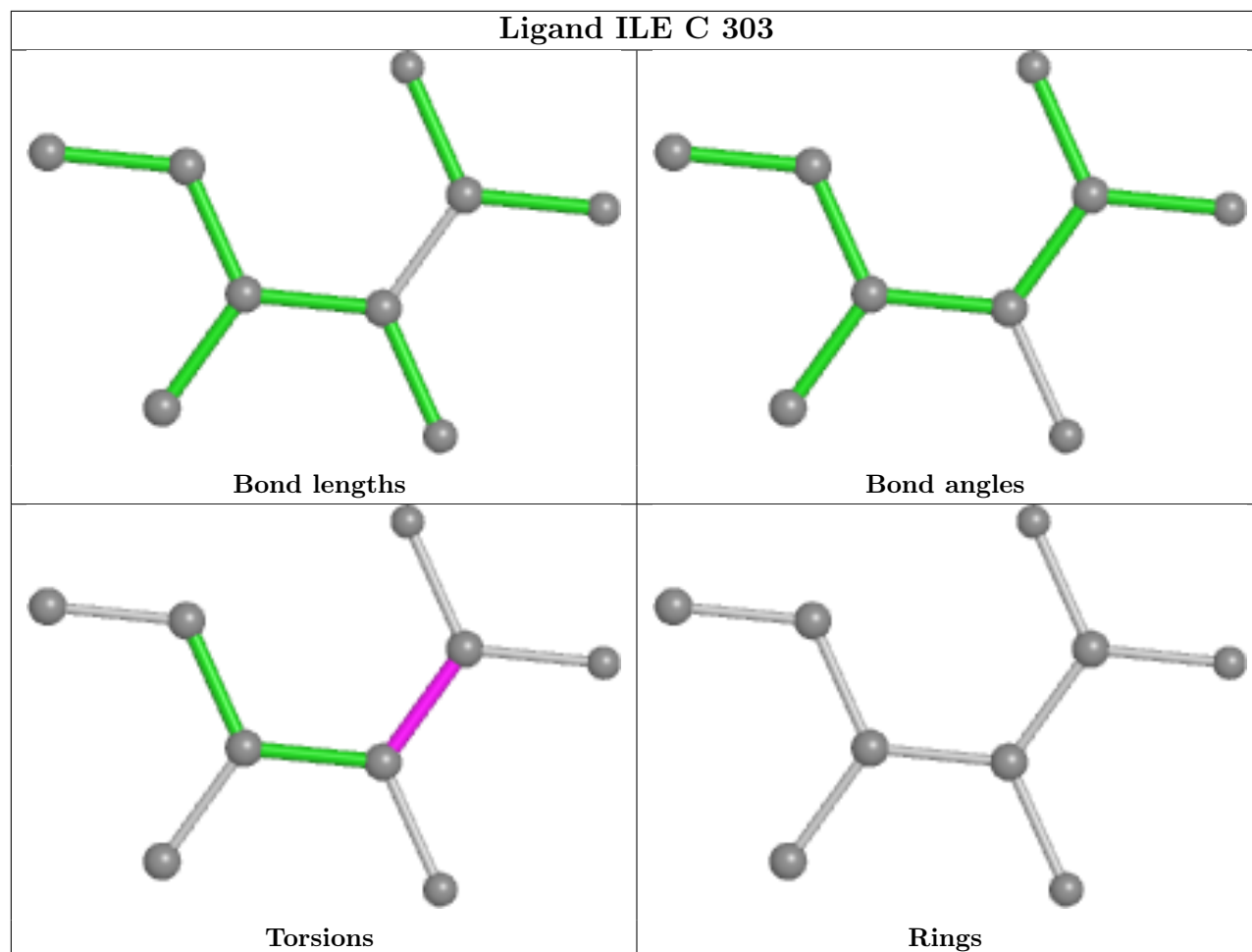


## Ligand ILE D 303

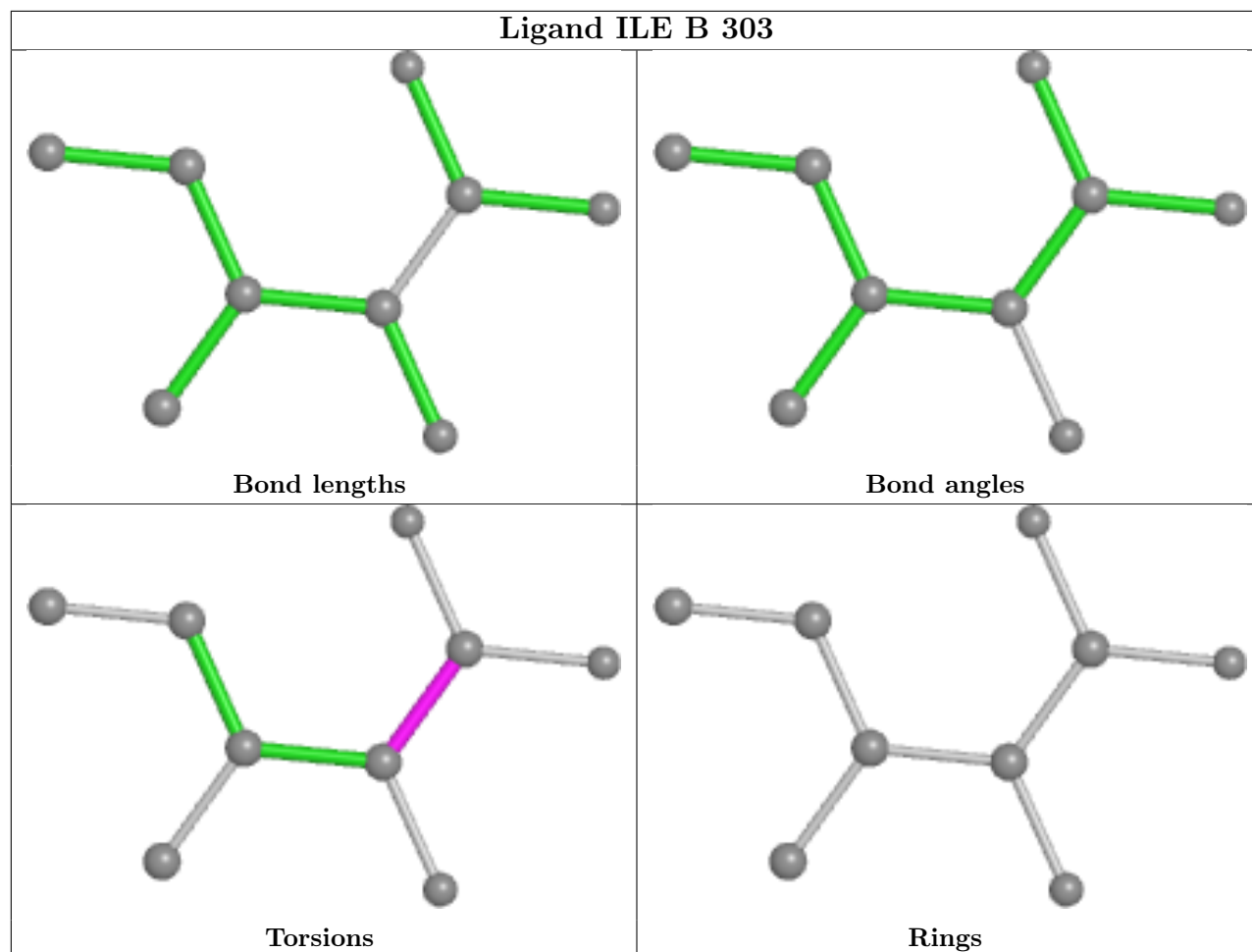




## Ligand ILE C 303







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	267/275 (97%)	-0.06	1 (0%) 89 86	30, 52, 76, 90	0
1	B	269/275 (97%)	0.36	10 (3%) 45 39	30, 70, 106, 128	0
1	C	261/275 (94%)	0.43	8 (3%) 51 46	30, 71, 104, 119	0
1	D	262/275 (95%)	0.32	7 (2%) 56 50	30, 69, 101, 146	0
1	E	267/275 (97%)	0.07	5 (1%) 66 61	30, 59, 93, 140	0
1	F	252/275 (91%)	0.56	11 (4%) 39 33	30, 81, 113, 135	0
All	All	1578/1650 (95%)	0.28	42 (2%) 56 50	30, 65, 106, 146	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	221	GLY	3.5
1	C	266	GLU	3.4
1	A	261	ASP	3.3
1	C	28	LEU	3.2
1	B	52	ALA	3.2
1	B	293	GLY	3.0
1	B	51	ARG	3.0
1	F	242	THR	2.9
1	B	63	ALA	2.9
1	F	69	GLU	2.8
1	E	53	ASP	2.8
1	F	54	ASN	2.7
1	B	48	ARG	2.6
1	F	74	ILE	2.5
1	B	247	GLN	2.4
1	E	294	HIS	2.4
1	C	229	ASP	2.4
1	F	129	ALA	2.4
1	E	28	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	64	GLU	2.3
1	F	231	LEU	2.3
1	D	241	GLU	2.3
1	D	54	ASN	2.3
1	B	53	ASP	2.3
1	D	251	GLU	2.3
1	E	104	ASP	2.2
1	C	30	ALA	2.2
1	D	224	LEU	2.2
1	F	213	LEU	2.2
1	F	56	PHE	2.2
1	C	99	ARG	2.2
1	D	31	ALA	2.2
1	F	283	LEU	2.2
1	E	55	ALA	2.2
1	B	270	THR	2.1
1	D	242	THR	2.1
1	F	261	ASP	2.1
1	C	211	ARG	2.0
1	F	214	TYR	2.0
1	B	226	ALA	2.0
1	C	152	VAL	2.0
1	C	153	LEU	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, 95<sup>th</sup> 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.

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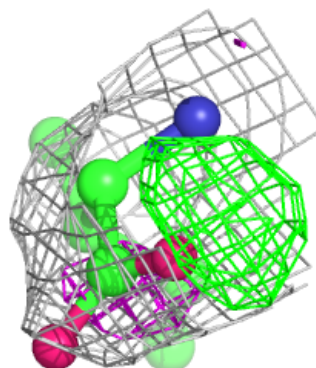
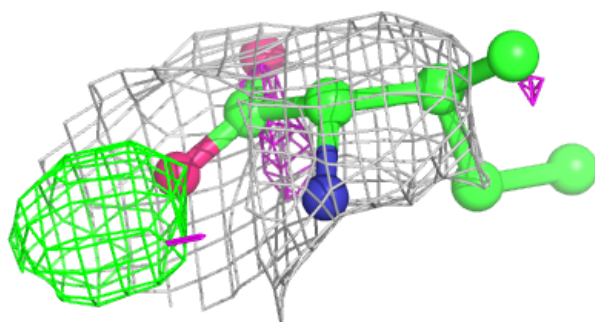
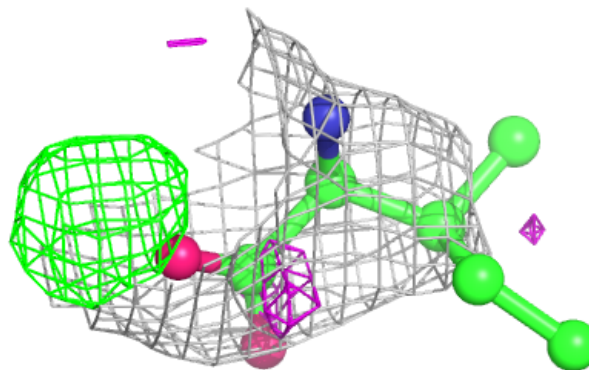
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE2	F	301	1/1	0.81	0.17	148,148,148,148	0
2	FE2	B	301	1/1	0.82	0.13	76,76,76,76	0
2	FE2	D	302	1/1	0.84	0.11	106,106,106,106	0
2	FE2	A	302	1/1	0.85	0.10	63,63,63,63	0
2	FE2	B	302	1/1	0.86	0.12	145,145,145,145	0
2	FE2	E	301	1/1	0.87	0.09	65,65,65,65	0
2	FE2	E	302	1/1	0.87	0.10	99,99,99,99	0
2	FE2	C	302	1/1	0.87	0.11	77,77,77,77	0
2	FE2	F	302	1/1	0.87	0.10	87,87,87,87	0
3	ILE	D	303	9/9	0.87	0.17	62,67,69,70	0
3	ILE	F	303	9/9	0.87	0.15	71,77,82,82	0
2	FE2	D	301	1/1	0.88	0.10	69,69,69,69	0
2	FE2	A	301	1/1	0.89	0.09	66,66,66,66	0
3	ILE	B	303	9/9	0.89	0.16	67,72,76,78	0
3	ILE	A	303	9/9	0.90	0.25	61,64,66,67	0
3	ILE	C	303	9/9	0.90	0.17	68,73,76,77	0
2	FE2	C	301	1/1	0.92	0.07	66,66,66,66	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.

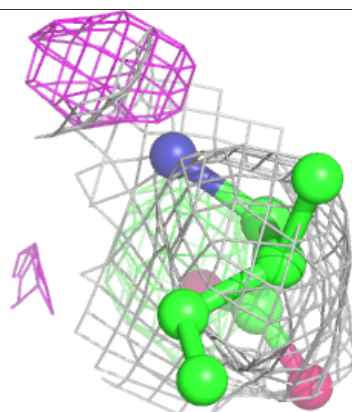
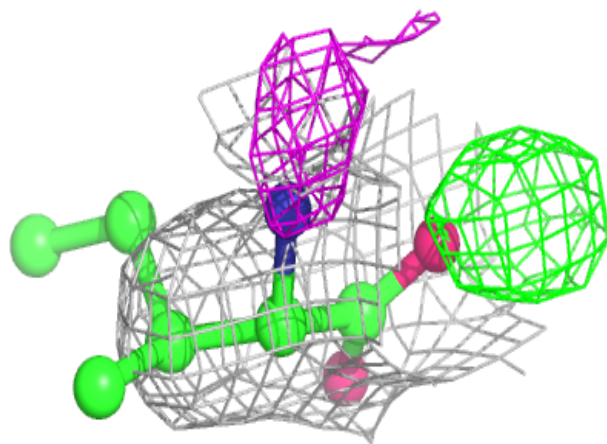
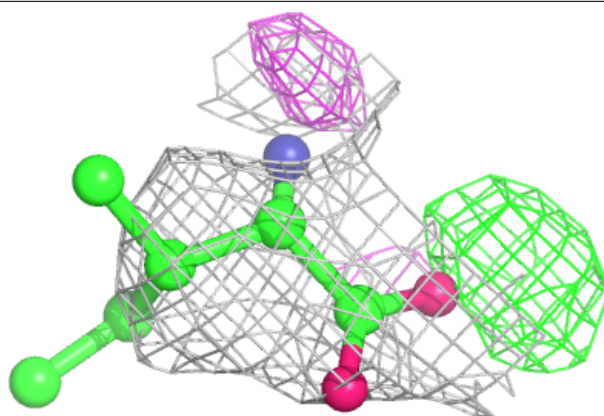
**Electron density around ILE D 303:**

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



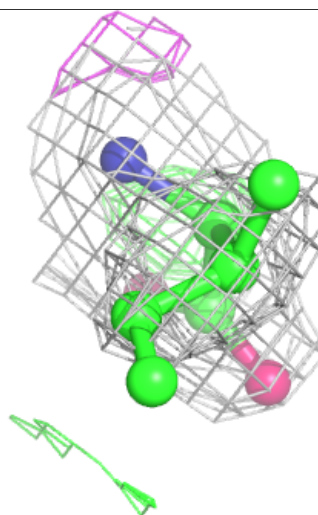
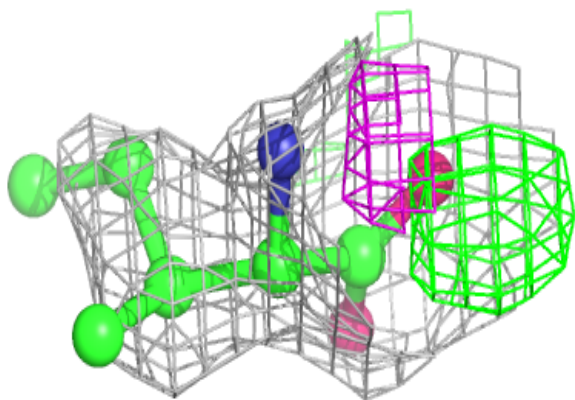
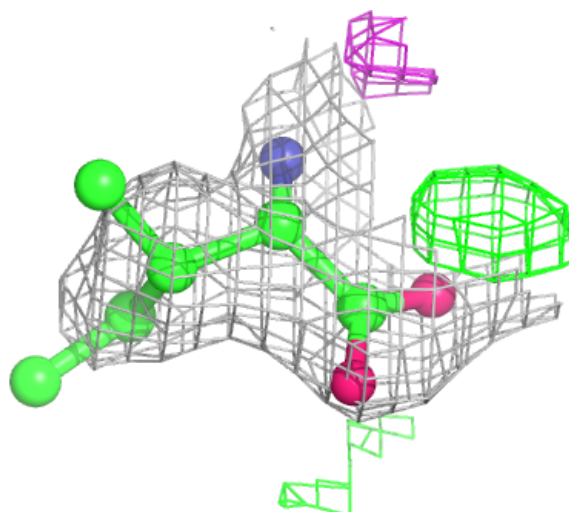
**Electron density around ILE F 303:**

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



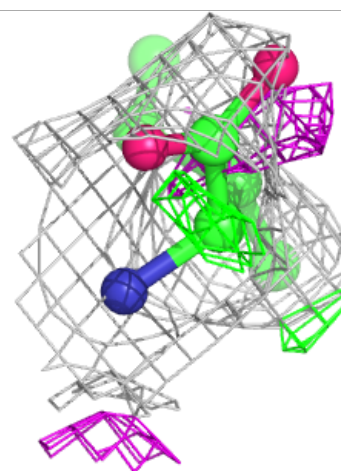
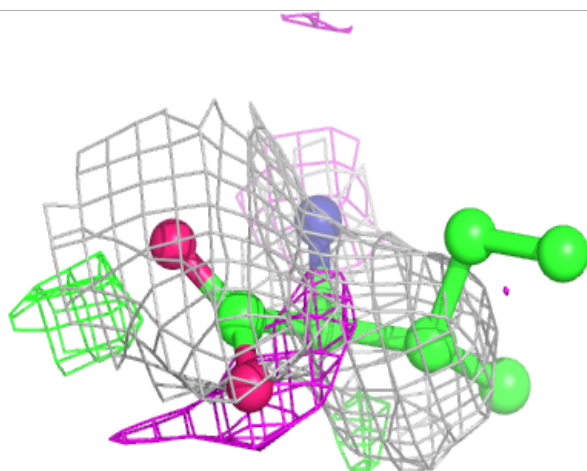
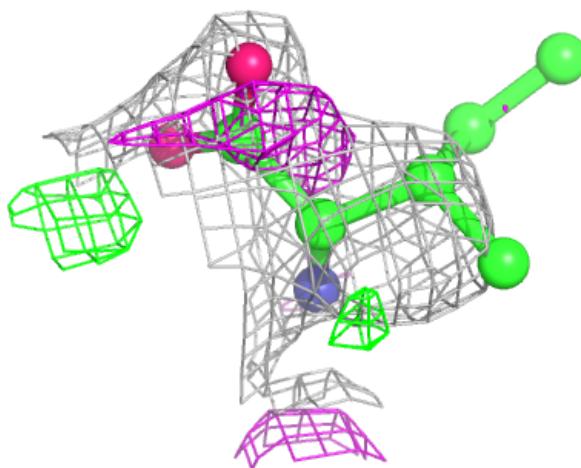
**Electron density around ILE B 303:**

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



**Electron density around ILE A 303:**

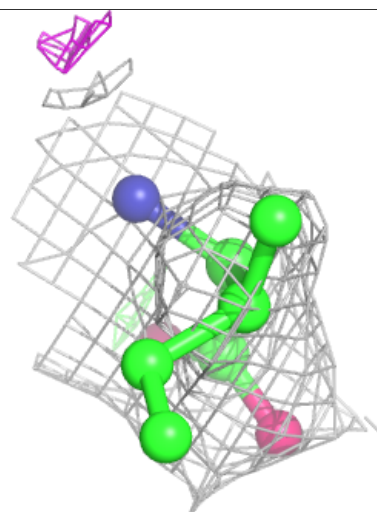
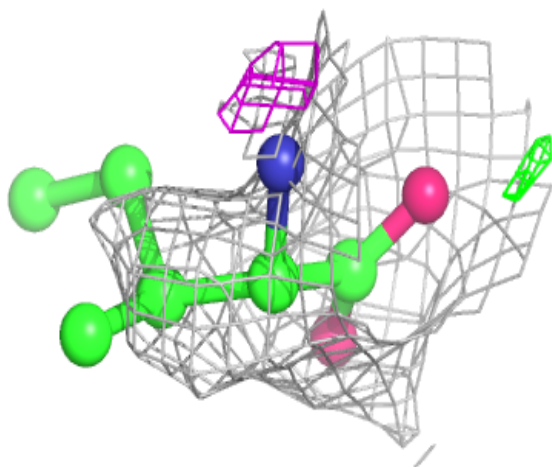
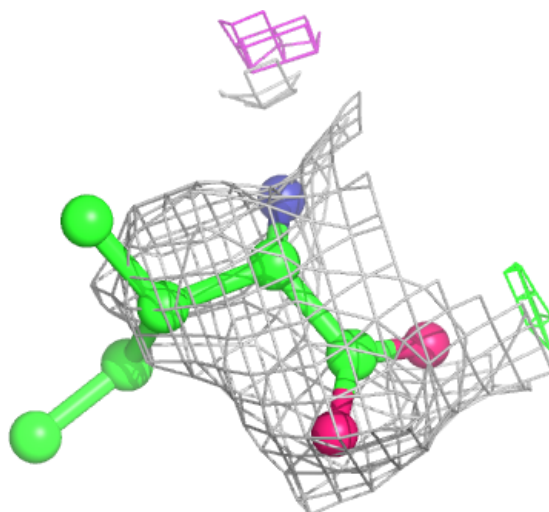
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around ILE C 303:**

$2mF_o-DF_c$  (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.