



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 05:18 AM JST

PDB ID : 5GGX / pdb_00005ggx
Title : Crystal Structure of Fe³⁺ - Desferal bound siderophore binding protein FhuD from *Vibrio cholerae*
Authors : Agarwal, S.; Dey, S.; Ghosh, B.; Dasgupta, J.
Deposited on : 2016-06-16
Resolution : 3.40 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	:	1.8.5 (274361), CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

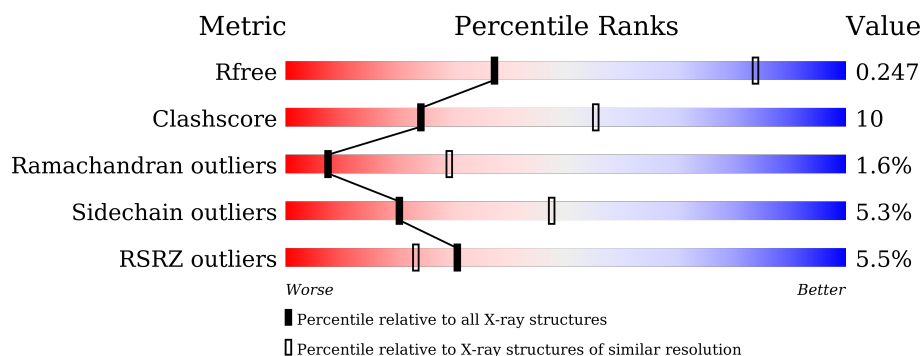
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	282	4% 69% 22% • 6%
1	B	282	8% 67% 25% • 6%
1	C	282	4% 69% 23% •• 6%
1	D	282	5% 71% 21% • 5%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DEF	A	401	X	-	-	-
2	DEF	B	401	X	-	-	-
2	DEF	C	401	X	-	-	-
2	DEF	D	401	X	-	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8438 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 Iron(III) ABC transporter, periplasmic iron-compound-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2071	1340	346	381	4			
1	B	266	Total	C	N	O	S	0	0	0
			2076	1343	347	382	4			
1	C	266	Total	C	N	O	S	0	0	0
			2076	1343	347	382	4			
1	D	267	Total	C	N	O	S	0	0	0
			2075	1342	346	383	4			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	HIS	-	expression tag	UNP A0A0H3AJ03
A	39	HIS	-	expression tag	UNP A0A0H3AJ03
A	40	HIS	-	expression tag	UNP A0A0H3AJ03
A	41	HIS	-	expression tag	UNP A0A0H3AJ03
A	42	HIS	-	expression tag	UNP A0A0H3AJ03
A	43	HIS	-	expression tag	UNP A0A0H3AJ03
A	44	SER	-	expression tag	UNP A0A0H3AJ03
A	45	SER	-	expression tag	UNP A0A0H3AJ03
A	46	GLY	-	expression tag	UNP A0A0H3AJ03
A	47	LEU	-	expression tag	UNP A0A0H3AJ03
A	48	VAL	-	expression tag	UNP A0A0H3AJ03
A	49	PRO	-	expression tag	UNP A0A0H3AJ03
A	50	ARG	-	expression tag	UNP A0A0H3AJ03
A	51	GLY	-	expression tag	UNP A0A0H3AJ03
A	52	SER	-	expression tag	UNP A0A0H3AJ03
A	53	HIS	-	expression tag	UNP A0A0H3AJ03
A	54	MET	-	expression tag	UNP A0A0H3AJ03
B	38	HIS	-	expression tag	UNP A0A0H3AJ03
B	39	HIS	-	expression tag	UNP A0A0H3AJ03
B	40	HIS	-	expression tag	UNP A0A0H3AJ03

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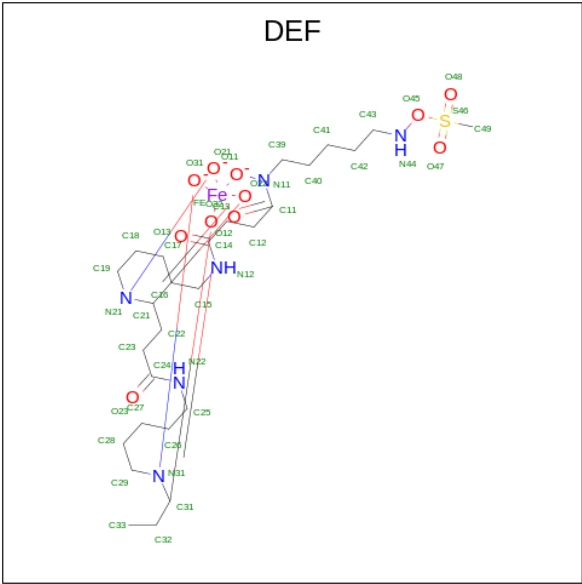
Chain	Residue	Modelled	Actual	Comment	Reference
B	41	HIS	-	expression tag	UNP A0A0H3AJ03
B	42	HIS	-	expression tag	UNP A0A0H3AJ03
B	43	HIS	-	expression tag	UNP A0A0H3AJ03
B	44	SER	-	expression tag	UNP A0A0H3AJ03
B	45	SER	-	expression tag	UNP A0A0H3AJ03
B	46	GLY	-	expression tag	UNP A0A0H3AJ03
B	47	LEU	-	expression tag	UNP A0A0H3AJ03
B	48	VAL	-	expression tag	UNP A0A0H3AJ03
B	49	PRO	-	expression tag	UNP A0A0H3AJ03
B	50	ARG	-	expression tag	UNP A0A0H3AJ03
B	51	GLY	-	expression tag	UNP A0A0H3AJ03
B	52	SER	-	expression tag	UNP A0A0H3AJ03
B	53	HIS	-	expression tag	UNP A0A0H3AJ03
B	54	MET	-	expression tag	UNP A0A0H3AJ03
C	38	HIS	-	expression tag	UNP A0A0H3AJ03
C	39	HIS	-	expression tag	UNP A0A0H3AJ03
C	40	HIS	-	expression tag	UNP A0A0H3AJ03
C	41	HIS	-	expression tag	UNP A0A0H3AJ03
C	42	HIS	-	expression tag	UNP A0A0H3AJ03
C	43	HIS	-	expression tag	UNP A0A0H3AJ03
C	44	SER	-	expression tag	UNP A0A0H3AJ03
C	45	SER	-	expression tag	UNP A0A0H3AJ03
C	46	GLY	-	expression tag	UNP A0A0H3AJ03
C	47	LEU	-	expression tag	UNP A0A0H3AJ03
C	48	VAL	-	expression tag	UNP A0A0H3AJ03
C	49	PRO	-	expression tag	UNP A0A0H3AJ03
C	50	ARG	-	expression tag	UNP A0A0H3AJ03
C	51	GLY	-	expression tag	UNP A0A0H3AJ03
C	52	SER	-	expression tag	UNP A0A0H3AJ03
C	53	HIS	-	expression tag	UNP A0A0H3AJ03
C	54	MET	-	expression tag	UNP A0A0H3AJ03
D	38	HIS	-	expression tag	UNP A0A0H3AJ03
D	39	HIS	-	expression tag	UNP A0A0H3AJ03
D	40	HIS	-	expression tag	UNP A0A0H3AJ03
D	41	HIS	-	expression tag	UNP A0A0H3AJ03
D	42	HIS	-	expression tag	UNP A0A0H3AJ03
D	43	HIS	-	expression tag	UNP A0A0H3AJ03
D	44	SER	-	expression tag	UNP A0A0H3AJ03
D	45	SER	-	expression tag	UNP A0A0H3AJ03
D	46	GLY	-	expression tag	UNP A0A0H3AJ03
D	47	LEU	-	expression tag	UNP A0A0H3AJ03
D	48	VAL	-	expression tag	UNP A0A0H3AJ03

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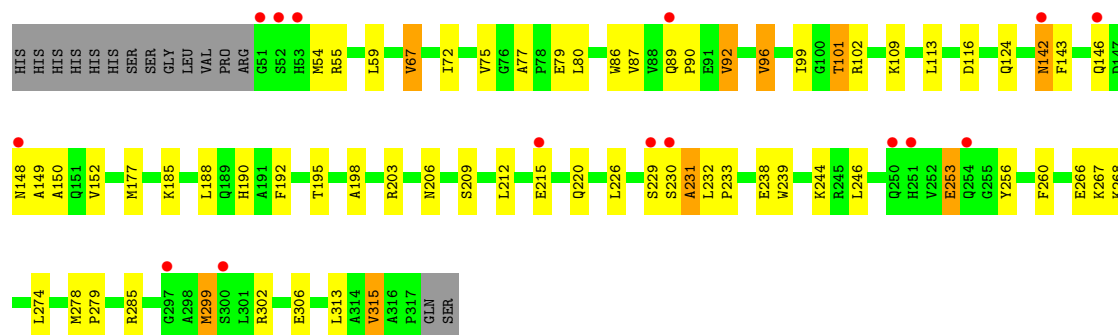
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Chain	Residue	Modelled	Actual	Comment	Reference
D	49	PRO	-	expression tag	UNP A0A0H3AJ03
D	50	ARG	-	expression tag	UNP A0A0H3AJ03
D	51	GLY	-	expression tag	UNP A0A0H3AJ03
D	52	SER	-	expression tag	UNP A0A0H3AJ03
D	53	HIS	-	expression tag	UNP A0A0H3AJ03
D	54	MET	-	expression tag	UNP A0A0H3AJ03

- Molecule 2 is DEFEROXAMINE MESYLATE FE(III) COMPLEX (CCD ID: DEF) (formula: C₂₇H₄₉FeN₆O₁₁S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			35	21	1	5	8		
2	B	1	Total	C	Fe	N	O	0	0
			35	21	1	5	8		
2	C	1	Total	C	Fe	N	O	0	0
			35	21	1	5	8		
2	D	1	Total	C	Fe	N	O	0	0
			35	21	1	5	8		



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	191.15Å 191.15Å 129.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.05 – 3.40 43.05 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.05-3.40) 99.8 (43.05-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.200 , 0.236 0.216 , 0.247	Depositor DCC
R_{free} test set	2018 reflections (5.35%)	wwPDB-VP
Wilson B-factor (Å ²)	82.5	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8438	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: DEF

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	0.33	0/2122	0.77	2/2898 (0.1%)
1	B	0.33	0/2127	0.77	4/2905 (0.1%)
1	C	0.34	0/2127	0.79	1/2905 (0.0%)
1	D	0.32	0/2125	0.76	1/2902 (0.0%)
All	All	0.33	0/8501	0.77	8/11610 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	254	GLN	N-CA-C	7.21	122.01	112.13
1	A	89	GLN	CA-C-N	-6.28	111.98	119.84
1	A	89	GLN	C-N-CA	-6.28	111.98	119.84
1	D	143	PHE	N-CA-C	5.87	118.46	110.06
1	B	89	GLN	CA-C-N	-5.74	112.67	119.84
1	B	89	GLN	C-N-CA	-5.74	112.67	119.84
1	B	196	LEU	CA-C-N	5.13	125.14	120.21
1	B	196	LEU	C-N-CA	5.13	125.14	120.21

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	2071	0	2092	33	0
1	B	2076	0	2095	41	0
1	C	2076	0	2095	46	0
1	D	2075	0	2093	39	0
2	A	35	0	30	3	0
2	B	35	0	30	8	0
2	C	35	0	30	4	0
2	D	35	0	30	4	0
All	All	8438	0	8495	169	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 10.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:DEF:N31	2:D:401:DEF:C31	1.78	1.46
2:B:401:DEF:N31	2:B:401:DEF:C31	1.79	1.45
2:A:401:DEF:N31	2:A:401:DEF:C31	1.78	1.45
2:C:401:DEF:C31	2:C:401:DEF:N31	1.78	1.44
2:D:401:DEF:N31	2:D:401:DEF:O31	1.59	1.35
2:C:401:DEF:N31	2:C:401:DEF:O31	1.59	1.33
2:A:401:DEF:N31	2:A:401:DEF:O31	1.59	1.32
2:B:401:DEF:N31	2:B:401:DEF:O31	1.59	1.29
1:C:89:GLN:HB2	1:C:90:PRO:HD3	1.56	0.86
1:C:253:GLU:C	1:C:254:GLN:HE21	1.82	0.86
1:C:193:GLY:O	1:C:195:THR:N	2.14	0.81
1:A:55:ARG:NH1	1:A:113:LEU:O	2.15	0.79
1:C:254:GLN:HE21	1:C:254:GLN:N	1.84	0.76
1:C:89:GLN:CB	1:C:90:PRO:HD3	2.18	0.73
1:D:142:ASN:O	1:D:142:ASN:ND2	2.23	0.71
1:C:89:GLN:OE1	1:C:290:ARG:NH1	2.29	0.65
1:B:148:ASN:O	1:B:150:ALA:N	2.30	0.65
1:D:148:ASN:O	1:D:150:ALA:N	2.31	0.64
1:C:148:ASN:O	1:C:150:ALA:N	2.32	0.63
1:A:148:ASN:O	1:A:150:ALA:N	2.32	0.62
1:D:206:ASN:ND2	1:D:209:SER:OG	2.33	0.62
1:B:89:GLN:NE2	1:B:291:PRO:O	2.23	0.62
1:B:75:VAL:HG23	1:B:113:LEU:HD13	1.82	0.61
1:A:290:ARG:NH1	1:A:310:GLU:OE2	2.34	0.59
1:D:80:LEU:HD22	1:D:92:VAL:HG21	1.84	0.59
1:A:214:THR:HA	1:A:234:GLN:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:VAL:HG13	1:B:72:ILE:HB	1.83	0.59
1:A:87:VAL:HB	1:A:293:TRP:HB2	1.84	0.59
1:A:62:ASP:OD2	1:A:63:LEU:N	2.36	0.59
1:D:302:ARG:NH1	1:D:306:GLU:OE1	2.36	0.58
1:B:77:ALA:HB3	1:B:80:LEU:HD21	1.85	0.58
1:D:55:ARG:NH1	1:D:113:LEU:O	2.36	0.58
1:B:62:ASP:OD1	1:B:63:LEU:N	2.36	0.57
1:C:77:ALA:HB3	1:C:80:LEU:HD21	1.86	0.57
1:D:67:VAL:HG13	1:D:72:ILE:HB	1.87	0.57
1:D:89:GLN:HB2	1:D:90:PRO:HD3	1.87	0.55
1:D:79:GLU:HG3	1:D:101:THR:HA	1.88	0.55
2:B:401:DEF:O31	2:B:401:DEF:H221	2.06	0.55
1:B:212:LEU:HD21	1:B:249:LEU:HD21	1.89	0.55
1:D:77:ALA:HB3	1:D:80:LEU:HD21	1.90	0.54
1:D:230:SER:C	1:D:232:LEU:H	2.16	0.54
1:C:73:GLN:NE2	1:C:95:SER:OG	2.32	0.54
1:D:101:THR:OG1	1:D:102:ARG:N	2.41	0.54
1:B:200:VAL:HG23	1:B:231:ALA:HB3	1.89	0.54
1:D:253:GLU:HA	1:D:279:PRO:HB2	1.90	0.54
1:C:177:MET:HG3	1:C:302:ARG:HB2	1.90	0.53
1:A:245:ARG:H	1:A:245:ARG:HD2	1.74	0.53
1:D:177:MET:HG3	1:D:302:ARG:HB2	1.89	0.53
1:C:79:GLU:HG3	1:C:101:THR:HA	1.91	0.53
2:D:401:DEF:H162	2:D:401:DEF:O13	2.10	0.52
1:C:180:ARG:O	1:C:184:LEU:HD22	2.09	0.52
1:D:230:SER:O	1:D:232:LEU:N	2.38	0.52
1:A:77:ALA:HB3	1:A:80:LEU:HD21	1.92	0.52
1:D:299:MET:HE3	1:D:302:ARG:HD2	1.91	0.51
1:C:55:ARG:NH1	1:C:113:LEU:O	2.44	0.51
1:D:238:GLU:HG2	1:D:239:TRP:CD1	2.45	0.51
1:B:188:LEU:HD13	1:B:309:THR:HG23	1.93	0.51
1:C:205:ALA:HB1	1:D:195:THR:HG23	1.93	0.51
1:A:215:GLU:HA	1:A:220:GLN:HG2	1.92	0.50
1:C:87:VAL:HA	1:C:293:TRP:HB2	1.93	0.50
1:B:79:GLU:HG3	1:B:101:THR:HA	1.94	0.50
1:B:196:LEU:HB3	1:B:228:LEU:HD23	1.93	0.49
1:C:109:LYS:O	1:C:113:LEU:HD23	2.11	0.49
1:D:190:HIS:C	1:D:192:PHE:H	2.20	0.49
1:A:66:GLN:NE2	1:A:153:ALA:O	2.43	0.49
1:A:263:PHE:CZ	1:A:265:GLU:HB2	2.48	0.49
1:D:80:LEU:HD11	1:D:96:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ALA:HB2	1:B:134:ILE:HD12	1.95	0.49
1:D:54:MET:HG2	1:D:116:ASP:HB2	1.95	0.49
1:C:200:VAL:HG23	1:C:231:ALA:HB3	1.95	0.48
1:C:145:GLU:HG2	1:C:237:LYS:HA	1.95	0.48
1:C:203:ARG:NH1	1:C:294:SER:OG	2.47	0.48
1:B:177:MET:HG3	1:B:302:ARG:HB2	1.96	0.48
1:C:215:GLU:HA	1:C:220:GLN:HG2	1.94	0.48
2:B:401:DEF:H222	2:B:401:DEF:H171	1.96	0.48
1:A:79:GLU:HG3	1:A:101:THR:HA	1.95	0.48
1:D:266:GLU:HG3	1:D:267:LYS:N	2.29	0.48
1:B:241:ILE:HD13	2:B:401:DEF:H262	1.95	0.47
1:B:87:VAL:HG12	1:B:90:PRO:HD2	1.95	0.47
1:D:198:ALA:HB1	1:D:231:ALA:HB2	1.96	0.47
1:B:83:TYR:OH	1:B:90:PRO:HG2	2.14	0.47
1:C:59:LEU:O	1:C:124:GLN:NE2	2.48	0.47
1:C:93:PRO:HG2	1:C:96:VAL:HG23	1.96	0.47
1:C:299:MET:HE3	1:C:302:ARG:HD2	1.97	0.47
1:A:154:ILE:HG22	1:A:158:LYS:HE3	1.97	0.47
1:A:162:THR:HA	1:A:167:GLU:HG2	1.96	0.46
1:B:67:VAL:HG11	1:B:74:PRO:HG3	1.97	0.46
1:B:171:GLN:HE21	1:B:171:GLN:HB3	1.54	0.46
1:B:154:ILE:HG22	1:B:158:LYS:HE3	1.97	0.46
1:C:274:LEU:HD22	1:D:233:PRO:HG3	1.98	0.46
1:D:59:LEU:O	1:D:124:GLN:NE2	2.49	0.46
1:A:200:VAL:HG23	1:A:231:ALA:HB3	1.97	0.46
1:B:161:ALA:HB1	1:B:167:GLU:HA	1.97	0.46
1:C:75:VAL:HG23	1:C:113:LEU:HD12	1.97	0.46
1:D:246:LEU:HD23	1:D:274:LEU:HD23	1.99	0.45
1:D:313:LEU:HD23	1:D:313:LEU:HA	1.85	0.45
1:A:238:GLU:HG2	1:A:239:TRP:CD1	2.52	0.45
1:C:80:LEU:HD22	1:C:92:VAL:HG21	1.97	0.45
1:B:193:GLY:C	1:B:195:THR:H	2.26	0.44
1:D:99:ILE:H	1:D:99:ILE:HG13	1.67	0.44
1:B:59:LEU:O	1:B:124:GLN:NE2	2.50	0.44
1:C:65:GLU:HG3	1:C:90:PRO:HG2	1.99	0.44
1:C:238:GLU:HG2	1:C:239:TRP:CD1	2.52	0.44
1:A:196:LEU:HB3	1:A:228:LEU:HD23	1.99	0.44
1:D:99:ILE:HA	1:D:109:LYS:HE2	1.98	0.44
1:A:212:LEU:HB2	1:A:242:VAL:HG23	2.00	0.44
1:B:215:GLU:HA	1:B:220:GLN:HG2	1.99	0.44
1:C:63:LEU:HD13	1:C:119:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:C	1:A:78:PRO:HG3	2.43	0.43
1:A:99:ILE:H	1:A:99:ILE:HG13	1.63	0.43
1:A:180:ARG:HE	1:A:184:LEU:HD21	1.83	0.43
1:C:254:GLN:N	1:C:254:GLN:NE2	2.60	0.43
1:D:87:VAL:O	1:D:89:GLN:N	2.41	0.43
1:A:67:VAL:HG22	1:A:72:ILE:HB	2.00	0.43
1:B:293:TRP:HH2	2:B:401:DEF:C21	2.32	0.43
1:D:75:VAL:HG23	1:D:113:LEU:HD13	2.00	0.43
1:B:102:ARG:C	1:B:104:GLU:H	2.26	0.43
1:C:207:PRO:HA	1:C:269:VAL:HG22	2.00	0.43
1:A:147:ASP:HB3	1:A:152:VAL:HG21	2.01	0.43
1:B:65:GLU:CD	1:B:297:GLY:H	2.26	0.43
1:B:295:TYR:OH	2:B:401:DEF:H252	2.17	0.43
1:C:59:LEU:C	1:C:78:PRO:HG3	2.44	0.43
1:C:102:ARG:NH2	2:C:401:DEF:O32	2.52	0.43
1:D:188:LEU:O	1:D:192:PHE:HB2	2.18	0.43
1:B:55:ARG:HD3	1:B:114:LYS:O	2.19	0.42
1:B:59:LEU:C	1:B:78:PRO:HG3	2.44	0.42
1:C:313:LEU:HD23	1:C:313:LEU:HA	1.84	0.42
1:B:314:ALA:O	1:B:315:VAL:HG22	2.20	0.42
1:A:249:LEU:HB3	1:A:280:PHE:HE2	1.84	0.42
1:D:86:TRP:CZ2	2:D:401:DEF:H172	2.55	0.42
1:D:274:LEU:HG	1:D:278:MET:HE2	2.01	0.42
1:C:193:GLY:C	1:C:195:THR:H	2.25	0.42
1:C:89:GLN:CB	1:C:90:PRO:CD	2.94	0.42
1:C:314:ALA:O	1:C:315:VAL:HG22	2.20	0.42
1:A:65:GLU:CD	1:A:300:SER:HG	2.28	0.42
1:C:237:LYS:HG3	1:C:242:VAL:HG22	2.02	0.42
1:D:215:GLU:HA	1:D:220:GLN:HG2	2.02	0.42
1:A:59:LEU:O	1:A:124:GLN:NE2	2.52	0.41
1:B:278:MET:HA	1:B:279:PRO:HD3	1.92	0.41
1:B:302:ARG:O	1:B:306:GLU:HG2	2.20	0.41
1:A:80:LEU:HD22	1:A:92:VAL:HG21	2.02	0.41
1:D:212:LEU:HD12	1:D:244:LYS:HG3	2.01	0.41
2:A:401:DEF:O13	2:A:401:DEF:H162	2.19	0.41
1:A:314:ALA:O	1:A:315:VAL:HG22	2.21	0.41
1:C:89:GLN:HB2	1:C:90:PRO:CD	2.40	0.41
1:C:92:VAL:O	1:C:92:VAL:HG13	2.19	0.41
1:C:139:TYR:CZ	1:C:141:PRO:HB3	2.55	0.41
1:C:196:LEU:HB3	1:C:228:LEU:HD23	2.03	0.41
1:C:241:ILE:HD13	2:C:401:DEF:H271	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LYS:HG3	1:D:226:LEU:O	2.21	0.41
1:A:73:GLN:HA	1:A:74:PRO:HD2	1.95	0.41
1:A:200:VAL:HB	1:A:257:VAL:HG22	2.03	0.41
1:B:211:PHE:CD2	2:B:401:DEF:H251	2.55	0.41
1:B:242:VAL:HG11	1:B:244:LYS:HE2	2.03	0.41
1:B:306:GLU:HG2	1:B:306:GLU:H	1.66	0.41
1:C:67:VAL:HG13	1:C:72:ILE:HB	2.01	0.41
1:D:256:TYR:CD1	1:D:285:ARG:HB3	2.56	0.41
1:A:65:GLU:OE1	1:A:300:SER:OG	2.36	0.40
1:A:246:LEU:HD23	1:A:274:LEU:HD23	2.04	0.40
1:B:69:GLU:O	1:B:173:LYS:NZ	2.46	0.40
1:C:143:PHE:HB3	1:C:239:TRP:HA	2.03	0.40
1:C:147:ASP:HB3	1:C:152:VAL:HG21	2.03	0.40
1:D:203:ARG:HG2	1:D:260:PHE:HB2	2.03	0.40
1:B:313:LEU:HD23	1:B:313:LEU:HA	1.86	0.40
1:A:92:VAL:HA	1:A:93:PRO:HD3	1.95	0.40
1:B:143:PHE:HB3	1:B:239:TRP:HA	2.03	0.40
1:B:202:LEU:O	1:B:259:TYR:HA	2.21	0.40
1:B:297:GLY:O	1:B:300:SER:HB3	2.22	0.40
1:B:206:ASN:ND2	1:B:208:THR:H	2.19	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	263/282 (93%)	244 (93%)	14 (5%)	5 (2%)	6	26
1	B	264/282 (94%)	245 (93%)	15 (6%)	4 (2%)	8	30
1	C	264/282 (94%)	245 (93%)	15 (6%)	4 (2%)	8	30
1	D	265/282 (94%)	246 (93%)	15 (6%)	4 (2%)	8	30
All	All	1056/1128 (94%)	980 (93%)	59 (6%)	17 (2%)	7	29

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	ALA
1	B	149	ALA
1	B	191	ALA
1	C	149	ALA
1	C	191	ALA
1	C	194	ASP
1	D	149	ALA
1	D	231	ALA
1	A	193	GLY
1	A	102	ARG
1	D	142	ASN
1	B	194	ASP
1	D	315	VAL
1	A	315	VAL
1	C	315	VAL
1	A	88	VAL
1	B	315	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	224/239 (94%)	210 (94%)	14 (6%)	16	42
1	B	224/239 (94%)	213 (95%)	11 (5%)	22	49
1	C	224/239 (94%)	213 (95%)	11 (5%)	22	49
1	D	223/239 (93%)	212 (95%)	11 (5%)	22	49
All	All	895/956 (94%)	848 (95%)	47 (5%)	20	47

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	VAL
1	A	88	VAL
1	A	89	GLN

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Mol	Chain	Res	Type
1	A	92	VAL
1	A	103	THR
1	A	146	GLN
1	A	152	VAL
1	A	195	THR
1	A	210	VAL
1	A	237	LYS
1	A	241	ILE
1	A	245	ARG
1	A	253	GLU
1	A	315	VAL
1	B	53	HIS
1	B	67	VAL
1	B	109	LYS
1	B	117	VAL
1	B	146	GLN
1	B	171	GLN
1	B	195	THR
1	B	210	VAL
1	B	271	LYS
1	B	306	GLU
1	B	315	VAL
1	C	67	VAL
1	C	113	LEU
1	C	117	VAL
1	C	145	GLU
1	C	146	GLN
1	C	184	LEU
1	C	210	VAL
1	C	254	GLN
1	C	292	VAL
1	C	299	MET
1	C	315	VAL
1	D	67	VAL
1	D	92	VAL
1	D	96	VAL
1	D	101	THR
1	D	146	GLN
1	D	152	VAL
1	D	229	SER
1	D	253	GLU
1	D	268	LYS

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Mol	Chain	Res	Type
1	D	299	MET
1	D	315	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	220	GLN
1	A	234	GLN
1	B	73	GLN
1	B	106	ASN
1	B	171	GLN
1	C	73	GLN
1	C	206	ASN
1	C	254	GLN
1	C	287	ASN
1	D	171	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](#)

4 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	DEF	A	401	-	39,39,50	5.66	15 (38%)	39,61,75	4.04	14 (35%)
2	DEF	D	401	-	39,39,50	5.73	15 (38%)	39,61,75	4.10	13 (33%)
2	DEF	C	401	-	39,39,50	5.66	15 (38%)	39,61,75	3.96	12 (30%)
2	DEF	B	401	-	39,39,50	5.68	14 (35%)	39,61,75	4.33	16 (41%)

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	DEF	A	401	-	2/2/9/13	10/28/82/95	0/3/5/5
2	DEF	D	401	-	1/1/9/13	10/28/82/95	0/3/5/5
2	DEF	C	401	-	2/2/9/13	10/28/82/95	0/3/5/5
2	DEF	B	401	-	2/2/9/13	6/28/82/95	0/3/5/5

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	DEF	C31-N31	15.72	1.79	1.31
2	C	401	DEF	C31-N31	15.61	1.78	1.31
2	D	401	DEF	C31-N31	15.58	1.78	1.31
2	A	401	DEF	C31-N31	15.53	1.78	1.31
2	D	401	DEF	O12-C11	14.60	1.52	1.28
2	B	401	DEF	O12-C11	14.57	1.52	1.28
2	C	401	DEF	O12-C11	14.16	1.51	1.28
2	A	401	DEF	O12-C11	14.08	1.51	1.28
2	D	401	DEF	C11-N11	13.39	1.50	1.31
2	B	401	DEF	C11-N11	13.01	1.50	1.31
2	A	401	DEF	C11-N11	12.87	1.50	1.31
2	C	401	DEF	C11-N11	12.68	1.49	1.31
2	C	401	DEF	O31-N31	12.62	1.59	1.38
2	A	401	DEF	O31-N31	12.56	1.59	1.38
2	D	401	DEF	O31-N31	12.39	1.59	1.38
2	B	401	DEF	O31-N31	12.28	1.59	1.38
2	C	401	DEF	C21-N21	9.75	1.46	1.31
2	B	401	DEF	O32-C31	9.75	1.47	1.28
2	D	401	DEF	O32-C31	9.75	1.47	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	DEF	C21-N21	9.69	1.46	1.31
2	A	401	DEF	O32-C31	9.61	1.47	1.28
2	C	401	DEF	O32-C31	9.57	1.47	1.28
2	D	401	DEF	C21-N21	9.56	1.46	1.31
2	B	401	DEF	C21-N21	9.37	1.46	1.31
2	B	401	DEF	O32-FE	-9.26	1.78	2.04
2	D	401	DEF	O32-FE	-9.15	1.78	2.04
2	A	401	DEF	O32-FE	-9.10	1.78	2.04
2	C	401	DEF	O32-FE	-9.05	1.78	2.04
2	C	401	DEF	O22-C21	8.47	1.42	1.28
2	A	401	DEF	O22-C21	8.43	1.41	1.28
2	D	401	DEF	O22-C21	8.38	1.41	1.28
2	B	401	DEF	O22-C21	8.18	1.41	1.28
2	D	401	DEF	C14-N12	5.53	1.46	1.33
2	A	401	DEF	C14-N12	5.31	1.45	1.33
2	C	401	DEF	C14-N12	5.08	1.44	1.33
2	B	401	DEF	C22-C21	-5.06	1.36	1.51
2	A	401	DEF	C22-C21	-5.03	1.36	1.51
2	D	401	DEF	O31-FE	-4.94	1.88	1.99
2	C	401	DEF	C22-C21	-4.92	1.37	1.51
2	B	401	DEF	O31-FE	-4.89	1.88	1.99
2	B	401	DEF	C12-C11	-4.86	1.37	1.51
2	D	401	DEF	C24-N22	4.82	1.44	1.33
2	D	401	DEF	C22-C21	-4.82	1.37	1.51
2	C	401	DEF	C24-N22	4.82	1.44	1.33
2	D	401	DEF	C12-C11	-4.79	1.37	1.51
2	B	401	DEF	C14-N12	4.76	1.44	1.33
2	C	401	DEF	C12-C11	-4.75	1.37	1.51
2	A	401	DEF	C24-N22	4.72	1.44	1.33
2	A	401	DEF	C12-C11	-4.64	1.38	1.51
2	A	401	DEF	O31-FE	-4.60	1.89	1.99
2	C	401	DEF	O31-FE	-4.58	1.89	1.99
2	B	401	DEF	C24-N22	4.46	1.43	1.33
2	A	401	DEF	C32-C31	-2.70	1.36	1.53
2	B	401	DEF	C32-C31	-2.69	1.36	1.53
2	C	401	DEF	C32-C31	-2.68	1.36	1.53
2	D	401	DEF	C32-C31	-2.68	1.36	1.53
2	C	401	DEF	O22-FE	2.13	2.10	2.04
2	D	401	DEF	O22-FE	2.04	2.10	2.04
2	A	401	DEF	O22-FE	2.02	2.10	2.04

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	DEF	O12-C11-N11	-14.51	107.31	118.38
2	C	401	DEF	O12-C11-N11	-14.32	107.45	118.38
2	D	401	DEF	C13-C12-C11	10.42	122.35	112.27
2	D	401	DEF	O12-C11-N11	-10.09	110.68	118.38
2	B	401	DEF	C23-C22-C21	9.56	121.52	112.27
2	B	401	DEF	O12-C11-N11	-9.54	111.10	118.38
2	C	401	DEF	C13-C12-C11	9.11	121.08	112.27
2	A	401	DEF	C13-C12-C11	9.08	121.05	112.27
2	D	401	DEF	O31-N31-C29	8.91	129.03	114.13
2	D	401	DEF	C23-C22-C21	8.85	120.83	112.27
2	B	401	DEF	C13-C12-C11	8.75	120.73	112.27
2	B	401	DEF	O11-N11-C11	8.53	121.99	116.42
2	D	401	DEF	O11-N11-C11	8.49	121.97	116.42
2	C	401	DEF	C23-C22-C21	8.49	120.49	112.27
2	A	401	DEF	O31-N31-C29	8.40	128.18	114.13
2	D	401	DEF	C19-N21-C21	-8.24	119.14	128.89
2	B	401	DEF	C19-N21-C21	-8.11	119.30	128.89
2	B	401	DEF	O31-N31-C29	8.08	127.63	114.13
2	C	401	DEF	O31-N31-C29	8.05	127.58	114.13
2	D	401	DEF	O31-N31-C31	-7.93	103.92	116.68
2	A	401	DEF	C19-N21-C21	-7.89	119.55	128.89
2	B	401	DEF	O31-N31-C31	-7.69	104.29	116.68
2	C	401	DEF	C19-N21-C21	-7.30	120.26	128.89
2	B	401	DEF	O22-C21-N21	-7.02	113.02	118.38
2	A	401	DEF	C23-C22-C21	6.71	118.76	112.27
2	C	401	DEF	O31-N31-C31	-6.70	105.89	116.68
2	A	401	DEF	O31-N31-C31	-6.57	106.10	116.68
2	B	401	DEF	C22-C21-N21	-6.15	113.38	121.07
2	B	401	DEF	O21-N21-C21	-5.77	112.65	116.42
2	A	401	DEF	O11-N11-C11	5.45	119.98	116.42
2	B	401	DEF	O22-C21-C22	-4.18	115.72	120.13
2	B	401	DEF	O21-N21-C19	4.15	121.06	114.13
2	A	401	DEF	O12-C11-C12	4.13	124.47	120.13
2	C	401	DEF	O11-N11-C11	3.92	118.98	116.42
2	D	401	DEF	O21-N21-C19	3.90	120.65	114.13
2	C	401	DEF	O12-C11-C12	3.77	124.10	120.13
2	C	401	DEF	O21-N21-C19	3.57	120.09	114.13
2	A	401	DEF	O21-N21-C19	3.47	119.92	114.13
2	D	401	DEF	O13-C14-C13	-3.42	115.77	122.02
2	D	401	DEF	C15-N12-C14	3.39	129.13	122.84
2	D	401	DEF	O21-N21-C21	-3.20	114.33	116.42
2	B	401	DEF	O12-C11-C12	3.11	123.41	120.13
2	A	401	DEF	C12-C11-N11	2.98	125.87	121.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	DEF	C39-N11-C11	-2.98	119.35	128.55
2	C	401	DEF	C39-N11-C11	-2.91	119.56	128.55
2	C	401	DEF	C12-C11-N11	2.89	125.72	121.34
2	A	401	DEF	O21-N21-C21	-2.86	114.55	116.42
2	A	401	DEF	C13-C14-N12	2.80	121.14	116.42
2	A	401	DEF	O13-C14-C13	-2.71	117.06	122.02
2	B	401	DEF	C39-N11-C11	-2.70	120.23	128.55
2	B	401	DEF	C25-N22-C24	-2.65	117.91	122.84
2	D	401	DEF	C39-N11-C11	-2.30	121.44	128.55
2	D	401	DEF	C13-C14-N12	2.29	120.27	116.42
2	B	401	DEF	C23-C24-N22	2.17	120.08	116.42
2	C	401	DEF	C13-C14-N12	2.16	120.05	116.42

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	401	DEF	N31
2	A	401	DEF	N21
2	B	401	DEF	N31
2	B	401	DEF	N21
2	C	401	DEF	N31
2	C	401	DEF	N21
2	D	401	DEF	N31

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	DEF	O12-C11-C12-C13
2	A	401	DEF	N11-C11-C12-C13
2	A	401	DEF	C28-C29-N31-O31
2	A	401	DEF	C28-C29-N31-C31
2	B	401	DEF	O12-C11-C12-C13
2	B	401	DEF	C18-C19-N21-O21
2	B	401	DEF	C21-C22-C23-C24
2	C	401	DEF	O12-C11-C12-C13
2	C	401	DEF	N11-C11-C12-C13
2	C	401	DEF	C28-C29-N31-O31
2	C	401	DEF	C28-C29-N31-C31
2	D	401	DEF	O12-C11-C12-C13
2	D	401	DEF	C11-C12-C13-C14
2	D	401	DEF	C28-C29-N31-O31
2	D	401	DEF	C28-C29-N31-C31

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Mol	Chain	Res	Type	Atoms
2	D	401	DEF	C16-C15-N12-C14
2	A	401	DEF	C16-C15-N12-C14
2	D	401	DEF	N12-C15-C16-C17
2	C	401	DEF	C16-C15-N12-C14
2	B	401	DEF	N22-C25-C26-C27
2	C	401	DEF	C15-C16-C17-C18
2	D	401	DEF	C15-C16-C17-C18
2	C	401	DEF	C26-C27-C28-C29
2	D	401	DEF	C16-C17-C18-C19
2	A	401	DEF	C26-C27-C28-C29
2	B	401	DEF	C25-C26-C27-C28
2	D	401	DEF	C26-C27-C28-C29
2	A	401	DEF	C15-C16-C17-C18
2	B	401	DEF	C15-C16-C17-C18
2	C	401	DEF	C21-C22-C23-C24
2	C	401	DEF	C12-C13-C14-O13
2	D	401	DEF	C17-C18-C19-N21
2	A	401	DEF	C12-C13-C14-O13
2	C	401	DEF	C12-C13-C14-N12
2	A	401	DEF	C21-C22-C23-C24
2	A	401	DEF	C12-C13-C14-N12

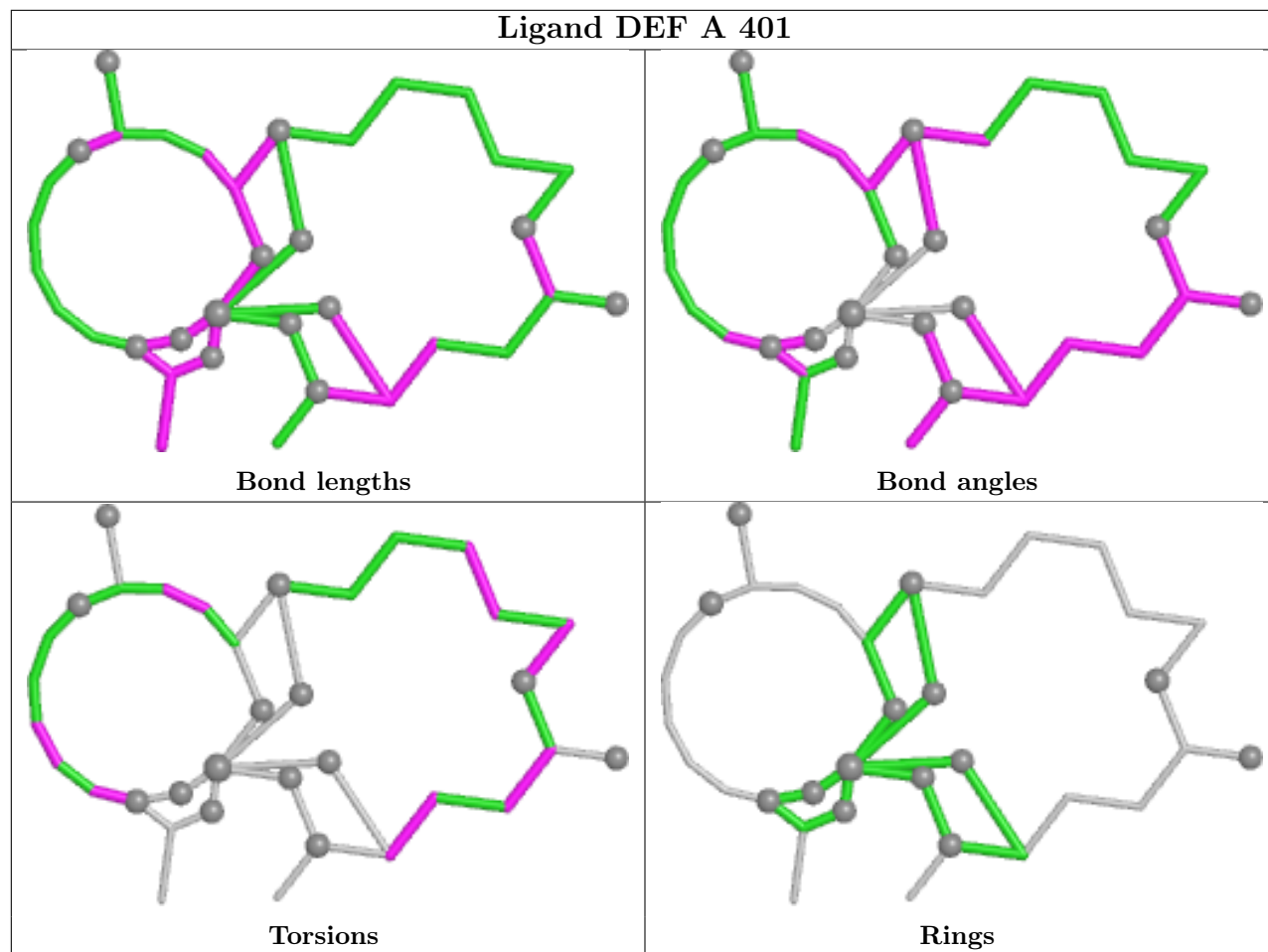
There are no ring outliers.

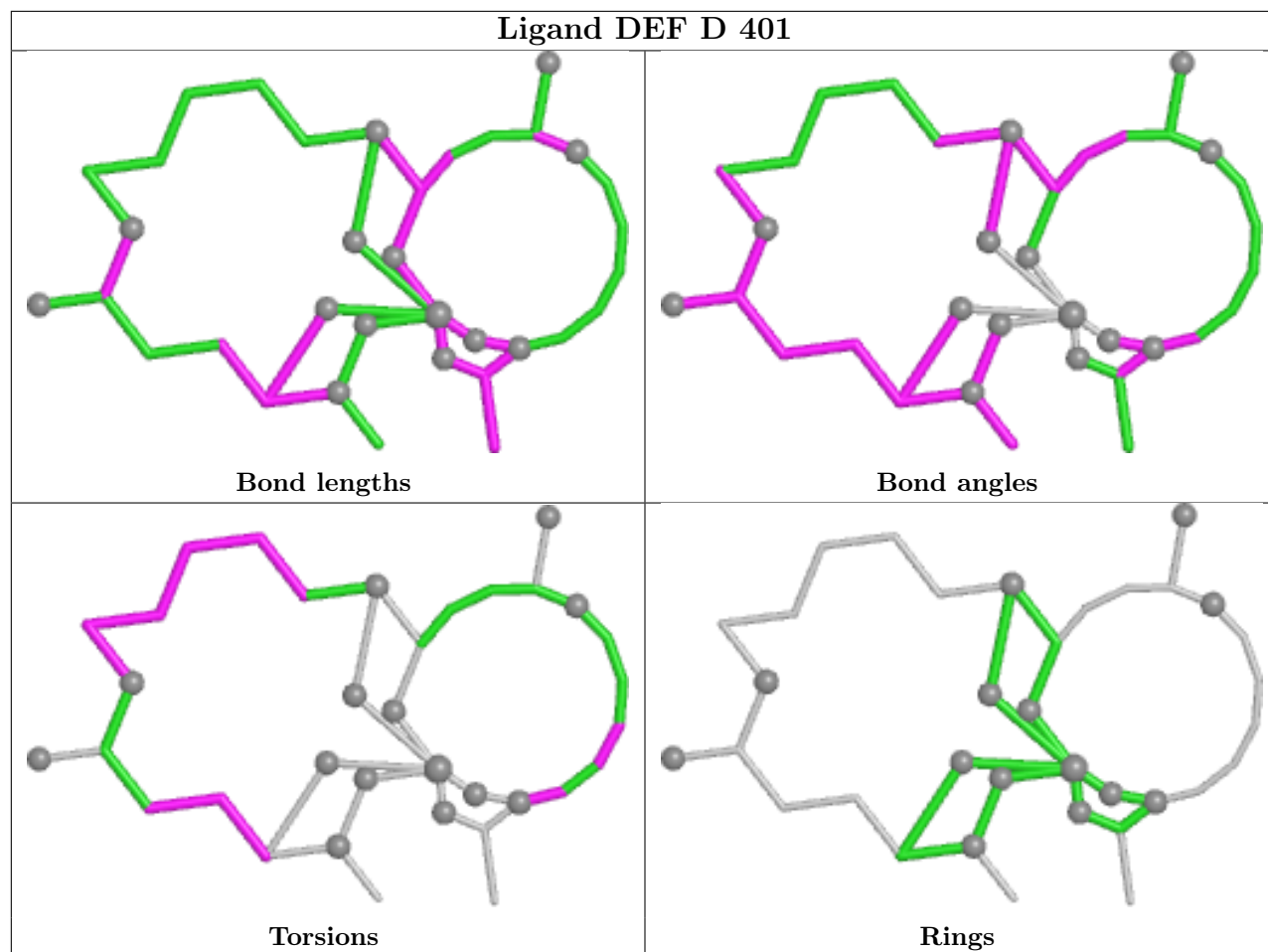
4 monomers are involved in 19 short contacts:

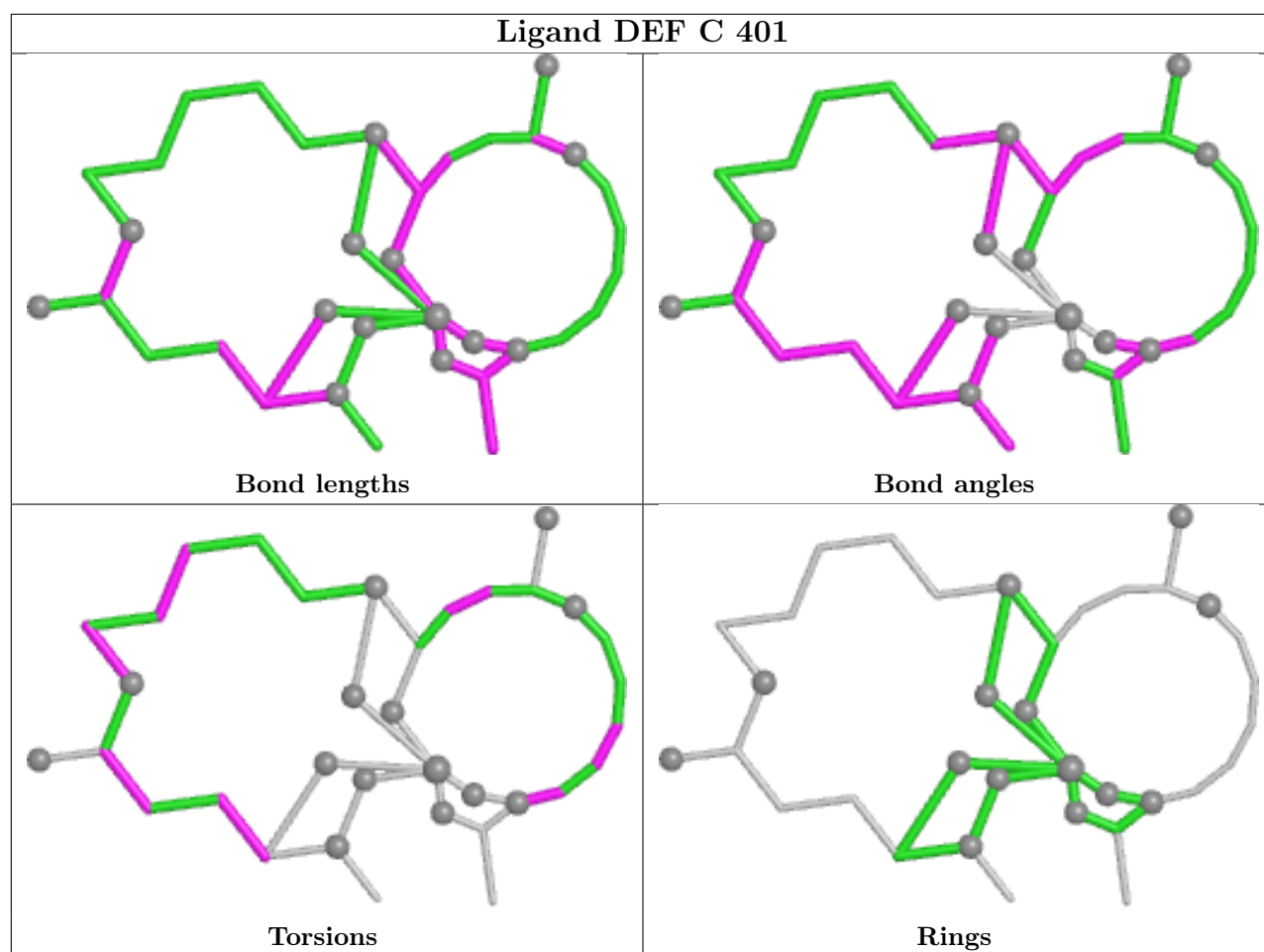
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	DEF	3	0
2	D	401	DEF	4	0
2	C	401	DEF	4	0
2	B	401	DEF	8	0

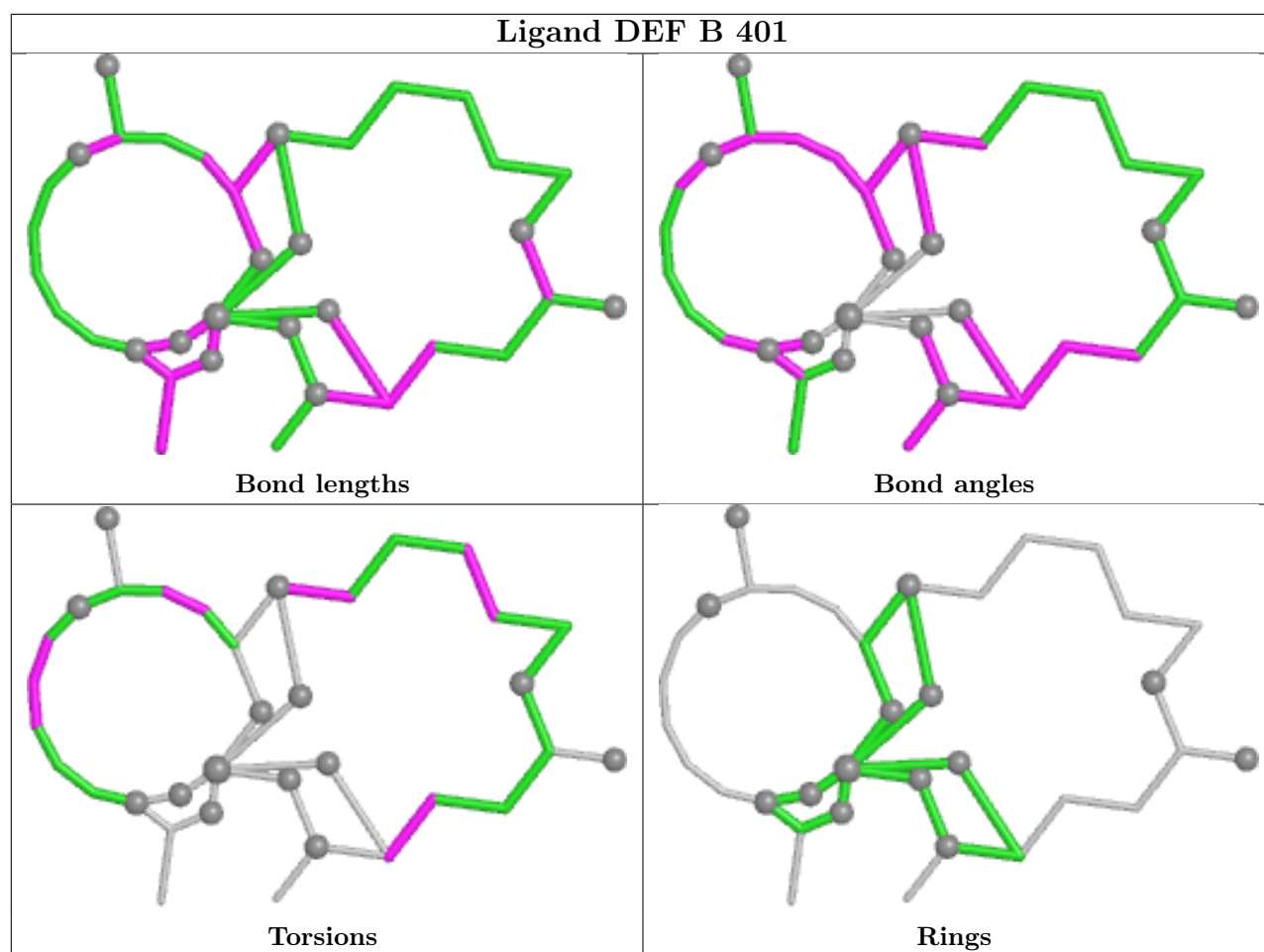
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	265/282 (93%)	0.28	11 (4%) 40 29	44, 72, 104, 148	0
1	B	266/282 (94%)	0.44	22 (8%) 17 15	52, 79, 113, 168	0
1	C	266/282 (94%)	0.25	10 (3%) 44 31	42, 67, 96, 144	0
1	D	267/282 (94%)	0.31	15 (5%) 30 23	45, 69, 104, 151	0
All	All	1064/1128 (94%)	0.32	58 (5%) 30 23	42, 72, 107, 168	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	52	SER	7.9
1	C	52	SER	6.8
1	B	52	SER	5.5
1	C	254	GLN	5.0
1	A	273	VAL	4.3
1	B	254	GLN	4.2
1	D	251	HIS	4.0
1	B	251	HIS	3.8
1	B	89	GLN	3.6
1	A	89	GLN	3.4
1	D	142	ASN	3.2
1	B	144	SER	3.2
1	A	250	GLN	3.2
1	C	53	HIS	3.0
1	B	148	ASN	3.0
1	C	206	ASN	3.0
1	D	250	GLN	2.9
1	D	215	GLU	2.9
1	C	190	HIS	2.9
1	A	194	ASP	2.9
1	A	53	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	271	LYS	2.9
1	C	85	GLN	2.8
1	B	53	HIS	2.8
1	D	230	SER	2.8
1	B	103	THR	2.8
1	B	146	GLN	2.7
1	B	317	PRO	2.7
1	D	53	HIS	2.6
1	B	194	ASP	2.6
1	B	193	GLY	2.5
1	B	235	PRO	2.5
1	C	89	GLN	2.5
1	B	273	VAL	2.5
1	C	148	ASN	2.5
1	C	251	HIS	2.5
1	B	271	LYS	2.4
1	D	254	GLN	2.4
1	D	300	SER	2.4
1	B	151	GLN	2.4
1	B	255	GLY	2.3
1	D	89	GLN	2.3
1	A	133	ARG	2.3
1	B	276	ARG	2.3
1	B	253	GLU	2.2
1	A	193	GLY	2.2
1	C	255	GLY	2.2
1	D	297	GLY	2.2
1	A	162	THR	2.2
1	B	84	VAL	2.2
1	D	51	GLY	2.1
1	B	315	VAL	2.1
1	B	300	SER	2.1
1	A	267	LYS	2.1
1	D	148	ASN	2.1
1	A	251	HIS	2.1
1	D	229	SER	2.0
1	D	146	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

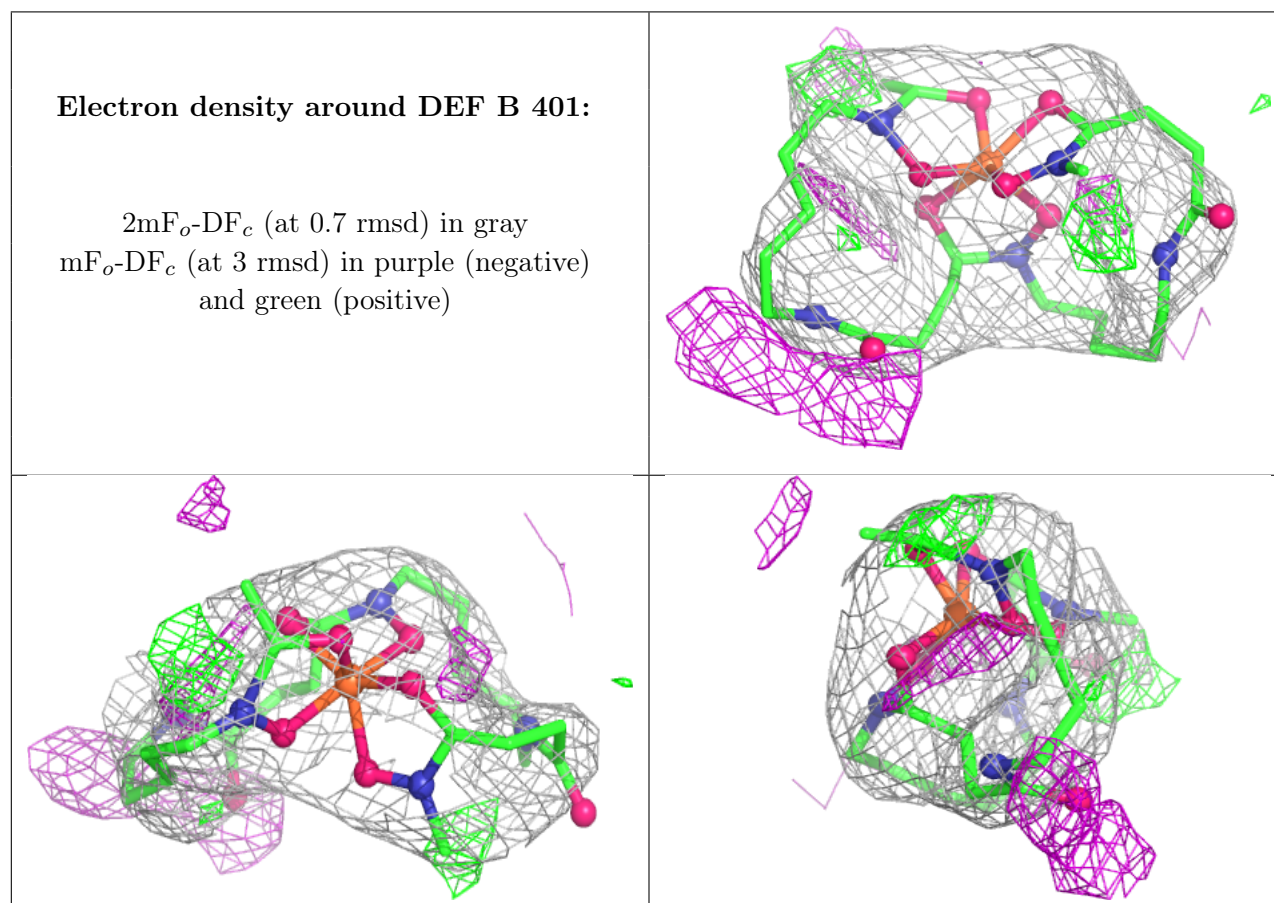
There are no oligosaccharides in this entry.

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.

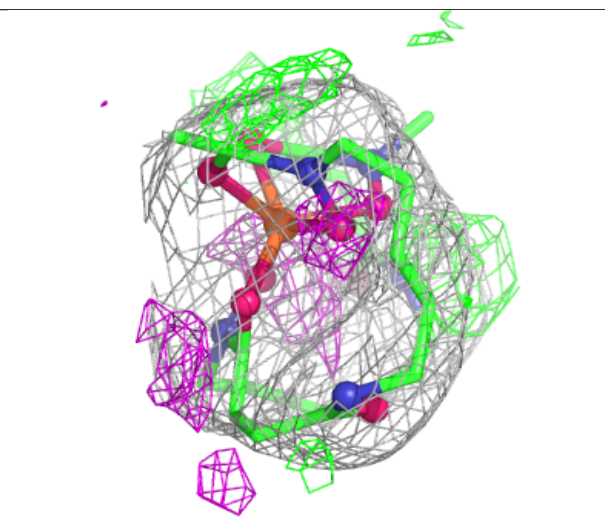
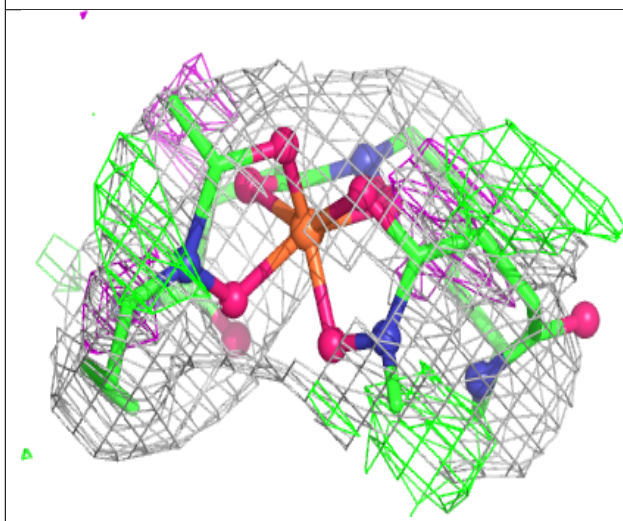
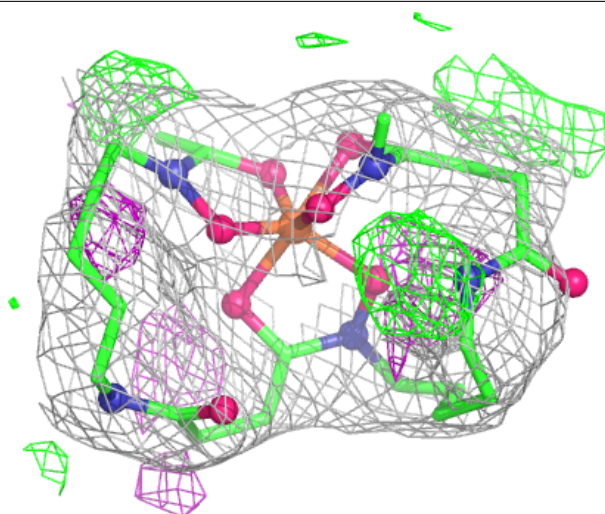
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DEF	B	401	35/46	0.92	0.17	59,95,116,129	0
2	DEF	A	401	35/46	0.94	0.15	29,80,102,107	0
2	DEF	C	401	35/46	0.94	0.17	29,85,104,110	0
2	DEF	D	401	35/46	0.94	0.14	49,96,112,122	0

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.



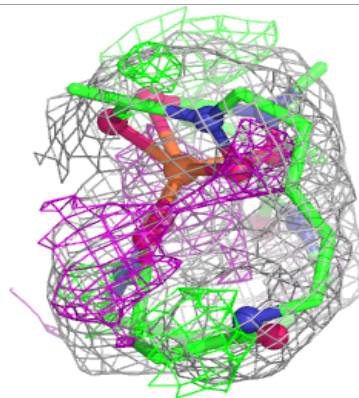
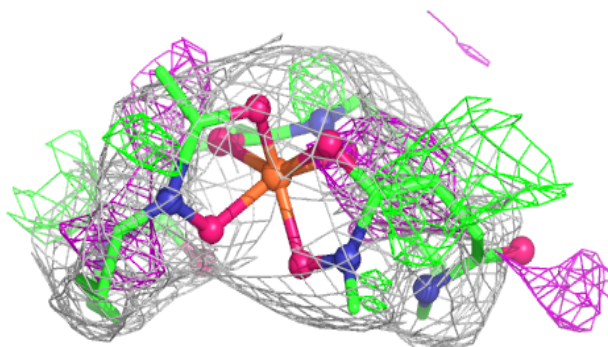
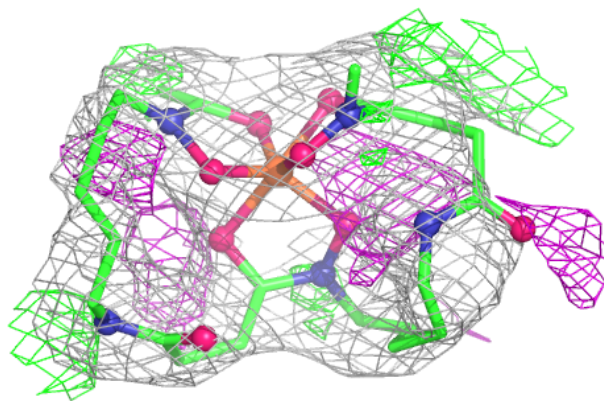
Electron density around DEF A 401:

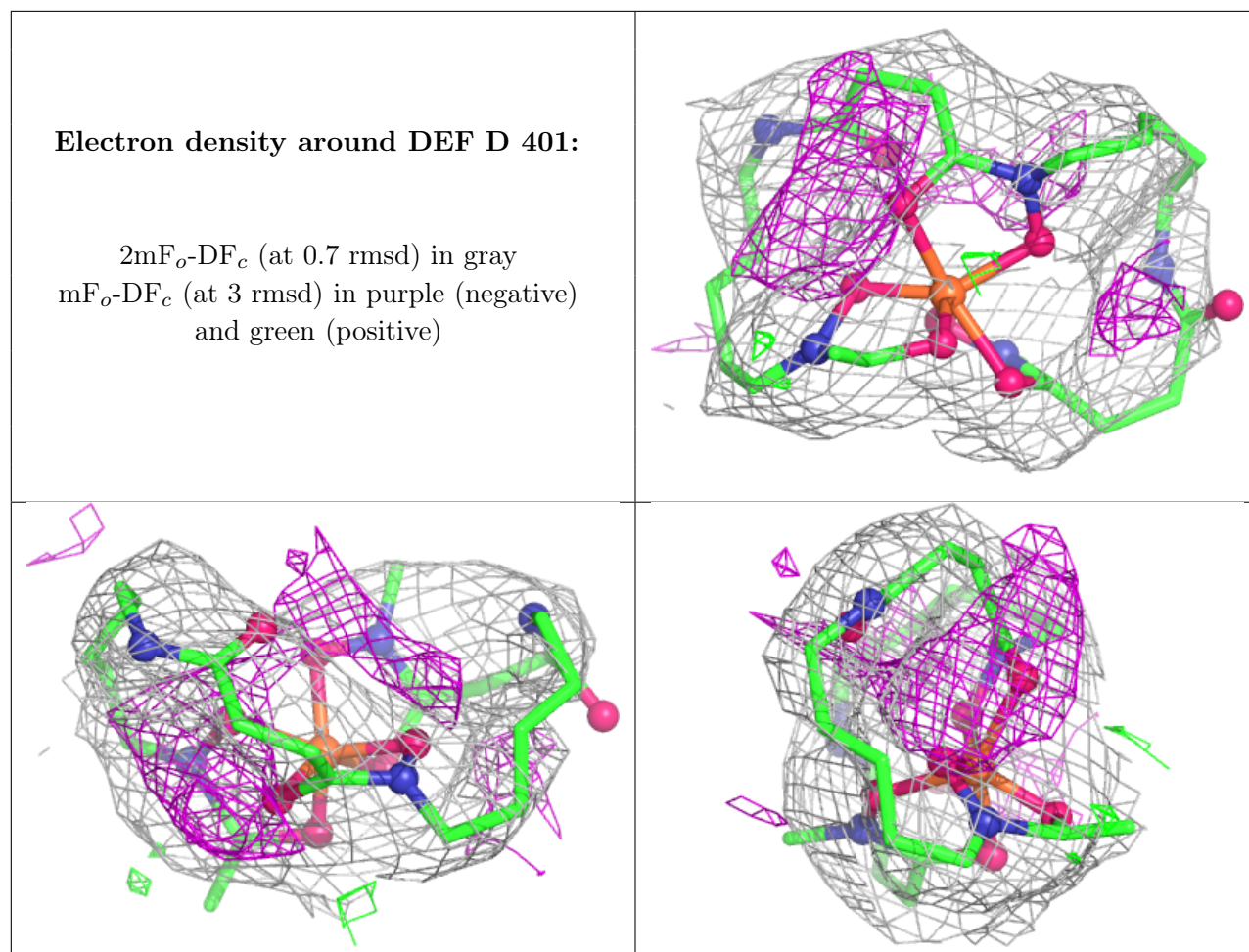
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DEF 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.