



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:56 AM GMT

PDB ID : 3GL2
Title : Crystal structure of dicamba monooxygenase bound to dicamba
Authors : Wilson, M.A.; Dumitru, R.; Jiang, W.Z.; Weeks, D.P.
Deposited on : 2009-03-11
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

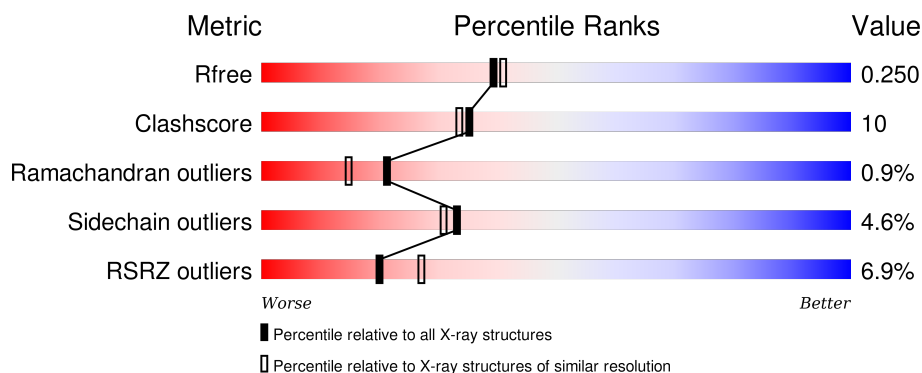
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	349	<div> <div>3%</div> <div>83% 13% ..</div> </div>
1	B	349	<div> <div>9%</div> <div>74% 17% . .</div> </div>
1	C	349	<div> <div>7%</div> <div>75% 13% • 10%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8156 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 DdmC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2633	1659	473	488	13			
1	B	334	Total	C	N	O	S	0	0	0
			2590	1634	463	480	13			
1	C	315	Total	C	N	O	S	0	1	0
			2440	1545	428	454	13			

There are 33 discrepancies between the modelled and reference sequences:

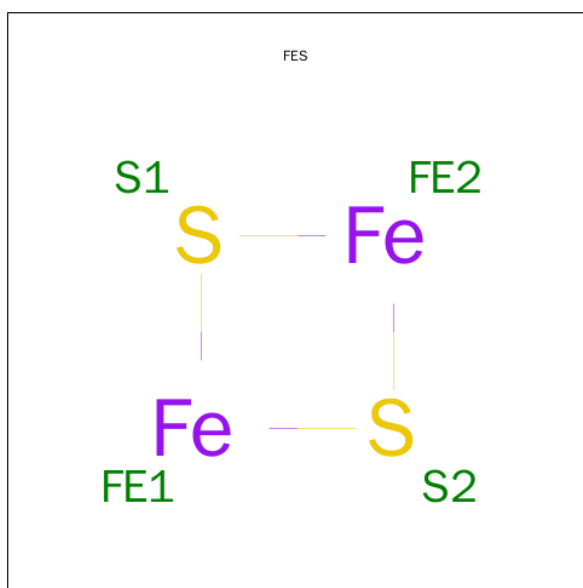
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INSERTION	UNP Q5S3I3
A	2	ALA	-	INSERTION	UNP Q5S3I3
A	341	ARG	-	INSERTION	UNP Q5S3I3
A	342	LEU	-	EXPRESSION TAG	UNP Q5S3I3
A	343	GLU	-	EXPRESSION TAG	UNP Q5S3I3
A	344	HIS	-	EXPRESSION TAG	UNP Q5S3I3
A	345	HIS	-	EXPRESSION TAG	UNP Q5S3I3
A	346	HIS	-	EXPRESSION TAG	UNP Q5S3I3
A	347	HIS	-	EXPRESSION TAG	UNP Q5S3I3
A	348	HIS	-	EXPRESSION TAG	UNP Q5S3I3
A	349	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	1	MET	-	INSERTION	UNP Q5S3I3
B	2	ALA	-	INSERTION	UNP Q5S3I3
B	341	ARG	-	INSERTION	UNP Q5S3I3
B	342	LEU	-	EXPRESSION TAG	UNP Q5S3I3
B	343	GLU	-	EXPRESSION TAG	UNP Q5S3I3
B	344	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	345	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	346	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	347	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	348	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	349	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	1	MET	-	INSERTION	UNP Q5S3I3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	-	INSERTION	UNP Q5S3I3
C	341	ARG	-	INSERTION	UNP Q5S3I3
C	342	LEU	-	EXPRESSION TAG	UNP Q5S3I3
C	343	GLU	-	EXPRESSION TAG	UNP Q5S3I3
C	344	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	345	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	346	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	347	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	348	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	349	HIS	-	EXPRESSION TAG	UNP Q5S3I3

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 4 2 2	0	0
2	B	1	Total Fe S 4 2 2	0	0
2	C	1	Total Fe S 4 2 2	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

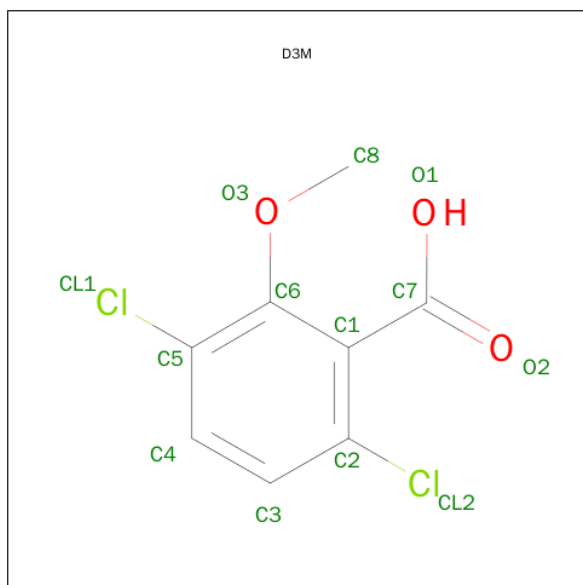
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Fe 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		

- Molecule 4 is 3,6-DICHLORO-2-METHOXYBENZOIC ACID (three-letter code: D3M) (formula: $C_8H_6Cl_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	O	0	0
			13	8	2	3		
4	B	1	Total	C	Cl	O	0	0
			13	8	2	3		

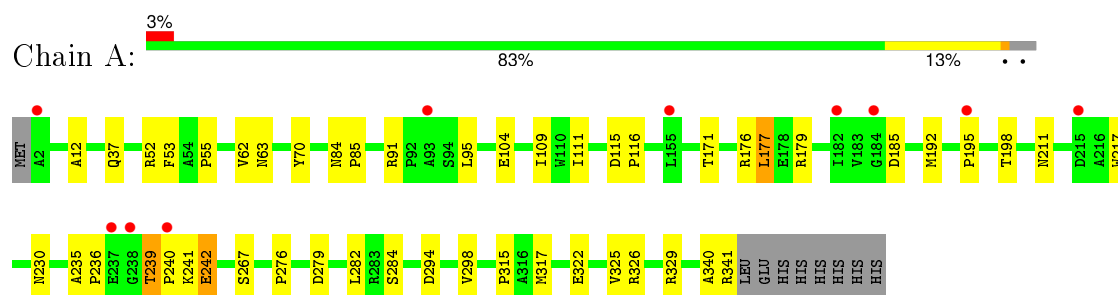
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	155	Total	O	0	0
			155	155		
5	B	142	Total	O	0	0
			142	142		
5	C	156	Total	O	0	0
			156	156		

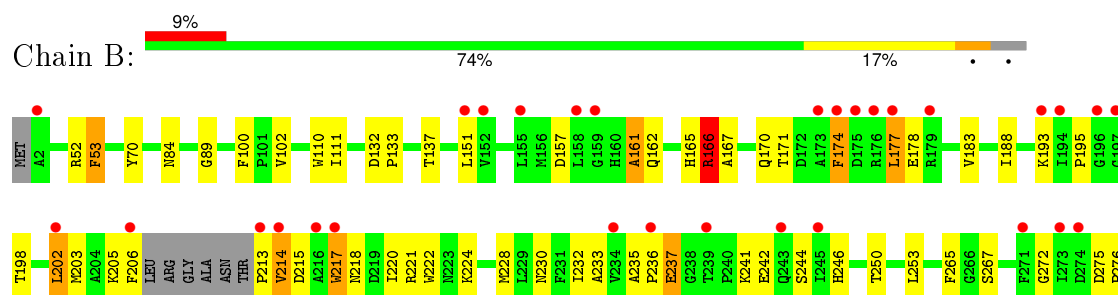
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

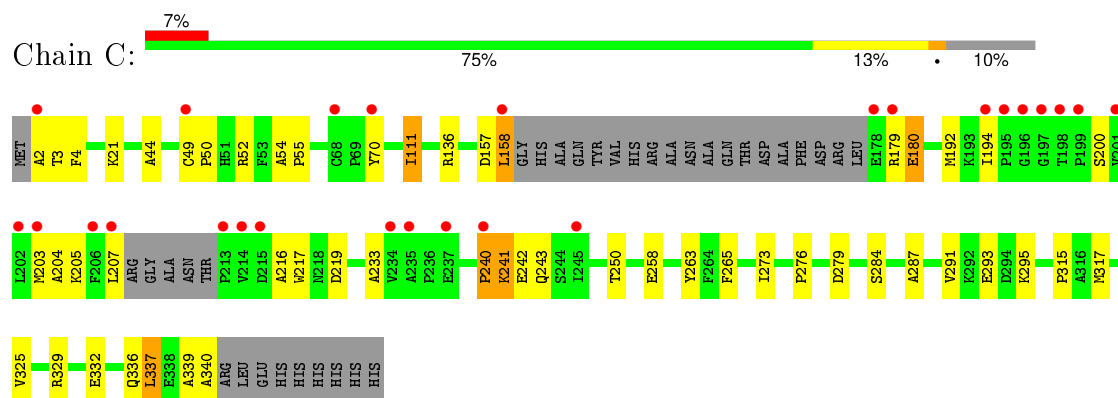
• Molecule 1: DdmC



• Molecule 1: DdmC



• Molecule 1: DdmC



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	81.32Å 81.32Å 159.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.00 – 2.10 36.21 – 2.11	Depositor EDS
% Data completeness (in resolution range)	98.4 (36.00-2.10) 98.4 (36.21-2.11)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.247 0.194 , 0.250	Depositor DCC
R_{free} test set	3338 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.7	EDS
Estimated twinning fraction	0.000 for -h,-k,l 0.034 for h,-h-k,-l 0.013 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 67158 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8156	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: D3M, FE, FES

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	0.46	0/2698	0.53	0/3674
1	B	0.47	0/2654	0.55	0/3612
1	C	0.45	0/2502	0.54	0/3405
All	All	0.46	0/7854	0.54	0/10691

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	A	0	1
1	B	0	2
1	C	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	340	ALA	Peptide
1	B	205	LYS	Peptide
1	B	213	PRO	Peptide
1	C	339	ALA	Peptide

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	2633	0	2566	35	0
1	B	2590	0	2521	76	0
1	C	2440	0	2386	40	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	13	0	5	0	0
4	B	13	0	5	0	0
5	A	155	0	0	3	0
5	B	142	0	0	4	0
5	C	156	0	0	7	0
All	All	8156	0	7483	148	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 (148) 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:236:PRO:O	1:A:239:THR:HG23	1.42	1.20
1:C:158:LEU:CD1	1:C:158:LEU:C	2.19	1.10
1:B:174:PHE:HA	1:B:177:LEU:CD2	1.85	1.07
1:B:174:PHE:HA	1:B:177:LEU:HD21	1.38	1.05
1:B:291:VAL:HG12	1:B:291:VAL:O	1.54	1.05
1:B:174:PHE:CA	1:B:177:LEU:HD21	1.90	1.00
1:C:340:ALA:HB2	5:C:461:HOH:O	1.65	0.95
1:C:136:ARG:HB2	1:C:273:ILE:HG23	1.49	0.95
1:C:158:LEU:HD12	1:C:158:LEU:C	1.86	0.95
1:C:158:LEU:HD13	1:C:158:LEU:C	1.92	0.90
1:B:102:VAL:HG13	1:B:111:ILE:CD1	2.03	0.88
1:B:102:VAL:HG13	1:B:111:ILE:HD11	1.56	0.85
1:B:291:VAL:CG1	1:B:291:VAL:O	2.29	0.81
1:A:12:ALA:CB	1:A:111:ILE:HD12	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ALA:HB1	1:C:4:PHE:CE2	2.17	0.79
1:A:236:PRO:O	1:A:239:THR:CG2	2.28	0.79
1:C:284:SER:HB3	1:C:287:ALA:HB3	1.66	0.78
1:B:110:TRP:C	1:B:111:ILE:HD13	2.04	0.78
1:C:295:LYS:NZ	5:C:395:HOH:O	2.18	0.77
1:B:337:LEU:O	1:B:340:ALA:HB3	1.86	0.76
1:B:110:TRP:O	1:B:111:ILE:HD13	1.87	0.75
1:C:325:VAL:O	1:C:329:ARG:HG2	1.86	0.74
1:B:206:PHE:O	5:B:355:HOH:O	2.07	0.73
1:C:2:ALA:HA	1:C:258:GLU:CG	2.21	0.70
1:B:174:PHE:HA	1:B:177:LEU:HD23	1.73	0.69
1:A:267:SER:CB	1:A:282:LEU:HD23	2.23	0.69
1:B:217:TRP:CD1	1:B:217:TRP:N	2.60	0.68
1:A:177:LEU:HD21	1:A:192:MET:HB3	1.75	0.68
1:B:157:ASP:O	5:B:482:HOH:O	2.11	0.67
1:B:162:GLN:HG3	1:B:174:PHE:CG	2.31	0.65
1:A:12:ALA:HB2	1:A:111:ILE:HD12	1.76	0.65
1:B:174:PHE:O	1:B:177:LEU:HG	1.97	0.64
1:B:174:PHE:C	1:B:177:LEU:HD21	2.18	0.64
1:B:174:PHE:O	1:B:177:LEU:HD21	1.99	0.63
1:B:166:ARG:O	1:B:170:GLN:HB2	1.99	0.62
1:B:162:GLN:HG3	1:B:174:PHE:CD1	2.35	0.61
1:B:340:ALA:O	1:B:341:ARG:C	2.39	0.61
1:C:217:TRP:HB2	1:C:233:ALA:HB3	1.81	0.60
1:A:55:PRO:HG3	1:B:300:ALA:HB1	1.82	0.60
1:B:183:VAL:HG13	1:B:188:ILE:HG12	1.83	0.60
1:C:340:ALA:CB	5:C:461:HOH:O	2.36	0.60
1:B:174:PHE:O	1:B:177:LEU:CD2	2.50	0.60
1:C:250:THR:O	1:C:265:PHE:HA	2.02	0.60
1:B:137:THR:HA	1:B:267:SER:O	2.02	0.59
1:A:276:PRO:O	1:A:279:ASP:HB2	2.03	0.59
1:A:267:SER:OG	1:A:282:LEU:CD2	2.51	0.58
1:B:174:PHE:CA	1:B:177:LEU:CD2	2.62	0.58
1:C:2:ALA:HA	1:C:258:GLU:HG2	1.85	0.58
1:B:174:PHE:O	1:B:177:LEU:CG	2.52	0.58
1:B:102:VAL:HG22	1:B:111:ILE:HD12	1.86	0.57
1:A:267:SER:OG	1:A:282:LEU:HD23	2.04	0.57
1:B:195:PRO:HA	1:B:215:ASP:OD1	2.04	0.57
1:B:236:PRO:O	1:B:237:GLU:C	2.42	0.56
1:C:315:PRO:HB2	1:C:317:MET:CE	2.35	0.56
1:B:174:PHE:CE1	1:B:177:LEU:HD11	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ASN:OD1	1:B:232:ILE:CD1	2.55	0.55
1:A:176:ARG:NH2	5:A:474:HOH:O	2.39	0.54
1:B:203:MET:O	1:B:206:PHE:C	2.47	0.53
1:C:340:ALA:HB1	5:C:399:HOH:O	2.07	0.53
1:B:218:ASN:OD1	1:B:232:ILE:HD12	2.08	0.53
1:B:272:GLY:O	1:B:275:ASP:HB3	2.08	0.52
1:B:217:TRP:CZ3	1:B:241:LYS:HB2	2.43	0.52
1:B:165:HIS:O	1:B:167:ALA:N	2.42	0.52
1:C:192:MET:HE2	1:C:194:ILE:HD11	1.90	0.52
1:B:161:ALA:HA	1:B:165:HIS:CD2	2.45	0.52
1:C:44:ALA:HB2	1:C:111:ILE:HD11	1.92	0.51
1:C:240:PRO:HG2	1:C:243:GLN:OE1	2.10	0.51
1:A:325:VAL:O	1:A:329:ARG:HG3	2.11	0.51
1:B:52:ARG:O	1:B:53:PHE:HB2	2.11	0.51
1:C:192:MET:CE	1:C:194:ILE:HD11	2.40	0.51
1:C:315:PRO:HB2	1:C:317:MET:HE1	1.93	0.50
1:A:294:ASP:O	1:A:298:VAL:HG22	2.12	0.50
1:B:174:PHE:C	1:B:177:LEU:CD2	2.81	0.49
1:B:174:PHE:CD1	1:B:177:LEU:HD11	2.47	0.49
1:A:84:ASN:C	1:A:84:ASN:OD1	2.50	0.49
1:C:340:ALA:CB	5:C:399:HOH:O	2.60	0.49
1:C:194:ILE:HB	1:C:216:ALA:HB3	1.95	0.49
1:C:157:ASP:O	1:C:158:LEU:HB3	2.12	0.48
1:A:176:ARG:NH1	1:A:195:PRO:O	2.46	0.48
1:B:132:ASP:OD1	1:B:133:PRO:HD2	2.13	0.48
1:B:292:LYS:O	1:B:296:VAL:HG23	2.14	0.48
1:A:84:ASN:ND2	1:B:318:LEU:HD22	2.29	0.47
1:A:315:PRO:HB2	1:A:317:MET:CE	2.44	0.47
1:B:336:GLN:HB3	5:B:474:HOH:O	2.13	0.47
1:C:291:VAL:HG13	1:C:293:GLU:H	1.80	0.47
1:A:177:LEU:HD22	1:A:179:ARG:HG3	1.96	0.47
1:A:91:ARG:HA	1:A:95:LEU:HD12	1.98	0.47
1:B:174:PHE:CB	1:B:177:LEU:HD21	2.44	0.46
1:B:193:LYS:NZ	1:B:195:PRO:HB3	2.30	0.46
1:A:217:TRP:CD1	1:A:241:LYS:HD2	2.50	0.46
1:B:217:TRP:HD1	1:B:233:ALA:O	1.99	0.46
1:C:332:GLU:O	1:C:336:GLN:HG3	2.16	0.46
1:B:233:ALA:HB2	1:B:246:HIS:HB3	1.99	0.45
1:B:165:HIS:CD2	5:B:366:HOH:O	2.69	0.45
1:C:203:MET:O	1:C:204:ALA:C	2.55	0.45
1:B:340:ALA:O	1:B:341:ARG:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLY:O	1:B:275:ASP:CB	2.64	0.45
1:B:202:LEU:HD13	1:B:203:MET:CE	2.47	0.44
1:B:202:LEU:HD13	1:B:203:MET:HE2	1.99	0.44
1:B:222:TRP:CZ2	1:B:224:LYS:HA	2.52	0.44
1:C:242:GLU:HG3	5:C:427:HOH:O	2.17	0.44
1:C:44:ALA:CB	1:C:111:ILE:CD1	2.96	0.44
1:A:37:GLN:NE2	5:A:467:HOH:O	2.50	0.44
1:A:104:GLU:HG3	1:A:109:ILE:HD13	2.00	0.44
1:B:250:THR:O	1:B:265:PHE:HA	2.18	0.44
1:A:52:ARG:O	1:A:53:PHE:HB2	2.18	0.44
1:C:44:ALA:CB	1:C:111:ILE:HD11	2.47	0.43
1:B:233:ALA:HB1	1:B:244:SER:OG	2.18	0.43
1:C:158:LEU:HD13	1:C:158:LEU:O	2.17	0.43
1:B:288:GLN:O	1:B:292:LYS:HB3	2.18	0.43
1:A:230:ASN:C	1:A:230:ASN:OD1	2.57	0.43
1:C:179:ARG:O	1:C:180:GLU:HB2	2.18	0.43
1:A:282:LEU:HD22	5:A:392:HOH:O	2.19	0.43
1:B:294:ASP:O	1:B:298:VAL:HG22	2.19	0.42
1:B:193:LYS:O	1:B:195:PRO:HD3	2.20	0.42
1:B:267:SER:CB	1:B:282:LEU:HD22	2.49	0.42
1:C:315:PRO:HB2	1:C:317:MET:HE3	1.99	0.42
1:B:52:ARG:HD2	5:C:483:HOH:O	2.18	0.42
1:B:165:HIS:O	1:B:166:ARG:C	2.57	0.42
1:B:100:PHE:O	1:B:102:VAL:HG23	2.19	0.42
1:A:211:ASN:OD1	1:A:211:ASN:N	2.50	0.42
1:A:322:GLU:O	1:A:326:ARG:HG3	2.19	0.42
1:A:84:ASN:HA	1:A:85:PRO:HD3	1.82	0.41
1:C:276:PRO:O	1:C:279:ASP:HB2	2.20	0.41
1:B:84:ASN:O	1:B:89:GLY:HA2	2.19	0.41
1:A:62:VAL:O	1:A:63:ASN:HB2	2.19	0.41
1:C:52:ARG:HG2	1:C:52:ARG:HH11	1.85	0.41
1:A:235:ALA:O	1:A:236:PRO:C	2.58	0.41
1:C:219:ASP:OD2	1:C:241:LYS:NZ	2.47	0.41
1:B:221:ARG:O	1:B:228:MET:HA	2.20	0.41
1:B:111:ILE:HD13	1:B:111:ILE:N	2.31	0.41
1:C:337:LEU:HD22	1:C:337:LEU:HA	1.90	0.41
1:A:84:ASN:HD21	1:B:318:LEU:HD22	1.84	0.41
1:B:206:PHE:CD1	1:B:206:PHE:C	2.94	0.41
1:A:115:ASP:HA	1:A:116:PRO:HD2	1.88	0.41
1:A:315:PRO:HB2	1:A:317:MET:HE3	2.03	0.41
1:A:240:PRO:HB3	1:A:242:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ALA:HA	1:C:258:GLU:HG3	2.02	0.40
1:C:49:CYS:HA	1:C:50:PRO:HD3	1.89	0.40
1:B:214:VAL:HG22	1:B:235:ALA:O	2.21	0.40
1:B:52:ARG:O	1:B:53:PHE:CB	2.69	0.40
1:B:151:LEU:HD13	1:B:253:LEU:HD21	2.03	0.40
1:B:174:PHE:CG	1:B:177:LEU:HD21	2.57	0.40
1:A:267:SER:HB3	1:A:282:LEU:HD23	2.00	0.40
1:B:220:ILE:HA	1:B:230:ASN:HA	2.04	0.40
1:B:183:VAL:HG13	1:B:188:ILE:CG1	2.51	0.40
1:B:230:ASN:OD1	1:B:230:ASN:C	2.60	0.40
1:C:54:ALA:HB1	1:C:55:PRO:HD2	2.03	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	338/349 (97%)	324 (96%)	14 (4%)	0	100	100
1	B	330/349 (95%)	303 (92%)	20 (6%)	7 (2%)	9	3
1	C	310/349 (89%)	292 (94%)	16 (5%)	2 (1%)	30	24
All	All	978/1047 (93%)	919 (94%)	50 (5%)	9 (1%)	21	15

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	166	ARG
1	B	340	ALA
1	B	237	GLU
1	B	292	LYS
1	C	180	GLU
1	B	53	PHE

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Mol	Chain	Res	Type
1	B	161	ALA
1	B	291	VAL
1	C	240	PRO

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	275/284 (97%)	266 (97%)	9 (3%)	45	47
1	B	271/284 (95%)	254 (94%)	17 (6%)	22	18
1	C	258/284 (91%)	247 (96%)	11 (4%)	35	34
All	All	804/852 (94%)	767 (95%)	37 (5%)	33	31

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	TYR
1	A	171	THR
1	A	177	LEU
1	A	185	ASP
1	A	198	THR
1	A	239	THR
1	A	242	GLU
1	A	284	SER
1	A	341	ARG
1	B	70	TYR
1	B	166	ARG
1	B	171	THR
1	B	174	PHE
1	B	177	LEU
1	B	178	GLU
1	B	198	THR
1	B	202	LEU
1	B	214	VAL
1	B	217	TRP

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Mol	Chain	Res	Type
1	B	242	GLU
1	B	276	PRO
1	B	282	LEU
1	B	295	LYS
1	B	320	CYS
1	B	337	LEU
1	B	341	ARG
1	C	3	THR
1	C	21	LYS
1	C	70	TYR
1	C	111	ILE
1	C	158	LEU
1	C	200	SER
1	C	205	LYS
1	C	207	LEU
1	C	241	LYS
1	C	263	TYR
1	C	337	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 2 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
2	FES	A	500	1	0,4,4	0.00	-	0,4,4	0.00	-
4	D3M	A	600	-	10,13,13	1.21	2 (20%)	11,18,18	1.04	0
2	FES	B	500	1	0,4,4	0.00	-	0,4,4	0.00	-
4	D3M	B	600	-	10,13,13	1.23	2 (20%)	11,18,18	1.34	2 (18%)
2	FES	C	500	1	0,4,4	0.00	-	0,4,4	0.00	-

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	FES	A	500	1	-	0/0/4/4	0/1/1/1
4	D3M	A	600	-	-	0/2/6/6	0/1/1/1
2	FES	B	500	1	-	0/0/4/4	0/1/1/1
4	D3M	B	600	-	-	0/2/6/6	0/1/1/1
2	FES	C	500	1	-	0/0/4/4	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	D3M	C2-CL2	2.00	1.78	1.73
4	B	600	D3M	C2-CL2	2.17	1.78	1.73
4	A	600	D3M	C5-CL1	2.22	1.79	1.73
4	B	600	D3M	C5-CL1	2.69	1.80	1.73

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	D3M	C6-C5-CL1	2.32	121.28	118.43
4	B	600	D3M	C8-O3-C6	3.08	122.92	114.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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	340/349 (97%)	-0.00	10 (2%) 55 63	41, 56, 86, 110	0
1	B	334/349 (95%)	0.34	32 (9%) 10 14	39, 57, 112, 138	0
1	C	315/349 (90%)	0.23	26 (8%) 14 19	39, 55, 116, 145	0
All	All	989/1047 (94%)	0.19	68 (6%) 20 27	39, 56, 107, 145	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	201	VAL	7.2
1	C	198	THR	6.5
1	B	214	VAL	6.1
1	B	194	ILE	5.5
1	C	207	LEU	5.3
1	B	216	ALA	4.8
1	C	195	PRO	4.7
1	C	213	PRO	4.5
1	C	196	GLY	4.4
1	B	177	LEU	4.3
1	C	197	GLY	4.2
1	C	202	LEU	4.1
1	B	213	PRO	4.1
1	B	174	PHE	3.9
1	B	339	ALA	3.7
1	B	234	VAL	3.6
1	C	206	PHE	3.6
1	B	206	PHE	3.5
1	B	2	ALA	3.4
1	C	237	GLU	3.2
1	B	243	GLN	3.2
1	C	179	ARG	3.1
1	B	176	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	155	LEU	3.0
1	B	273	ILE	3.0
1	B	175	ASP	3.0
1	B	217	TRP	3.0
1	B	193	LYS	2.9
1	B	173	ALA	2.9
1	A	195	PRO	2.9
1	B	197	GLY	2.9
1	A	2	ALA	2.9
1	C	178	GLU	2.8
1	B	274	ASP	2.7
1	A	240	PRO	2.7
1	B	152	VAL	2.6
1	B	158	LEU	2.6
1	A	215	ASP	2.6
1	A	93	ALA	2.6
1	B	196	GLY	2.6
1	B	245	ILE	2.6
1	C	203	MET	2.6
1	C	235	ALA	2.5
1	B	271	PHE	2.5
1	A	155	LEU	2.5
1	B	159	GLY	2.5
1	C	158	LEU	2.5
1	B	151	LEU	2.4
1	B	239	THR	2.4
1	C	49	CYS	2.4
1	B	202	LEU	2.4
1	B	291	VAL	2.4
1	B	236	PRO	2.4
1	C	234	VAL	2.3
1	B	179	ARG	2.3
1	C	68	CYS	2.3
1	C	214	VAL	2.3
1	C	245	ILE	2.3
1	C	240	PRO	2.3
1	C	70	TYR	2.3
1	A	184	GLY	2.2
1	A	238	GLY	2.2
1	C	199	PRO	2.2
1	A	182	ILE	2.2
1	C	2	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	215	ASP	2.1
1	A	237	GLU	2.1
1	C	194	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	FE	A	501	1/1	0.99	0.17	0.49	48,48,48,48	0
3	FE	B	501	1/1	0.99	0.16	0.29	64,64,64,64	0
2	FES	A	500	4/4	0.99	0.10	-0.27	46,47,49,53	0
4	D3M	A	600	13/13	0.97	0.09	-0.61	46,53,60,69	0
2	FES	B	500	4/4	1.00	0.08	-0.65	41,44,44,47	0
2	FES	C	500	4/4	0.99	0.16	-0.94	41,43,44,50	0
4	D3M	B	600	13/13	0.94	0.11	-1.11	57,72,76,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.