



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2017 – 07:05 PM EDT

PDB ID : 1ZXI  
Title : Reconstituted CO dehydrogenase from Oligotropha carboxidovorans  
Authors : Resch, M.; Dobbek, H.; Meyer, O.  
Deposited on : unknown  
Resolution : 1.70 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

<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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

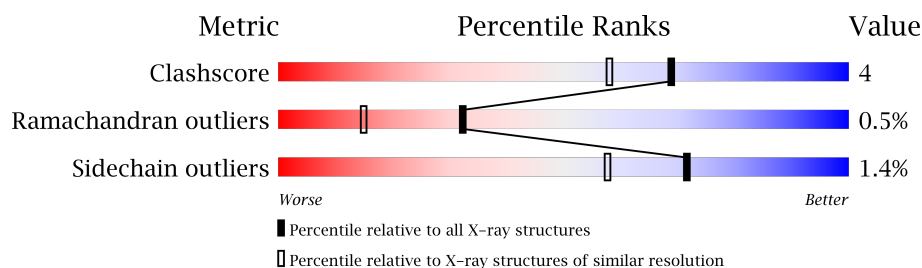
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	166	
1	D	166	
2	B	809	
2	E	809	
3	C	288	
3	F	288	

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 21735 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 Carbon monoxide dehydrogenase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	2	0	0
			1204	746	215	228	15			
1	D	158	Total	C	N	O	S	5	0	0
			1175	727	212	221	15			

- Molecule 2 is a protein called Carbon monoxide dehydrogenase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	804	Total	C	N	O	S	73	0	0
			6198	3934	1061	1162	41			
2	E	795	Total	C	N	O	S	61	0	0
			6130	3894	1049	1146	41			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	670	ILE	VAL	CONFLICT	UNP P19919
E	670	ILE	VAL	CONFLICT	UNP P19919

- Molecule 3 is a protein called Carbon monoxide dehydrogenase medium chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	287	Total	C	N	O	S	26	0	0
			2112	1333	372	396	11			
3	F	286	Total	C	N	O	S	26	0	0
			2103	1327	370	395	11			

There are 2 discrepancies between the modelled and reference sequences:

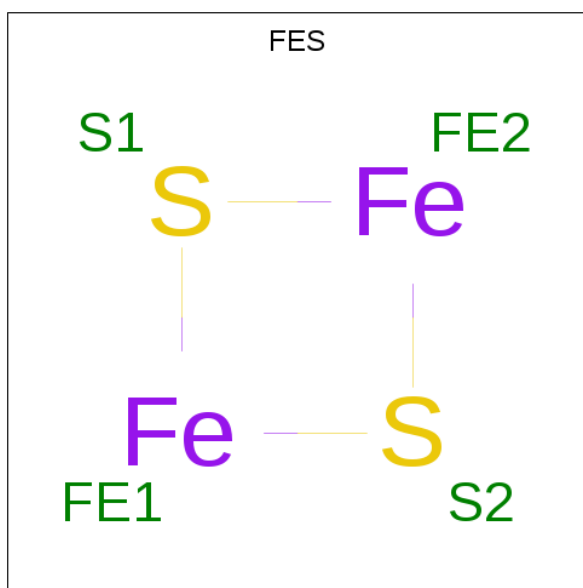
Chain	Residue	Modelled	Actual	Comment	Reference
C	211	SER	THR	CONFLICT	UNP P19920
F	211	SER	THR	CONFLICT	UNP P19920

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $\text{O}_4\text{P}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



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

*Continued on next page...*

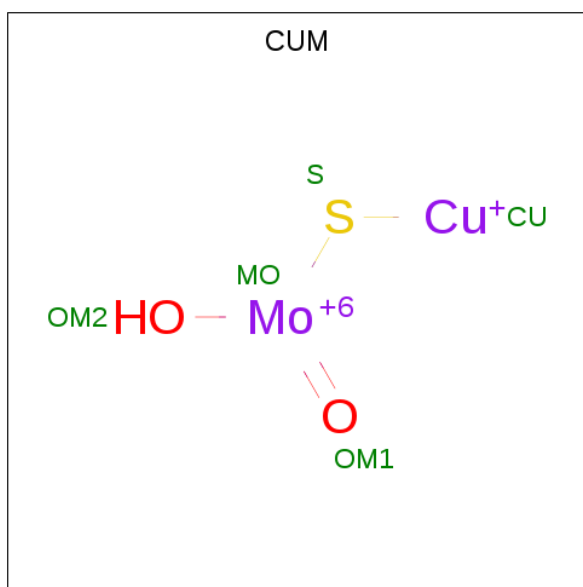
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	Fe	S	0	0
			4	2	2		
5	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

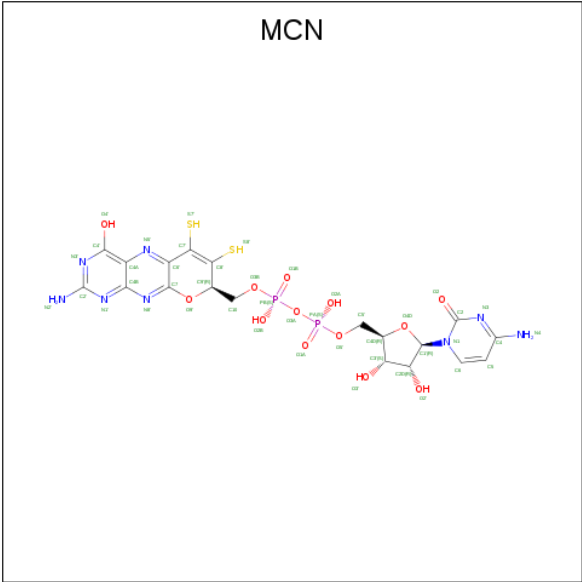
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cu	0	0
			1	1		
6	E	1	Total	Cu	0	1
			1	1		

- Molecule 7 is CU(I)-S-MO(VI)(=O)OH CLUSTER (three-letter code: CUM) (formula: CuHMoO<sub>2</sub>S).



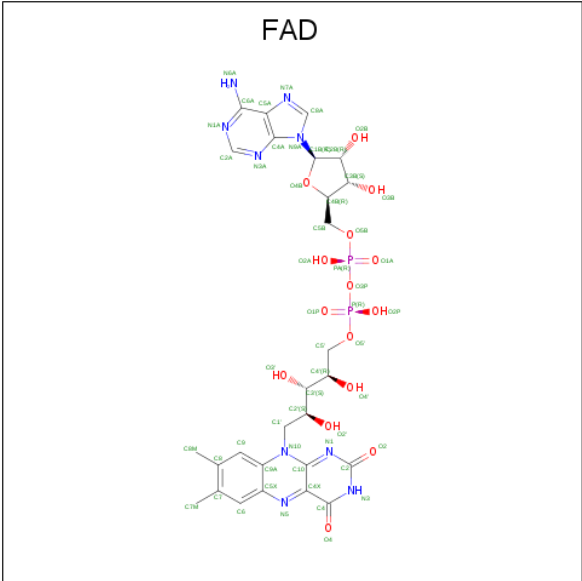
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	Cu	Mo	O	S	0	0
			5	1	1	2	1		
7	E	1	Total	Cu	Mo	O	S	0	1
			5	1	1	2	1		

- Molecule 8 is PTERIN CYTOSINE DINUCLEOTIDE (three-letter code: MCN) (formula: C<sub>19</sub>H<sub>22</sub>N<sub>8</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	S	0	0
			44	19	8	13	2	2		
8	E	1	Total	C	N	O	P	S	0	0
			44	19	8	13	2	2		

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 10 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	190	Total	O	0	0
			190	190		
10	B	804	Total	O	0	0
			804	804		
10	C	342	Total	O	0	0
			342	342		
10	D	189	Total	O	0	0
			189	189		
10	E	749	Total	O	0	0
			749	749		
10	F	312	Total	O	0	0
			312	312		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.


Note EDS was not executed.

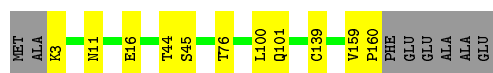
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain A: 




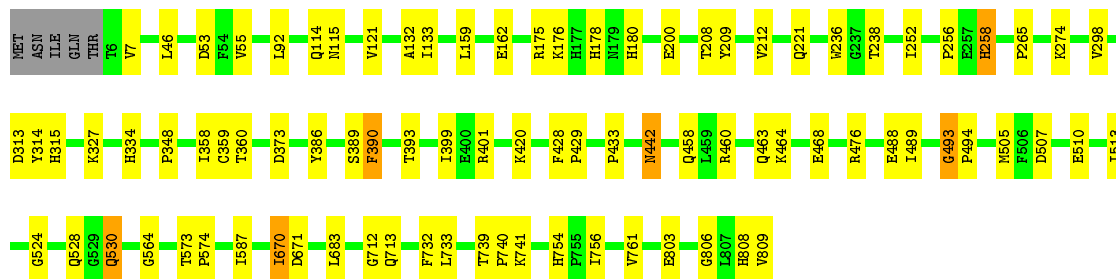
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain D: 




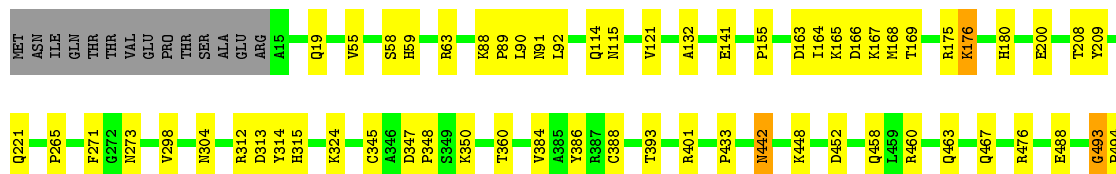
- Molecule 2: Carbon monoxide dehydrogenase large chain

Chain B: 



- Molecule 2: Carbon monoxide dehydrogenase large chain

Chain E: 







● Molecule 3: Carbon monoxide dehydrogenase medium chain



● Molecule 3: Carbon monoxide dehydrogenase medium chain



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.84Å 131.32Å 159.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.166 , 0.194	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21735	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MCN, PO4, FES, FAD, CUM, CU

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	0.53	0/1225	0.71	0/1656
1	D	0.53	0/1195	0.74	0/1616
2	B	0.51	0/6351	0.74	2/8617 (0.0%)
2	E	0.51	0/6282	0.73	2/8522 (0.0%)
3	C	0.43	0/2149	0.70	0/2918
3	F	0.45	0/2140	0.71	0/2907
All	All	0.50	0/19342	0.73	4/26236 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	55	VAL	N-CA-C	-6.30	94.00	111.00
2	B	55	VAL	N-CA-C	-6.02	94.75	111.00
2	E	348	PRO	N-CA-C	-5.27	98.39	112.10
2	B	348	PRO	N-CA-C	-5.16	98.69	112.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1204	0	1178	10	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1175	0	1157	5	0
2	B	6198	0	6072	61	0
2	E	6130	0	6007	60	0
3	C	2112	0	2170	11	0
3	F	2103	0	2157	15	0
4	A	5	0	0	0	0
5	A	8	0	0	0	0
5	D	8	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
7	B	5	0	0	1	0
7	E	5	0	0	0	0
8	B	44	0	17	0	0
8	E	44	0	17	1	0
9	C	53	0	31	1	0
9	F	53	0	31	0	0
10	A	190	0	0	2	0
10	B	804	0	0	6	0
10	C	342	0	0	0	0
10	D	189	0	0	1	0
10	E	749	0	0	5	0
10	F	312	0	0	2	0
All	All	21735	0	18837	159	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (159) 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:E:537:ALA:HB2	2:E:553:ILE:HD11	1.49	0.92
2:B:528:GLN:H	2:B:530:GLN:HE22	1.20	0.86
1:D:11:ASN:HD21	1:D:76:THR:H	1.23	0.86
2:E:460:ARG:HH11	2:E:463:GLN:HE22	1.25	0.84
2:E:670:ILE:HD12	2:E:671:ASP:N	1.94	0.83
2:E:208:THR:H	2:E:790:GLN:HE22	1.25	0.82
2:B:476:ARG:O	2:B:670:ILE:HD12	1.80	0.82
2:E:476:ARG:NH2	2:E:670:ILE:HD11	1.96	0.80
2:B:458:GLN:HA	2:B:458:GLN:HE21	1.47	0.80
2:E:155:PRO:HA	2:E:169:THR:HB	1.65	0.79
1:A:82:ALA:HB3	1:A:86:THR:HG22	1.65	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:537:ALA:HB2	2:E:553:ILE:CD1	2.15	0.77
1:D:3:LYS:N	10:D:4009:HOH:O	2.17	0.76
2:B:92:LEU:HD21	2:B:252:ILE:CG2	2.16	0.76
2:B:530:GLN:HE21	2:B:530:GLN:H	1.34	0.75
2:E:670:ILE:C	2:E:670:ILE:HD12	2.10	0.72
3:F:240:LYS:HG2	3:F:241:PRO:HD3	1.71	0.72
2:E:458:GLN:HG3	10:E:4134:HOH:O	1.89	0.71
2:B:528:GLN:H	2:B:530:GLN:NE2	1.88	0.71
2:E:593:MET:HG2	2:E:603:GLU:OE2	1.90	0.71
2:E:273:ASN:HD21	2:E:304:ASN:HD21	1.37	0.71
2:E:754:HIS:HD2	2:E:756:ILE:H	1.39	0.71
2:B:92:LEU:HD21	2:B:252:ILE:HG23	1.75	0.69
2:E:176:LYS:HB3	2:E:180:HIS:ND1	2.08	0.68
2:B:458:GLN:HA	2:B:458:GLN:NE2	2.08	0.68
2:E:168:MET:HG2	2:E:175:ARG:O	1.95	0.67
2:B:460:ARG:HH11	2:B:463:GLN:HE22	1.39	0.67
2:B:803:GLU:OE1	2:B:808:HIS:HD2	1.78	0.66
3:F:43:THR:OG1	3:F:45:LEU:HG	1.96	0.66
3:F:121:PRO:HD2	10:F:5179:HOH:O	1.95	0.65
2:E:476:ARG:HH21	2:E:670:ILE:HD11	1.61	0.64
2:E:90:LEU:O	2:E:92:LEU:HD13	1.97	0.63
2:B:53:ASP:HB3	2:B:133:ILE:HD11	1.80	0.63
2:E:88:LYS:HB2	2:E:89:PRO:HD3	1.81	0.62
2:B:212:VAL:HB	10:B:4369:HOH:O	2.01	0.60
2:B:530:GLN:H	2:B:530:GLN:NE2	1.99	0.59
2:B:670:ILE:O	2:B:808:HIS:HE1	1.86	0.59
7:B:3920:CUM:OM1	7:B:3920:CUM:MO	1.73	0.58
2:B:754:HIS:HD2	2:B:756:ILE:H	1.51	0.58
3:C:240:LYS:HB3	3:C:241:PRO:HD3	1.85	0.58
2:B:493:GLY:HA2	2:B:505:MET:O	2.04	0.58
2:E:754:HIS:CD2	2:E:756:ILE:H	2.21	0.58
2:B:358:ILE:HD12	2:B:489:ILE:HB	1.85	0.57
2:B:458:GLN:HG2	10:B:4217:HOH:O	2.05	0.57
1:A:125:GLU:OE2	2:B:741:LYS:HD3	2.05	0.57
1:A:20:GLU:HG3	10:A:4028:HOH:O	2.05	0.56
3:F:221:ASN:N	3:F:221:ASN:HD22	2.02	0.56
10:A:4006:HOH:O	2:B:741:LYS:HD2	2.06	0.56
2:B:573:THR:HB	2:B:574:PRO:HD3	1.88	0.56
1:A:135:ASN:HD21	3:C:105:GLN:HE22	1.53	0.55
2:E:476:ARG:NH2	2:E:670:ILE:CD1	2.68	0.55
2:E:788:HIS:HE2	2:E:790:GLN:NE2	2.05	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:200:GLU:HB3	2:E:324:LYS:HE3	1.87	0.55
2:B:238:THR:HB	2:B:274:LYS:HD3	1.90	0.55
3:F:221:ASN:ND2	10:F:5097:HOH:O	2.39	0.55
3:F:221:ASN:H	3:F:221:ASN:HD22	1.55	0.54
3:F:197:ALA:HB3	3:F:217:THR:HB	1.89	0.54
1:A:135:ASN:ND2	3:C:105:GLN:HE22	2.05	0.54
2:E:350:LYS:HE3	10:E:4572:HOH:O	2.08	0.54
2:B:114:GLN:O	2:B:115:ASN:HB2	2.09	0.53
2:B:713:GLN:HG3	2:B:732:PHE:O	2.08	0.53
2:E:164:ILE:HG13	2:E:165:LYS:HG2	1.91	0.53
2:B:334:HIS:HE1	2:B:373:ASP:OD2	1.90	0.53
3:C:197:ALA:HB3	3:C:217:THR:HB	1.90	0.53
2:B:754:HIS:CD2	2:B:756:ILE:H	2.27	0.52
2:E:493:GLY:HA2	2:E:505:MET:O	2.08	0.52
2:E:476:ARG:CZ	2:E:670:ILE:HD11	2.39	0.52
2:B:803:GLU:OE1	2:B:808:HIS:CD2	2.62	0.52
2:E:770:VAL:HB	2:E:771:PRO:HD3	1.92	0.51
2:E:670:ILE:C	2:E:670:ILE:CD1	2.79	0.51
2:B:208:THR:OG1	2:B:315:HIS:HD2	1.94	0.51
3:C:275:LEU:HD23	3:C:275:LEU:C	2.30	0.50
2:B:159:LEU:HD21	2:B:162:GLU:HG2	1.94	0.50
2:B:713:GLN:NE2	2:B:733:LEU:HD23	2.27	0.50
1:A:84:ASP:OD1	1:A:86:THR:HG22	2.11	0.50
2:E:524:GLY:HA3	2:E:564:GLY:HA3	1.93	0.49
2:B:683:LEU:HD23	2:B:683:LEU:C	2.32	0.49
2:E:208:THR:OG1	2:E:315:HIS:HD2	1.96	0.49
2:E:573:THR:HB	2:E:574:PRO:HD3	1.94	0.49
2:B:713:GLN:OE1	10:B:4369:HOH:O	2.19	0.49
2:B:46:LEU:HD11	2:B:236:TRP:CZ3	2.48	0.49
1:A:5:HIS:NE2	1:A:16:GLU:HG3	2.27	0.48
2:B:493:GLY:CA	2:B:505:MET:O	2.62	0.48
2:E:114:GLN:O	2:E:115:ASN:HB2	2.13	0.48
3:F:239:ASP:CG	3:F:241:PRO:HD2	2.33	0.48
2:B:464:LYS:O	2:B:468:GLU:HG3	2.14	0.47
1:A:115:ARG:O	1:A:119:GLU:HG3	2.13	0.47
2:E:553:ILE:N	2:E:553:ILE:HD12	2.28	0.47
2:E:442:ASN:HD22	2:E:442:ASN:C	2.17	0.47
2:E:476:ARG:HH21	2:E:670:ILE:CD1	2.26	0.47
2:B:442:ASN:C	2:B:442:ASN:HD22	2.18	0.47
2:E:463:GLN:O	2:E:467:GLN:HG3	2.15	0.47
3:C:103:ASP:HB2	3:C:104:PRO:CD	2.45	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:19:GLN:NE2	10:E:4402:HOH:O	2.48	0.47
3:F:214:ILE:HD13	3:F:275:LEU:HD11	1.97	0.46
2:B:200:GLU:HG3	10:B:4461:HOH:O	2.15	0.46
3:F:138:LEU:HD23	3:F:167:LEU:HA	1.96	0.46
2:E:208:THR:H	2:E:790:GLN:NE2	2.03	0.46
2:E:665:ILE:N	2:E:665:ILE:HD12	2.31	0.46
3:F:8:TYR:OH	3:F:10:ARG:HD3	2.16	0.46
2:B:176:LYS:HG2	2:B:180:HIS:ND1	2.30	0.46
2:B:327:LYS:HG2	2:B:420:LYS:HE3	1.97	0.46
2:E:63:ARG:HG2	2:E:63:ARG:HH11	1.80	0.46
2:E:121:VAL:HG11	2:E:132:ALA:HB3	1.98	0.46
3:F:240:LYS:CG	3:F:241:PRO:HD3	2.42	0.46
3:C:115:ASN:OD1	3:C:125:MET:HB2	2.15	0.46
3:F:239:ASP:OD1	3:F:241:PRO:HD2	2.16	0.45
2:B:493:GLY:HA2	2:B:505:MET:HB2	1.98	0.45
3:C:118:ASN:HD22	9:C:4932:FAD:H4B	1.82	0.45
2:B:221:GLN:HB3	2:B:298:VAL:HA	1.99	0.45
2:B:493:GLY:O	2:B:494:PRO:C	2.51	0.45
2:B:809:VAL:OXT	2:B:809:VAL:HG23	2.17	0.45
3:C:204:MET:HG3	3:C:286:ALA:HB1	1.97	0.45
2:E:345:CYS:SG	2:E:384:VAL:HG23	2.57	0.45
2:B:713:GLN:HB3	10:B:4369:HOH:O	2.16	0.45
3:C:204:MET:HG3	3:C:286:ALA:CB	2.47	0.45
3:C:138:LEU:HD23	3:C:167:LEU:HA	1.98	0.45
2:E:384:VAL:HG13	2:E:388:CYS:SG	2.57	0.45
2:E:493:GLY:O	2:E:494:PRO:C	2.54	0.44
2:B:670:ILE:HD13	2:B:671:ASP:N	2.31	0.44
2:B:159:LEU:CD2	2:B:162:GLU:HG2	2.48	0.44
2:B:175:ARG:NH2	2:B:178:HIS:O	2.51	0.44
2:B:524:GLY:HA3	2:B:564:GLY:HA3	2.00	0.44
2:E:166:ASP:O	2:E:168:MET:N	2.51	0.44
2:B:121:VAL:HG11	2:B:132:ALA:HB3	1.98	0.44
2:B:389:SER:O	2:B:390:PHE:HB2	2.18	0.44
2:E:360:THR:HG21	2:E:433:PRO:HG2	2.00	0.43
2:E:522:ARG:NH1	10:E:4339:HOH:O	2.43	0.43
2:B:360:THR:HG21	2:B:433:PRO:HG2	2.00	0.43
2:E:537:ALA:CB	2:E:553:ILE:HD11	2.35	0.43
2:E:505:MET:HA	2:E:565:LEU:HG	2.00	0.43
2:E:200:GLU:OE1	2:E:324:LYS:HG2	2.18	0.43
2:B:513:ILE:HD11	2:B:587:ILE:HG21	2.01	0.43
1:D:101:GLN:HB2	1:D:139:CYS:HB3	1.99	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:163:ASP:OD2	2:E:164:ILE:HG23	2.18	0.43
2:E:683:LEU:HD23	2:E:683:LEU:C	2.39	0.43
1:A:8:LEU:HD23	1:A:8:LEU:N	2.34	0.42
2:B:713:GLN:HE21	2:B:733:LEU:HD23	1.84	0.42
2:E:347:ASP:HB2	10:E:4020:HOH:O	2.18	0.42
2:E:448:LYS:HE3	2:E:452:ASP:OD2	2.19	0.42
2:B:739:THR:HA	2:B:740:PRO:HD3	1.92	0.42
2:E:63:ARG:HD2	2:E:141:GLU:OE1	2.20	0.42
2:E:623:LYS:HD3	2:E:623:LYS:HA	1.88	0.42
2:B:510:GLU:OE2	2:E:510:GLU:OE2	2.37	0.42
2:B:806:GLY:O	2:B:809:VAL:HG22	2.19	0.41
1:D:159:VAL:HB	1:D:160:PRO:HD3	2.02	0.41
2:B:358:ILE:CD1	2:B:489:ILE:HB	2.49	0.41
2:E:176:LYS:HG3	2:E:176:LYS:H	1.48	0.41
1:D:44:THR:O	1:D:45:SER:HB2	2.20	0.41
2:E:221:GLN:HB3	2:E:298:VAL:HA	2.03	0.41
2:E:271:PHE:HA	8:E:3923:MCN:S7'	2.60	0.41
2:E:58:SER:OG	2:E:59:HIS:HD2	2.03	0.41
2:B:315:HIS:HE1	10:B:4008:HOH:O	2.04	0.41
2:B:359:CYS:O	2:B:399:ILE:HB	2.21	0.41
2:B:428:PHE:HA	2:B:429:PRO:C	2.41	0.41
3:F:35:HIS:HD2	3:F:106:ILE:HG12	1.85	0.41
1:A:63:THR:HG22	1:A:63:THR:O	2.21	0.41
2:B:256:PRO:HB2	2:B:258:HIS:CD2	2.57	0.40
3:F:65:GLU:HB2	3:F:86:PHE:HZ	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	159/166 (96%)	156 (98%)	3 (2%)	0	100	100

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	156/166 (94%)	153 (98%)	3 (2%)	0	100	100
2	B	802/809 (99%)	775 (97%)	22 (3%)	5 (1%)	28	12
2	E	793/809 (98%)	761 (96%)	25 (3%)	7 (1%)	20	5
3	C	285/288 (99%)	280 (98%)	5 (2%)	0	100	100
3	F	284/288 (99%)	280 (99%)	4 (1%)	0	100	100
All	All	2479/2526 (98%)	2405 (97%)	62 (2%)	12 (0%)	32	15

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	176	LYS
2	E	167	LYS
2	B	493	GLY
2	B	712	GLY
2	E	493	GLY
2	E	712	GLY
2	B	265	PRO
2	E	265	PRO
2	B	390	PHE
2	E	312	ARG
2	E	761	VAL
2	B	761	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	129/131 (98%)	129 (100%)	0	100	100
1	D	126/131 (96%)	124 (98%)	2 (2%)	68	53
2	B	648/653 (99%)	635 (98%)	13 (2%)	60	42
2	E	640/653 (98%)	628 (98%)	12 (2%)	62	45
3	C	211/212 (100%)	211 (100%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	210/212 (99%)	209 (100%)	1 (0%)	91	87
All	All	1964/1992 (99%)	1936 (99%)	28 (1%)	71	58

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	209	TYR
2	B	258	HIS
2	B	313	ASP
2	B	314	TYR
2	B	386	TYR
2	B	393	THR
2	B	401	ARG
2	B	442	ASN
2	B	488	GLU
2	B	507	ASP
2	B	530	GLN
2	B	670	ILE
1	D	16	GLU
1	D	100	LEU
2	E	91	ASN
2	E	209	TYR
2	E	313	ASP
2	E	314	TYR
2	E	386	TYR
2	E	393	THR
2	E	401	ARG
2	E	442	ASN
2	E	488	GLU
2	E	507	ASP
2	E	639	ASN
2	E	790	GLN
3	F	221	ASN

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

Mol	Chain	Res	Type
1	A	34	ASN
1	A	135	ASN
2	B	115	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	172	HIS
2	B	258	HIS
2	B	273	ASN
2	B	304	ASN
2	B	315	HIS
2	B	334	HIS
2	B	442	ASN
2	B	458	GLN
2	B	463	GLN
2	B	530	GLN
2	B	592	GLN
2	B	639	ASN
2	B	698	GLN
2	B	754	HIS
2	B	808	HIS
3	C	118	ASN
3	C	221	ASN
1	D	11	ASN
2	E	19	GLN
2	E	59	HIS
2	E	91	ASN
2	E	115	ASN
2	E	273	ASN
2	E	315	HIS
2	E	334	HIS
2	E	442	ASN
2	E	463	GLN
2	E	592	GLN
2	E	597	HIS
2	E	698	GLN
2	E	713	GLN
2	E	754	HIS
2	E	790	GLN
2	E	804	GLN
3	F	78	GLN
3	F	118	ASN
3	F	221	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\# Z  > 2$
4	PO4	A	3001	-	4,4,4	0.97	0	6,6,6	0.41	0
5	FES	A	3907	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FES	A	3908	1	0,4,4	0.00	-	0,4,4	0.00	-
7	CUM	B	3920	8,2,6	0,4,4	0.00	-	0,4,4	0.00	-
8	MCN	B	3921	7	36,48,48	3.92	15 (41%)	37,74,74	2.40	11 (29%)
9	FAD	C	4932	-	51,58,58	2.11	19 (37%)	54,89,89	1.74	9 (16%)
5	FES	D	3907	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FES	D	3908	1	0,4,4	0.00	-	0,4,4	0.00	-
7	CUM	E	3922[B]	2	0,4,4	0.00	-	0,4,4	0.00	-
8	MCN	E	3923	7	36,48,48	3.78	13 (36%)	37,74,74	2.41	11 (29%)
9	FAD	F	4931	-	51,58,58	2.05	18 (35%)	54,89,89	1.77	7 (12%)

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
4	PO4	A	3001	-	-	0/0/0/0	0/0/0/0
5	FES	A	3907	1	-	0/0/4/4	0/1/1/1
5	FES	A	3908	1	-	0/0/4/4	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CUM	B	3920	8,2,6	-	0/0/2/2	0/0/0/0
8	MCN	B	3921	7	-	0/18/54/54	0/5/5/5
9	FAD	C	4932	-	-	0/28/50/50	0/6/6/6
5	FES	D	3907	1	-	0/0/4/4	0/1/1/1
5	FES	D	3908	1	-	0/0/4/4	0/1/1/1
7	CUM	E	3922[B]	2	-	0/0/2/2	0/0/0/0
8	MCN	E	3923	7	-	0/18/54/54	0/5/5/5
9	FAD	F	4931	-	-	0/28/50/50	0/6/6/6

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	4931	FAD	PA-O2A	-3.55	1.37	1.55
9	C	4932	FAD	PA-O2A	-3.53	1.37	1.55
9	C	4932	FAD	P-O2P	-2.62	1.41	1.55
9	F	4931	FAD	P-O2P	-2.56	1.42	1.55
9	F	4931	FAD	C2B-C1B	-2.35	1.49	1.53
9	C	4932	FAD	C2-N1	-2.30	1.33	1.38
9	F	4931	FAD	C2-N1	-2.25	1.33	1.38
8	B	3921	MCN	C4-N3	2.01	1.38	1.35
9	F	4931	FAD	C2A-N3A	2.11	1.35	1.32
8	B	3921	MCN	O9'-C9'	2.12	1.48	1.44
8	B	3921	MCN	C5'-C4D	2.16	1.58	1.51
9	C	4932	FAD	C5B-C4B	2.20	1.58	1.51
8	B	3921	MCN	O4D-C4D	2.24	1.50	1.45
9	F	4931	FAD	C10-N1	2.27	1.36	1.33
9	F	4931	FAD	C2-N3	2.35	1.42	1.38
9	C	4932	FAD	C4'-C3'	2.37	1.58	1.53
9	C	4932	FAD	O4B-C4B	2.38	1.50	1.45
8	E	3923	MCN	C4-N3	2.41	1.39	1.35
8	E	3923	MCN	O3'-C3'	2.44	1.48	1.43
9	F	4931	FAD	C5B-C4B	2.45	1.59	1.51
8	E	3923	MCN	C4B-N1'	2.45	1.41	1.36
8	B	3921	MCN	C4'-N3'	2.48	1.43	1.36
8	B	3921	MCN	O3'-C3'	2.48	1.48	1.43
8	E	3923	MCN	C4'-N3'	2.51	1.43	1.36
9	C	4932	FAD	C4A-N3A	2.53	1.39	1.35
9	C	4932	FAD	C2A-N1A	2.57	1.38	1.33
9	F	4931	FAD	O5'-C5'	2.59	1.55	1.44
9	F	4931	FAD	C4-C4X	2.64	1.46	1.41
9	F	4931	FAD	C5X-N5	2.65	1.39	1.35
8	E	3923	MCN	O9'-C9'	2.72	1.49	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	4932	FAD	C4-C4X	2.76	1.46	1.41
9	C	4932	FAD	C2A-N3A	2.76	1.36	1.32
8	B	3921	MCN	C4B-N8'	2.77	1.41	1.36
8	E	3923	MCN	C5-C4	2.83	1.48	1.41
8	B	3921	MCN	C5-C4	2.84	1.48	1.41
9	F	4931	FAD	C8-C7	2.88	1.48	1.41
9	C	4932	FAD	C4X-N5	2.93	1.37	1.33
8	E	3923	MCN	C4B-N8'	2.94	1.42	1.36
9	C	4932	FAD	O5'-C5'	2.98	1.56	1.44
9	F	4931	FAD	C4A-N3A	3.01	1.40	1.35
9	C	4932	FAD	C8-C7	3.02	1.48	1.41
8	B	3921	MCN	C4B-N1'	3.05	1.42	1.36
9	F	4931	FAD	C4X-N5	3.12	1.37	1.33
9	C	4932	FAD	C5X-N5	3.15	1.40	1.35
9	F	4931	FAD	C4-N3	3.30	1.39	1.33
8	B	3921	MCN	C4A-N5'	3.37	1.44	1.37
8	E	3923	MCN	C4A-N5'	3.40	1.44	1.37
9	C	4932	FAD	C10-N1	3.49	1.38	1.33
9	C	4932	FAD	C4X-C10	3.51	1.47	1.41
9	F	4931	FAD	O4B-C1B	4.11	1.46	1.41
9	C	4932	FAD	O4B-C1B	4.18	1.47	1.41
9	F	4931	FAD	C4X-C10	4.57	1.49	1.41
9	C	4932	FAD	C4-N3	4.62	1.41	1.33
9	C	4932	FAD	C9A-N10	4.79	1.45	1.38
8	E	3923	MCN	O9'-C7	4.80	1.41	1.35
8	E	3923	MCN	C2D-C1'	5.35	1.62	1.53
8	B	3921	MCN	C2D-C1'	5.40	1.62	1.53
8	E	3923	MCN	C6-N1	5.84	1.43	1.35
9	F	4931	FAD	C9A-N10	5.89	1.46	1.38
8	B	3921	MCN	O9'-C7	5.91	1.42	1.35
8	B	3921	MCN	C6-N1	6.99	1.45	1.35
8	B	3921	MCN	C7-N8'	7.36	1.48	1.30
8	E	3923	MCN	C7-N8'	7.62	1.49	1.30
8	E	3923	MCN	C6'-N5'	17.03	1.54	1.32
8	B	3921	MCN	C6'-N5'	17.47	1.55	1.32

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	3921	MCN	C7'-C6'-N5'	-7.57	101.99	119.23
8	E	3923	MCN	C7'-C6'-N5'	-7.55	102.03	119.23
8	B	3921	MCN	C6'-N5'-C4A	-5.82	106.63	118.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	3923	MCN	C6'-N5'-C4A	-5.74	106.79	118.19
9	F	4931	FAD	C4X-C4-N3	-4.64	116.88	123.48
8	E	3923	MCN	O9'-C7-N8'	-4.47	108.05	114.82
9	C	4932	FAD	C4X-C4-N3	-4.36	117.28	123.48
8	B	3921	MCN	O9'-C7-N8'	-4.08	108.64	114.82
9	F	4931	FAD	C4-C4X-C10	-3.47	117.16	119.96
9	C	4932	FAD	C4-C4X-C10	-3.34	117.26	119.96
8	E	3923	MCN	C5-C4-N3	-3.03	118.07	121.68
8	E	3923	MCN	N1'-C2'-N3'	-2.90	123.23	127.46
8	B	3921	MCN	C5-C4-N3	-2.84	118.30	121.68
8	B	3921	MCN	N1'-C2'-N3'	-2.75	123.44	127.46
9	C	4932	FAD	N3A-C2A-N1A	-2.67	126.54	128.86
9	C	4932	FAD	C4X-C10-N10	-2.59	118.72	120.52
9	F	4931	FAD	C4X-C10-N10	-2.58	118.73	120.52
9	C	4932	FAD	O5B-PA-O1A	-2.45	99.38	109.25
9	C	4932	FAD	C5X-C9A-N10	-2.44	115.85	117.66
9	F	4931	FAD	O5B-PA-O1A	-2.15	100.58	109.25
9	C	4932	FAD	O3'-C3'-C2'	-2.07	103.69	108.82
9	C	4932	FAD	C2A-N1A-C6A	2.07	122.39	118.77
9	F	4931	FAD	C2A-N1A-C6A	2.12	122.48	118.77
9	F	4931	FAD	C1'-N10-C10	2.30	120.86	118.50
8	E	3923	MCN	C4A-C4B-N1'	2.50	126.04	122.07
8	B	3921	MCN	O2'-C2D-C3'	2.54	119.98	111.83
8	E	3923	MCN	O2'-C2D-C3'	2.57	120.06	111.83
8	B	3921	MCN	C6-N1-C2	2.59	125.47	121.28
8	B	3921	MCN	C4A-C4B-N1'	2.62	126.22	122.07
8	E	3923	MCN	C6-N1-C2	2.78	125.79	121.28
8	B	3921	MCN	N4-C4-N3	2.83	121.40	116.64
8	E	3923	MCN	N4-C4-N3	2.86	121.46	116.64
8	E	3923	MCN	C2'-N3'-C4'	3.79	125.88	116.59
8	B	3921	MCN	C2'-N3'-C4'	3.84	126.00	116.59
8	B	3921	MCN	O4'-C4'-C4A	3.93	127.25	119.71
8	E	3923	MCN	O4'-C4'-C4A	4.22	127.81	119.71
9	C	4932	FAD	C4-N3-C2	7.56	121.77	115.16
9	F	4931	FAD	C4-N3-C2	8.35	122.46	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	3920	CUM	1	0
9	C	4932	FAD	1	0
8	E	3923	MCN	1	0

## 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.