



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:52 PM UTC

PDB ID : 1DGJ / pdb_00001dgj
Title : CRYSTAL STRUCTURE OF THE ALDEHYDE OXIDOREDUCTASE
FROM DESULFOVIBRIO DESULFURICANS ATCC 27774
Authors : Rebelo, J.M.; Macieira, S.; Dias, J.M.; Huber, R.; Romao, M.J.
Deposited on : 1999-11-24
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

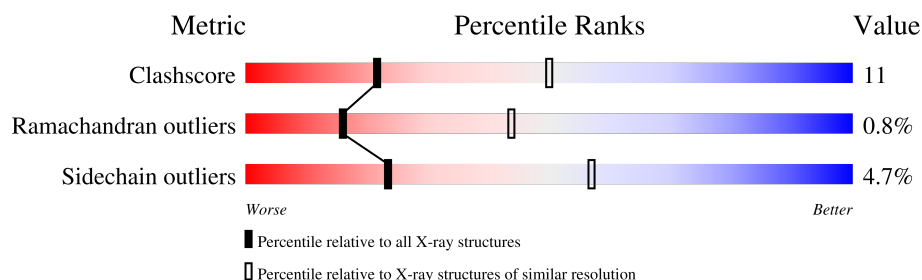
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	907	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FES	A	909	-	-	X	-

2 Entry composition [i](#)

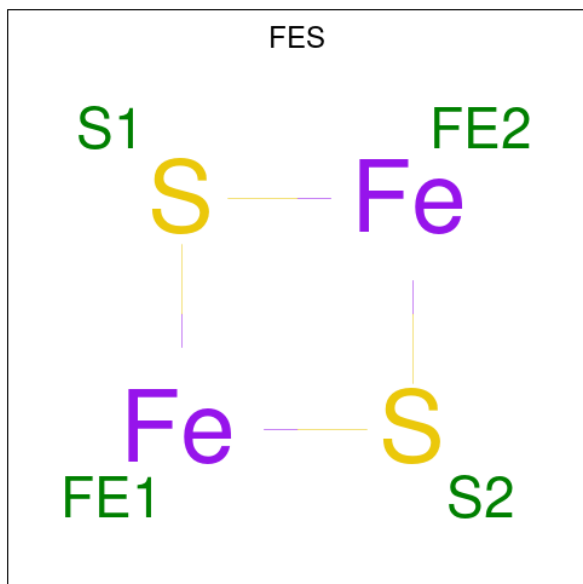
There are 5 unique types of molecules in this entry. The entry contains 7102 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALDEHYDE OXIDOREDUCTASE.

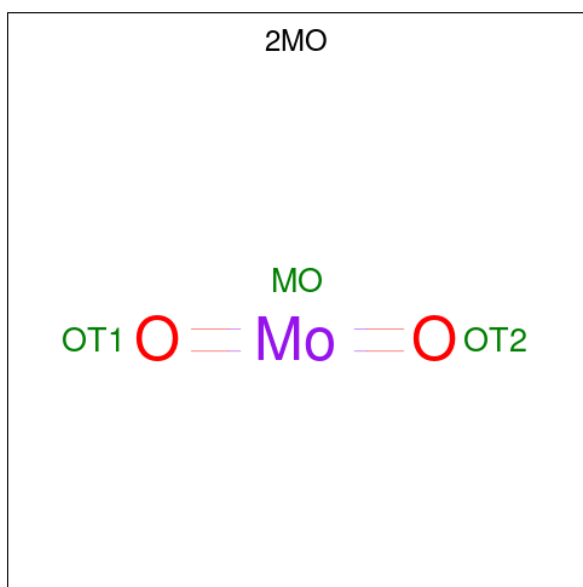
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	906	6854	4312	1187	1306	49	45	0	0

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



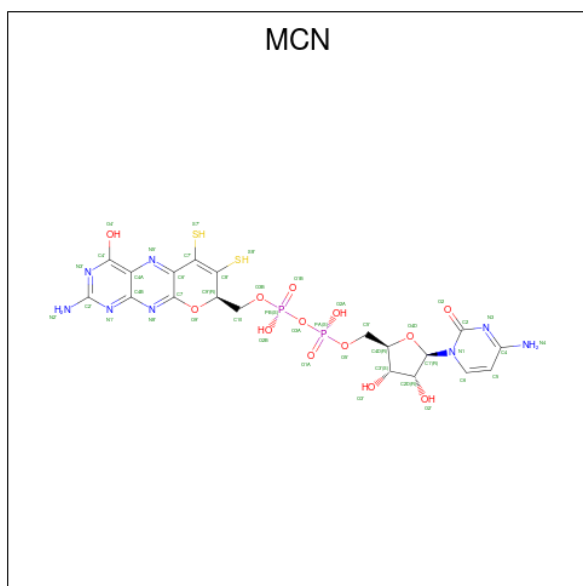
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0

- Molecule 3 is MOLYBDENUM (IV)OXIDE (CCD ID: 2MO) (formula: MoO_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Mo	O	0	0
			3	1	2		

- Molecule 4 is PTERIN CYTOSINE DINUCLEOTIDE (CCD ID: MCN) (formula: $C_{19}H_{22}N_8O_{13}P_2S_2$).



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

- Molecule 5 is water.

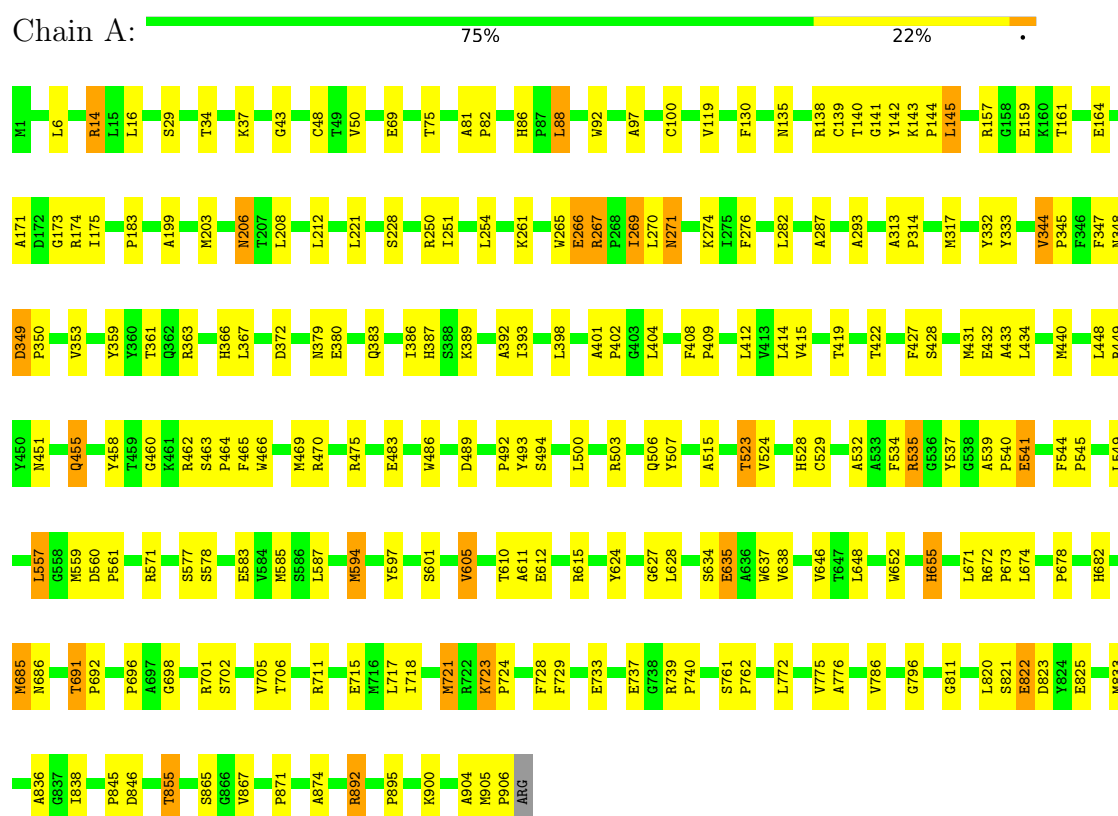
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	193	Total 193	O 193	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: ALDEHYDE OXIDOREDUCTASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	156.64Å 156.64Å 177.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.80 – 2.80	Depositor
% Data completeness (in resolution range)	98.2 (24.80-2.80)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.164 , 0.224	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7102	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: FES, MCN, 2MO

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	0.64	2/7003 (0.0%)	1.09	39/9496 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	721	MET	SD-CE	-6.16	1.64	1.79
1	A	594	MET	SD-CE	-5.02	1.67	1.79

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	821	SER	N-CA-C	9.51	125.46	114.62
1	A	427	PHE	N-CA-C	-9.45	101.02	112.54
1	A	494	SER	N-CA-C	9.37	124.25	113.01
1	A	507	TYR	N-CA-C	9.06	125.50	113.72
1	A	140	THR	N-CA-C	8.89	122.14	111.82
1	A	820	LEU	N-CA-C	8.08	123.26	113.41
1	A	655	HIS	N-CA-C	-7.28	104.37	113.18
1	A	141	GLY	N-CA-C	-7.25	105.20	115.43
1	A	393	ILE	N-CA-C	7.11	118.72	110.62
1	A	515	ALA	N-CA-C	6.99	118.90	111.28
1	A	686	ASN	N-CA-C	6.82	119.54	111.02
1	A	455	GLN	N-CA-C	-6.52	104.18	111.28
1	A	139	CYS	N-CA-C	6.33	121.09	112.68
1	A	29	SER	N-CA-C	6.32	119.15	111.82
1	A	171	ALA	CA-C-N	6.11	128.74	120.44
1	A	171	ALA	C-N-CA	6.11	128.74	120.44
1	A	269	ILE	N-CA-C	-5.98	105.02	110.82
1	A	855	THR	N-CA-C	-5.94	102.16	109.65
1	A	761	SER	CA-C-N	5.88	125.75	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	761	SER	C-N-CA	5.88	125.75	119.28
1	A	100	CYS	N-CA-C	-5.84	105.41	112.54
1	A	691	THR	CA-C-N	5.80	126.61	120.11
1	A	691	THR	C-N-CA	5.80	126.61	120.11
1	A	349	ASP	CA-C-N	5.75	125.45	119.82
1	A	349	ASP	C-N-CA	5.75	125.45	119.82
1	A	822	GLU	N-CA-C	5.74	118.98	110.48
1	A	458	TYR	N-CA-C	5.73	117.77	110.61
1	A	462	ARG	N-CA-C	-5.72	101.81	110.28
1	A	451	ASN	N-CA-C	-5.65	102.40	110.59
1	A	723	LYS	N-CA-C	-5.52	102.69	109.65
1	A	846	ASP	N-CA-C	-5.52	105.80	112.54
1	A	578	SER	N-CA-C	-5.50	106.56	113.72
1	A	728	PHE	N-CA-C	5.48	118.02	109.52
1	A	412	LEU	N-CA-C	5.35	118.17	109.24
1	A	228	SER	N-CA-C	5.32	120.09	111.37
1	A	685	MET	N-CA-C	5.20	117.58	109.52
1	A	173	GLY	N-CA-C	-5.20	108.45	115.21
1	A	270	LEU	N-CA-C	-5.13	99.92	108.34
1	A	762	PRO	N-CA-C	5.11	120.55	113.65

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	6854	0	6766	146	0
2	A	8	0	0	2	0
3	A	3	0	0	0	0
4	A	44	0	17	3	0
5	A	193	0	0	10	0
All	All	7102	0	6783	146	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 11.

All (146) 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:610:THR:HG22	1:A:612:GLU:H	1.37	0.89
1:A:594:MET:HE3	1:A:597:TYR:HB2	1.65	0.79
1:A:271:ASN:HD22	1:A:271:ASN:H	1.34	0.75
1:A:206:ASN:H	1:A:206:ASN:HD22	1.34	0.75
1:A:786:VAL:O	1:A:845:PRO:HG3	1.87	0.74
1:A:627:GLY:HA2	1:A:701:ARG:HB3	1.70	0.72
1:A:206:ASN:HD22	1:A:206:ASN:N	1.88	0.72
1:A:372:ASP:H	1:A:455:GLN:HE21	1.37	0.71
1:A:379:ASN:ND2	1:A:383:GLN:HE21	1.87	0.71
1:A:344:VAL:HG12	1:A:345:PRO:HD3	1.74	0.68
1:A:43:GLY:HA2	2:A:909:FES:S1	2.36	0.66
1:A:637:TRP:CD1	1:A:692:PRO:HD3	2.31	0.66
1:A:392:ALA:HB2	1:A:696:PRO:HB3	1.79	0.64
1:A:500:LEU:O	1:A:503:ARG:HB2	1.98	0.64
1:A:635:GLU:HB3	1:A:692:PRO:HB2	1.81	0.63
1:A:389:LYS:HE3	1:A:419:THR:HG23	1.81	0.62
1:A:464:PRO:HG2	1:A:489:ASP:HB3	1.81	0.62
1:A:267:ARG:HD3	5:A:1072:HOH:O	2.00	0.61
1:A:717:LEU:HG	1:A:721:MET:HE2	1.82	0.60
1:A:465:PHE:CE1	1:A:541:GLU:HG3	2.38	0.59
1:A:161:THR:CG2	1:A:164:GLU:HB2	2.33	0.59
1:A:528:HIS:CD2	1:A:529:CYS:H	2.21	0.59
1:A:528:HIS:HD2	1:A:529:CYS:H	1.51	0.59
1:A:627:GLY:HA2	1:A:701:ARG:CB	2.33	0.59
1:A:585:MET:HE3	5:A:1162:HOH:O	2.02	0.58
1:A:97:ALA:HB1	1:A:145:LEU:HD12	1.84	0.58
1:A:359:TYR:CE2	1:A:892:ARG:HD2	2.40	0.57
1:A:361:THR:HG21	1:A:541:GLU:HA	1.86	0.57
1:A:138:ARG:HD2	5:A:1055:HOH:O	2.04	0.57
1:A:682:HIS:HB3	5:A:1117:HOH:O	2.05	0.56
1:A:460:GLY:HA3	1:A:532:ALA:HB2	1.88	0.56
1:A:372:ASP:H	1:A:455:GLN:NE2	2.04	0.55
1:A:865:SER:O	4:A:914:MCN:H5	2.07	0.55
1:A:81:ALA:HB1	1:A:82:PRO:HD2	1.88	0.55
1:A:610:THR:HG21	1:A:612:GLU:HG2	1.89	0.55
1:A:372:ASP:N	1:A:455:GLN:HE21	2.02	0.54
1:A:702:SER:O	1:A:706:THR:HB	2.08	0.54
1:A:540:PRO:HD2	1:A:541:GLU:OE1	2.08	0.54
1:A:711:ARG:O	1:A:715:GLU:HG3	2.07	0.54
1:A:698:GLY:HA2	4:A:914:MCN:S8'	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:THR:CG2	1:A:612:GLU:HG2	2.39	0.53
1:A:367:LEU:HD13	1:A:838:ILE:HB	1.91	0.53
1:A:634:SER:HB2	1:A:705:VAL:HG12	1.91	0.52
1:A:539:ALA:HB3	1:A:540:PRO:HD3	1.91	0.52
1:A:557:LEU:HB3	1:A:559:MET:HE3	1.90	0.52
1:A:610:THR:HG22	1:A:611:ALA:N	2.24	0.52
1:A:833:MET:HG2	1:A:838:ILE:HG21	1.92	0.52
1:A:470:ARG:HA	1:A:549:LEU:HD21	1.90	0.52
1:A:161:THR:HG22	1:A:164:GLU:HB2	1.91	0.52
1:A:333:TYR:HB3	1:A:523:THR:OG1	2.09	0.52
1:A:379:ASN:HB3	1:A:383:GLN:H	1.75	0.52
1:A:571:ARG:HH11	1:A:571:ARG:HG3	1.75	0.52
1:A:130:PHE:HA	1:A:135:ASN:HD22	1.74	0.51
1:A:251:ILE:HD12	1:A:267:ARG:HD2	1.93	0.51
1:A:271:ASN:H	1:A:271:ASN:ND2	2.03	0.51
1:A:271:ASN:HB2	1:A:282:LEU:HD22	1.91	0.51
1:A:402:PRO:HD2	5:A:1142:HOH:O	2.10	0.51
1:A:534:PHE:HD1	1:A:535:ARG:N	2.08	0.51
1:A:717:LEU:CD1	1:A:721:MET:HE2	2.41	0.51
1:A:601:SER:O	1:A:605:VAL:HB	2.10	0.51
1:A:655:HIS:HB3	4:A:914:MCN:O4'	2.10	0.51
1:A:313:ALA:O	1:A:317:MET:HG3	2.12	0.50
1:A:892:ARG:CG	1:A:892:ARG:HH11	2.25	0.50
1:A:142:TYR:HA	1:A:145:LEU:HD22	1.93	0.50
1:A:389:LYS:CE	1:A:419:THR:HG23	2.42	0.50
1:A:503:ARG:HD3	1:A:506:GLN:NE2	2.27	0.50
1:A:638:VAL:HG12	1:A:717:LEU:HD22	1.95	0.49
1:A:448:LEU:HD12	1:A:449:ARG:N	2.28	0.49
1:A:637:TRP:NE1	1:A:692:PRO:HD3	2.27	0.49
1:A:267:ARG:HG3	1:A:493:TYR:CG	2.48	0.49
1:A:14:ARG:HD3	5:A:1119:HOH:O	2.13	0.49
1:A:143:LYS:HB3	1:A:144:PRO:HD3	1.95	0.48
1:A:199:ALA:O	1:A:203:MET:HG3	2.13	0.48
1:A:717:LEU:CG	1:A:721:MET:HE2	2.43	0.48
1:A:363:ARG:NH2	1:A:825:GLU:OE1	2.47	0.48
1:A:539:ALA:HB2	1:A:624:TYR:CD2	2.48	0.48
1:A:652:TRP:NE1	1:A:702:SER:HB3	2.28	0.48
1:A:372:ASP:N	1:A:455:GLN:NE2	2.61	0.48
1:A:594:MET:CE	1:A:597:TYR:HB2	2.38	0.47
1:A:739:ARG:HD3	1:A:740:PRO:HD2	1.97	0.47
1:A:174:ARG:HG2	1:A:672:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ALA:HB3	1:A:314:PRO:HD3	1.97	0.47
1:A:652:TRP:CE2	1:A:702:SER:HB3	2.49	0.47
1:A:266:GLU:HG3	5:A:1145:HOH:O	2.15	0.46
1:A:379:ASN:HD22	1:A:383:GLN:HE21	1.62	0.46
1:A:822:GLU:HA	1:A:836:ALA:O	2.15	0.46
1:A:392:ALA:CB	1:A:696:PRO:HB3	2.45	0.46
1:A:615:ARG:HH11	1:A:776:ALA:CB	2.28	0.46
1:A:174:ARG:NH1	5:A:1139:HOH:O	2.49	0.46
1:A:175:ILE:HD13	1:A:678:PRO:HG3	1.98	0.46
1:A:344:VAL:HG22	1:A:348:ASN:ND2	2.31	0.46
1:A:796:GLY:HA2	1:A:855:THR:O	2.16	0.46
1:A:161:THR:HG23	1:A:164:GLU:HB2	1.98	0.45
1:A:261:LYS:HD3	1:A:332:TYR:C	2.41	0.45
1:A:206:ASN:N	1:A:206:ASN:ND2	2.58	0.45
1:A:610:THR:CG2	1:A:611:ALA:N	2.79	0.45
1:A:206:ASN:H	1:A:206:ASN:ND2	2.08	0.45
1:A:37:LYS:O	1:A:48:CYS:HB3	2.17	0.45
1:A:386:ILE:HD13	1:A:432:GLU:O	2.17	0.45
1:A:344:VAL:HG22	1:A:348:ASN:HD21	1.81	0.44
1:A:723:LYS:HA	1:A:729:PHE:CE1	2.51	0.44
1:A:269:ILE:HD13	1:A:433:ALA:HB1	1.99	0.44
1:A:349:ASP:HA	1:A:350:PRO:HD3	1.82	0.44
1:A:733:GLU:O	1:A:737:GLU:HG2	2.17	0.44
1:A:43:GLY:CA	2:A:909:FES:S1	3.05	0.44
1:A:50:VAL:HG12	1:A:75:THR:HG22	2.00	0.44
1:A:92:TRP:CD1	1:A:97:ALA:HB3	2.53	0.44
1:A:674:LEU:HD11	1:A:721:MET:HE3	1.99	0.44
1:A:130:PHE:HD2	1:A:135:ASN:HD22	1.65	0.44
1:A:460:GLY:HA3	1:A:532:ALA:CB	2.47	0.44
1:A:401:ALA:HB3	1:A:402:PRO:HD3	1.99	0.43
1:A:811:GLY:HA3	1:A:871:PRO:HG2	2.01	0.43
1:A:287:ALA:HB3	1:A:293:ALA:HB2	2.00	0.43
1:A:534:PHE:O	1:A:535:ARG:C	2.61	0.43
1:A:347:PHE:CE1	1:A:483:GLU:HG3	2.53	0.43
1:A:221:LEU:HD23	1:A:274:LYS:HG2	2.00	0.43
1:A:673:PRO:HG2	1:A:718:ILE:HD13	2.00	0.43
1:A:904:ALA:O	1:A:906:PRO:HD3	2.18	0.43
1:A:544:PHE:N	1:A:545:PRO:HD2	2.35	0.42
1:A:615:ARG:NH1	1:A:776:ALA:CB	2.83	0.42
1:A:276:PHE:HB3	1:A:492:PRO:CB	2.50	0.42
1:A:314:PRO:HA	1:A:317:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:LEU:HD23	1:A:587:LEU:HA	1.79	0.42
1:A:905:MET:HE3	1:A:905:MET:HB2	1.89	0.42
1:A:628:LEU:HD23	1:A:628:LEU:HA	1.93	0.42
1:A:157:ARG:HD2	1:A:159:GLU:OE2	2.19	0.42
1:A:344:VAL:CG1	1:A:345:PRO:HD3	2.46	0.42
1:A:466:TRP:O	1:A:486:TRP:HA	2.20	0.42
1:A:463:SER:HB3	1:A:489:ASP:O	2.20	0.41
1:A:469:MET:HE3	1:A:469:MET:HB2	1.87	0.41
1:A:685:MET:HA	1:A:691:THR:HG21	2.01	0.41
1:A:366:HIS:CD2	1:A:366:HIS:H	2.39	0.41
1:A:366:HIS:HD2	5:A:1026:HOH:O	2.03	0.41
1:A:408:PHE:HA	1:A:409:PRO:HA	1.78	0.41
1:A:387:HIS:HA	1:A:415:VAL:O	2.21	0.41
1:A:822:GLU:O	1:A:823:ASP:HB2	2.21	0.41
1:A:895:PRO:O	1:A:900:LYS:HD2	2.21	0.41
1:A:86:HIS:ND1	1:A:88:LEU:HB2	2.35	0.41
1:A:250:ARG:HD2	1:A:265:TRP:O	2.21	0.41
1:A:560:ASP:HA	1:A:561:PRO:HD3	1.94	0.41
1:A:615:ARG:HH11	1:A:776:ALA:HB2	1.85	0.41
1:A:892:ARG:HH11	1:A:892:ARG:HG2	1.86	0.41
1:A:353:VAL:HG21	1:A:557:LEU:CD1	2.50	0.40
1:A:212:LEU:HD21	1:A:434:LEU:HD13	2.02	0.40
1:A:404:LEU:O	1:A:440:MET:HE1	2.21	0.40
1:A:380:GLU:HB3	5:A:1040:HOH:O	2.22	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	904/907 (100%)	860 (95%)	37 (4%)	7 (1%)	16 44

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	535	ARG
1	A	34	THR
1	A	254	LEU
1	A	537	TYR
1	A	874	ALA
1	A	724	PRO
1	A	867	VAL

5.3.2 Protein sidechains [i](#)

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	719/720 (100%)	685 (95%)	34 (5%)	23	57

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	14	ARG
1	A	16	LEU
1	A	69	GLU
1	A	88	LEU
1	A	119	VAL
1	A	145	LEU
1	A	183	PRO
1	A	206	ASN
1	A	208	LEU
1	A	266	GLU
1	A	267	ARG
1	A	271	ASN
1	A	344	VAL
1	A	398	LEU
1	A	414	LEU
1	A	422	THR
1	A	428	SER

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Mol	Chain	Res	Type
1	A	431	MET
1	A	475	ARG
1	A	523	THR
1	A	524	VAL
1	A	541	GLU
1	A	557	LEU
1	A	577	SER
1	A	583	GLU
1	A	605	VAL
1	A	635	GLU
1	A	646	VAL
1	A	648	LEU
1	A	671	LEU
1	A	772	LEU
1	A	775	VAL
1	A	892	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	44	GLN
1	A	90	HIS
1	A	118	ASN
1	A	135	ASN
1	A	206	ASN
1	A	271	ASN
1	A	348	ASN
1	A	366	HIS
1	A	383	GLN
1	A	394	HIS
1	A	417	ASN
1	A	455	GLN
1	A	456	GLN
1	A	506	GLN
1	A	528	HIS
1	A	641	ASN
1	A	680	ASN
1	A	682	HIS
1	A	703	GLN
1	A	807	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	FES	A	908	1	0,4,4	-	-	-		
2	FES	A	909	1	0,4,4	-	-	-		
4	MCN	A	914	3	42,48,48	2.59	9 (21%)	55,74,74	2.07	10 (18%)
3	2MO	A	910	5,4	0,2,2	-	-	-		

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	908	1	-	-	0/1/1/1
2	FES	A	909	1	-	-	0/1/1/1
4	MCN	A	914	3	-	1/22/54/54	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	914	MCN	C6'-N5'	11.63	1.48	1.32
4	A	914	MCN	C6'-C7	5.24	1.52	1.43
4	A	914	MCN	C2'-N3'	5.11	1.44	1.35
4	A	914	MCN	C7-N8'	4.75	1.41	1.30
4	A	914	MCN	O5'-C5'	3.26	1.57	1.44
4	A	914	MCN	C4A-N5'	3.17	1.43	1.37
4	A	914	MCN	PA-O3A	3.12	1.62	1.59
4	A	914	MCN	C7'-S7'	-3.11	1.69	1.76
4	A	914	MCN	C5-C4	2.01	1.47	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	914	MCN	N1'-C2'-N3'	-7.47	117.72	127.21
4	A	914	MCN	C2'-N1'-C4B	5.94	121.88	115.48
4	A	914	MCN	O9'-C7-N8'	-5.13	108.35	115.12
4	A	914	MCN	O9'-C7-C6'	-4.28	114.29	120.97
4	A	914	MCN	N2'-C2'-N1'	4.09	124.18	117.79
4	A	914	MCN	C5-C4-N4	-3.85	113.89	120.63
4	A	914	MCN	N4-C4-N3	3.64	124.43	117.91
4	A	914	MCN	C7-N8'-C4B	-2.17	114.15	117.01
4	A	914	MCN	C2'-N3'-C4'	2.12	120.87	116.31
4	A	914	MCN	O2B-PB-O1B	2.06	122.04	112.44

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	914	MCN	C9'-C10-O3B-PB

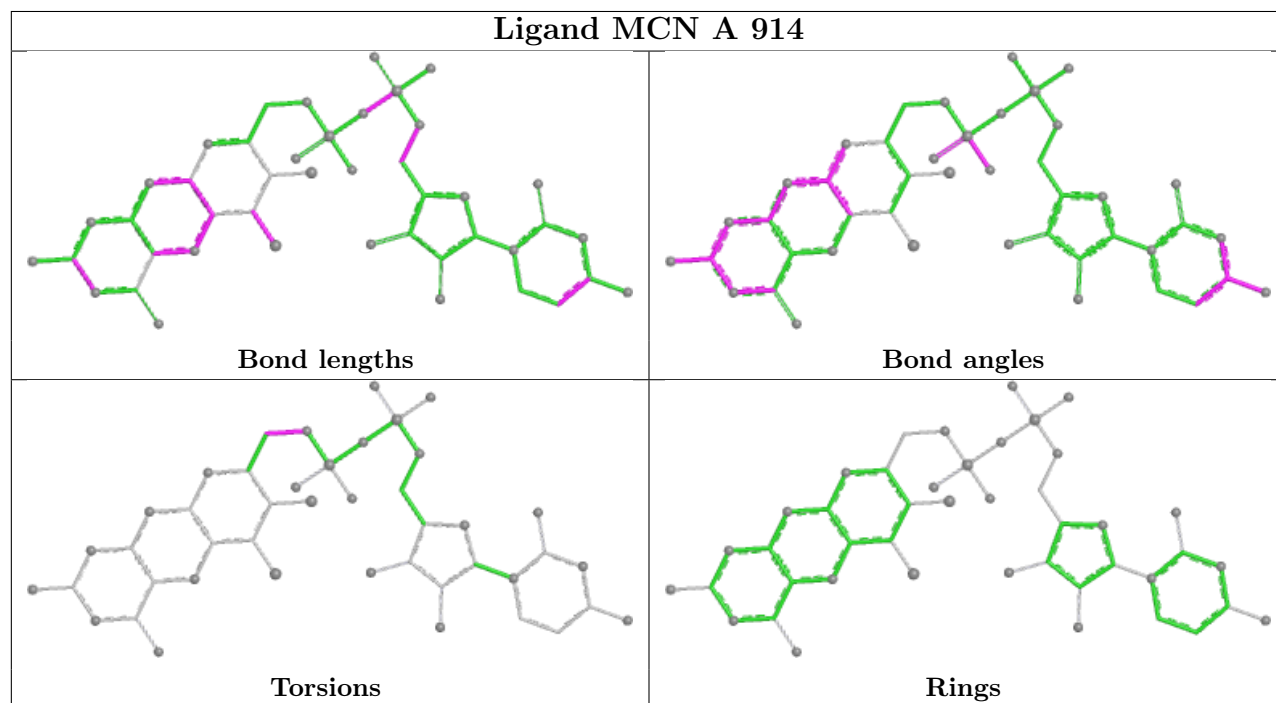
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	909	FES	2	0
4	A	914	MCN	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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.