Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2026 – 12:59 am BST

PDB ID	:	2IV2 / pdb_00002iv2
Title	:	Reinterpretation of reduced form of formate dehydrogenase H from E. coli
Authors	:	Raaijmakers, H.C.A.; Romao, M.J.
Deposited on	:	2006-06-08
Resolution	:	2.27 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:

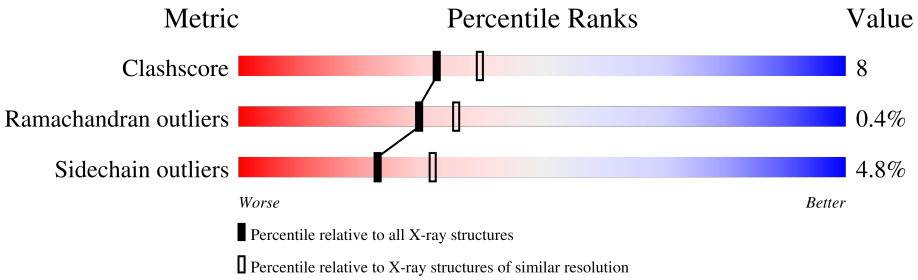
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	X	715	79% 17%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2MD	X	801	X	-	-	-

2 Entry composition

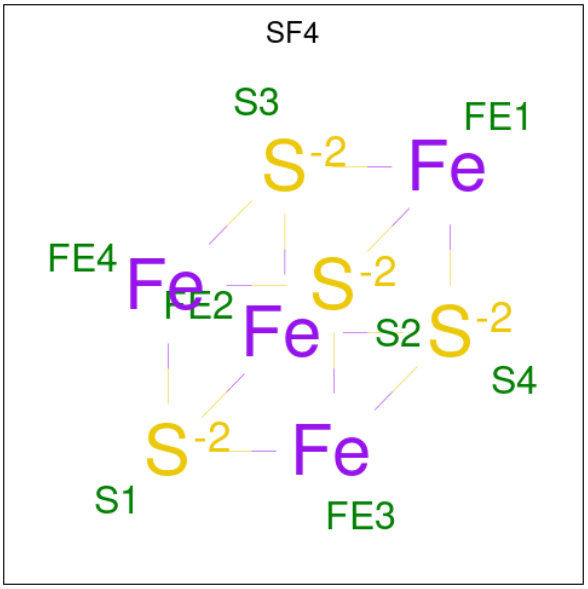
There are 7 unique types of molecules in this entry. The entry contains 5817 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Formate dehydrogenase H.

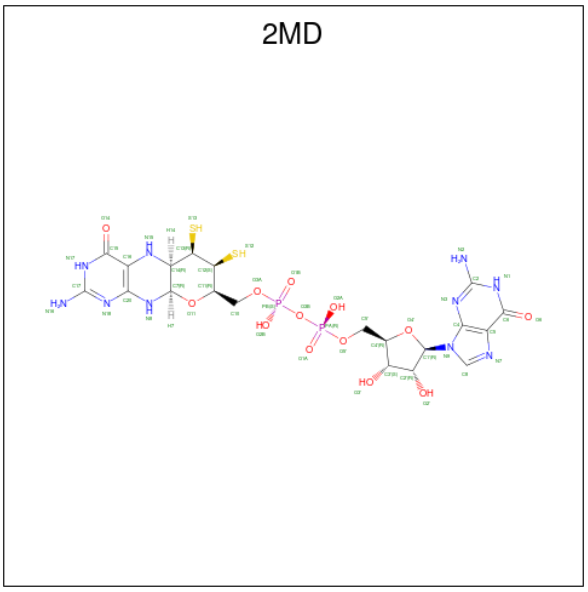
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	X	697	5446	3428	952	1032	33	1	0	1	0

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



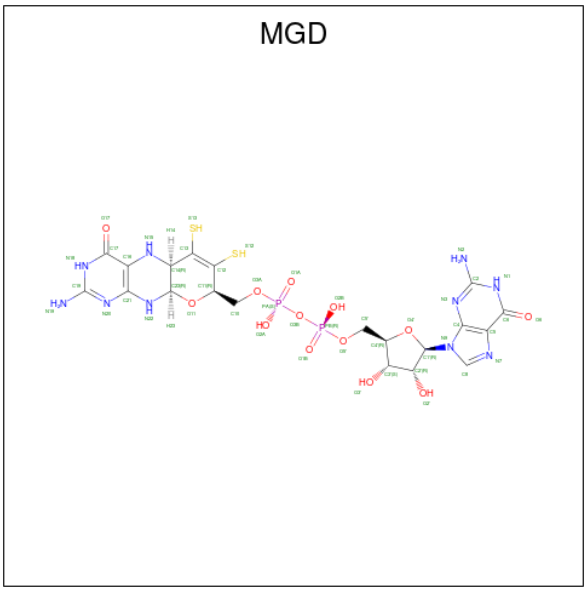
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Fe	S			
2	X	1	8	4	4		0	0

- Molecule 3 is GUANYLATE-O'-PHOSPHORIC ACID MONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,5,6,7,8A,9,10,10A-OCTAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (CCD ID: 2MD) (formula: $C_{20}H_{28}N_{10}O_{13}P_2S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	X	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 4 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA -1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	X	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 5 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	X	1	Total Mo 1 1	0	0

- Molecule 6 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	X	1	Total X 1 1	0	0

- Molecule 7 is water.

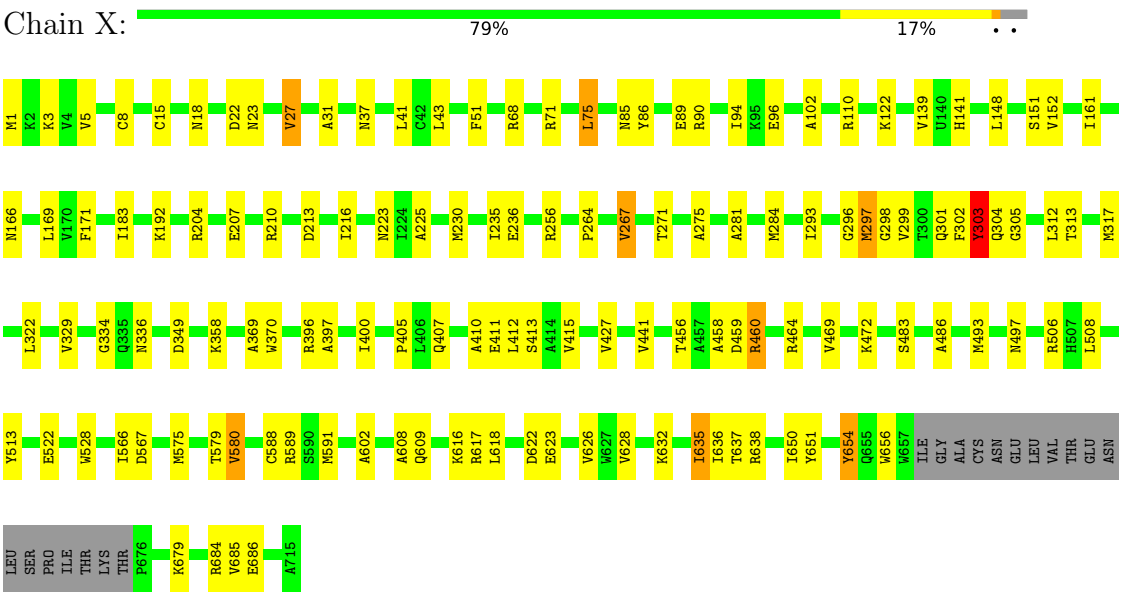
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	X	267	Total O 267 267	0	0

3 Residue-property plots (i)

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: Formate dehydrogenase H



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	146.40Å 146.40Å 81.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.50 – 2.27	Depositor
% Data completeness (in resolution range)	88.5 (34.50-2.27)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.175 , 0.226	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5817	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MD, UNX, MGD, MO, SF4, SEC

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	X	0.72	0/5563	0.86	3/7542 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	297	MET	N-CA-C	7.12	121.59	112.34
1	X	303	TYR	N-CA-C	5.47	122.46	110.80
1	X	223	ASN	N-CA-C	5.06	116.49	111.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	297	MET	Peptide
1	X	303	TYR	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	X	5446	0	5319	85	0
2	X	8	0	0	1	0
3	X	47	0	24	3	0
4	X	47	0	22	2	0
5	X	1	0	0	0	0
6	X	1	0	0	0	0
7	X	267	0	0	8	0
All	All	5817	0	5365	86	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (86) 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:X:588[B]:CYS:SG	1:X:588[B]:CYS:CB	2.20	1.30
1:X:110:ARG:HA	1:X:336:ASN:HD21	1.41	0.85
1:X:68:ARG:HB2	1:X:75:LEU:HD13	1.65	0.79
1:X:141:HIS:NE2	1:X:349:ASP:OD1	2.16	0.79
1:X:296:GLY:C	1:X:298:GLY:HA3	2.13	0.73
1:X:299:VAL:HA	1:X:302:PHE:CE1	2.24	0.72
1:X:575:MET:CE	1:X:650:ILE:HG23	2.21	0.71
1:X:588[B]:CYS:HB3	3:X:801:2MD:O1A	1.91	0.70
1:X:51:PHE:CZ	1:X:591:MET:HE3	2.26	0.70
1:X:216:ILE:HD11	1:X:281:ALA:CB	2.24	0.67
1:X:141:HIS:HE2	1:X:349:ASP:CG	2.03	0.66
1:X:464:ARG:HD3	7:X:2204:HOH:O	1.95	0.66
1:X:575:MET:HE2	1:X:650:ILE:HG23	1.77	0.66
1:X:303:TYR:HA	1:X:305:GLY:N	2.11	0.65
1:X:483:SER:HA	1:X:493:MET:HE3	1.78	0.64
1:X:102:ALA:HB1	1:X:396:ARG:HG2	1.80	0.63
1:X:575:MET:HE2	1:X:650:ILE:CG2	2.29	0.61
1:X:204:ARG:HH11	1:X:609:GLN:HE22	1.49	0.60
1:X:303:TYR:CG	1:X:304:GLN:N	2.66	0.60
1:X:303:TYR:HA	1:X:305:GLY:H	1.65	0.60
1:X:486:ALA:CB	1:X:493:MET:HE2	2.32	0.60
1:X:299:VAL:HG22	1:X:302:PHE:CE1	2.37	0.59
1:X:299:VAL:HG22	1:X:302:PHE:HE1	1.69	0.58
1:X:460:ARG:HB2	1:X:528:TRP:NE1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:296:GLY:O	1:X:299:VAL:N	2.36	0.56
1:X:296:GLY:O	1:X:298:GLY:HA3	2.05	0.56
1:X:405:PRO:HB2	1:X:415:VAL:HG11	1.87	0.56
1:X:608:ALA:HB2	1:X:637:THR:HG21	1.88	0.55
1:X:299:VAL:HA	1:X:302:PHE:CZ	2.41	0.55
1:X:636:ILE:HG22	7:X:2253:HOH:O	2.06	0.55
1:X:322:LEU:HD21	1:X:329:VAL:HG22	1.89	0.54
1:X:267:VAL:HG13	1:X:271:THR:HG23	1.88	0.54
1:X:166:ASN:ND2	7:X:2079:HOH:O	2.26	0.54
1:X:456:THR:CG2	1:X:460:ARG:HA	2.38	0.54
1:X:506:ARG:HD2	1:X:513:TYR:O	2.08	0.53
1:X:301:GLN:C	1:X:303:TYR:H	2.18	0.52
1:X:588[A]:CYS:HB2	3:X:801:2MD:O1A	2.11	0.51
1:X:313:THR:HG22	1:X:317:MET:HE3	1.94	0.50
1:X:86:TYR:CE2	1:X:90:ARG:NH2	2.80	0.50
1:X:456:THR:HG22	1:X:460:ARG:HA	1.94	0.50
1:X:602:ALA:HB1	1:X:656:TRP:CZ2	2.47	0.49
1:X:216:ILE:HD11	1:X:281:ALA:HB1	1.93	0.49
1:X:575:MET:CE	1:X:650:ILE:CG2	2.90	0.49
1:X:22:ASP:HB3	1:X:27:VAL:HG21	1.96	0.48
1:X:110:ARG:HA	1:X:336:ASN:ND2	2.21	0.48
1:X:96:GLU:HG2	7:X:2048:HOH:O	2.14	0.47
1:X:169:LEU:CD1	1:X:284:MET:HG2	2.45	0.47
1:X:216:ILE:HD11	1:X:281:ALA:HB2	1.97	0.46
1:X:369:ALA:CB	1:X:508:LEU:HD21	2.45	0.46
1:X:204:ARG:CZ	1:X:580:VAL:HG21	2.45	0.46
1:X:302:PHE:CE2	1:X:679:LYS:HD2	2.50	0.46
1:X:579:THR:HG22	1:X:654:TYR:HB2	1.97	0.45
1:X:235:ILE:HG21	1:X:256:ARG:HG3	1.97	0.45
1:X:369:ALA:HB2	1:X:508:LEU:HD21	1.98	0.44
1:X:31:ALA:HB2	1:X:41:LEU:HG	2.00	0.44
1:X:122:LYS:HE3	1:X:370:TRP:CD1	2.52	0.44
1:X:148:LEU:HD22	1:X:152:VAL:CG2	2.48	0.44
1:X:267:VAL:HG13	1:X:271:THR:CG2	2.48	0.44
1:X:407:GLN:O	1:X:412:LEU:HD21	2.17	0.44
1:X:334:GLY:HA3	4:X:802:MGD:C13	2.48	0.43
1:X:459:ASP:O	1:X:460:ARG:HG2	2.17	0.43
1:X:618:LEU:HD13	1:X:685:VAL:O	2.19	0.43
1:X:192:LYS:NZ	1:X:213:ASP:OD1	2.49	0.43
1:X:358:LYS:NZ	7:X:2137:HOH:O	2.51	0.43
1:X:684:ARG:HD3	7:X:2260:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:151:SER:HB3	1:X:317:MET:CE	2.49	0.43
1:X:171:PHE:CE2	1:X:230:MET:HE1	2.54	0.43
1:X:161:ILE:HD11	1:X:458:ALA:HB3	2.01	0.42
1:X:207:GLU:O	1:X:210:ARG:HB2	2.19	0.42
1:X:400:ILE:O	1:X:427:VAL:HA	2.19	0.42
1:X:15:CYS:SG	1:X:37:ASN:HB3	2.59	0.42
1:X:5:VAL:HG22	1:X:18:ASN:OD1	2.20	0.42
1:X:264:PRO:HB2	1:X:275:ALA:HB1	2.02	0.41
1:X:622:ASP:O	1:X:623:GLU:HB2	2.21	0.41
1:X:5:VAL:HG11	1:X:522:GLU:O	2.21	0.41
1:X:139:VAL:HG21	7:X:2128:HOH:O	2.21	0.41
1:X:628:VAL:HB	1:X:635:ILE:HG22	2.03	0.41
1:X:204:ARG:HD3	1:X:651:TYR:CG	2.55	0.41
1:X:602:ALA:HB1	1:X:656:TRP:HZ2	1.85	0.41
4:X:802:MGD:H8	7:X:2240:HOH:O	2.21	0.41
1:X:8:CYS:HB3	2:X:800:SF4:S1	2.61	0.40
1:X:225:ALA:HB1	1:X:267:VAL:HG22	2.03	0.40
1:X:410:ALA:CA	3:X:801:2MD:HNG2	2.34	0.40
1:X:85:ASN:O	1:X:89:GLU:HG3	2.21	0.40
1:X:293:ILE:HD13	1:X:312:LEU:HD22	2.03	0.40
1:X:94:ILE:HD13	1:X:397:ALA:HB2	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	X	693/715 (97%)	668 (96%)	22 (3%)	3 (0%)	30 36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	303	TYR
1	X	411	GLU
1	X	654	TYR

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	X	569/584 (97%)	542 (95%)	27 (5%)	23 33

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	1	MET
1	X	3	LYS
1	X	23	ASN
1	X	27	VAL
1	X	43	LEU
1	X	71	ARG
1	X	75	LEU
1	X	183	ILE
1	X	236	GLU
1	X	267	VAL
1	X	413	SER
1	X	441	VAL
1	X	460	ARG
1	X	469	VAL
1	X	472	LYS
1	X	497	ASN
1	X	566	ILE
1	X	567	ASP
1	X	580	VAL
1	X	589	ARG
1	X	616	LYS
1	X	617	ARG
1	X	626	VAL
1	X	632	LYS

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Mol	Chain	Res	Type
1	X	635	ILE
1	X	638	ARG
1	X	686	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	280	GLN
1	X	301	GLN
1	X	336	ASN
1	X	339	GLN
1	X	388	HIS
1	X	609	GLN
1	X	696	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)

Of 5 ligands modelled in this entry, 1 is monoatomic and 1 is unknown - leaving 3 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	MGD	X	802	5	45,52,52	1.38	9 (20%)	54,81,81	1.97	10 (18%)
3	2MD	X	801	5	46,52,52	1.68	10 (21%)	61,81,81	2.78	19 (31%)
2	SF4	X	800	1	0,12,12	-	-	-		

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	MGD	X	802	5	-	0/22/66/66	0/6/6/6
3	2MD	X	801	5	1/1/11/13	6/22/66/66	0/6/6/6
2	SF4	X	800	1	-	-	0/6/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	801	2MD	C7-N8	4.48	1.52	1.45
3	X	801	2MD	O11-C7	4.32	1.49	1.43
3	X	801	2MD	C16-C15	3.33	1.50	1.42
4	X	802	MGD	C5-C4	2.98	1.47	1.38
3	X	801	2MD	C5-C4	2.75	1.46	1.38
3	X	801	2MD	C5-N7	-2.74	1.33	1.39
4	X	802	MGD	C6-N1	-2.67	1.33	1.38
4	X	802	MGD	C5-N7	-2.61	1.34	1.39
3	X	801	2MD	C17-N16	2.56	1.40	1.34
3	X	801	2MD	C4-N9	-2.48	1.31	1.38
4	X	802	MGD	C21-N22	-2.43	1.33	1.35
3	X	801	2MD	C6-N1	-2.41	1.34	1.38
4	X	802	MGD	C19-N19	2.37	1.39	1.34
4	X	802	MGD	C16-C17	2.31	1.48	1.42
4	X	802	MGD	C2-N2	2.29	1.39	1.34
4	X	802	MGD	C17-N18	-2.20	1.34	1.38
3	X	801	2MD	C15-N17	-2.15	1.34	1.38
3	X	801	2MD	C11-C12	2.12	1.54	1.53
4	X	802	MGD	C4-N9	-2.09	1.32	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	X	801	2MD	C11-O11-C7	14.24	131.84	112.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	X	801	2MD	O11-C7-N8	5.91	114.64	108.57
4	X	802	MGD	PA-O3B-PB	-5.29	114.67	132.83
4	X	802	MGD	C5-C4-N3	-5.24	119.97	128.46
3	X	801	2MD	O11-C11-C10	5.01	116.78	106.67
4	X	802	MGD	C2-N3-C4	4.91	121.05	112.30
3	X	801	2MD	C10-C11-C12	-4.89	101.95	112.14
3	X	801	2MD	C17-N18-C20	4.76	122.03	113.43
3	X	801	2MD	C5-C4-N3	-4.71	120.83	128.46
4	X	802	MGD	N9-C4-N3	4.02	134.00	125.94
3	X	801	2MD	N9-C4-N3	3.98	133.94	125.94
3	X	801	2MD	C2-N3-C4	3.98	119.39	112.30
4	X	802	MGD	C19-N20-C21	3.86	120.39	113.43
4	X	802	MGD	C6-C5-N7	3.79	137.30	130.25
4	X	802	MGD	O17-C17-C16	-3.00	120.36	127.24
3	X	801	2MD	C6-C5-N7	2.71	135.29	130.25
4	X	802	MGD	C4'-O4'-C1'	-2.68	103.55	109.47
3	X	801	2MD	O6-C6-C5	-2.61	119.67	126.60
3	X	801	2MD	PA-O3B-PB	-2.49	124.28	132.83
3	X	801	2MD	C17-N17-C15	-2.43	120.67	125.10
4	X	802	MGD	C4-C5-N7	-2.43	106.88	110.72
3	X	801	2MD	O14-C15-C16	-2.39	121.77	127.24
3	X	801	2MD	C7-C14-N15	2.38	113.61	108.76
3	X	801	2MD	C4'-O4'-C1'	-2.27	104.46	109.47
3	X	801	2MD	O4'-C4'-C3'	2.26	109.58	105.11
4	X	802	MGD	O4'-C1'-C2'	-2.20	101.83	106.64
3	X	801	2MD	O2A-PA-O5'	2.08	117.40	107.75
3	X	801	2MD	C11-C12-S12	2.08	115.21	110.16
3	X	801	2MD	C8-N9-C4	2.06	109.97	106.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	X	801	2MD	C12

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	801	2MD	C5'-O5'-PA-O1A
3	X	801	2MD	C5'-O5'-PA-O2A
3	X	801	2MD	C11-C10-O3A-PB
3	X	801	2MD	C5'-O5'-PA-O3B
3	X	801	2MD	O4'-C4'-C5'-O5'

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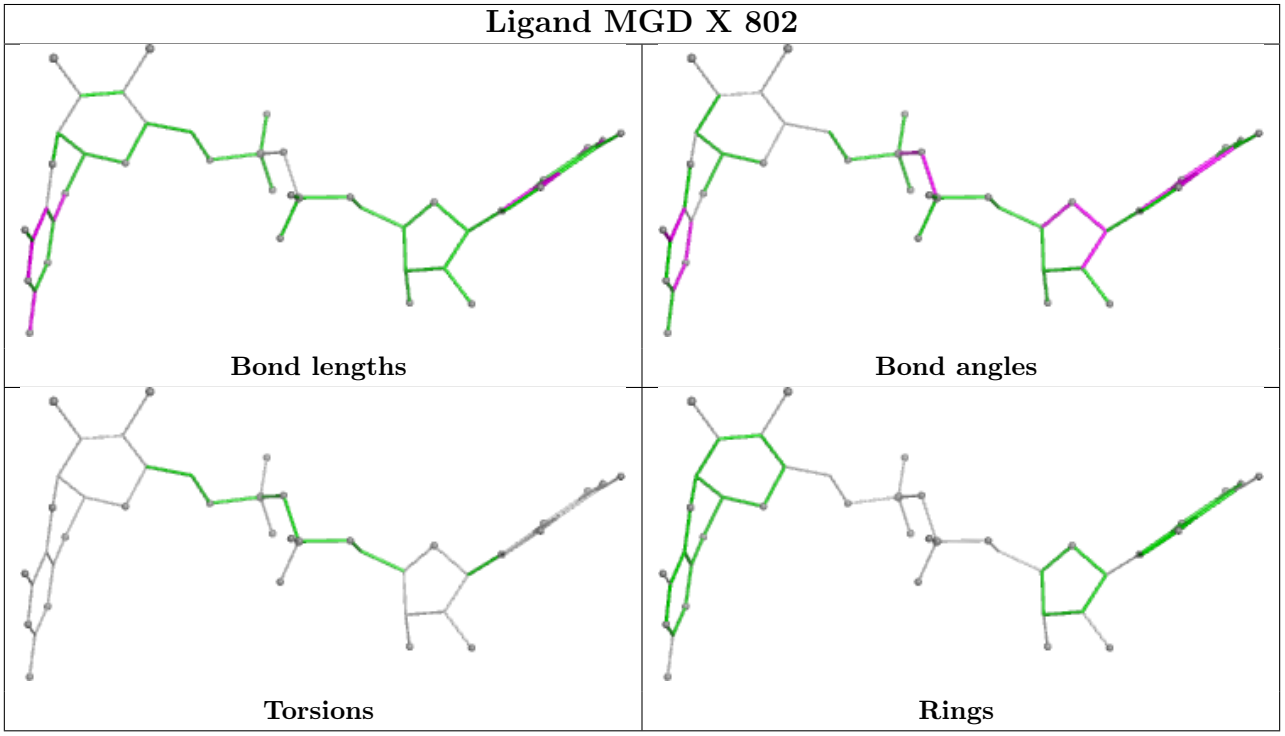
Mol	Chain	Res	Type	Atoms
3	X	801	2MD	PA-O3B-PB-O2B

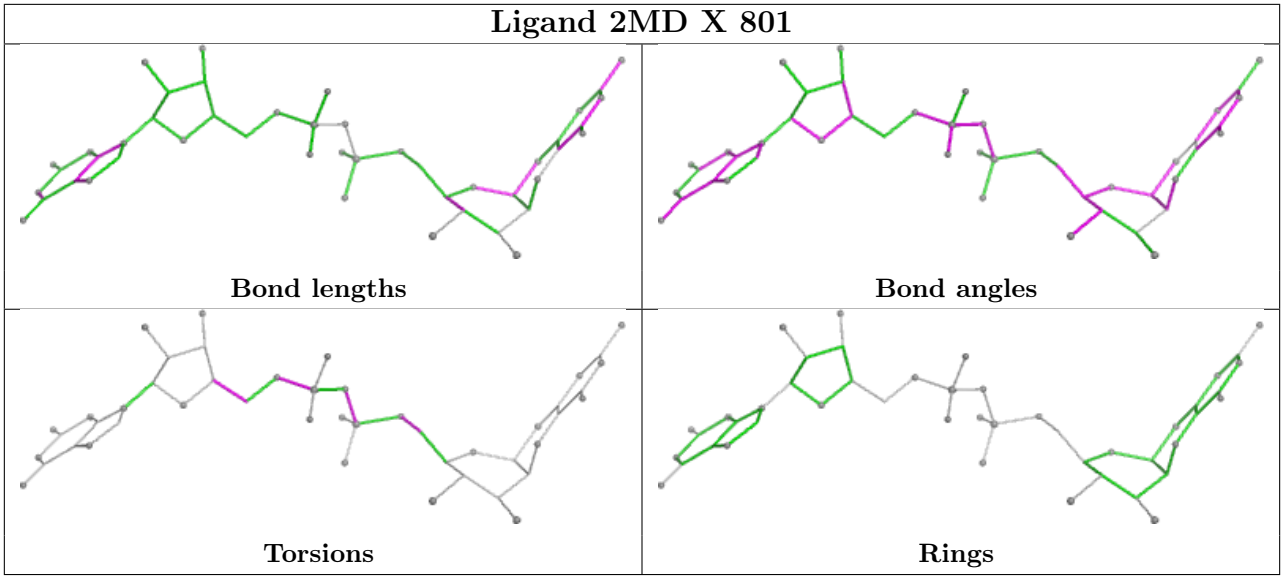
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	802	MGD	2	0
3	X	801	2MD	3	0
2	X	800	SF4	1	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 then 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.