



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 29, 2024 – 08:44 PM EST

PDB ID : 1FDO
Title : OXIDIZED FORM OF FORMATE DEHYDROGENASE H FROM E. COLI
Authors : Sun, P.D.; Boyington, J.C.
Deposited on : 1997-01-27
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

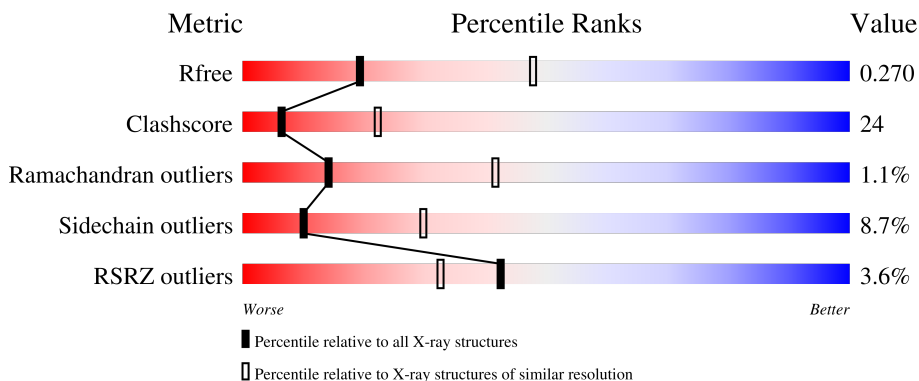
1 Overall quality at a glance

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))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 $\leq 5\%$. 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	715	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5742 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.

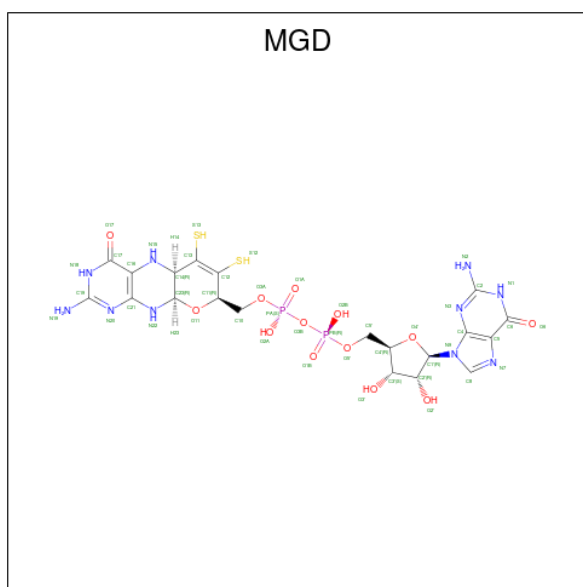
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	715	5575	3508	973	1060	33	1	0	0	0

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 3 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 (three-letter code: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



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

- Molecule 4 is MOLYBDENUM(VI) ION (three-letter code: 6MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mo	0	0
			1	1		

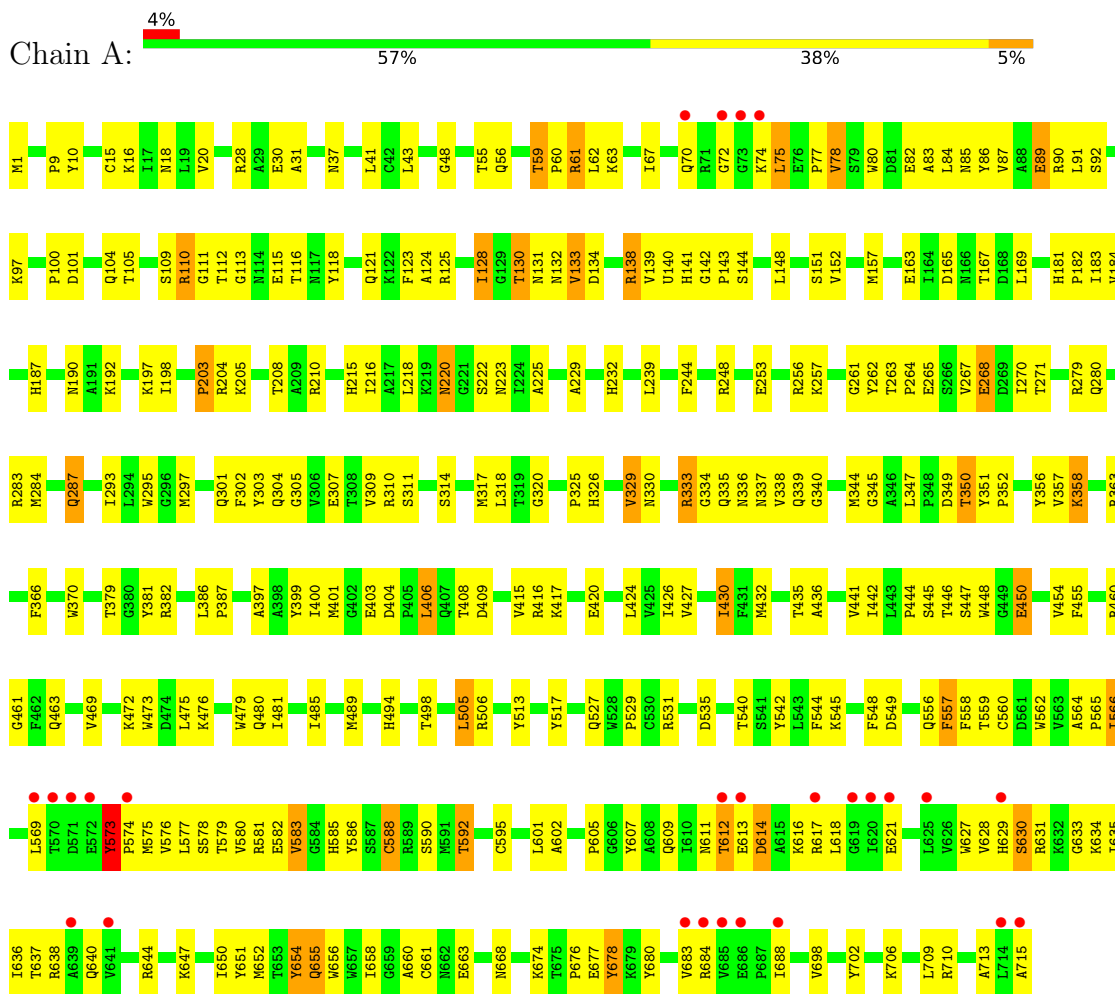
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	64	Total	O	0	0
			64	64		

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 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: FORMATE DEHYDROGENASE H



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	146.60Å 146.60Å 81.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80 41.86 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.0 (6.00-2.80) 93.5 (41.86-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.15 (at 2.81Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.192 , 0.281 0.214 , 0.270	Depositor DCC
R_{free} test set	978 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtrriage
Anisotropy	0.159	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5742	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6MO, MGD, SEC, SF4

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	0.56	0/5690	0.81	2/7719 (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	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	505	LEU	CA-CB-CG	7.11	131.65	115.30
1	A	75	LEU	CA-CB-CG	5.91	128.90	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	573	TYR	Sidechain
1	A	678	TYR	Sidechain

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	5575	0	5453	268	0
2	A	8	0	0	1	0
3	A	94	0	44	13	0
4	A	1	0	0	0	0
5	A	64	0	0	2	0
All	All	5742	0	5497	268	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 24.

All (268) 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:585:HIS:HA	1:A:592:THR:HG21	1.34	1.07
1:A:140:SEC:HA	1:A:297:MET:HE1	1.52	0.92
1:A:614:ASP:HB3	1:A:647:LYS:HE3	1.54	0.90
1:A:573:TYR:HD1	1:A:684:ARG:HB2	1.36	0.90
1:A:582:GLU:HG2	1:A:655:GLN:HE22	1.36	0.88
1:A:588:CYS:HB2	3:A:801:MGD:O1B	1.75	0.85
1:A:148:LEU:HD21	1:A:329:VAL:HG11	1.57	0.85
1:A:580:VAL:HG22	1:A:581:ARG:H	1.41	0.84
1:A:613:GLU:HB3	1:A:647:LYS:NZ	1.92	0.84
1:A:302:PHE:HA	1:A:677:GLU:HG3	1.56	0.84
1:A:59:THR:HG21	1:A:432:MET:O	1.79	0.81
1:A:16:LYS:HE2	1:A:463:GLN:NE2	1.94	0.81
1:A:239:LEU:HD22	1:A:287:GLN:HE22	1.46	0.80
1:A:167:THR:HG22	1:A:326:HIS:O	1.82	0.79
1:A:614:ASP:HB2	1:A:617:ARG:HH22	1.47	0.79
1:A:582:GLU:HG2	1:A:655:GLN:NE2	1.97	0.79
1:A:157:MET:HE3	1:A:330:ASN:HB3	1.63	0.79
1:A:139:VAL:HG13	1:A:678:TYR:HE2	1.48	0.78
1:A:110:ARG:HD2	1:A:336:ASN:HD21	1.51	0.76
1:A:573:TYR:CD1	1:A:684:ARG:HB2	2.23	0.72
1:A:305:GLY:O	1:A:309:VAL:HG23	1.90	0.72
1:A:232:HIS:CE1	1:A:263:THR:HG22	2.23	0.72
1:A:229:ALA:HB2	1:A:267:VAL:HG21	1.71	0.72
1:A:660:ALA:O	1:A:663:GLU:HB2	1.89	0.72
1:A:115:GLU:HG2	1:A:498:THR:HB	1.71	0.71
1:A:78:VAL:HG13	1:A:82:GLU:HB3	1.74	0.69
1:A:295:TRP:CZ2	1:A:309:VAL:HG13	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:THR:HG22	1:A:654:TYR:CD2	2.28	0.69
1:A:110:ARG:HD2	1:A:336:ASN:ND2	2.09	0.67
1:A:408:THR:HG22	1:A:654:TYR:HD2	1.59	0.67
1:A:479:TRP:CZ3	1:A:480:GLN:HG3	2.29	0.67
1:A:203:PRO:HG3	1:A:218:LEU:O	1.94	0.67
1:A:628:VAL:O	1:A:634:LYS:HA	1.94	0.67
1:A:333:ARG:HH11	1:A:333:ARG:HB3	1.60	0.67
1:A:139:VAL:HG13	1:A:678:TYR:CE2	2.30	0.66
1:A:613:GLU:HB3	1:A:647:LYS:HZ1	1.60	0.66
1:A:335:GLN:HG2	3:A:802:MGD:S13	2.36	0.66
1:A:134:ASP:OD2	1:A:138:ARG:HD2	1.96	0.66
1:A:151:SER:OG	1:A:310:ARG:HD3	1.96	0.65
1:A:239:LEU:HD22	1:A:287:GLN:NE2	2.11	0.65
1:A:140:SEC:HA	1:A:297:MET:CE	2.27	0.65
1:A:220:ASN:HD22	1:A:220:ASN:H	1.44	0.65
1:A:613:GLU:HB3	1:A:647:LYS:HZ2	1.60	0.65
1:A:256:ARG:HH12	1:A:257:LYS:HZ2	1.44	0.64
1:A:676:PRO:HG2	1:A:678:TYR:CE2	2.32	0.64
1:A:267:VAL:HG12	1:A:271:THR:HG23	1.81	0.63
1:A:279:ARG:HB3	1:A:283:ARG:NH1	2.13	0.62
1:A:573:TYR:CE1	1:A:684:ARG:HD2	2.34	0.62
1:A:43:LEU:HD21	1:A:601:LEU:HD11	1.82	0.62
1:A:110:ARG:HA	1:A:336:ASN:HD21	1.65	0.62
1:A:86:TYR:CE2	1:A:90:ARG:NH2	2.68	0.61
1:A:100:PRO:HB3	1:A:128:ILE:O	2.00	0.61
1:A:109:SER:HB3	1:A:338:VAL:HA	1.83	0.61
1:A:279:ARG:HB3	1:A:283:ARG:HH12	1.65	0.60
1:A:295:TRP:HZ3	1:A:329:VAL:HG22	1.65	0.60
1:A:351:TYR:CZ	1:A:357:VAL:HG12	2.36	0.60
1:A:630:SER:N	1:A:633:GLY:O	2.34	0.60
1:A:335:GLN:HA	1:A:586:TYR:OH	2.02	0.60
1:A:318:LEU:HD13	1:A:557:PHE:CZ	2.38	0.59
1:A:85:ASN:O	1:A:89:GLU:HB2	2.03	0.59
1:A:565:PRO:HG2	1:A:680:TYR:CD2	2.37	0.59
1:A:244:PHE:CE1	1:A:248:ARG:HD3	2.38	0.58
1:A:310:ARG:HB3	1:A:558:PHE:HD2	1.68	0.58
1:A:86:TYR:O	1:A:90:ARG:HG2	2.04	0.58
1:A:121:GLN:HA	1:A:133:VAL:HG11	1.86	0.58
1:A:485:ILE:HG22	1:A:489:MET:CE	2.34	0.58
1:A:350:THR:HG23	1:A:356:TYR:CD2	2.38	0.57
1:A:578:SER:HB3	1:A:651:TYR:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LYS:HE2	1:A:463:GLN:HE21	1.69	0.57
1:A:408:THR:HG21	3:A:801:MGD:O2A	2.05	0.57
1:A:318:LEU:HD13	1:A:557:PHE:HZ	1.69	0.57
1:A:607:TYR:CD1	1:A:640:GLN:HB2	2.40	0.57
1:A:573:TYR:HE1	1:A:684:ARG:HD2	1.70	0.57
1:A:183:ILE:O	1:A:187:HIS:HD2	1.88	0.56
1:A:256:ARG:HB3	1:A:256:ARG:NH1	2.21	0.56
1:A:506:ARG:HD2	1:A:513:TYR:O	2.04	0.56
1:A:629:HIS:CE1	1:A:634:LYS:HE3	2.40	0.56
1:A:18:ASN:HB2	1:A:30:GLU:HG3	1.86	0.56
1:A:566:ILE:HD12	1:A:668:ASN:HB3	1.86	0.56
1:A:629:HIS:CE1	1:A:634:LYS:HG3	2.41	0.56
1:A:123:PHE:CZ	1:A:128:ILE:HD11	2.41	0.55
1:A:279:ARG:O	1:A:283:ARG:HG3	2.06	0.55
1:A:256:ARG:HH22	1:A:257:LYS:NZ	2.04	0.55
1:A:204:ARG:HD2	1:A:651:TYR:CE2	2.41	0.55
1:A:404:ASP:CB	1:A:588:CYS:SG	2.95	0.55
1:A:460:ARG:O	1:A:527:GLN:HA	2.06	0.55
1:A:256:ARG:HB3	1:A:256:ARG:HH11	1.72	0.55
1:A:461:GLY:HA2	1:A:527:GLN:HA	1.88	0.55
1:A:15:CYS:SG	1:A:183:ILE:HG12	2.47	0.55
1:A:248:ARG:NH1	1:A:548:PHE:CE2	2.75	0.55
1:A:15:CYS:SG	1:A:37:ASN:HB3	2.46	0.54
1:A:401:MET:O	1:A:403:GLU:HG3	2.07	0.54
1:A:582:GLU:CG	1:A:655:GLN:HE22	2.15	0.54
1:A:101:ASP:HA	1:A:130:THR:CG2	2.37	0.54
1:A:629:HIS:HA	1:A:634:LYS:HA	1.90	0.54
1:A:650:ILE:HD11	1:A:683:VAL:HG21	1.89	0.54
1:A:253:GLU:HA	1:A:256:ARG:HH11	1.72	0.53
1:A:75:LEU:HD21	1:A:442:ILE:CD1	2.38	0.53
1:A:579:THR:HA	1:A:652:MET:O	2.09	0.53
1:A:333:ARG:HB3	1:A:333:ARG:NH1	2.24	0.53
1:A:430:ILE:HD12	1:A:445:SER:OG	2.07	0.53
1:A:585:HIS:NE2	1:A:602:ALA:HB3	2.24	0.53
1:A:637:THR:HG21	1:A:652:MET:HE3	1.91	0.53
1:A:426:ILE:HG12	1:A:441:VAL:HG13	1.90	0.53
1:A:109:SER:HB3	1:A:338:VAL:CA	2.38	0.53
1:A:617:ARG:CZ	1:A:617:ARG:HB3	2.39	0.53
1:A:169:LEU:HD12	1:A:197:LYS:CE	2.40	0.52
1:A:60:PRO:HG2	1:A:713:ALA:CB	2.39	0.52
1:A:163:GLU:OE1	1:A:325:PRO:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLY:HA2	1:A:455:PHE:CE1	2.45	0.52
1:A:31:ALA:HB2	1:A:41:LEU:HG	1.91	0.52
1:A:397:ALA:HA	1:A:424:LEU:O	2.10	0.52
1:A:627:TRP:CD1	1:A:688:ILE:HD11	2.45	0.52
1:A:192:LYS:HB2	1:A:198:ILE:HD11	1.92	0.52
1:A:702:TYR:CE1	1:A:706:LYS:HD2	2.44	0.51
1:A:311:SER:O	1:A:314:SER:HB2	2.10	0.51
1:A:637:THR:HG21	1:A:652:MET:CE	2.40	0.51
1:A:333:ARG:HG3	1:A:339:GLN:HE21	1.75	0.51
1:A:406:LEU:HD12	1:A:435:THR:HA	1.92	0.51
1:A:140:SEC:SE	1:A:141:HIS:HD2	2.44	0.51
1:A:264:PRO:HG2	1:A:279:ARG:NH1	2.26	0.51
1:A:169:LEU:HD12	1:A:197:LYS:HE3	1.93	0.51
1:A:583:VAL:HA	3:A:802:MGD:N19	2.25	0.51
1:A:87:VAL:HG11	1:A:485:ILE:HD13	1.93	0.50
1:A:581:ARG:HH11	3:A:802:MGD:H15	1.59	0.50
1:A:253:GLU:HA	1:A:256:ARG:NH1	2.27	0.50
1:A:485:ILE:HG22	1:A:489:MET:HE3	1.92	0.50
1:A:611:ASN:HB3	1:A:614:ASP:OD2	2.11	0.50
1:A:335:GLN:HA	1:A:586:TYR:HH	1.76	0.50
1:A:562:TRP:CH2	1:A:564:ALA:HB2	2.46	0.50
1:A:110:ARG:HD3	1:A:335:GLN:OE1	2.12	0.50
1:A:267:VAL:CG1	1:A:271:THR:HG23	2.41	0.50
1:A:386:LEU:HB3	1:A:387:PRO:HD3	1.94	0.50
1:A:220:ASN:HD22	1:A:220:ASN:N	2.10	0.50
1:A:280:GLN:O	1:A:284:MET:HB2	2.12	0.50
1:A:263:THR:O	1:A:267:VAL:HG23	2.12	0.49
1:A:334:GLY:HA3	3:A:802:MGD:S12	2.52	0.49
1:A:485:ILE:O	1:A:489:MET:HG3	2.12	0.49
1:A:513:TYR:HD2	1:A:531:ARG:O	1.94	0.49
1:A:223:ASN:HD22	1:A:223:ASN:H	1.59	0.49
1:A:479:TRP:NE1	1:A:498:THR:HG22	2.27	0.49
1:A:181:HIS:HB2	1:A:184:VAL:HB	1.93	0.49
1:A:297:MET:HE1	3:A:801:MGD:S13	2.53	0.49
1:A:628:VAL:O	1:A:635:ILE:N	2.45	0.49
1:A:430:ILE:HD11	1:A:446:THR:C	2.32	0.49
1:A:270:ILE:HD13	1:A:562:TRP:CZ3	2.48	0.49
1:A:566:ILE:HD12	1:A:668:ASN:CG	2.34	0.49
1:A:420:GLU:O	1:A:420:GLU:HG2	2.13	0.48
1:A:585:HIS:CD2	1:A:602:ALA:HB3	2.48	0.48
1:A:101:ASP:HA	1:A:130:THR:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:ASP:HB2	1:A:617:ARG:NH2	2.22	0.48
1:A:56:GLN:OE1	1:A:710:ARG:NH1	2.47	0.48
1:A:62:LEU:HB3	1:A:444:PRO:HB3	1.95	0.48
1:A:605:PRO:HG3	1:A:698:VAL:CG2	2.44	0.48
1:A:479:TRP:HE1	1:A:498:THR:HG22	1.79	0.48
1:A:583:VAL:HA	3:A:802:MGD:H191	1.79	0.48
1:A:203:PRO:HB3	1:A:220:ASN:ND2	2.28	0.47
1:A:609:GLN:HB2	1:A:651:TYR:HB2	1.95	0.47
1:A:337:ASN:OD1	1:A:340:GLY:HA3	2.13	0.47
1:A:404:ASP:HB2	1:A:588:CYS:SG	2.54	0.47
1:A:349:ASP:HB3	1:A:379:THR:HG23	1.97	0.47
1:A:144:SER:O	1:A:148:LEU:HB2	2.15	0.47
1:A:607:TYR:HA	1:A:638:ARG:O	2.14	0.47
1:A:658:ILE:HD11	1:A:702:TYR:HA	1.96	0.47
1:A:43:LEU:HD21	1:A:601:LEU:CD1	2.43	0.47
1:A:63:LYS:HG2	1:A:473:TRP:CE2	2.49	0.47
1:A:80:TRP:CE2	1:A:476:LYS:HD2	2.50	0.47
1:A:115:GLU:OE2	1:A:454:VAL:HG23	2.14	0.47
1:A:265:GLU:OE2	1:A:279:ARG:NH2	2.48	0.47
1:A:485:ILE:HG22	1:A:489:MET:HE2	1.97	0.47
1:A:366:PHE:HD2	1:A:370:TRP:CZ2	2.32	0.47
1:A:548:PHE:O	1:A:549:ASP:HB2	2.15	0.47
1:A:270:ILE:HD13	1:A:562:TRP:CE3	2.50	0.46
1:A:20:VAL:HG21	1:A:28:ARG:CZ	2.46	0.46
1:A:293:ILE:HG22	1:A:295:TRP:HE3	1.80	0.46
1:A:61:ARG:HH2	1:A:450:GLU:CD	2.19	0.46
1:A:430:ILE:HG12	1:A:447:SER:HB2	1.97	0.46
1:A:75:LEU:HD21	1:A:442:ILE:HD11	1.96	0.46
1:A:124:ALA:HA	1:A:128:ILE:HG13	1.96	0.46
1:A:244:PHE:CD2	1:A:320:GLY:HA2	2.50	0.46
1:A:436:ALA:O	1:A:442:ILE:HD11	2.16	0.46
1:A:430:ILE:HD13	3:A:801:MGD:C6	2.45	0.46
1:A:77:PRO:HD3	1:A:715:ALA:OXT	2.15	0.46
1:A:118:TYR:CD1	1:A:505:LEU:HD23	2.50	0.46
1:A:142:GLY:N	1:A:143:PRO:CD	2.79	0.46
1:A:203:PRO:HB3	1:A:220:ASN:HD21	1.81	0.46
1:A:566:ILE:HD12	1:A:668:ASN:CB	2.45	0.46
1:A:580:VAL:HG23	3:A:802:MGD:O1B	2.16	0.46
1:A:358:LYS:NZ	1:A:358:LYS:HB3	2.31	0.46
1:A:416:ARG:HD2	5:A:867:HOH:O	2.16	0.46
1:A:569:LEU:HB3	1:A:574:PRO:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:TYR:CE2	3:A:801:MGD:O11	2.70	0.45
1:A:577:LEU:HD11	1:A:652:MET:HB2	1.98	0.45
1:A:627:TRP:HB3	1:A:629:HIS:CE1	2.52	0.45
1:A:307:GLU:HG2	1:A:560:CYS:SG	2.57	0.45
1:A:357:VAL:O	1:A:363:ARG:NE	2.47	0.45
1:A:123:PHE:HE1	1:A:489:MET:HE3	1.82	0.45
1:A:131:ASN:ND2	1:A:357:VAL:HG21	2.31	0.45
1:A:350:THR:HA	1:A:356:TYR:HA	1.99	0.45
1:A:151:SER:HG	1:A:310:ARG:HD3	1.81	0.45
1:A:205:LYS:HG3	1:A:644:ARG:O	2.17	0.45
1:A:101:ASP:OD1	1:A:130:THR:HG23	2.17	0.45
1:A:614:ASP:CB	1:A:647:LYS:HE3	2.37	0.45
1:A:55:THR:O	1:A:56:GLN:HB2	2.17	0.44
1:A:152:VAL:O	1:A:548:PHE:O	2.35	0.44
1:A:573:TYR:C	1:A:575:MET:H	2.20	0.44
1:A:580:VAL:HG22	1:A:581:ARG:N	2.21	0.44
1:A:301:GLN:O	1:A:677:GLU:HA	2.17	0.44
1:A:223:ASN:H	1:A:223:ASN:ND2	2.16	0.44
1:A:544:PHE:HB3	1:A:548:PHE:CD1	2.52	0.44
1:A:59:THR:HG22	1:A:60:PRO:HD2	2.00	0.44
1:A:232:HIS:HE1	1:A:263:THR:HG22	1.78	0.44
1:A:529:PRO:HD2	1:A:540:THR:CB	2.47	0.44
1:A:635:ILE:HD13	1:A:635:ILE:HA	1.77	0.44
1:A:59:THR:HG22	1:A:432:MET:HB3	2.00	0.44
1:A:84:LEU:HD21	1:A:481:ILE:HG23	1.98	0.44
1:A:344:MET:O	1:A:352:PRO:HB3	2.18	0.44
1:A:569:LEU:HD21	1:A:576:VAL:HG22	2.00	0.44
1:A:123:PHE:CZ	1:A:489:MET:HE1	2.53	0.43
1:A:317:MET:HE3	5:A:826:HOH:O	2.17	0.43
1:A:169:LEU:HD12	1:A:197:LYS:NZ	2.33	0.43
1:A:311:SER:OG	1:A:559:THR:HG22	2.17	0.43
1:A:409:ASP:HB2	1:A:415:VAL:HG21	1.99	0.43
1:A:569:LEU:HD13	1:A:574:PRO:O	2.18	0.43
1:A:702:TYR:CZ	1:A:706:LYS:HD2	2.54	0.43
1:A:139:VAL:HG11	3:A:801:MGD:H23	2.00	0.43
1:A:210:ARG:HD2	1:A:210:ARG:HA	1.84	0.43
1:A:400:ILE:O	1:A:427:VAL:HA	2.19	0.43
1:A:118:TYR:O	1:A:121:GLN:HG3	2.18	0.43
1:A:205:LYS:HA	1:A:215:HIS:HE1	1.83	0.43
1:A:183:ILE:O	1:A:187:HIS:CD2	2.70	0.43
1:A:542:TYR:OH	1:A:545:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LEU:HD12	1:A:489:MET:CE	2.49	0.42
1:A:225:ALA:HB1	1:A:267:VAL:HG13	2.01	0.42
1:A:573:TYR:C	1:A:575:MET:N	2.72	0.42
1:A:581:ARG:HA	1:A:655:GLN:OE1	2.19	0.42
1:A:70:GLN:HG2	1:A:72:GLY:H	1.85	0.42
1:A:48:GLY:HA2	1:A:595:CYS:SG	2.59	0.42
1:A:582:GLU:OE2	1:A:656:TRP:HZ2	2.02	0.42
1:A:417:LYS:HD2	1:A:420:GLU:OE1	2.20	0.42
1:A:432:MET:O	1:A:709:LEU:HD22	2.19	0.42
1:A:358:LYS:O	1:A:363:ARG:NH2	2.52	0.42
1:A:105:THR:OG1	1:A:133:VAL:HG13	2.20	0.42
1:A:60:PRO:HG2	1:A:713:ALA:HB3	2.02	0.41
1:A:261:GLY:O	1:A:263:THR:HG23	2.19	0.41
1:A:661:CYS:SG	3:A:801:MGD:N19	2.93	0.41
1:A:612:THR:HG22	1:A:616:LYS:HE3	2.02	0.41
1:A:345:GLY:C	1:A:347:LEU:H	2.24	0.41
1:A:631:ARG:H	1:A:631:ARG:HG3	1.68	0.41
1:A:344:MET:HA	1:A:352:PRO:HB3	2.03	0.41
1:A:472:LYS:HD3	1:A:472:LYS:HA	1.80	0.41
1:A:9:PRO:HD3	1:A:448:TRP:CE2	2.55	0.41
1:A:215:HIS:HD2	1:A:216:ILE:N	2.18	0.41
1:A:310:ARG:HB3	1:A:558:PHE:CD2	2.52	0.41
1:A:67:ILE:HD11	1:A:83:ALA:HA	2.03	0.41
1:A:479:TRP:CE3	1:A:480:GLN:HG3	2.55	0.41
1:A:10:TYR:HB2	2:A:800:SF4:S3	2.61	0.41
1:A:60:PRO:CG	1:A:713:ALA:HB3	2.51	0.41
1:A:90:ARG:HB3	1:A:424:LEU:HD22	2.03	0.41
1:A:215:HIS:C	1:A:215:HIS:CD2	2.95	0.41
1:A:430:ILE:HD11	1:A:446:THR:O	2.21	0.41
1:A:138:ARG:HA	1:A:138:ARG:NE	2.35	0.40
1:A:627:TRP:HB3	1:A:629:HIS:HE1	1.85	0.40
1:A:347:LEU:HD23	1:A:347:LEU:HA	1.85	0.40
1:A:444:PRO:HB2	1:A:475:LEU:HD22	2.03	0.40
1:A:104:GLN:OE1	1:A:381:TYR:HB2	2.22	0.40
1:A:121:GLN:HB2	1:A:125:ARG:NH1	2.36	0.40
1:A:222:SER:HA	1:A:562:TRP:NE1	2.37	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	712/715 (100%)	644 (90%)	60 (8%)	8 (1%)	14 41

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	GLU
1	A	612	THR
1	A	262	TYR
1	A	74	LYS
1	A	111	GLY
1	A	132	ASN
1	A	406	LEU
1	A	566	ILE

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	584/584 (100%)	533 (91%)	51 (9%)	10 30

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	59	THR
1	A	61	ARG

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Mol	Chain	Res	Type
1	A	78	VAL
1	A	89	GLU
1	A	92	SER
1	A	97	LYS
1	A	110	ARG
1	A	112	THR
1	A	116	THR
1	A	128	ILE
1	A	130	THR
1	A	133	VAL
1	A	138	ARG
1	A	165	ASP
1	A	182	PRO
1	A	190	ASN
1	A	203	PRO
1	A	208	THR
1	A	220	ASN
1	A	268	GLU
1	A	287	GLN
1	A	303	TYR
1	A	304	GLN
1	A	329	VAL
1	A	333	ARG
1	A	350	THR
1	A	358	LYS
1	A	382	ARG
1	A	399	TYR
1	A	430	ILE
1	A	450	GLU
1	A	469	VAL
1	A	494	HIS
1	A	517	TYR
1	A	535	ASP
1	A	556	GLN
1	A	557	PHE
1	A	573	TYR
1	A	583	VAL
1	A	588	CYS
1	A	590	SER
1	A	592	THR
1	A	614	ASP
1	A	618	LEU

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Mol	Chain	Res	Type
1	A	621	GLU
1	A	630	SER
1	A	636	ILE
1	A	654	TYR
1	A	655	GLN
1	A	674	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	220	ASN
1	A	280	GLN
1	A	287	GLN
1	A	321	ASN
1	A	336	ASN
1	A	339	GLN
1	A	388	HIS
1	A	392	HIS
1	A	463	GLN
1	A	527	GLN
1	A	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - 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
3	MGD	A	802	4	41,52,52	1.64	5 (12%)	40,81,81	1.34	2 (5%)
3	MGD	A	801	4	41,52,52	1.18	4 (9%)	40,81,81	1.47	4 (10%)
2	SF4	A	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
3	MGD	A	802	4	-	1/18/66/66	0/6/6/6
3	MGD	A	801	4	-	7/18/66/66	0/6/6/6
2	SF4	A	800	1	-	-	0/6/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	MGD	C23-C14	-7.19	1.47	1.53
3	A	801	MGD	C5-C6	-3.50	1.40	1.47
3	A	802	MGD	O11-C23	-3.36	1.39	1.43
3	A	802	MGD	C5-C4	-3.28	1.34	1.43
3	A	802	MGD	C5-C6	-2.71	1.41	1.47
3	A	801	MGD	C16-C21	2.34	1.42	1.38
3	A	801	MGD	C23-C14	-2.22	1.51	1.53
3	A	802	MGD	C2'-C1'	-2.16	1.50	1.53
3	A	801	MGD	PA-O2A	-2.08	1.45	1.55

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	MGD	O11-C23-C14	5.50	112.63	108.96
3	A	801	MGD	C19-N20-C21	4.83	122.15	113.43
3	A	802	MGD	C19-N20-C21	4.74	121.99	113.43
3	A	802	MGD	O4'-C1'-C2'	-2.62	103.10	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	MGD	O17-C17-C16	-2.56	121.37	127.24
3	A	801	MGD	N18-C19-N20	-2.24	119.14	123.32

There are no chirality outliers.

All (8) torsion outliers are listed below:

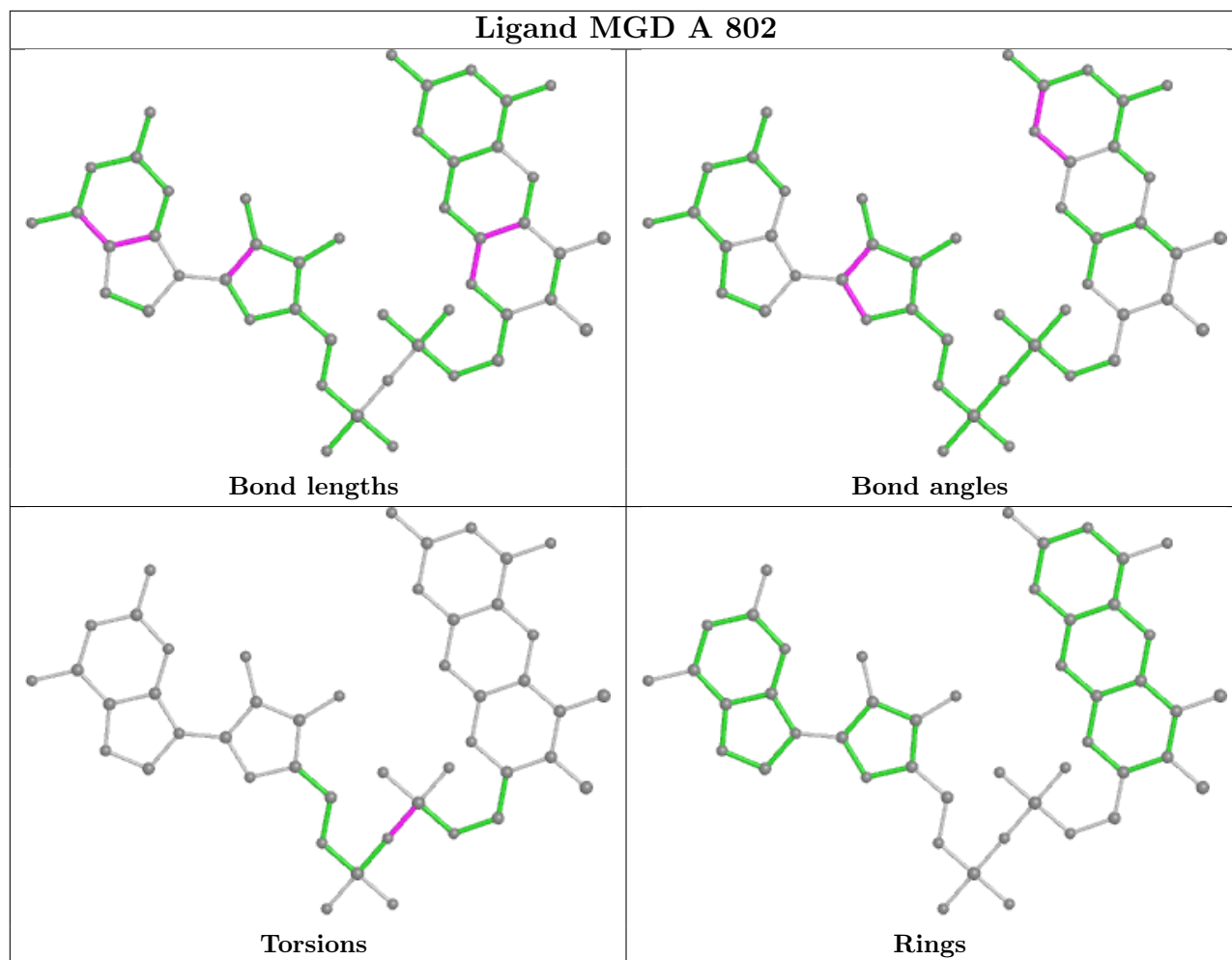
Mol	Chain	Res	Type	Atoms
3	A	801	MGD	C5'-O5'-PB-O1B
3	A	801	MGD	C5'-O5'-PB-O2B
3	A	801	MGD	O3A-C10-C11-O11
3	A	801	MGD	O3A-C10-C11-C12
3	A	801	MGD	C10-O3A-PA-O3B
3	A	802	MGD	PB-O3B-PA-O2A
3	A	801	MGD	O4'-C4'-C5'-O5'
3	A	801	MGD	C5'-O5'-PB-O3B

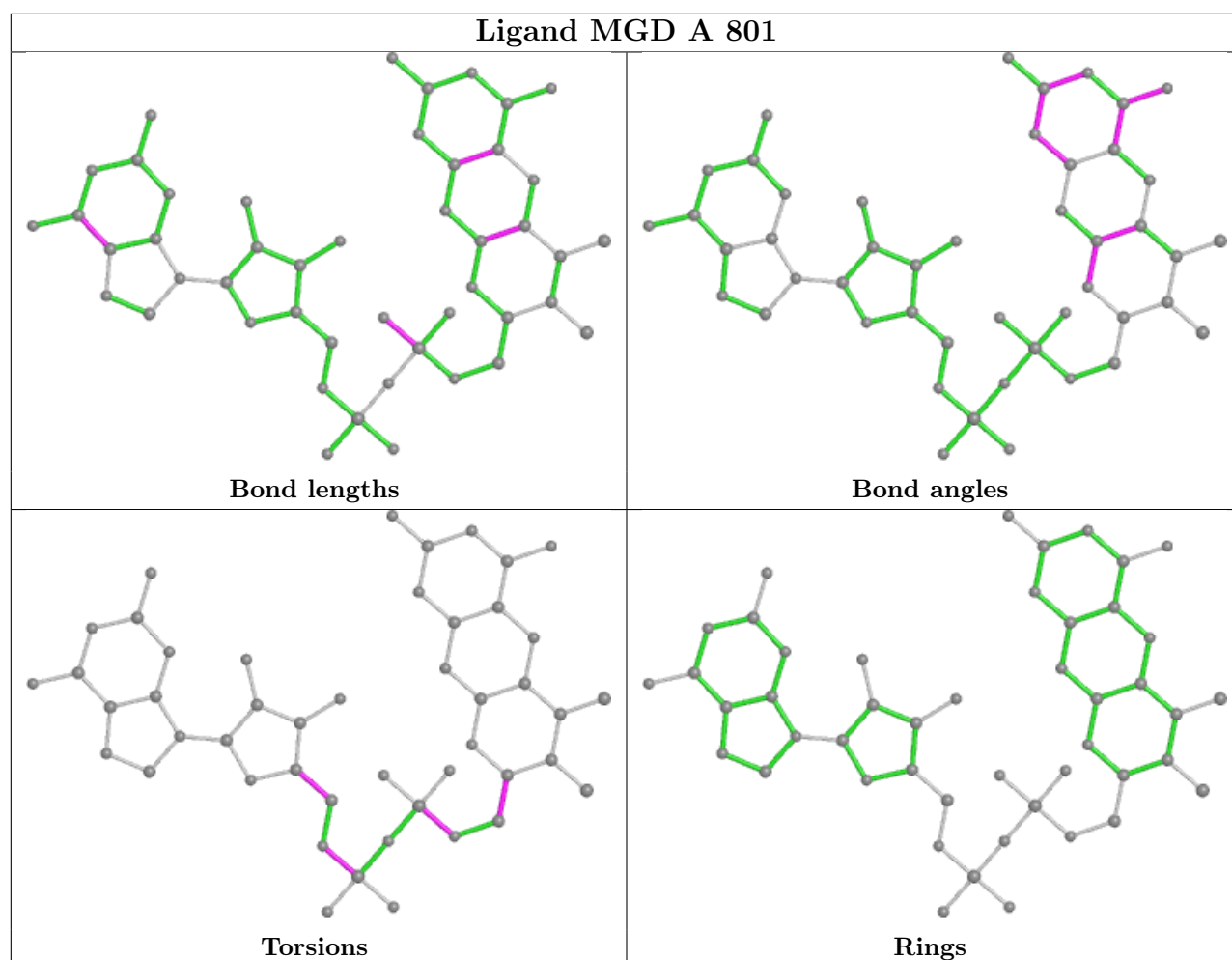
There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	MGD	6	0
3	A	801	MGD	7	0
2	A	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	714/715 (99%)	0.09	26 (3%) 42 32	5, 21, 42, 72	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	571	ASP	7.3
1	A	572	GLU	5.8
1	A	613	GLU	4.4
1	A	621	GLU	3.8
1	A	570	THR	3.7
1	A	574	PRO	3.6
1	A	72	GLY	3.6
1	A	641	VAL	3.2
1	A	625	LEU	3.2
1	A	688	ILE	3.1
1	A	629	HIS	2.9
1	A	715	ALA	2.8
1	A	714	LEU	2.7
1	A	73	GLY	2.7
1	A	686	GLU	2.6
1	A	74	LYS	2.5
1	A	70	GLN	2.4
1	A	684	ARG	2.4
1	A	569	LEU	2.4
1	A	620	ILE	2.4
1	A	685	VAL	2.3
1	A	612	THR	2.3
1	A	619	GLY	2.3
1	A	683	VAL	2.2
1	A	617	ARG	2.2
1	A	639	ALA	2.1

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 monosaccharides in this entry.

6.4 Ligands [i](#)

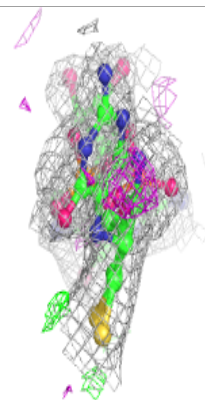
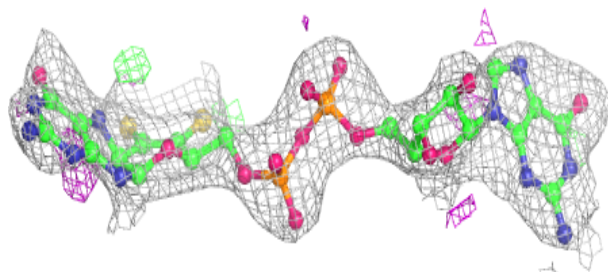
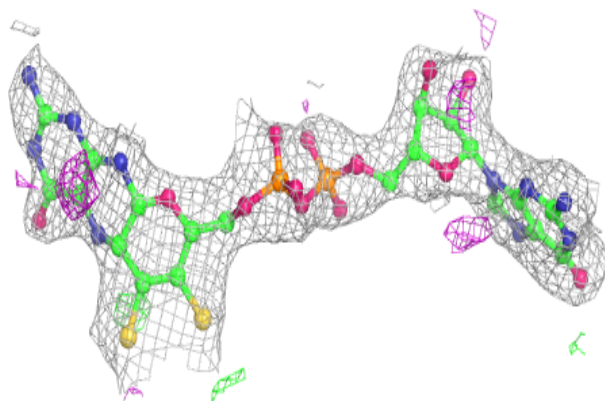
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MGD	A	801	47/47	0.96	0.16	12,21,26,26	0
3	MGD	A	802	47/47	0.96	0.15	17,22,25,27	0
4	6MO	A	803	1/1	0.97	0.08	25,25,25,25	0
2	SF4	A	800	8/8	0.98	0.15	11,13,14,14	0

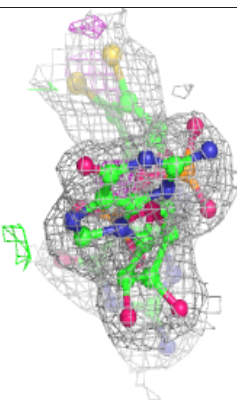
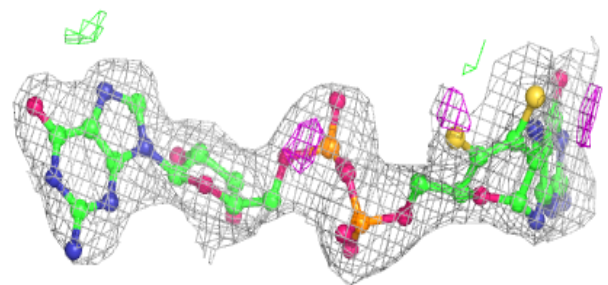
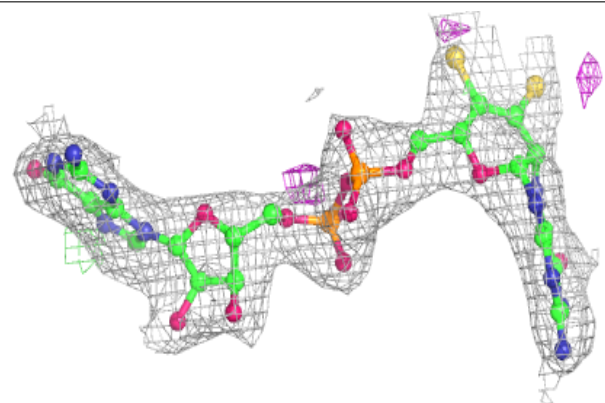
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MGD A 801:

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

**Electron density around MGD A 802:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.