Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 09:26 PM EST

PDB ID	:	1SQI
Title	:	Structural basis for inhibitor selectivity revealed by crystal structures of plant and mammalian 4-hydroxyphenylpyruvate dioxygenases
Authors	:	Yang, C.; Pflugrath, J.W.; Camper, D.L.; Foster, M.L.; Pernich, D.J.; Walsh, T.A.
Deposited on	:	2004-03-18
Resolution	:	2.15 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:

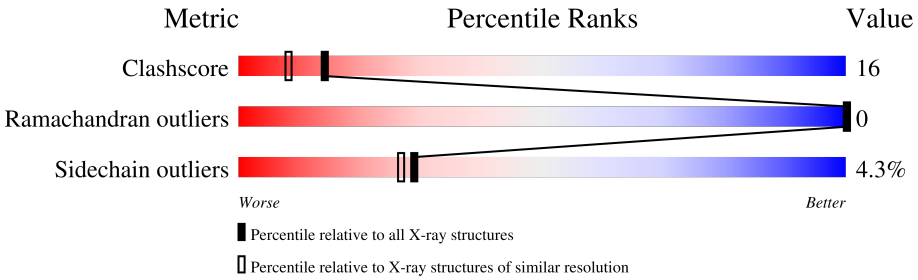
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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	A	393	66% 19% • 13%
1	B	393	64% 19% • 13%

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	869	A	1501	-	X	X	-
3	869	B	1502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6105 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.

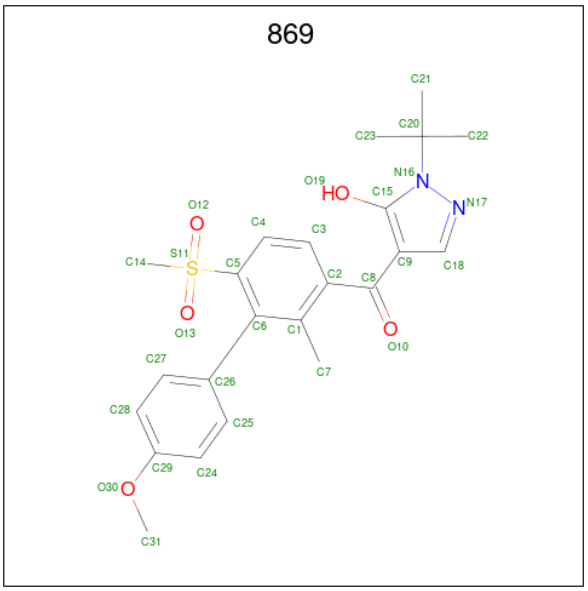
- Molecule 1 is a protein called 4-hydroxyphenylpyruvic acid dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	1	0
			2790	1786	483	510	11			
1	B	342	Total	C	N	O	S	0	1	0
			2786	1784	483	508	11			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		

- Molecule 3 is (1-TERT-BUTYL-5-HYDROXY-1H-PYRAZOL-4-YL)[6-(METHYLSULFONYL)-4'-METHOXY-2-METHYL-1,1'-BIPHENYL-3-YL]METHANONE (three-letter code: 869) (formula: $C_{23}H_{26}N_2O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			31	23	2	5	1		
3	B	1	Total	C	N	O	S	0	0
			31	23	2	5	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	228	Total	O	0	0
			228	228		
4	B	235	Total	O	0	0
			235	235		

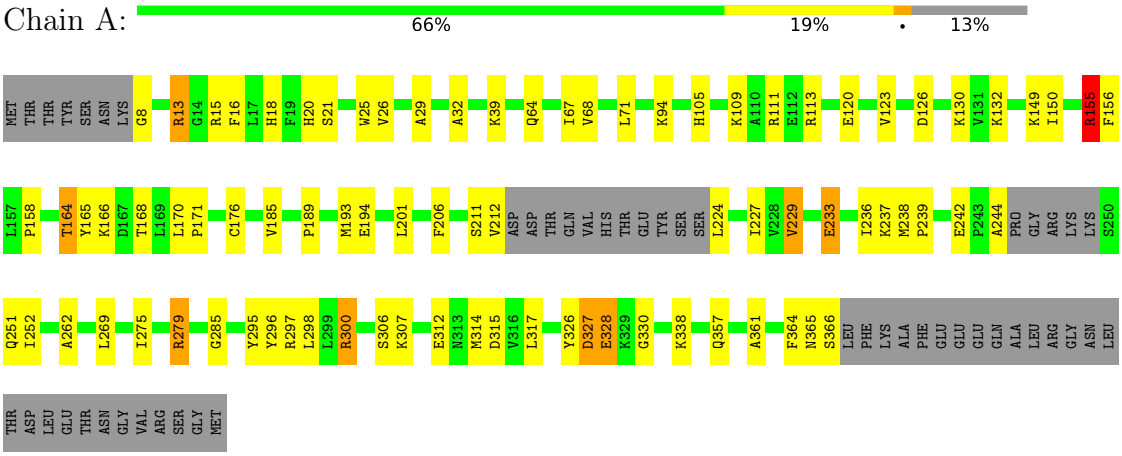
3 Residue-property plots (i)

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.

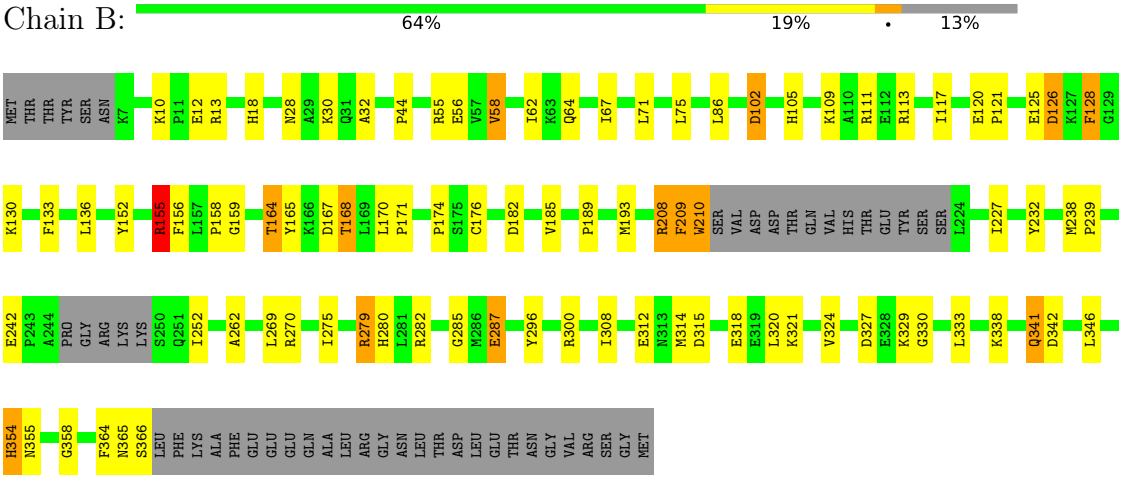
• Molecule 1: 4-hydroxyphenylpyruvic acid dioxygenase

Chain A:



• Molecule 1: 4-hydroxyphenylpyruvic acid dioxygenase

Chain B:



4 Data and refinement statistics (i)

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, α, β, γ	61.61Å 107.48Å 133.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.15	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.15)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6105	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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: 869, FE

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	0.36	0/2861	0.81	3/3863 (0.1%)
1	B	0.36	1/2857 (0.0%)	1.05	16/3856 (0.4%)
All	All	0.36	1/5718 (0.0%)	0.94	19/7719 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	155	ARG	C-N	7.49	1.51	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	208	ARG	NE-CZ-NH2	25.67	133.13	120.30
1	B	209	PHE	CB-CG-CD2	12.55	129.58	120.80
1	B	208	ARG	NE-CZ-NH1	-9.15	115.72	120.30
1	B	209	PHE	CB-CG-CD1	-8.99	114.51	120.80
1	B	102	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	B	209	PHE	N-CA-CB	7.60	124.28	110.60
1	B	208	ARG	NH1-CZ-NH2	-7.51	111.14	119.40
1	A	155	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	B	209	PHE	CB-CA-C	-7.34	95.71	110.40
1	B	279	ARG	CD-NE-CZ	7.30	133.82	123.60
1	B	155	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	B	210	TRP	CB-CG-CD1	6.30	135.19	127.00
1	B	354	HIS	CA-CB-CG	-6.27	102.94	113.60
1	B	128	PHE	CB-CG-CD1	5.97	124.98	120.80
1	B	102	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	328	GLU	O-C-N	5.70	131.81	122.70
1	A	327	ASP	N-CA-C	-5.57	95.96	111.00
1	B	209	PHE	O-C-N	5.35	131.26	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	128	PHE	CB-CG-CD2	-5.17	117.18	120.80

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	2790	0	2751	82	1
1	B	2786	0	2750	77	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	31	0	22	14	0
3	B	31	0	25	15	0
4	A	228	0	0	21	0
4	B	235	0	0	15	0
All	All	6105	0	5548	175	1

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 16.

All (175) 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)
3:B:1502:869:C31	3:B:1502:869:O30	1.79	1.29
3:A:1501:869:S11	3:A:1501:869:C14	1.20	1.28
3:A:1501:869:C14	3:A:1501:869:O13	1.90	1.19
3:B:1502:869:H313	3:B:1502:869:H24	1.26	1.12
1:B:155:ARG:HG2	1:B:156:PHE:N	1.67	1.10
1:A:233:GLU:HG3	4:A:1725:HOH:O	1.52	1.08
3:A:1501:869:C14	3:A:1501:869:O12	2.01	1.07
3:A:1501:869:O12	3:A:1501:869:C27	2.04	1.05
3:B:1502:869:C31	3:B:1502:869:C29	2.34	1.05
3:B:1502:869:C31	3:B:1502:869:C24	2.35	1.04
1:B:210:TRP:C	4:B:1725:HOH:O	1.96	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1501:869:C14	3:A:1501:869:C5	2.40	1.00
3:B:1502:869:C31	3:B:1502:869:H24	1.93	0.96
1:A:326:TYR:CE1	1:A:328:GLU:OE2	2.22	0.93
1:B:210:TRP:CA	4:B:1725:HOH:O	2.17	0.92
1:A:168:THR:HG22	1:B:285:GLY:HA2	1.56	0.88
1:A:326:TYR:HE1	1:A:328:GLU:OE2	1.54	0.87
1:B:155:ARG:HG2	1:B:156:PHE:H	1.39	0.83
1:A:314:MET:HE3	1:A:317:LEU:HB2	1.61	0.83
1:A:327:ASP:OD1	1:A:327:ASP:C	2.16	0.82
1:B:208:ARG:HH21	1:B:210:TRP:HZ2	1.23	0.82
3:A:1501:869:O12	3:A:1501:869:H27	1.77	0.82
1:B:210:TRP:HA	4:B:1725:HOH:O	1.80	0.81
1:B:209:PHE:O	1:B:210:TRP:HB3	1.80	0.80
1:A:237:LYS:NZ	4:A:1583:HOH:O	2.11	0.78
1:A:193:MET:HB2	1:A:242:GLU:HB2	1.66	0.78
1:B:64:GLN:HE22	1:B:176:CYS:HB2	1.50	0.77
3:B:1502:869:H313	3:B:1502:869:C24	2.01	0.76
1:A:126:ASP:HB2	1:A:158:PRO:HB3	1.67	0.75
1:A:64:GLN:HE22	1:A:176:CYS:HB2	1.52	0.74
1:A:307:LYS:N	1:A:328:GLU:OE1	2.20	0.74
1:A:224:LEU:HD13	1:A:252:ILE:HG13	1.70	0.73
1:A:296:TYR:O	1:A:300:ARG:HG3	1.89	0.72
1:A:211:SER:O	1:A:212:VAL:HB	1.89	0.71
1:A:155:ARG:CG	4:A:1678:HOH:O	2.36	0.71
1:A:164:THR:HG23	1:A:165:TYR:HD2	1.55	0.71
1:B:155:ARG:CG	1:B:156:PHE:N	2.52	0.71
1:B:287:GLU:HB2	1:B:338:LYS:HD3	1.72	0.70
1:A:327:ASP:OD1	1:A:327:ASP:O	2.09	0.69
3:B:1502:869:C27	3:B:1502:869:O12	2.42	0.68
1:B:209:PHE:O	1:B:210:TRP:CB	2.41	0.68
1:A:8:GLY:N	4:A:1677:HOH:O	2.27	0.67
1:A:224:LEU:N	4:A:1591:HOH:O	2.27	0.67
1:A:155:ARG:HG2	4:A:1678:HOH:O	1.94	0.67
1:A:67:ILE:HD13	1:A:269:LEU:HD22	1.77	0.67
1:B:300:ARG:NH2	1:B:318:GLU:OE2	2.25	0.66
3:A:1501:869:H71	3:A:1501:869:C25	2.26	0.65
1:B:300:ARG:HD2	4:B:1684:HOH:O	1.97	0.65
1:B:67:ILE:HD13	1:B:269:LEU:HD22	1.80	0.64
1:A:327:ASP:O	1:A:330:GLY:O	2.15	0.63
1:A:242:GLU:OE2	4:A:1593:HOH:O	2.15	0.63
1:A:109:LYS:HE3	1:A:113:ARG:HH21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:SER:HB2	1:A:328:GLU:OE2	2.00	0.62
1:A:39:LYS:HZ1	1:B:167:ASP:CG	2.03	0.61
3:A:1501:869:S11	3:A:1501:869:C27	2.87	0.61
1:A:155:ARG:HG3	4:A:1678:HOH:O	1.98	0.61
1:B:10:LYS:NZ	4:B:1669:HOH:O	2.13	0.60
1:B:330:GLY:HA3	1:B:354:HIS:O	2.02	0.60
1:B:308:ILE:HD12	1:B:308:ILE:O	2.02	0.60
1:A:130:LYS:HE2	1:A:150:ILE:HD12	1.84	0.60
1:A:123:VAL:HG13	1:A:130:LYS:HG3	1.83	0.60
1:A:68:VAL:HG11	1:A:156:PHE:CE2	2.37	0.59
1:B:300:ARG:NH1	1:B:314:MET:HG3	2.17	0.59
1:B:102:ASP:OD2	1:B:105[B]:HIS:ND1	2.36	0.59
1:A:239:PRO:HB3	3:A:1501:869:H221	1.84	0.59
1:A:365:ASN:ND2	1:A:365:ASN:H	2.00	0.59
1:B:329:LYS:HE2	1:B:355:ASN:HD22	1.68	0.59
3:A:1501:869:C25	3:A:1501:869:C7	2.79	0.58
1:A:312:GLU:OE2	4:A:1682:HOH:O	2.17	0.58
1:B:279:ARG:HD2	4:B:1556:HOH:O	2.03	0.57
1:A:338:LYS:NZ	4:A:1546:HOH:O	2.38	0.57
1:A:357:GLN:HG3	4:A:1724:HOH:O	2.04	0.57
1:B:321:LYS:HE3	4:B:1706:HOH:O	2.04	0.56
1:B:13:ARG:HB2	1:B:105[A]:HIS:CD2	2.41	0.56
1:B:238:MET:HE1	4:B:1561:HOH:O	2.05	0.55
1:A:364:PHE:CE1	3:A:1501:869:H18	2.41	0.55
1:B:365:ASN:O	1:B:366:SER:HB2	2.05	0.55
1:B:121:PRO:HA	1:B:133:PHE:O	2.06	0.55
1:B:193:MET:HB2	1:B:242:GLU:HB3	1.89	0.54
1:B:300:ARG:NH1	1:B:314:MET:CG	2.70	0.54
1:B:341:GLN:HE22	1:B:346:LEU:HB3	1.72	0.54
1:B:126:ASP:OD1	1:B:128:PHE:HB2	2.07	0.54
1:B:32:ALA:HB1	1:B:71:LEU:HD22	1.90	0.54
1:B:170:LEU:HB2	1:B:171:PRO:HD3	1.90	0.53
1:B:30:LYS:NZ	4:B:1598:HOH:O	2.42	0.53
1:A:123:VAL:HG21	1:A:130:LYS:HE3	1.90	0.53
1:A:193:MET:SD	1:A:227:ILE:HG12	2.49	0.52
1:A:13:ARG:HD3	1:A:105[B]:HIS:CG	2.45	0.52
1:A:364:PHE:HE1	3:A:1501:869:H18	1.76	0.51
1:A:164:THR:HG23	1:A:165:TYR:CD2	2.42	0.51
1:A:123:VAL:CG2	1:A:130:LYS:HE3	2.41	0.51
1:B:238:MET:CE	4:B:1561:HOH:O	2.59	0.50
1:A:238:MET:CE	4:A:1522:HOH:O	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ASP:OD2	1:A:158:PRO:HA	2.12	0.50
1:B:44:PRO:HB3	1:B:165:TYR:HE1	1.77	0.50
1:A:185:VAL:HG22	1:A:239:PRO:HG2	1.94	0.50
1:A:123:VAL:HG23	1:A:132:LYS:NZ	2.28	0.49
1:B:275:ILE:HD11	1:B:312:GLU:HB3	1.95	0.49
1:A:13:ARG:HB2	1:A:105[B]:HIS:CD2	2.46	0.49
1:A:194:GLU:HB2	4:A:1556:HOH:O	2.12	0.49
1:B:364:PHE:HD1	3:B:1502:869:H18	1.77	0.48
1:B:109:LYS:HE3	1:B:113:ARG:NH2	2.28	0.48
1:B:185:VAL:HG22	1:B:239:PRO:HB2	1.95	0.48
1:B:209:PHE:O	1:B:210:TRP:CD1	2.67	0.48
1:B:111:ARG:NH2	1:B:120:GLU:OE1	2.47	0.48
1:A:165:TYR:HE2	4:A:1638:HOH:O	1.95	0.48
1:B:159:GLY:HA3	4:B:1711:HOH:O	2.12	0.48
3:B:1502:869:C14	3:B:1502:869:C26	2.91	0.48
1:A:64:GLN:NE2	1:A:176:CYS:HB2	2.23	0.48
1:B:270:ARG:HD2	4:B:1519:HOH:O	2.14	0.47
1:B:126:ASP:OD2	1:B:158:PRO:HA	2.15	0.47
1:B:324:VAL:HG22	1:B:333:LEU:HD22	1.96	0.47
1:A:275:ILE:HD11	1:A:312:GLU:HB3	1.95	0.47
1:B:365:ASN:O	1:B:366:SER:CB	2.62	0.47
1:B:189:PRO:HD3	1:B:262:ALA:HB2	1.97	0.47
1:B:364:PHE:CD1	3:B:1502:869:H18	2.49	0.47
1:A:326:TYR:CD1	1:A:326:TYR:O	2.68	0.46
1:B:164:THR:HG1	1:B:165:TYR:HD2	1.55	0.46
1:B:174:PRO:HB2	1:B:280:HIS:CG	2.50	0.46
1:B:329:LYS:HG2	1:B:355:ASN:HD22	1.80	0.46
1:A:224:LEU:HD13	1:A:252:ILE:CG1	2.41	0.46
3:A:1501:869:H28	3:A:1501:869:H313	1.43	0.46
1:A:15:ARG:HG3	1:A:233:GLU:OE1	2.15	0.46
1:A:170:LEU:HD22	4:A:1547:HOH:O	2.16	0.46
1:A:26:VAL:HG11	1:A:32:ALA:HB2	1.98	0.45
1:A:189:PRO:HD3	1:A:262:ALA:HB2	1.97	0.45
1:A:295:TYR:CE1	1:A:366:SER:HB3	2.51	0.45
1:B:10:LYS:HB2	1:B:232:TYR:CZ	2.52	0.45
1:A:16:PHE:HB3	1:A:236:ILE:HD12	1.98	0.45
1:A:29:ALA:HB3	1:B:342:ASP:OD1	2.16	0.45
1:B:12:GLU:HG3	4:B:1666:HOH:O	2.17	0.45
1:B:182:ASP:OD1	1:B:270:ARG:NH1	2.48	0.45
1:A:206:PHE:HD2	1:A:229:VAL:HG13	1.82	0.45
1:B:329:LYS:HE2	1:B:355:ASN:ND2	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LYS:CE	4:A:1629:HOH:O	2.61	0.45
4:A:1575:HOH:O	1:B:168:THR:HG23	2.15	0.45
1:A:68:VAL:HG11	1:A:156:PHE:HE2	1.82	0.44
3:B:1502:869:C27	3:B:1502:869:S11	3.04	0.44
1:A:20:HIS:O	1:A:21:SER:HB3	2.18	0.44
1:A:285:GLY:HA2	1:B:168:THR:HG22	1.99	0.44
3:B:1502:869:O12	3:B:1502:869:H27	2.18	0.44
3:B:1502:869:O19	3:B:1502:869:H223	2.18	0.44
1:A:326:TYR:HD1	1:A:328:GLU:HG2	1.83	0.44
1:B:44:PRO:HB3	1:B:165:TYR:CE1	2.53	0.44
1:B:296:TYR:O	1:B:300:ARG:HG3	2.17	0.44
1:A:361:ALA:HB2	4:A:1553:HOH:O	2.18	0.43
1:B:111:ARG:HD2	4:B:1572:HOH:O	2.19	0.43
3:B:1502:869:O19	3:B:1502:869:C22	2.67	0.43
1:B:209:PHE:O	1:B:210:TRP:CG	2.71	0.43
1:B:32:ALA:CB	1:B:71:LEU:HD22	2.49	0.43
1:A:211:SER:O	1:A:212:VAL:CB	2.63	0.43
1:B:358:GLY:HA3	4:B:1735:HOH:O	2.19	0.43
1:A:39:LYS:NZ	1:B:167:ASP:OD2	2.51	0.42
1:A:32:ALA:HB1	1:A:71:LEU:HD22	2.02	0.42
1:B:44:PRO:HA	1:B:62:ILE:HG22	2.01	0.42
1:A:244:ALA:HB2	4:A:1591:HOH:O	2.18	0.42
1:B:239:PRO:CG	3:B:1502:869:H221	2.49	0.42
1:A:238:MET:HE3	4:A:1522:HOH:O	2.17	0.42
1:A:168:THR:HG21	1:B:282:ARG:O	2.20	0.42
1:A:25:TRP:CE2	1:A:94:LYS:HG2	2.55	0.41
1:A:171:PRO:HD3	4:A:1565:HOH:O	2.20	0.41
1:B:308:ILE:HG22	1:B:329:LYS:O	2.19	0.41
1:A:297:ARG:NH1	1:A:298:LEU:HD21	2.35	0.41
1:A:111:ARG:NH2	1:A:120:GLU:OE1	2.53	0.41
1:B:117:ILE:CD1	1:B:136:LEU:HD22	2.50	0.41
1:B:327:ASP:OD1	1:B:330:GLY:N	2.51	0.41
1:A:165:TYR:CD1	1:A:166:LYS:N	2.89	0.41
1:B:58:VAL:HG22	1:B:75:LEU:CD2	2.50	0.41
1:A:109:LYS:CE	1:A:113:ARG:HH21	2.31	0.41
1:B:109:LYS:HE3	1:B:113:ARG:HH22	1.85	0.41
1:A:185:VAL:HG22	1:A:239:PRO:HB2	2.03	0.40
1:A:201:LEU:HD21	1:A:229:VAL:HG22	2.02	0.40
1:A:239:PRO:CB	3:A:1501:869:H221	2.49	0.40
1:B:125:GLU:HB2	1:B:130:LYS:HG2	2.04	0.40
1:B:155:ARG:HE	1:B:155:ARG:HB3	1.75	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ARG:NH1	1:B:315:ASP:OD2[4_555]	2.02	0.18

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/393 (86%)	321 (95%)	17 (5%)	0	100	100
1	B	337/393 (86%)	323 (96%)	14 (4%)	0	100	100
All	All	675/786 (86%)	644 (95%)	31 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	303/346 (88%)	293 (97%)	10 (3%)	38	37
1	B	302/346 (87%)	286 (95%)	16 (5%)	22	19
All	All	605/692 (87%)	579 (96%)	26 (4%)	29	27

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	18	HIS
1	A	155	ARG
1	A	164	THR
1	A	229	VAL
1	A	233	GLU
1	A	251	GLN
1	A	279	ARG
1	A	300	ARG
1	A	315	ASP
1	B	18	HIS
1	B	28	ASN
1	B	55	ARG
1	B	56	GLU
1	B	58	VAL
1	B	86	LEU
1	B	126	ASP
1	B	152	TYR
1	B	155	ARG
1	B	164	THR
1	B	168	THR
1	B	227	ILE
1	B	252	ILE
1	B	287	GLU
1	B	320	LEU
1	B	341	GLN

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	64	GLN
1	A	89	HIS
1	A	365	ASN
1	B	28	ASN
1	B	64	GLN
1	B	89	HIS
1	B	144	HIS
1	B	187	ASN
1	B	253	GLN
1	B	259	ASN
1	B	341	GLN
1	B	355	ASN

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	869	A	1501	2	26,33,33	4.40	15 (57%)	35,51,51	4.72	27 (77%)
3	869	B	1502	2	26,33,33	3.10	12 (46%)	35,51,51	5.50	18 (51%)

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	869	A	1501	2	-	6/18/26/26	0/3/3/3
3	869	B	1502	2	-	2/18/26/26	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1501	869	C14-S11	-13.93	1.20	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1502	869	O30-C31	12.23	1.79	1.42
3	A	1501	869	C9-C8	-9.66	1.30	1.50
3	A	1501	869	O13-S11	-7.82	1.22	1.44
3	A	1501	869	C2-C8	6.04	1.62	1.50
3	A	1501	869	O10-C8	5.91	1.33	1.22
3	A	1501	869	C7-C1	-3.78	1.42	1.51
3	B	1502	869	C4-C5	3.64	1.41	1.37
3	B	1502	869	C7-C1	-3.22	1.43	1.51
3	A	1501	869	C22-C20	-3.13	1.48	1.52
3	B	1502	869	C9-C8	3.03	1.56	1.50
3	B	1502	869	C4-C3	2.93	1.44	1.38
3	A	1501	869	C4-C3	2.81	1.43	1.38
3	A	1501	869	O30-C29	2.61	1.43	1.37
3	B	1502	869	C2-C1	2.59	1.44	1.40
3	B	1502	869	O19-C15	2.48	1.39	1.32
3	A	1501	869	C4-C5	2.47	1.40	1.37
3	B	1502	869	C27-C28	2.45	1.41	1.36
3	A	1501	869	C2-C1	2.41	1.43	1.40
3	A	1501	869	C25-C24	2.33	1.41	1.36
3	B	1502	869	O12-S11	-2.23	1.37	1.44
3	A	1501	869	O12-S11	-2.22	1.37	1.44
3	B	1502	869	O30-C29	2.18	1.42	1.37
3	B	1502	869	C2-C8	2.12	1.54	1.50
3	A	1501	869	C23-C20	2.11	1.55	1.52
3	B	1502	869	O10-C8	2.11	1.26	1.22
3	A	1501	869	C27-C28	2.08	1.41	1.36

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1502	869	O10-C8-C2	14.41	145.03	119.82
3	B	1502	869	C9-C8-C2	-13.35	91.28	120.16
3	A	1501	869	C14-S11-C5	11.89	122.61	105.11
3	B	1502	869	C31-O30-C29	-11.27	93.06	117.51
3	A	1501	869	C18-C9-C8	10.35	146.08	127.45
3	A	1501	869	C3-C2-C1	-9.54	113.91	120.73
3	B	1502	869	O13-S11-C5	9.29	119.04	108.27
3	B	1502	869	C18-C9-C8	8.75	143.20	127.45
3	B	1502	869	C3-C2-C1	-8.50	114.65	120.73
3	B	1502	869	O12-S11-O13	-7.53	104.95	117.92
3	A	1501	869	O12-S11-O13	-7.40	105.17	117.92
3	A	1501	869	O10-C8-C9	7.14	132.31	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1502	869	O12-S11-C5	6.87	116.24	108.27
3	A	1501	869	C25-C26-C27	6.70	124.60	118.65
3	A	1501	869	C31-O30-C29	-5.86	104.80	117.51
3	B	1502	869	C18-N17-N16	5.43	109.88	104.23
3	A	1501	869	C23-C20-N16	5.41	117.36	108.80
3	B	1502	869	C2-C1-C6	5.39	123.51	117.50
3	B	1502	869	C22-C20-N16	5.33	117.22	108.80
3	B	1502	869	C23-C20-N16	4.93	116.59	108.80
3	A	1501	869	C2-C1-C6	4.80	122.86	117.50
3	B	1502	869	C14-S11-C5	-4.73	98.16	105.11
3	A	1501	869	C18-N17-N16	4.56	108.98	104.23
3	A	1501	869	O12-S11-C5	4.53	113.52	108.27
3	A	1501	869	C23-C20-C21	-4.26	102.32	110.05
3	B	1502	869	C21-C20-N16	-4.06	102.39	108.80
3	A	1501	869	O12-S11-C14	-4.06	102.66	108.49
3	A	1501	869	C9-C8-C2	-3.90	111.73	120.16
3	A	1501	869	O10-C8-C2	-3.81	113.15	119.82
3	B	1502	869	C7-C1-C2	-3.42	114.99	120.93
3	A	1501	869	C6-C5-S11	3.24	128.62	122.44
3	A	1501	869	O13-S11-C14	-3.08	104.07	108.49
3	A	1501	869	C21-C20-N16	-3.07	103.96	108.80
3	A	1501	869	C22-C20-N16	3.00	113.54	108.80
3	A	1501	869	C3-C2-C8	-2.91	112.23	118.71
3	A	1501	869	C23-C20-C22	-2.77	105.03	110.05
3	A	1501	869	C4-C5-C6	-2.74	115.92	120.16
3	B	1502	869	C22-C20-C21	-2.72	105.11	110.05
3	A	1501	869	C24-C25-C26	-2.53	116.91	120.82
3	B	1502	869	C4-C5-C6	-2.48	116.32	120.16
3	A	1501	869	C22-C20-C21	2.41	114.43	110.05
3	B	1502	869	C25-C26-C27	2.24	120.63	118.65
3	A	1501	869	C7-C1-C2	-2.20	117.11	120.93
3	A	1501	869	C28-C27-C26	-2.18	117.44	120.82
3	A	1501	869	C4-C3-C2	2.17	124.45	120.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1501	869	C24-C29-O30-C31
3	A	1501	869	C28-C29-O30-C31
3	B	1502	869	C28-C29-O30-C31
3	B	1502	869	C24-C29-O30-C31

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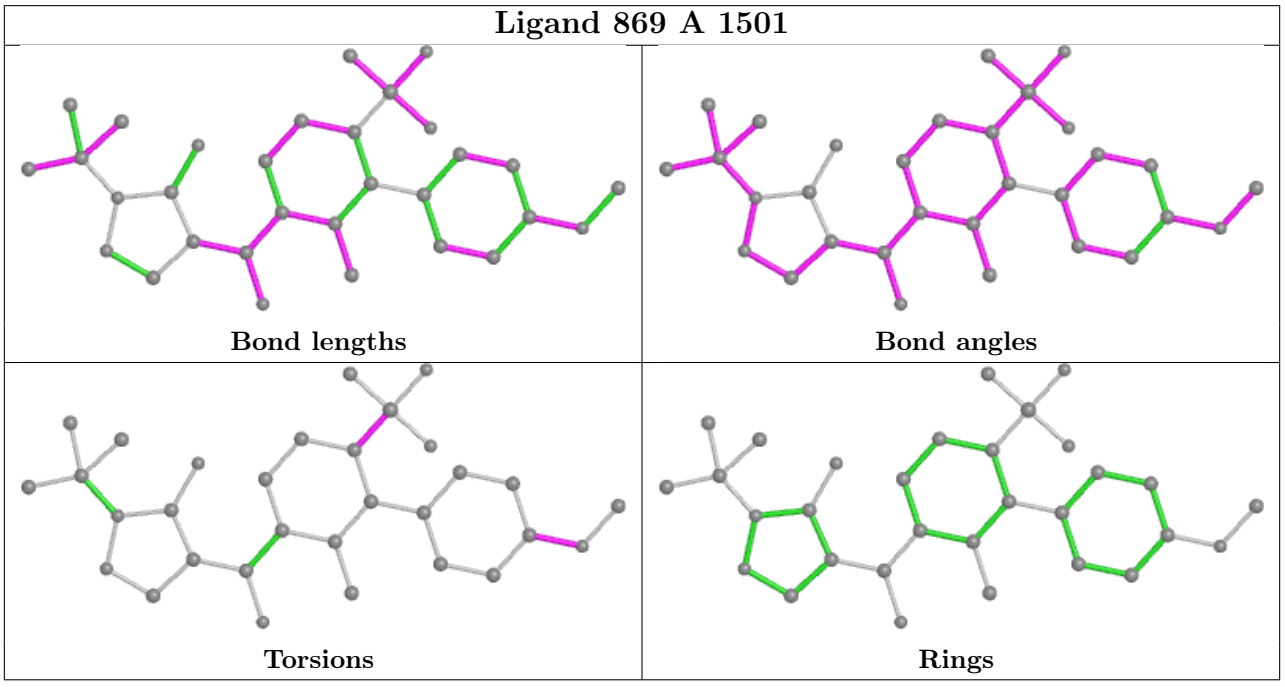
Mol	Chain	Res	Type	Atoms
3	A	1501	869	C6-C5-S11-O13
3	A	1501	869	C4-C5-S11-O13
3	A	1501	869	C4-C5-S11-C14
3	A	1501	869	C6-C5-S11-C14

There are no ring outliers.

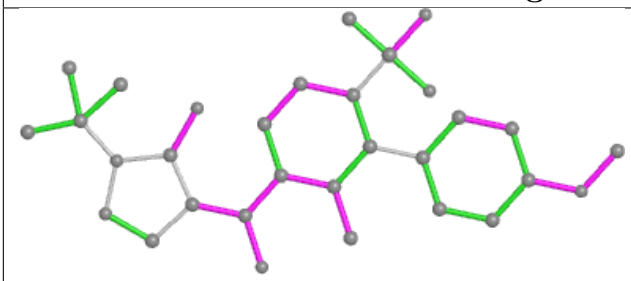
2 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1501	869	14	0
3	B	1502	869	15	0

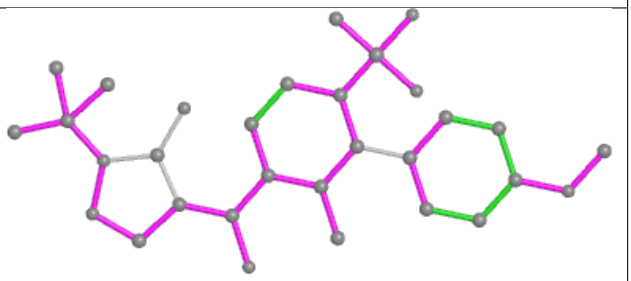
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



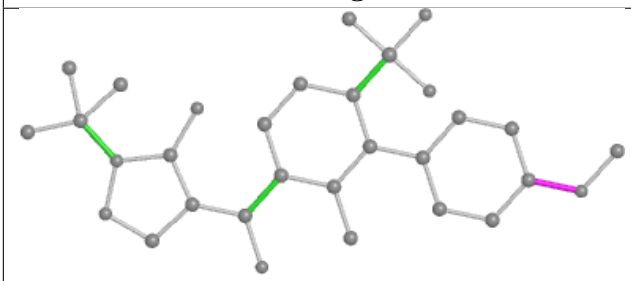
Ligand 869 B 1502



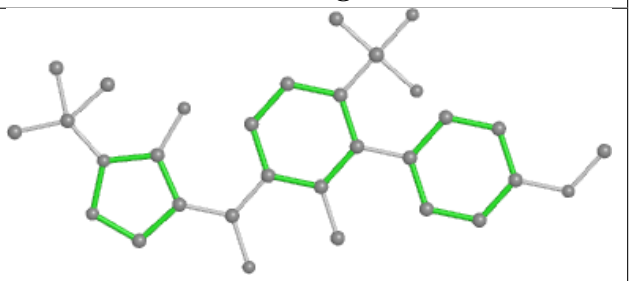
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.