



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:11 am BST

PDB ID : 2BT4
Title : Type II Dehydroquinase inhibitor complex
Authors : Toscano, M.D.; Stewart, K.A.; Coggins, J.R.; Lapthorn, A.J.; Abell, C.
Deposited on : 2005-05-26
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (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) : 2.11

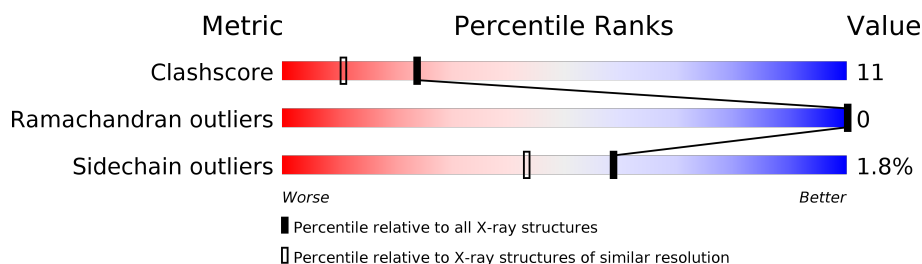
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	157	84% 10% • 5%
1	B	157	85% 8% • 5%
1	C	157	87% 7% • 5%
1	D	157	83% 10% • 5%
1	E	157	81% 11% • 5%
1	F	157	81% 13% • 5%
1	G	157	86% 8% • 5%
1	H	157	84% 10% • 5%

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Mol	Chain	Length	Quality of chain
1	I	157	 80% 15% 5%
1	J	157	 82% 11% 5%
1	K	157	 83% 12% 5%
1	L	157	 82% 12% 5%

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	PO4	A	2401	-	-	X	-
5	GOL	B	2414	-	-	X	-
5	GOL	C	2415	-	-	X	-
5	GOL	D	2416	-	-	X	-
5	GOL	E	2419	-	-	X	-
5	GOL	E	2422	-	-	X	-
5	GOL	F	2418	-	-	X	-
5	GOL	G	2417	-	-	X	-
5	GOL	H	2411	-	-	X	-
5	GOL	I	2420	-	-	X	-
5	GOL	J	2412	-	-	X	-
5	GOL	K	2421	-	-	X	-

2 Entry composition

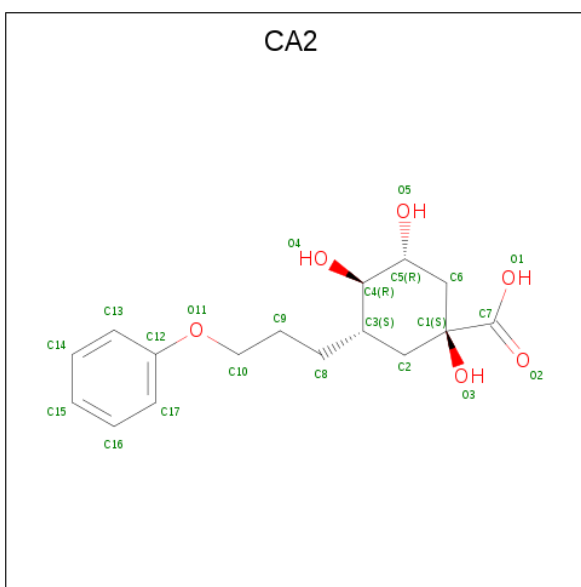
There are 6 unique types of molecules in this entry. The entry contains 15641 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-DEHYDROQUINATE DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	B	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	C	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	D	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	E	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	F	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	G	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	H	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	I	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	J	149	Total	C	N	O	S	0	2	0
			1132	704	213	210	5			
1	K	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	L	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			

- Molecule 2 is (1S,3R,4R,5S)-1,3,4-TRIHIDROXY-5-(3-PHENOXYPROPYL)CYCLOHEXANECARBOXYLIC ACID (three-letter code: CA2) (formula: C₁₆H₂₂O₆).



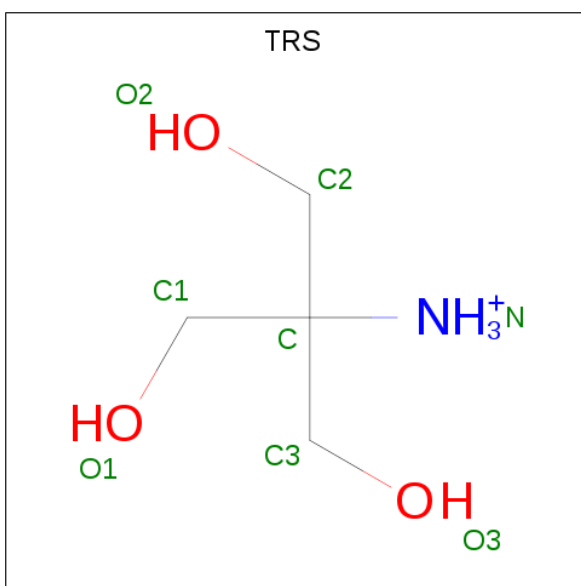
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			22	16	6		
2	B	1	Total	C	O	0	0
			22	16	6		
2	C	1	Total	C	O	0	0
			22	16	6		
2	D	1	Total	C	O	0	0
			22	16	6		
2	E	1	Total	C	O	0	0
			22	16	6		
2	F	1	Total	C	O	0	0
			22	16	6		
2	G	1	Total	C	O	0	0
			22	16	6		
2	H	1	Total	C	O	0	0
			22	16	6		
2	I	1	Total	C	O	0	0
			22	16	6		
2	J	1	Total	C	O	0	0
			22	16	6		
2	K	1	Total	C	O	0	0
			22	16	6		
2	L	1	Total	C	O	0	0
			22	16	6		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



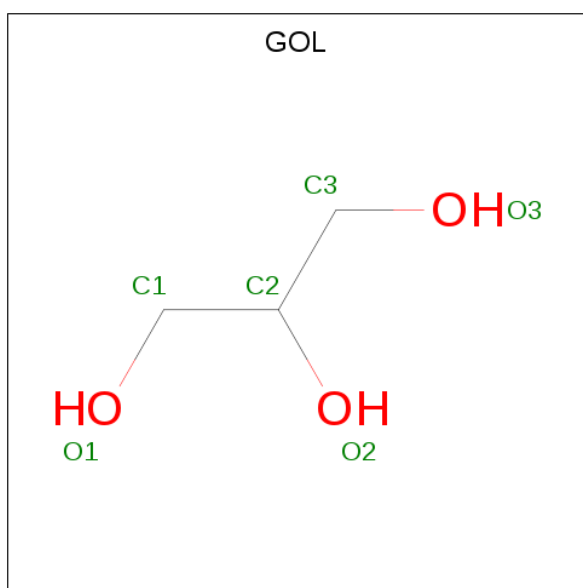
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 8 4 1 3	0	0
4	F	1	Total C N O 8 4 1 3	0	0
4	H	1	Total C N O 8 4 1 3	0	0
4	L	1	Total C N O 8 4 1 3	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	135	Total	O	0	0
			135	135		
6	B	152	Total	O	0	0
			152	152		
6	C	146	Total	O	0	0
			146	146		
6	D	146	Total	O	0	0
			146	146		
6	E	186	Total	O	0	0
			186	186		
6	F	146	Total	O	0	0
			146	146		
6	G	148	Total	O	0	0
			148	148		
6	H	124	Total	O	0	0
			124	124		
6	I	156	Total	O	0	0
			156	156		
6	J	120	Total	O	0	0
			120	120		
6	K	123	Total	O	0	0
			123	123		
6	L	149	Total	O	0	0
			149	149		

3 Residue-property plots [i](#)

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

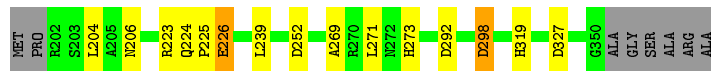
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain A: 



• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain B: 




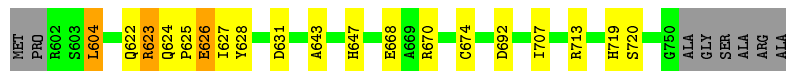
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain C: 




• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain D: 

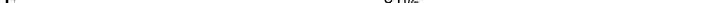


• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain E: 




• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain F:  81% 13% • 5%

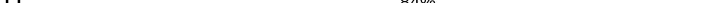


- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain G:  86% 8% • 5%

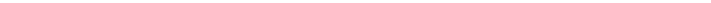


- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain H:  84% 10% • 5%




- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain I:  80% 15% 5%




- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain J:  82% 11% • 5%



- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain K:  83% 12% 5%



- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain L: 82% 12% • 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	196.62Å 196.49Å 240.63Å 65.91° 65.91° 90.01°	Depositor
Resolution (Å)	27.00 – 1.70	Depositor
% Data completeness (in resolution range)	75.8 (27.00-1.70)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.197 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15641	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: GOL, PO4, TRS, CA2

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	1.02	0/1161	1.04	4/1582 (0.3%)
1	B	1.05	0/1155	0.99	4/1574 (0.3%)
1	C	1.01	0/1155	0.95	3/1574 (0.2%)
1	D	1.05	0/1161	0.95	2/1582 (0.1%)
1	E	1.01	2/1155 (0.2%)	0.94	3/1574 (0.2%)
1	F	1.06	1/1155 (0.1%)	1.02	6/1574 (0.4%)
1	G	1.03	1/1161 (0.1%)	1.01	3/1582 (0.2%)
1	H	1.04	0/1155	1.02	2/1574 (0.1%)
1	I	1.00	0/1155	0.96	2/1574 (0.1%)
1	J	1.02	1/1166 (0.1%)	0.98	3/1588 (0.2%)
1	K	1.00	0/1155	0.93	0/1574
1	L	1.02	0/1161	0.98	3/1582 (0.2%)
All	All	1.03	5/13895 (0.0%)	0.98	35/18934 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1083	TYR	CD1-CE1	6.32	1.48	1.39
1	G	1305	VAL	CB-CG2	-5.66	1.41	1.52
1	E	828	TYR	CD2-CE2	-5.37	1.31	1.39
1	E	939	VAL	CB-CG1	-5.24	1.41	1.52
1	J	1940	PHE	CD2-CE2	5.09	1.49	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1527	ASP	CB-CG-OD2	13.19	130.17	118.30
1	G	1327	ASP	CB-CG-OD2	8.20	125.68	118.30
1	C	527	ASP	CB-CG-OD2	7.63	125.17	118.30
1	B	252	ASP	CB-CG-OD1	7.24	124.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	631	ASP	CB-CG-OD2	7.06	124.65	118.30
1	C	525	ARG	NE-CZ-NH1	-6.91	116.85	120.30
1	J	1927	ASP	CB-CG-OD2	6.89	124.50	118.30
1	A	127	ASP	CB-CG-OD2	6.78	124.40	118.30
1	B	327	ASP	CB-CG-OD2	6.64	124.28	118.30
1	L	2327	ASP	CB-CG-OD2	6.41	124.06	118.30
1	A	92	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	292	ASP	CB-CG-OD1	6.33	123.99	118.30
1	A	64	ASP	CB-CG-OD2	6.31	123.98	118.30
1	F	1031	ASP	CB-CG-OD2	6.17	123.86	118.30
1	I	1631	ASP	CB-CG-OD2	6.14	123.83	118.30
1	G	1254	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	G	1231	ASP	CB-CG-OD2	6.06	123.75	118.30
1	F	1098	ASP	CB-CG-OD2	6.05	123.74	118.30
1	F	1035	ASP	CB-CG-OD2	5.94	123.64	118.30
1	C	431	ASP	CB-CG-OD2	5.87	123.58	118.30
1	I	1692	ASP	CB-CG-OD1	5.84	123.55	118.30
1	A	31	ASP	CB-CG-OD2	5.81	123.53	118.30
1	J	1831	ASP	CB-CG-OD2	5.72	123.45	118.30
1	F	1127	ASP	CB-CG-OD2	5.70	123.43	118.30
1	H	1431	ASP	CB-CG-OD2	5.52	123.27	118.30
1	F	1117	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	E	835	ASP	CB-CG-OD2	5.42	123.18	118.30
1	L	2231	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	692	ASP	CB-CG-OD1	5.37	123.14	118.30
1	E	839	LEU	CB-CG-CD1	-5.28	102.03	111.00
1	F	1020	LEU	CB-CG-CD2	-5.26	102.05	111.00
1	J	1880	PRO	N-CD-CG	-5.26	95.31	103.20
1	E	831	ASP	CB-CG-OD2	5.22	123.00	118.30
1	L	2252	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	298	ASP	CB-CG-OD2	5.12	122.91	118.30

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	1127	0	1093	20	0
1	B	1126	0	1092	14	0
1	C	1126	0	1092	17	0
1	D	1127	0	1093	18	0
1	E	1126	0	1092	38	0
1	F	1126	0	1092	36	0
1	G	1127	0	1093	16	0
1	H	1126	0	1092	27	0
1	I	1126	0	1092	41	0
1	J	1132	0	1102	19	0
1	K	1126	0	1092	20	0
1	L	1127	0	1093	22	0
2	A	22	0	21	1	0
2	B	22	0	21	2	0
2	C	22	0	21	0	0
2	D	22	0	21	0	0
2	E	22	0	21	2	0
2	F	22	0	21	2	0
2	G	22	0	21	1	0
2	H	22	0	21	1	0
2	I	22	0	21	0	0
2	J	22	0	21	1	0
2	K	22	0	21	0	0
2	L	22	0	21	0	0
3	A	5	0	0	2	0
3	D	5	0	0	1	0
3	I	5	0	0	1	0
3	L	5	0	0	0	0
4	A	8	0	12	0	0
4	F	8	0	12	0	0
4	H	8	0	12	0	0
4	L	8	0	12	0	0
5	A	6	0	8	1	0
5	B	6	0	8	6	0
5	C	6	0	8	9	0
5	D	6	0	8	9	0
5	E	12	0	16	15	0
5	F	6	0	8	13	0
5	G	6	0	8	7	0
5	H	6	0	8	7	0
5	I	6	0	8	21	0
5	J	6	0	8	4	0
5	K	6	0	8	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	135	0	0	10	0
6	B	152	0	0	8	0
6	C	146	0	0	10	0
6	D	146	0	0	5	0
6	E	186	0	0	17	0
6	F	146	0	0	10	0
6	G	148	0	0	0	0
6	H	124	0	0	18	0
6	I	156	0	0	22	0
6	J	120	0	0	13	0
6	K	123	0	0	2	0
6	L	149	0	0	13	0
All	All	15641	0	13514	305	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 (305) 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:I:1719[A]:HIS:CD2	5:I:2420:GOL:H11	1.62	1.33
1:F:1098:ASP:CB	6:F:2109:HOH:O	1.68	1.31
1:H:1519[A]:HIS:CD2	5:H:2411:GOL:H12	1.72	1.25
5:B:2414:GOL:C1	6:B:2150:HOH:O	1.88	1.22
1:I:1602:ARG:N	6:I:2022:HOH:O	1.76	1.18
5:C:2415:GOL:H11	6:C:2146:HOH:O	1.03	1.18
1:J:1821:GLY:O	6:J:2016:HOH:O	1.56	1.17
1:J:1842:LYS:HE2	6:J:2046:HOH:O	1.41	1.17
1:B:271:LEU:CD2	6:B:2095:HOH:O	1.93	1.14
1:C:513:ARG:HG2	6:C:2111:HOH:O	1.43	1.13
1:F:1120:SER:H	5:F:2418:GOL:H12	1.05	1.12
1:F:1098:ASP:HB2	6:F:2109:HOH:O	1.32	1.12
5:D:2416:GOL:O1	6:D:2145:HOH:O	1.65	1.11
1:I:1750:GLY:HA3	6:I:2149:HOH:O	1.51	1.11
1:I:1719[A]:HIS:CD2	5:I:2420:GOL:C1	2.34	1.09
1:J:1821:GLY:C	6:J:2016:HOH:O	1.87	1.08
5:C:2415:GOL:C1	6:C:2146:HOH:O	1.64	1.08
1:F:1098:ASP:O	6:F:2109:HOH:O	1.70	1.07
1:E:914:GLU:CD	6:E:2155:HOH:O	1.91	1.06
5:B:2414:GOL:H11	6:B:2150:HOH:O	1.46	1.06
1:J:1842:LYS:HG2	6:J:2043:HOH:O	1.55	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2319[B]:HIS:HD2	6:L:2101:HOH:O	1.39	1.05
1:F:1071:LEU:HD12	6:F:2083:HOH:O	1.58	1.03
1:G:1320:SER:H	5:G:2417:GOL:H12	1.20	1.02
1:L:2225:PRO:HB3	6:L:2047:HOH:O	1.61	1.01
1:I:1719[A]:HIS:CG	5:I:2420:GOL:H11	1.97	0.99
1:L:2225:PRO:CB	6:L:2047:HOH:O	2.07	0.99
5:E:2419:GOL:H2	6:E:2184:HOH:O	1.61	0.98
1:I:1750:GLY:CA	6:I:2149:HOH:O	2.04	0.98
1:C:425:PRO:HD2	1:C:426:GLU:OE2	1.62	0.97
1:F:1098:ASP:C	6:F:2109:HOH:O	1.85	0.95
5:H:2411:GOL:H32	6:H:2123:HOH:O	1.64	0.95
1:H:1519[A]:HIS:HD2	5:H:2411:GOL:H12	1.30	0.94
1:H:1519[A]:HIS:CD2	5:H:2411:GOL:C1	2.51	0.94
1:H:1442:LYS:HG2	6:H:2046:HOH:O	1.65	0.94
1:J:1842:LYS:HG3	6:J:2044:HOH:O	1.67	0.93
5:B:2414:GOL:H12	6:B:2150:HOH:O	1.59	0.93
1:I:1719[A]:HIS:HD2	5:I:2420:GOL:C2	1.81	0.92
1:A:25:PRO:HB3	6:A:2023:HOH:O	1.68	0.92
1:H:1442:LYS:HE3	6:H:2046:HOH:O	1.71	0.91
1:G:1225:PRO:HD2	1:G:1226:GLU:OE2	1.69	0.91
1:F:1120:SER:N	5:F:2418:GOL:H12	1.87	0.89
5:H:2411:GOL:C3	6:H:2123:HOH:O	2.17	0.89
1:F:1119[A]:HIS:CD2	5:F:2418:GOL:H31	2.07	0.89
1:C:513:ARG:CD	6:C:2111:HOH:O	2.19	0.88
3:D:2402:PO4:O2	6:D:2144:HOH:O	1.90	0.88
1:E:919[A]:HIS:HD2	5:E:2419:GOL:C3	1.86	0.88
1:B:319[A]:HIS:HD2	5:B:2414:GOL:H32	1.37	0.86
6:B:2151:HOH:O	5:G:2417:GOL:H32	1.75	0.86
1:I:1719[A]:HIS:CD2	5:I:2420:GOL:C2	2.58	0.86
1:I:1750:GLY:N	6:I:2149:HOH:O	2.06	0.86
1:E:919[A]:HIS:HD2	5:E:2419:GOL:H31	1.40	0.84
1:C:513:ARG:NE	6:C:2111:HOH:O	2.10	0.84
1:F:1052:ASP:OD1	6:F:2062:HOH:O	1.95	0.83
1:L:2225:PRO:HG3	6:L:2047:HOH:O	1.79	0.83
1:H:1442:LYS:HG3	6:H:2048:HOH:O	1.78	0.82
1:A:111:HIS:HD1	5:D:2416:GOL:HO2	1.26	0.81
1:A:25:PRO:CB	6:A:2023:HOH:O	2.26	0.81
1:K:2120:SER:H	5:K:2421:GOL:C1	1.93	0.81
5:E:2422:GOL:H12	1:L:2319[B]:HIS:ND1	1.97	0.80
1:H:1519[A]:HIS:HD2	5:H:2411:GOL:C1	1.88	0.80
1:I:1719[A]:HIS:HD2	5:I:2420:GOL:C3	1.94	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1749:ALA:C	6:I:2149:HOH:O	2.20	0.79
1:A:25:PRO:CG	6:A:2023:HOH:O	2.31	0.79
1:E:822:GLN:HE21	1:F:1070:ARG:HH22	1.29	0.78
1:H:1442:LYS:CE	6:H:2047:HOH:O	2.31	0.78
1:D:720:SER:H	5:D:2416:GOL:C1	1.96	0.78
1:D:720:SER:H	5:D:2416:GOL:H12	1.49	0.77
1:G:1320:SER:N	5:G:2417:GOL:H12	1.98	0.77
1:D:628:TYR:OH	1:D:713:ARG:NH1	2.17	0.77
1:E:914:GLU:OE2	6:E:2154:HOH:O	2.02	0.77
1:E:914:GLU:CG	6:E:2155:HOH:O	2.32	0.76
1:I:1668:GLU:OE1	6:I:2089:HOH:O	2.03	0.76
1:C:513:ARG:CG	6:C:2111:HOH:O	2.08	0.76
1:B:319[A]:HIS:CD2	5:B:2414:GOL:H32	2.21	0.75
1:E:919[A]:HIS:CD2	5:E:2419:GOL:H12	2.21	0.75
1:L:2247:HIS:CE1	6:L:2068:HOH:O	2.40	0.75
1:I:1674:CYS:O	6:I:2096:HOH:O	2.04	0.75
5:J:2412:GOL:C1	6:J:2098:HOH:O	2.35	0.74
1:F:1119[A]:HIS:HD2	5:F:2418:GOL:H31	1.50	0.74
1:G:1225:PRO:CD	1:G:1226:GLU:OE2	2.35	0.74
5:E:2422:GOL:H2	6:E:2149:HOH:O	1.88	0.73
1:L:2225:PRO:CG	6:L:2047:HOH:O	2.27	0.73
1:F:1119[A]:HIS:HD2	5:F:2418:GOL:C3	2.00	0.73
1:B:226:GLU:CD	1:B:226:GLU:H	1.91	0.73
1:B:271:LEU:HD23	6:B:2095:HOH:O	1.75	0.72
5:E:2419:GOL:C2	6:E:2184:HOH:O	2.29	0.72
1:G:1319[A]:HIS:ND1	5:G:2417:GOL:H31	2.04	0.72
1:I:1642:LYS:CE	6:I:2061:HOH:O	2.39	0.71
1:E:914:GLU:HG2	6:E:2155:HOH:O	1.91	0.71
1:F:1068:GLU:CD	6:F:2088:HOH:O	2.28	0.71
1:E:919[A]:HIS:CD2	5:E:2419:GOL:H31	2.24	0.70
1:F:1119[B]:HIS:HB3	5:F:2418:GOL:H31	1.72	0.70
1:H:1442:LYS:NZ	6:H:2047:HOH:O	2.09	0.70
1:L:2349:ALA:O	6:L:2147:HOH:O	2.09	0.69
1:L:2224:GLN:HA	1:L:2226:GLU:OE2	1.92	0.69
5:I:2420:GOL:H2	6:I:2155:HOH:O	1.91	0.69
5:E:2422:GOL:C1	1:L:2319[B]:HIS:ND1	2.55	0.69
1:C:519[B]:HIS:CD2	5:C:2415:GOL:H12	2.28	0.69
1:D:670:ARG:O	6:D:2097:HOH:O	2.11	0.69
1:L:2319[B]:HIS:CD2	6:L:2101:HOH:O	2.25	0.68
1:E:919[A]:HIS:CD2	5:E:2419:GOL:C3	2.74	0.68
1:F:1068:GLU:OE1	6:F:2088:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1642:LYS:HE2	6:I:2061:HOH:O	1.94	0.67
1:K:2119[A]:HIS:CD2	5:K:2421:GOL:C1	2.78	0.67
1:L:2203:SER:HB2	6:L:2027:HOH:O	1.95	0.66
1:D:668:GLU:OE1	6:D:2094:HOH:O	2.14	0.66
1:H:1442:LYS:HE2	6:H:2047:HOH:O	1.92	0.65
1:D:719[B]:HIS:ND1	6:D:2122:HOH:O	2.20	0.65
5:A:2413:GOL:O1	6:A:2135:HOH:O	2.08	0.65
6:A:2096:HOH:O	5:D:2416:GOL:H2	1.98	0.64
1:K:2002:ARG:NH1	1:K:2071:LEU:O	2.32	0.63
1:I:1719[A]:HIS:CD2	5:I:2420:GOL:H2	2.33	0.62
1:E:822:GLN:NE2	1:F:1070:ARG:HH22	1.98	0.62
1:I:1642:LYS:HE3	6:I:2059:HOH:O	1.99	0.61
1:A:25:PRO:CD	6:A:2023:HOH:O	2.48	0.60
1:H:1430:SER:HB3	6:H:2005:HOH:O	2.01	0.60
1:I:1719[B]:HIS:ND1	5:I:2420:GOL:H31	2.17	0.60
1:I:1719[A]:HIS:HD2	5:I:2420:GOL:H31	1.65	0.60
1:E:802:ARG:NH1	6:E:2053:HOH:O	2.33	0.59
1:D:626:GLU:H	1:D:626:GLU:CD	2.05	0.59
5:J:2412:GOL:H11	6:J:2098:HOH:O	1.99	0.59
1:C:448:GLY:HA3	6:C:2061:HOH:O	2.02	0.59
1:H:1442:LYS:CE	6:H:2046:HOH:O	2.39	0.59
1:L:2348:LEU:C	1:L:2350:GLY:H	2.05	0.59
1:J:1842:LYS:CG	6:J:2043:HOH:O	2.30	0.58
1:K:2120:SER:H	5:K:2421:GOL:H11	1.65	0.58
1:F:1119[A]:HIS:CG	5:F:2418:GOL:H31	2.39	0.58
1:E:935:VAL:HG22	6:E:2171:HOH:O	2.04	0.58
5:J:2412:GOL:H12	6:J:2098:HOH:O	2.02	0.57
1:D:670:ARG:HH22	1:F:1022:GLN:HE21	1.51	0.57
1:E:823:ARG:NE	1:F:1098:ASP:OD2	2.36	0.57
1:H:1442:LYS:CG	6:H:2046:HOH:O	2.38	0.57
1:C:519[A]:HIS:ND1	5:C:2415:GOL:H31	2.19	0.57
1:I:1719[A]:HIS:CD2	5:I:2420:GOL:H31	2.40	0.57
1:K:2119[A]:HIS:CD2	5:K:2421:GOL:H11	2.40	0.56
1:J:1842:LYS:CD	6:J:2046:HOH:O	2.50	0.56
1:G:1319[A]:HIS:ND1	5:G:2417:GOL:C3	2.68	0.56
5:C:2415:GOL:H12	6:C:2146:HOH:O	1.62	0.56
1:A:25:PRO:HD3	6:A:2023:HOH:O	2.05	0.56
1:H:1544:ARG:NH2	6:H:2117:HOH:O	2.15	0.56
1:E:839:LEU:HD22	6:E:2093:HOH:O	2.07	0.55
1:I:1627:ILE:HD13	6:I:2116:HOH:O	2.06	0.55
5:I:2420:GOL:C2	6:I:2155:HOH:O	2.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:2026:GLU:H	1:K:2026:GLU:CD	2.10	0.55
1:A:24:GLN:HA	1:A:26:GLU:OE2	2.07	0.55
1:A:124:GLN:HE22	1:C:516:PHE:HE2	1.54	0.54
1:I:1719[A]:HIS:CG	5:I:2420:GOL:C1	2.76	0.54
1:E:822:GLN:HE22	1:F:1070:ARG:HH12	1.56	0.54
1:E:914:GLU:OE2	6:E:2155:HOH:O	2.09	0.54
1:L:2284:SER:OG	1:L:2306:HIS:HE1	1.91	0.54
1:H:1430:SER:CB	6:H:2017:HOH:O	2.55	0.54
1:I:1602:ARG:C	6:I:2022:HOH:O	2.47	0.54
1:F:1068:GLU:OE2	6:F:2088:HOH:O	2.18	0.53
1:A:113:ARG:HG2	6:A:2101:HOH:O	2.09	0.53
1:E:802:ARG:NH2	6:E:2053:HOH:O	2.41	0.53
1:I:1642:LYS:CE	6:I:2059:HOH:O	2.55	0.52
1:E:822:GLN:HE21	1:F:1070:ARG:NH2	2.03	0.52
1:F:1022:GLN:NE2	6:F:2030:HOH:O	2.41	0.52
1:I:1720:SER:H	5:I:2420:GOL:C1	2.22	0.52
3:A:2401:PO4:O4	1:C:458:HIS:ND1	2.40	0.52
1:I:1719[B]:HIS:HB3	5:I:2420:GOL:H11	1.91	0.52
1:K:2025:PRO:HD2	1:K:2026:GLU:OE2	2.10	0.52
1:D:720:SER:N	5:D:2416:GOL:H12	2.21	0.52
1:E:831:ASP:HB2	6:E:2078:HOH:O	2.10	0.52
1:J:1842:LYS:HE3	6:J:2043:HOH:O	2.09	0.52
1:J:1822:GLN:HE21	1:K:2070:ARG:HH22	1.58	0.51
1:H:1424:GLN:HA	1:H:1426:GLU:OE2	2.10	0.51
1:G:1222:GLN:HE21	1:H:1470:ARG:HH22	1.57	0.51
1:E:919[A]:HIS:HD2	5:E:2419:GOL:C2	2.22	0.51
1:B:319[A]:HIS:CD2	5:B:2414:GOL:H12	2.45	0.51
1:K:2004:LEU:CD1	1:K:2149:ALA:HB3	2.40	0.51
1:I:1642:LYS:HG2	6:I:2059:HOH:O	2.09	0.51
5:K:2421:GOL:H2	6:K:3122:HOH:O	2.10	0.51
1:A:2:ARG:NH2	6:A:2001:HOH:O	2.44	0.51
1:G:1319[B]:HIS:HD2	5:G:2417:GOL:H2	1.77	0.50
1:L:2315:PRO:HB2	6:L:2125:HOH:O	2.10	0.50
1:L:2319[B]:HIS:CE1	6:L:2128:HOH:O	2.64	0.50
1:G:1222:GLN:NE2	1:H:1470:ARG:HH22	2.09	0.50
1:K:2119[A]:HIS:HD2	5:K:2421:GOL:C2	2.24	0.50
1:H:1544:ARG:NE	6:H:2117:HOH:O	2.42	0.50
1:J:1884:SER:OG	1:J:1906:HIS:HE1	1.95	0.50
1:G:1281:ALA:HA	2:G:1360:CA2:HA	1.94	0.50
1:B:224:GLN:N	1:B:225:PRO:CD	2.75	0.49
1:G:1319[B]:HIS:CD2	5:G:2417:GOL:H2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:804:LEU:HD23	1:E:849:GLY:HA3	1.95	0.49
1:G:1270:ARG:HH22	1:I:1622:GLN:HE21	1.60	0.49
1:J:1826:GLU:CD	1:J:1826:GLU:H	2.16	0.49
1:I:1604:LEU:O	6:I:2024:HOH:O	2.20	0.49
1:E:828:TYR:CG	2:E:960:CA2:H13	2.48	0.48
1:F:1119[A]:HIS:HD2	5:F:2418:GOL:C2	2.26	0.48
1:A:111:HIS:ND1	5:D:2416:GOL:O2	2.31	0.48
1:E:919[A]:HIS:CD2	5:E:2419:GOL:C1	2.93	0.48
1:F:1028:TYR:CD1	2:F:1160:CA2:H13	2.48	0.48
1:K:2011:ILE:HD13	1:K:2077:VAL:HB	1.95	0.48
1:H:1519[A]:HIS:CG	5:H:2411:GOL:H12	2.38	0.48
1:A:28:TYR:OH	1:A:113:ARG:NH1	2.47	0.48
1:K:2015:PRO:O	1:K:2016:ASN:HB2	2.14	0.48
1:D:622:GLN:HE21	1:E:870:ARG:HH22	1.62	0.47
1:F:1025:PRO:HD2	1:F:1026:GLU:OE2	2.14	0.47
1:J:1842:LYS:HD3	6:J:2046:HOH:O	2.13	0.47
1:C:430:SER:HB3	6:C:2044:HOH:O	2.13	0.47
1:F:1119[A]:HIS:HB2	5:F:2418:GOL:H31	1.95	0.47
1:G:1226:GLU:CD	1:G:1226:GLU:H	2.14	0.47
1:I:1602:ARG:CA	6:I:2022:HOH:O	2.47	0.47
1:A:58:HIS:ND1	3:A:2401:PO4:O2	2.29	0.47
1:B:271:LEU:HD22	6:B:2095:HOH:O	1.85	0.47
1:K:2015:PRO:HD2	1:K:2081:ALA:HB3	1.95	0.47
1:I:1624:GLN:N	1:I:1625:PRO:CD	2.78	0.47
1:I:1642:LYS:NZ	6:I:2061:HOH:O	2.48	0.47
5:C:2415:GOL:O1	6:C:2144:HOH:O	2.21	0.47
1:E:828:TYR:CD1	2:E:960:CA2:H13	2.49	0.46
5:E:2422:GOL:H11	1:L:2319[B]:HIS:ND1	2.31	0.46
1:I:1658:HIS:HD1	3:I:2403:PO4:P	2.38	0.46
1:I:1627:ILE:O	6:I:2041:HOH:O	2.21	0.46
1:C:433:LEU:HA	1:C:433:LEU:HD12	1.87	0.46
1:F:1120:SER:H	5:F:2418:GOL:C1	1.98	0.46
1:G:1225:PRO:N	1:G:1226:GLU:OE2	2.49	0.46
1:D:604:LEU:HD12	1:D:674:CYS:SG	2.57	0.45
1:D:623:ARG:CD	1:E:896:THR:HA	2.47	0.45
1:I:1719[B]:HIS:HB3	5:I:2420:GOL:C1	2.47	0.45
1:J:1821:GLY:CA	6:J:2016:HOH:O	2.53	0.45
1:H:1428:TYR:CD1	2:H:1560:CA2:H13	2.51	0.45
1:L:2202:ARG:NH2	6:L:2098:HOH:O	2.39	0.45
1:E:927:ASP:OD1	6:E:2169:HOH:O	2.20	0.45
1:I:1701:PRO:HB2	1:I:1745:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1026:GLU:CD	1:F:1026:GLU:H	2.19	0.44
1:C:426:GLU:CD	1:C:426:GLU:H	2.20	0.44
1:L:2226:GLU:H	1:L:2226:GLU:CD	2.21	0.44
1:B:223:ARG:HG2	2:B:360:CA2:H15	1.99	0.44
1:H:1519[A]:HIS:ND1	6:H:2098:HOH:O	2.14	0.44
1:I:1643:ALA:O	1:I:1647:HIS:HD2	2.01	0.44
5:K:2421:GOL:C2	6:K:3122:HOH:O	2.65	0.44
1:A:25:PRO:HG3	6:A:2023:HOH:O	2.10	0.44
1:F:1125:ARG:HD2	1:F:1125:ARG:O	2.18	0.44
1:I:1716:PHE:CB	6:I:2018:HOH:O	2.66	0.44
1:G:1324:GLN:HE22	1:I:1716:PHE:HE2	1.65	0.44
1:B:269:ALA:HA	1:B:273:HIS:ND1	2.34	0.43
1:H:1513:ARG:NH2	6:H:2029:HOH:O	2.51	0.43
1:E:826:GLU:H	1:E:826:GLU:CD	2.21	0.43
1:J:1824:GLN:N	1:J:1825:PRO:CD	2.81	0.43
1:L:2228:TYR:OH	1:L:2313:ARG:NH1	2.44	0.43
1:A:24:GLN:N	1:A:25:PRO:CD	2.82	0.43
1:B:226:GLU:CD	1:B:226:GLU:N	2.67	0.43
1:J:1919[B]:HIS:ND1	5:J:2412:GOL:H31	2.33	0.43
1:D:622:GLN:HE22	1:E:870:ARG:HH12	1.66	0.43
1:D:643:ALA:O	1:D:647:HIS:HD2	2.02	0.43
1:J:1869:ALA:HA	1:J:1873:HIS:ND1	2.33	0.43
1:J:1815:PRO:HD2	1:J:1881:ALA:HB3	2.01	0.42
1:A:23:ARG:NH2	1:B:298:ASP:OD1	2.35	0.42
1:D:707:ILE:HD13	1:D:707:ILE:HG21	1.84	0.42
1:H:1443:ALA:O	1:H:1447:HIS:HD2	2.03	0.42
1:D:624:GLN:N	1:D:625:PRO:CD	2.83	0.42
1:D:627:ILE:HD13	1:D:627:ILE:HG21	1.83	0.42
1:L:2348:LEU:C	1:L:2350:GLY:N	2.72	0.42
1:E:911:HIS:HD1	5:E:2422:GOL:HO2	1.62	0.42
1:A:2:ARG:HD3	1:A:7:ALA:HB2	2.02	0.42
1:A:98:ASP:OD2	1:C:423:ARG:NE	2.40	0.42
1:B:223:ARG:HD3	6:B:2036:HOH:O	2.19	0.42
1:B:223:ARG:NH1	1:B:224:GLN:OE1	2.53	0.42
1:G:1254:ARG:HB3	1:G:1265:TRP:CZ3	2.55	0.42
1:K:2114:GLU:CD	1:K:2114:GLU:H	2.22	0.42
1:K:2119[A]:HIS:HD2	5:K:2421:GOL:H31	1.84	0.42
1:A:2:ARG:HB3	1:A:6:ASN:HD21	1.85	0.41
1:J:1916:PHE:HE2	1:K:2124:GLN:HE22	1.68	0.41
1:K:2119[A]:HIS:HD2	5:K:2421:GOL:C3	2.33	0.41
1:C:519[B]:HIS:HD2	5:C:2415:GOL:H12	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:950:GLY:CA	6:E:2181:HOH:O	2.68	0.41
1:C:425:PRO:CD	1:C:426:GLU:OE2	2.51	0.41
1:E:918:HIS:HE1	6:E:2158:HOH:O	2.03	0.41
1:H:1430:SER:HB2	6:H:2017:HOH:O	2.17	0.41
1:E:914:GLU:CD	6:E:2154:HOH:O	2.56	0.41
1:F:1119[A]:HIS:HD2	5:F:2418:GOL:H2	1.85	0.41
1:H:1402:ARG:HD3	1:H:1407:ALA:HB2	2.02	0.41
1:H:1498:ASP:OD1	6:H:2083:HOH:O	2.22	0.41
1:K:2119[A]:HIS:CD2	5:K:2421:GOL:C2	3.04	0.41
1:L:2202:ARG:HA	6:L:2026:HOH:O	2.20	0.41
1:E:919[A]:HIS:CD2	5:E:2419:GOL:C2	3.04	0.41
1:E:824:GLN:HA	1:E:826:GLU:OE2	2.21	0.41
2:J:1960:CA2:O4	1:K:2092:ASP:OD2	2.37	0.41
2:A:160:CA2:H102	2:A:160:CA2:H17	1.83	0.41
1:C:519[A]:HIS:ND1	5:C:2415:GOL:C3	2.83	0.40
1:J:1925:ARG:O	1:J:1926:ALA:C	2.59	0.40
1:F:1028:TYR:CG	2:F:1160:CA2:H13	2.56	0.40
1:I:1749:ALA:O	6:I:2149:HOH:O	2.21	0.40
1:E:822:GLN:NE2	1:F:1070:ARG:NH2	2.65	0.40
1:E:914:GLU:HA	1:E:915:PRO:HD3	1.84	0.40
1:F:1002:ARG:HD3	1:F:1007:ALA:HB2	2.04	0.40
1:I:1720:SER:H	5:I:2420:GOL:H11	1.85	0.40
1:K:2007:ALA:HB1	1:K:2008:PRO:HD2	2.03	0.40
1:F:1114:GLU:HA	1:F:1115:PRO:HD3	1.93	0.40
1:A:26:GLU:CD	1:A:26:GLU:H	2.24	0.40
2:B:360:CA2:H2C1	2:B:360:CA2:H9C2	1.89	0.40
1:D:670:ARG:HH22	1:F:1022:GLN:NE2	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	149/157 (95%)	146 (98%)	3 (2%)	0	100	100
1	B	148/157 (94%)	145 (98%)	3 (2%)	0	100	100
1	C	148/157 (94%)	145 (98%)	3 (2%)	0	100	100
1	D	149/157 (95%)	146 (98%)	3 (2%)	0	100	100
1	E	148/157 (94%)	144 (97%)	4 (3%)	0	100	100
1	F	148/157 (94%)	145 (98%)	3 (2%)	0	100	100
1	G	149/157 (95%)	145 (97%)	4 (3%)	0	100	100
1	H	148/157 (94%)	145 (98%)	3 (2%)	0	100	100
1	I	148/157 (94%)	145 (98%)	3 (2%)	0	100	100
1	J	148/157 (94%)	144 (97%)	4 (3%)	0	100	100
1	K	148/157 (94%)	145 (98%)	3 (2%)	0	100	100
1	L	149/157 (95%)	145 (97%)	4 (3%)	0	100	100
All	All	1780/1884 (94%)	1740 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	119/121 (98%)	117 (98%)	2 (2%)	60	46
1	B	118/121 (98%)	114 (97%)	4 (3%)	37	18
1	C	118/121 (98%)	116 (98%)	2 (2%)	60	46
1	D	119/121 (98%)	116 (98%)	3 (2%)	47	29
1	E	118/121 (98%)	116 (98%)	2 (2%)	60	46
1	F	118/121 (98%)	117 (99%)	1 (1%)	81	74
1	G	119/121 (98%)	117 (98%)	2 (2%)	60	46
1	H	118/121 (98%)	116 (98%)	2 (2%)	60	46
1	I	118/121 (98%)	116 (98%)	2 (2%)	60	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	119/121 (98%)	117 (98%)	2 (2%)	60	46
1	K	118/121 (98%)	118 (100%)	0	100	100
1	L	119/121 (98%)	116 (98%)	3 (2%)	47	29
All	All	1421/1452 (98%)	1396 (98%)	25 (2%)	59	43

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	26	GLU
1	B	204	LEU
1	B	206	ASN
1	B	226	GLU
1	B	239	LEU
1	C	426	GLU
1	C	430	SER
1	D	604	LEU
1	D	623	ARG
1	D	626	GLU
1	E	823	ARG
1	E	826	GLU
1	F	1026	GLU
1	G	1211	ILE
1	G	1226	GLU
1	H	1426	GLU
1	H	1439	LEU
1	I	1623	ARG
1	I	1626	GLU
1	J	1826	GLU
1	J	1842	LYS
1	L	2211	ILE
1	L	2223	ARG
1	L	2226	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	124	GLN
1	B	247	HIS

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Mol	Chain	Res	Type
1	C	422	GLN
1	C	447	HIS
1	D	622	GLN
1	D	724	GLN
1	E	822	GLN
1	F	1022	GLN
1	F	1047	HIS
1	F	1124	GLN
1	G	1222	GLN
1	G	1247	HIS
1	G	1324	GLN
1	H	1422	GLN
1	H	1524	GLN
1	I	1606	ASN
1	I	1622	GLN
1	I	1647	HIS
1	J	1822	GLN
1	J	1924	GLN
1	K	2022	GLN
1	K	2047	HIS
1	K	2124	GLN
1	L	2222	GLN
1	L	2324	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

32 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$
3	PO4	L	2404	-	4,4,4	1.06	0	6,6,6	2.15	2 (33%)
2	CA2	G	1360	-	20,23,23	1.68	3 (15%)	23,32,32	2.12	6 (26%)
5	GOL	J	2412	-	5,5,5	0.51	0	5,5,5	1.01	0
2	CA2	L	2360	-	20,23,23	1.02	1 (5%)	23,32,32	1.58	4 (17%)
5	GOL	C	2415	-	5,5,5	0.77	0	5,5,5	0.80	0
3	PO4	A	2401	-	4,4,4	1.62	1 (25%)	6,6,6	1.78	2 (33%)
5	GOL	E	2422	-	5,5,5	0.92	0	5,5,5	0.43	0
3	PO4	D	2402	-	4,4,4	1.50	1 (25%)	6,6,6	0.76	0
2	CA2	B	360	-	20,23,23	1.03	2 (10%)	23,32,32	2.34	8 (34%)
5	GOL	K	2421	-	5,5,5	0.64	0	5,5,5	0.91	0
5	GOL	D	2416	-	5,5,5	0.56	0	5,5,5	0.55	0
4	TRS	F	2406	-	7,7,7	0.62	0	9,9,9	0.69	0
2	CA2	K	2160	-	20,23,23	0.65	0	23,32,32	1.91	5 (21%)
2	CA2	A	160	-	20,23,23	1.46	3 (15%)	23,32,32	2.14	5 (21%)
2	CA2	F	1160	-	20,23,23	1.05	1 (5%)	23,32,32	1.54	5 (21%)
5	GOL	E	2419	-	5,5,5	0.72	0	5,5,5	0.86	0
2	CA2	E	960	-	20,23,23	1.19	1 (5%)	23,32,32	2.08	6 (26%)
4	TRS	L	2408	-	7,7,7	0.45	0	9,9,9	0.97	0
5	GOL	H	2411	-	5,5,5	0.41	0	5,5,5	0.60	0
2	CA2	I	1760	-	20,23,23	1.18	2 (10%)	23,32,32	1.54	5 (21%)
5	GOL	B	2414	-	5,5,5	0.53	0	5,5,5	0.49	0
5	GOL	G	2417	-	5,5,5	0.77	0	5,5,5	1.41	1 (20%)
4	TRS	A	2405	-	7,7,7	0.68	0	9,9,9	1.47	3 (33%)
2	CA2	C	560	-	20,23,23	0.94	1 (5%)	23,32,32	1.42	4 (17%)
2	CA2	J	1960	-	20,23,23	1.36	3 (15%)	23,32,32	1.46	4 (17%)
2	CA2	D	760	-	20,23,23	0.96	1 (5%)	23,32,32	2.21	7 (30%)
2	CA2	H	1560	-	20,23,23	1.20	2 (10%)	23,32,32	1.86	5 (21%)
5	GOL	F	2418	-	5,5,5	0.96	0	5,5,5	1.97	3 (60%)
4	TRS	H	2407	-	7,7,7	0.91	0	9,9,9	0.83	0
5	GOL	A	2413	-	5,5,5	0.76	0	5,5,5	0.69	0
3	PO4	I	2403	-	4,4,4	1.40	1 (25%)	6,6,6	1.67	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	I	2420	-	5,5,5	0.55	0	5,5,5	0.77	0

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	CA2	G	1360	-	-	0/7/31/31	0/2/2/2
5	GOL	J	2412	-	-	4/4/4/4	-
2	CA2	L	2360	-	-	2/7/31/31	0/2/2/2
5	GOL	C	2415	-	-	3/4/4/4	-
5	GOL	E	2422	-	-	4/4/4/4	-
2	CA2	B	360	-	-	1/7/31/31	0/2/2/2
5	GOL	K	2421	-	-	2/4/4/4	-
2	CA2	I	1760	-	-	1/7/31/31	0/2/2/2
4	TRS	F	2406	-	-	0/9/9/9	-
2	CA2	K	2160	-	-	2/7/31/31	0/2/2/2
2	CA2	A	160	-	-	0/7/31/31	0/2/2/2
2	CA2	F	1160	-	-	1/7/31/31	0/2/2/2
5	GOL	E	2419	-	-	2/4/4/4	-
2	CA2	E	960	-	-	0/7/31/31	0/2/2/2
4	TRS	L	2408	-	-	0/9/9/9	-
5	GOL	H	2411	-	-	0/4/4/4	-
5	GOL	D	2416	-	-	4/4/4/4	-
5	GOL	B	2414	-	-	2/4/4/4	-
5	GOL	G	2417	-	-	1/4/4/4	-
4	TRS	A	2405	-	-	0/9/9/9	-
2	CA2	C	560	-	-	3/7/31/31	0/2/2/2
2	CA2	J	1960	-	-	1/7/31/31	0/2/2/2
2	CA2	D	760	-	-	0/7/31/31	0/2/2/2
2	CA2	H	1560	-	-	2/7/31/31	0/2/2/2
5	GOL	F	2418	-	-	0/4/4/4	-
4	TRS	H	2407	-	-	0/9/9/9	-
5	GOL	A	2413	-	-	4/4/4/4	-
5	GOL	I	2420	-	-	3/4/4/4	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1360	CA2	C2-C1	-5.30	1.48	1.53
2	A	160	CA2	O3-C1	4.39	1.50	1.43
2	E	960	CA2	O3-C1	4.03	1.49	1.43
2	I	1760	CA2	C6-C1	-3.89	1.50	1.53
2	B	360	CA2	C2-C1	-3.40	1.50	1.53
2	L	2360	CA2	C2-C1	-3.21	1.50	1.53
2	H	1560	CA2	C2-C1	-3.11	1.50	1.53
2	J	1960	CA2	C2-C1	-2.81	1.51	1.53
3	A	2401	PO4	P-O2	-2.79	1.46	1.54
2	J	1960	CA2	O5-C5	2.75	1.49	1.43
2	C	560	CA2	C5-C4	-2.61	1.48	1.52
3	I	2403	PO4	P-O3	-2.54	1.47	1.54
2	H	1560	CA2	C6-C1	-2.49	1.51	1.53
2	D	760	CA2	C6-C5	2.45	1.56	1.53
2	G	1360	CA2	O3-C1	-2.36	1.39	1.43
2	F	1160	CA2	C6-C5	2.34	1.56	1.53
2	G	1360	CA2	C6-C5	-2.31	1.49	1.53
2	A	160	CA2	C3-C4	2.23	1.56	1.53
3	D	2402	PO4	P-O4	-2.15	1.48	1.54
2	A	160	CA2	O4-C4	2.13	1.48	1.43
2	J	1960	CA2	C3-C4	-2.11	1.50	1.53
2	B	360	CA2	O5-C5	2.01	1.47	1.43
2	I	1760	CA2	C6-C5	2.01	1.56	1.53

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	160	CA2	C2-C3-C4	6.46	117.40	109.20
2	H	1560	CA2	C2-C3-C4	6.01	116.83	109.20
2	K	2160	CA2	C6-C5-C4	-5.51	105.45	110.84
2	B	360	CA2	C6-C1-C2	5.49	115.99	110.43
2	D	760	CA2	C6-C5-C4	-5.33	105.62	110.84
2	G	1360	CA2	C2-C3-C8	-5.23	102.23	111.99
2	L	2360	CA2	C2-C3-C4	4.99	115.54	109.20
2	D	760	CA2	C2-C3-C4	4.81	115.31	109.20
2	B	360	CA2	O5-C5-C6	4.50	120.38	109.91
2	A	160	CA2	O3-C1-C2	4.42	116.69	108.42
2	E	960	CA2	O3-C1-C6	4.40	116.66	108.42
3	L	2404	PO4	O2-P-O1	-4.32	95.08	110.89
2	E	960	CA2	O4-C4-C3	-4.29	102.84	110.08
2	G	1360	CA2	C6-C5-C4	-4.23	106.70	110.84
2	E	960	CA2	C2-C3-C4	4.17	114.50	109.20
2	D	760	CA2	C2-C3-C8	-3.97	104.59	111.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	960	CA2	C6-C1-C2	-3.90	106.48	110.43
2	K	2160	CA2	C6-C1-C2	3.88	114.36	110.43
2	B	360	CA2	C2-C3-C4	3.80	114.02	109.20
2	G	1360	CA2	C2-C3-C4	3.78	114.00	109.20
2	G	1360	CA2	C6-C1-C2	3.69	114.17	110.43
2	F	1160	CA2	C2-C3-C4	3.67	113.86	109.20
2	B	360	CA2	O5-C5-C4	-3.61	102.90	110.14
2	A	160	CA2	C6-C5-C4	-3.53	107.38	110.84
2	D	760	CA2	O4-C4-C5	-3.53	103.24	109.99
2	B	360	CA2	C1-C6-C5	-3.48	106.32	112.38
2	I	1760	CA2	O4-C4-C5	-3.47	103.35	109.99
2	J	1960	CA2	C2-C3-C4	3.42	113.54	109.20
2	C	560	CA2	O5-C5-C4	-3.31	103.52	110.14
2	B	360	CA2	O4-C4-C5	-3.29	103.70	109.99
2	D	760	CA2	C6-C1-C2	3.28	113.75	110.43
2	I	1760	CA2	C6-C5-C4	3.26	114.02	110.84
2	K	2160	CA2	C2-C3-C4	3.22	113.29	109.20
2	K	2160	CA2	O4-C4-C5	-3.21	103.84	109.99
3	A	2401	PO4	O3-P-O2	3.20	118.22	107.97
2	H	1560	CA2	O3-C1-C2	3.13	114.28	108.42
2	J	1960	CA2	O3-C1-C2	3.10	114.22	108.42
2	A	160	CA2	O5-C5-C4	-3.09	103.94	110.14
2	I	1760	CA2	O5-C5-C4	-3.00	104.12	110.14
5	F	2418	GOL	O1-C1-C2	2.88	124.03	110.20
2	H	1560	CA2	O4-C4-C5	-2.87	104.50	109.99
2	F	1160	CA2	O5-C5-C6	2.80	116.43	109.91
2	G	1360	CA2	O4-C4-C3	2.77	114.77	110.08
2	K	2160	CA2	C2-C3-C8	-2.70	106.96	111.99
2	F	1160	CA2	C6-C1-C2	-2.70	107.70	110.43
4	A	2405	TRS	O1-C1-C	2.66	119.42	111.00
2	J	1960	CA2	C6-C1-C2	2.66	113.12	110.43
5	G	2417	GOL	O1-C1-C2	2.65	122.91	110.20
2	H	1560	CA2	O5-C5-C4	-2.59	104.95	110.14
2	C	560	CA2	O4-C4-C5	-2.55	105.11	109.99
2	L	2360	CA2	O4-C4-C5	-2.54	105.13	109.99
3	A	2401	PO4	O3-P-O1	-2.54	101.59	110.89
2	D	760	CA2	C10-O11-C12	2.54	124.55	117.93
2	J	1960	CA2	O5-C5-C4	-2.50	105.13	110.14
2	I	1760	CA2	O3-C1-C2	2.49	113.09	108.42
2	L	2360	CA2	O3-C1-C2	2.47	113.05	108.42
2	F	1160	CA2	O5-C5-C4	-2.46	105.22	110.14
2	G	1360	CA2	C8-C9-C10	-2.45	105.54	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	760	CA2	O3-C1-C6	-2.44	103.86	108.42
2	C	560	CA2	C2-C3-C8	-2.40	107.51	111.99
2	B	360	CA2	C6-C5-C4	-2.39	108.50	110.84
2	H	1560	CA2	C1-C6-C5	2.35	116.48	112.38
2	A	160	CA2	O4-C4-C5	-2.34	105.51	109.99
2	E	960	CA2	O3-C1-C2	2.31	112.75	108.42
2	I	1760	CA2	C10-O11-C12	2.29	123.92	117.93
3	I	2403	PO4	O3-P-O2	2.25	115.20	107.97
3	I	2403	PO4	O4-P-O1	2.20	118.96	110.89
2	L	2360	CA2	O5-C5-C4	-2.20	105.73	110.14
4	A	2405	TRS	C3-C-N	2.18	114.48	107.98
4	A	2405	TRS	O3-C3-C	2.14	117.78	111.00
2	F	1160	CA2	O3-C1-C2	2.09	112.34	108.42
5	F	2418	GOL	O2-C2-C3	-2.08	99.96	109.12
2	E	960	CA2	O4-C4-C5	-2.08	106.01	109.99
5	F	2418	GOL	C3-C2-C1	2.06	119.72	111.70
2	C	560	CA2	C2-C3-C4	2.06	111.81	109.20
3	L	2404	PO4	O4-P-O1	2.01	118.26	110.89
2	B	360	CA2	C9-C8-C3	-2.00	108.38	115.17

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	2412	GOL	O1-C1-C2-C3
5	J	2412	GOL	C1-C2-C3-O3
5	C	2415	GOL	C1-C2-C3-O3
5	E	2422	GOL	O1-C1-C2-C3
5	E	2422	GOL	C1-C2-C3-O3
5	E	2422	GOL	O2-C2-C3-O3
5	K	2421	GOL	O1-C1-C2-C3
5	E	2419	GOL	C1-C2-C3-O3
5	B	2414	GOL	C1-C2-C3-O3
5	A	2413	GOL	C1-C2-C3-O3
5	I	2420	GOL	O1-C1-C2-C3
5	K	2421	GOL	O1-C1-C2-O2
5	C	2415	GOL	O1-C1-C2-C3
5	D	2416	GOL	O1-C1-C2-C3
5	G	2417	GOL	O1-C1-C2-C3
5	A	2413	GOL	O1-C1-C2-C3
2	B	360	CA2	O11-C10-C9-C8
5	J	2412	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	J	2412	GOL	O2-C2-C3-O3
5	E	2422	GOL	O1-C1-C2-O2
5	B	2414	GOL	O2-C2-C3-O3
5	A	2413	GOL	O1-C1-C2-O2
5	A	2413	GOL	O2-C2-C3-O3
5	E	2419	GOL	O2-C2-C3-O3
5	D	2416	GOL	O1-C1-C2-O2
2	F	1160	CA2	O11-C10-C9-C8
2	J	1960	CA2	O11-C10-C9-C8
5	I	2420	GOL	O1-C1-C2-O2
2	I	1760	CA2	O11-C10-C9-C8
5	D	2416	GOL	O2-C2-C3-O3
2	K	2160	CA2	O11-C10-C9-C8
2	C	560	CA2	O11-C10-C9-C8
2	H	1560	CA2	C13-C12-O11-C10
5	I	2420	GOL	C1-C2-C3-O3
2	C	560	CA2	C13-C12-O11-C10
2	C	560	CA2	C17-C12-O11-C10
2	H	1560	CA2	C17-C12-O11-C10
5	C	2415	GOL	O2-C2-C3-O3
2	L	2360	CA2	C13-C12-O11-C10
2	L	2360	CA2	C17-C12-O11-C10
5	D	2416	GOL	C1-C2-C3-O3
2	K	2160	CA2	C13-C12-O11-C10

There are no ring outliers.

22 monomers are involved in 118 short contacts:

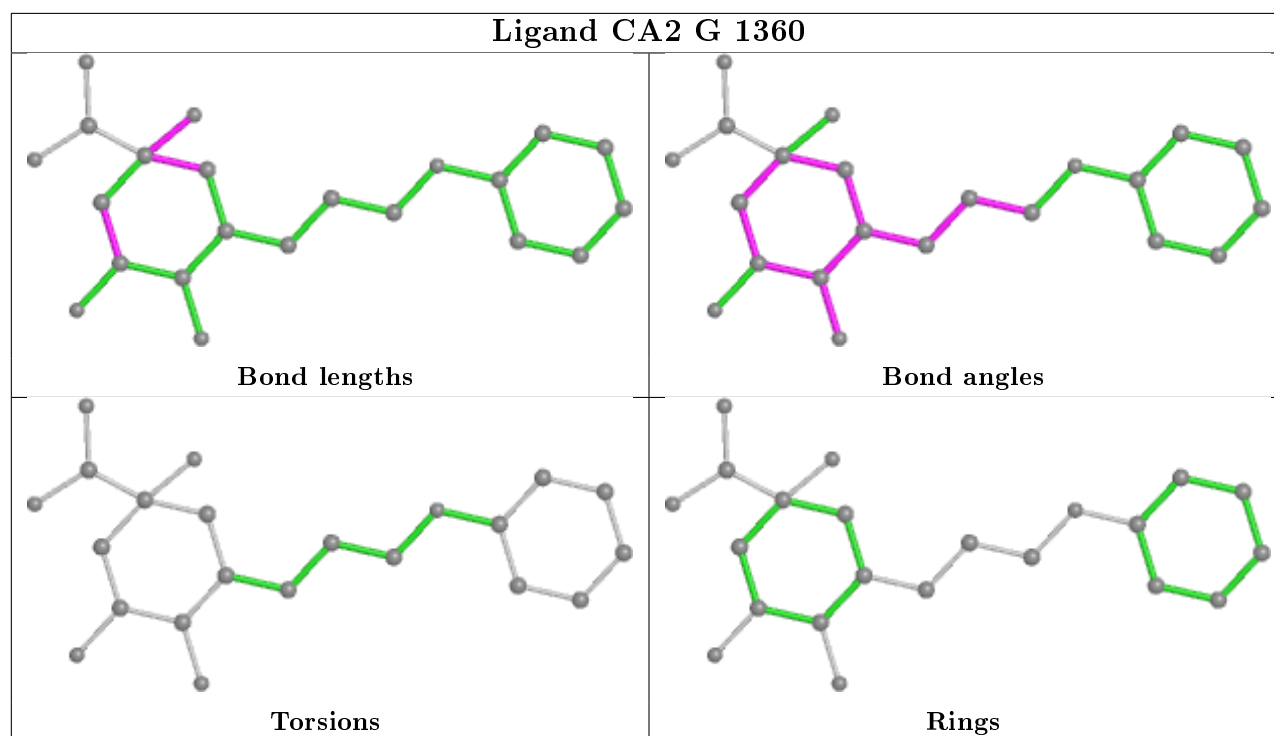
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1360	CA2	1	0
5	J	2412	GOL	4	0
5	C	2415	GOL	9	0
3	A	2401	PO4	2	0
5	E	2422	GOL	5	0
3	D	2402	PO4	1	0
2	B	360	CA2	2	0
5	K	2421	GOL	12	0
5	D	2416	GOL	9	0
2	A	160	CA2	1	0
2	F	1160	CA2	2	0
5	E	2419	GOL	10	0
2	E	960	CA2	2	0

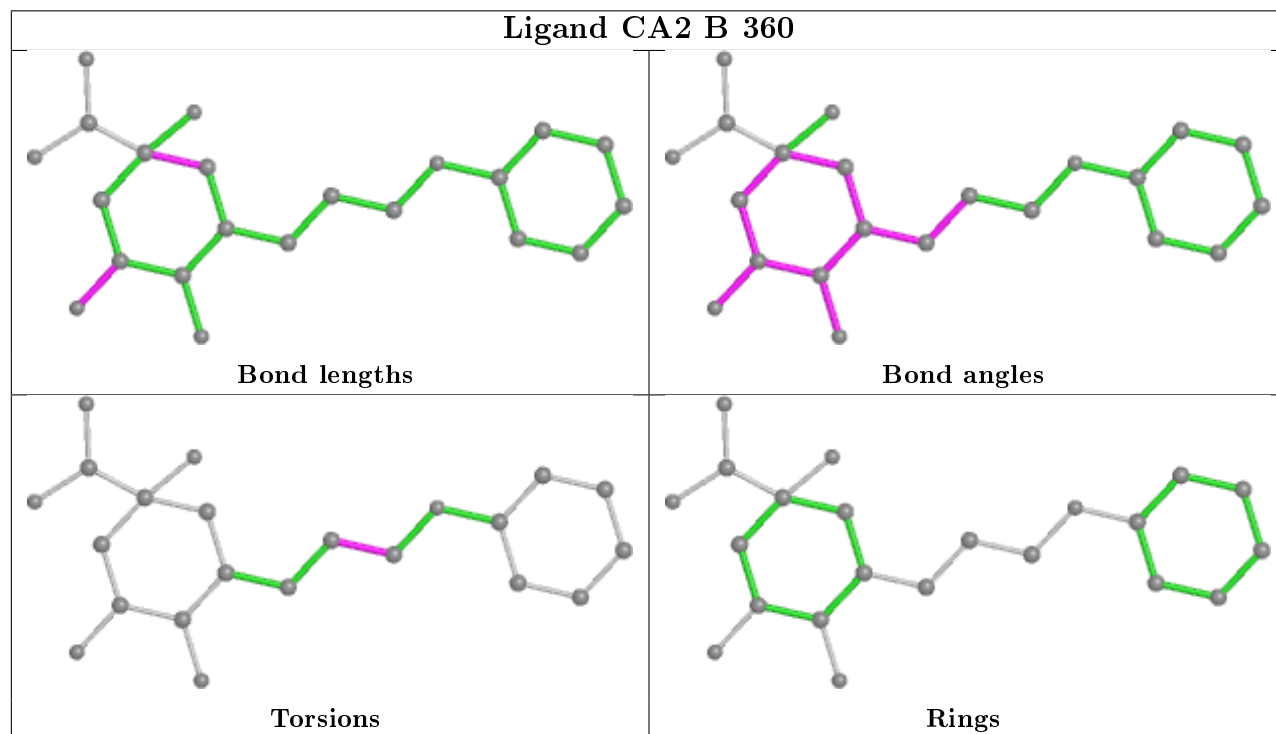
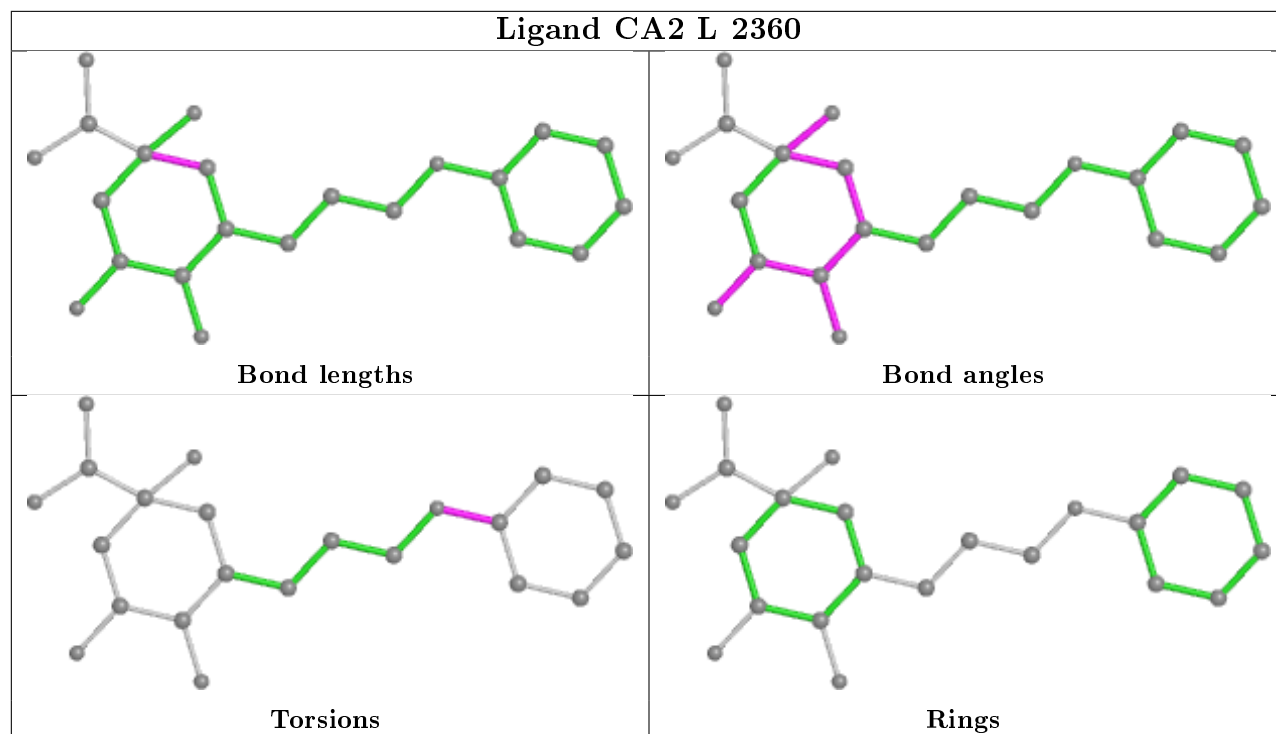
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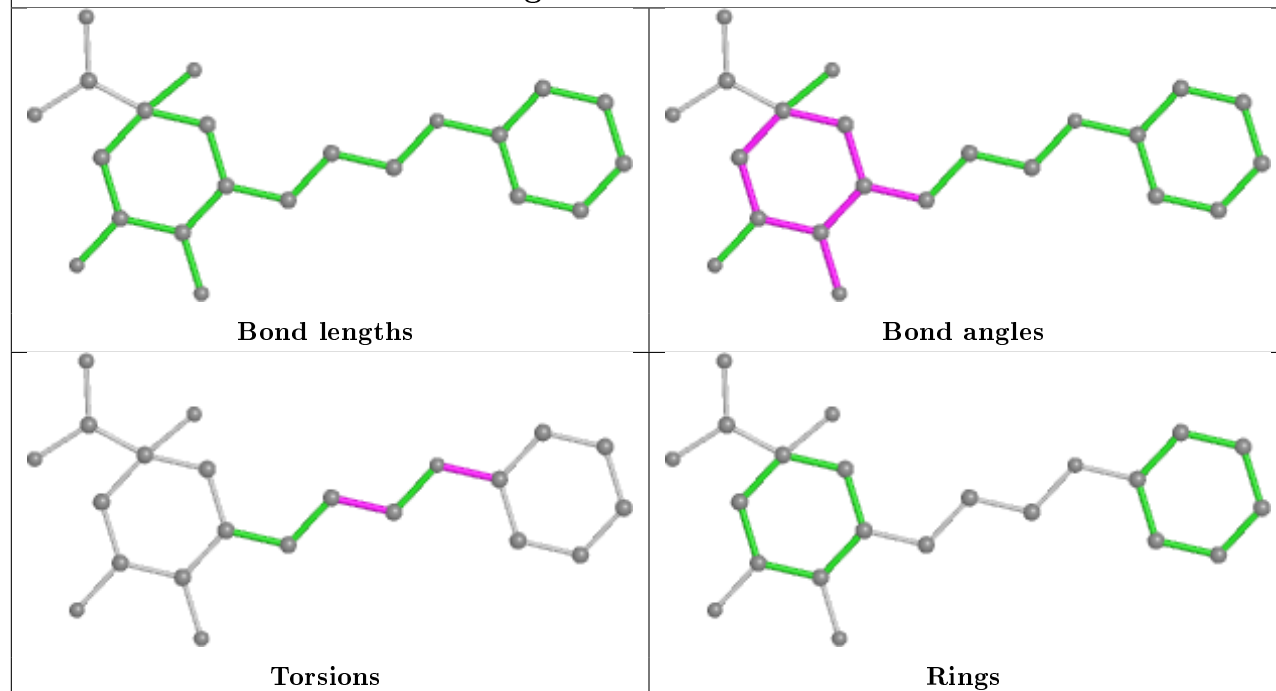
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	2411	GOL	7	0
5	B	2414	GOL	6	0
5	G	2417	GOL	7	0
2	J	1960	CA2	1	0
2	H	1560	CA2	1	0
5	F	2418	GOL	13	0
5	A	2413	GOL	1	0
3	I	2403	PO4	1	0
5	I	2420	GOL	21	0

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.

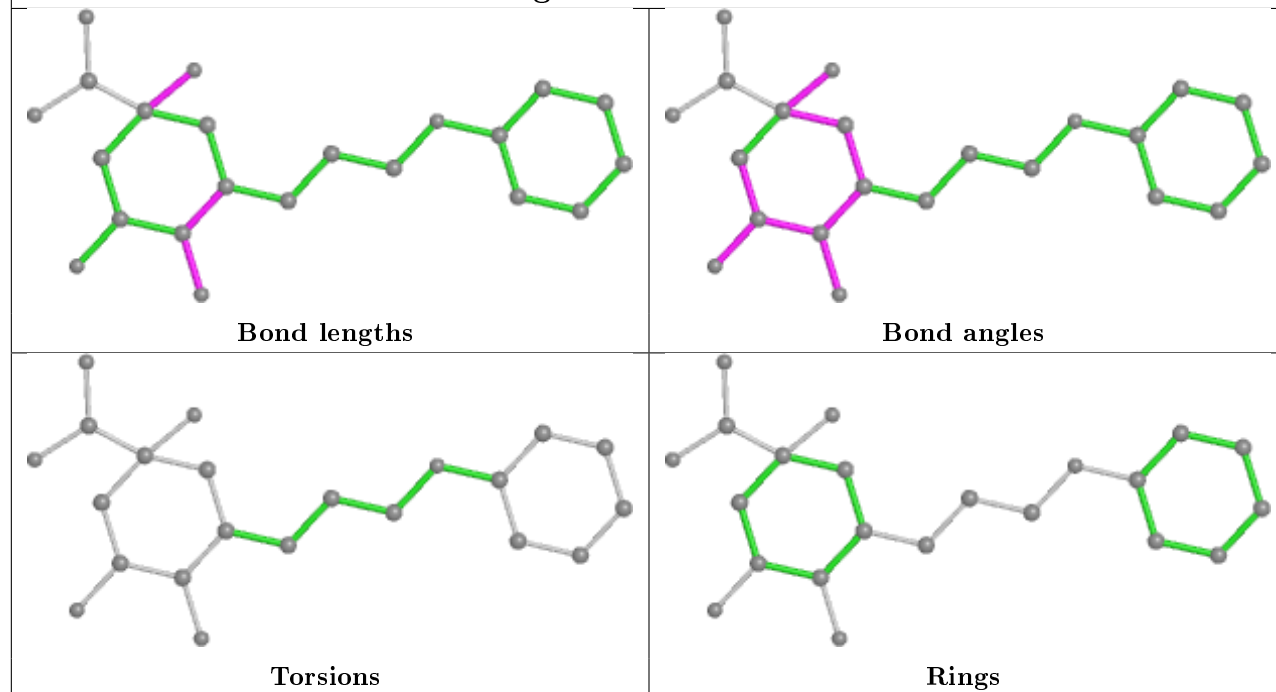




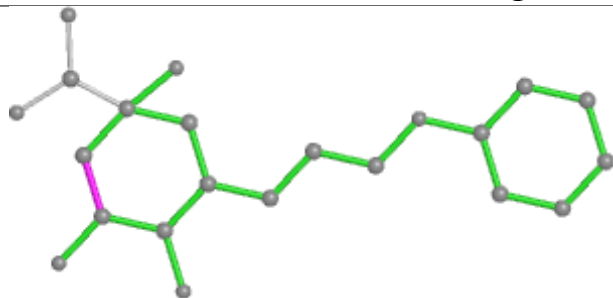
Ligand CA2 K 2160



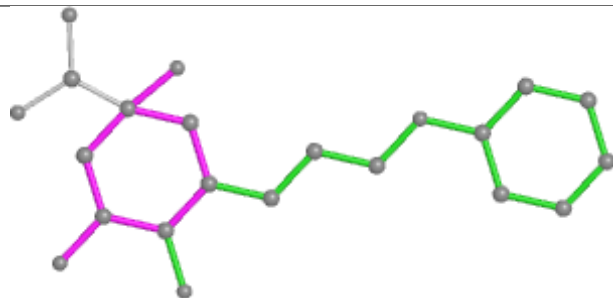
Ligand CA2 A 160



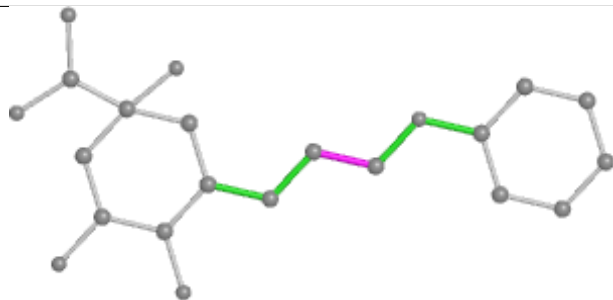
Ligand CA2 F 1160



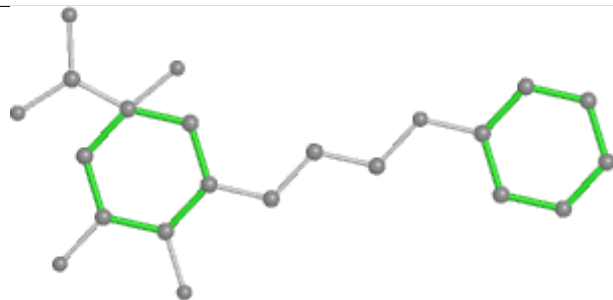
Bond lengths



Bond angles

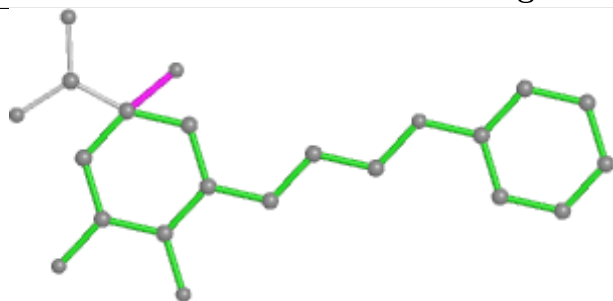


Torsions

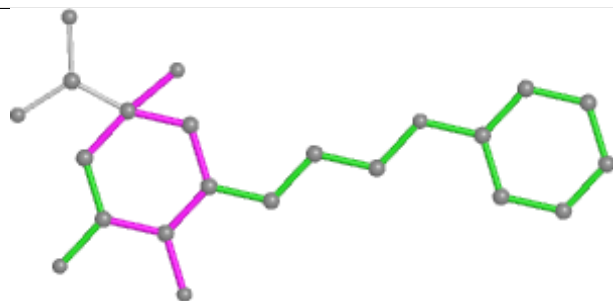


Rings

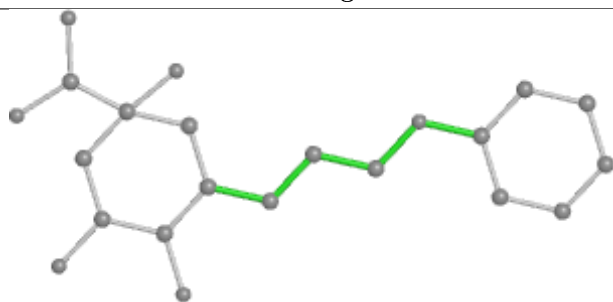
Ligand CA2 E 960



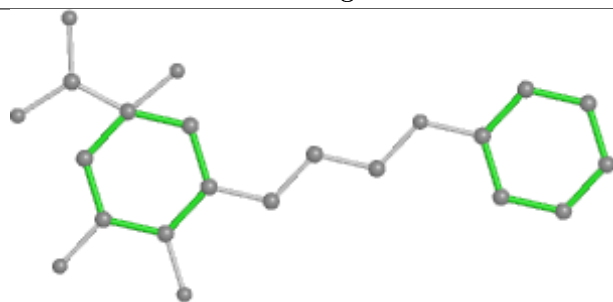
Bond lengths



Bond angles

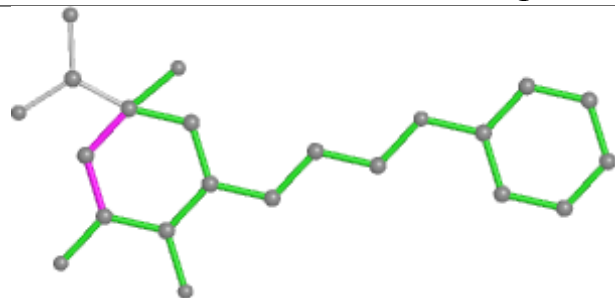


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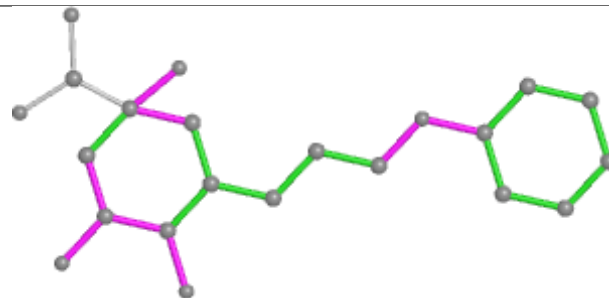


Rings

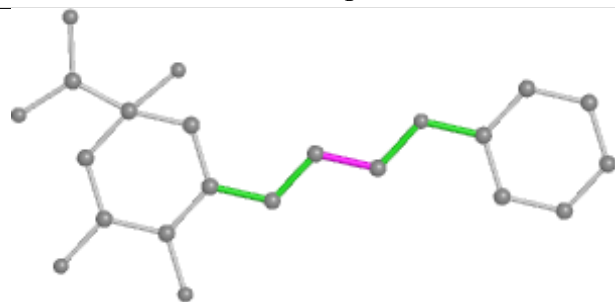
Ligand CA2 I 1760



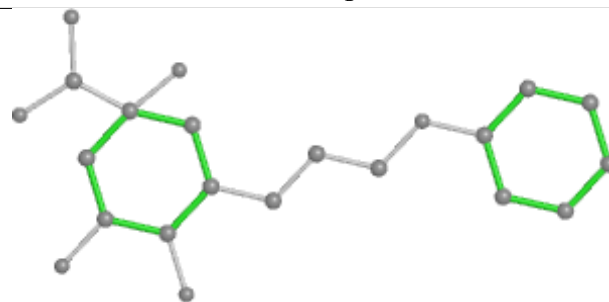
Bond lengths



Bond angles

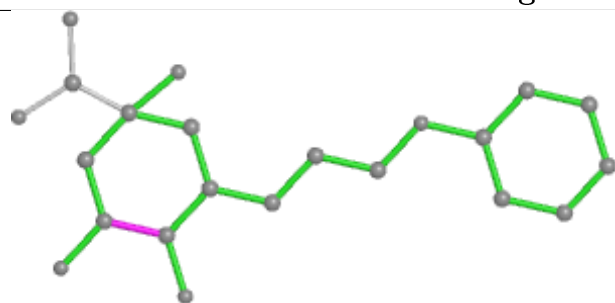


Torsions

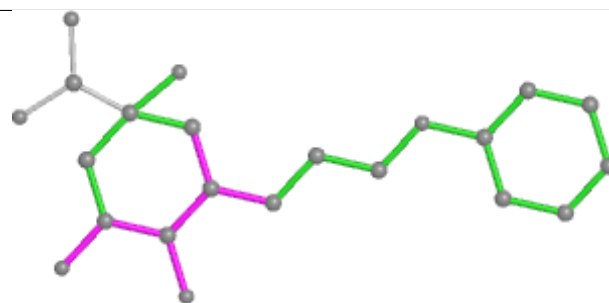


Rings

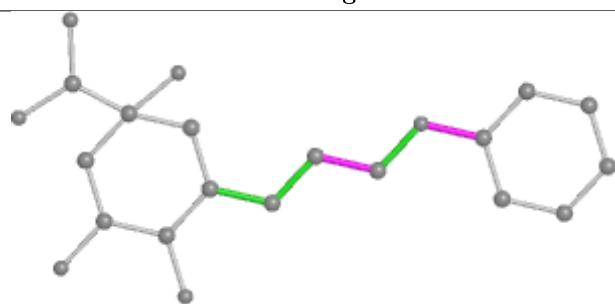
Ligand CA2 C 560



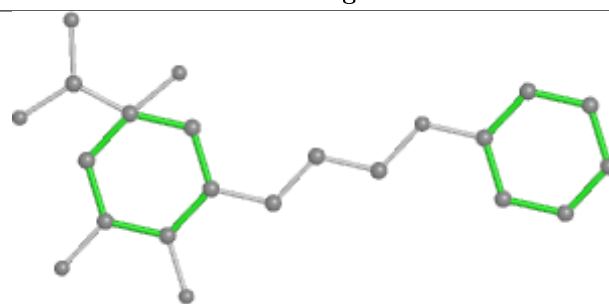
Bond lengths



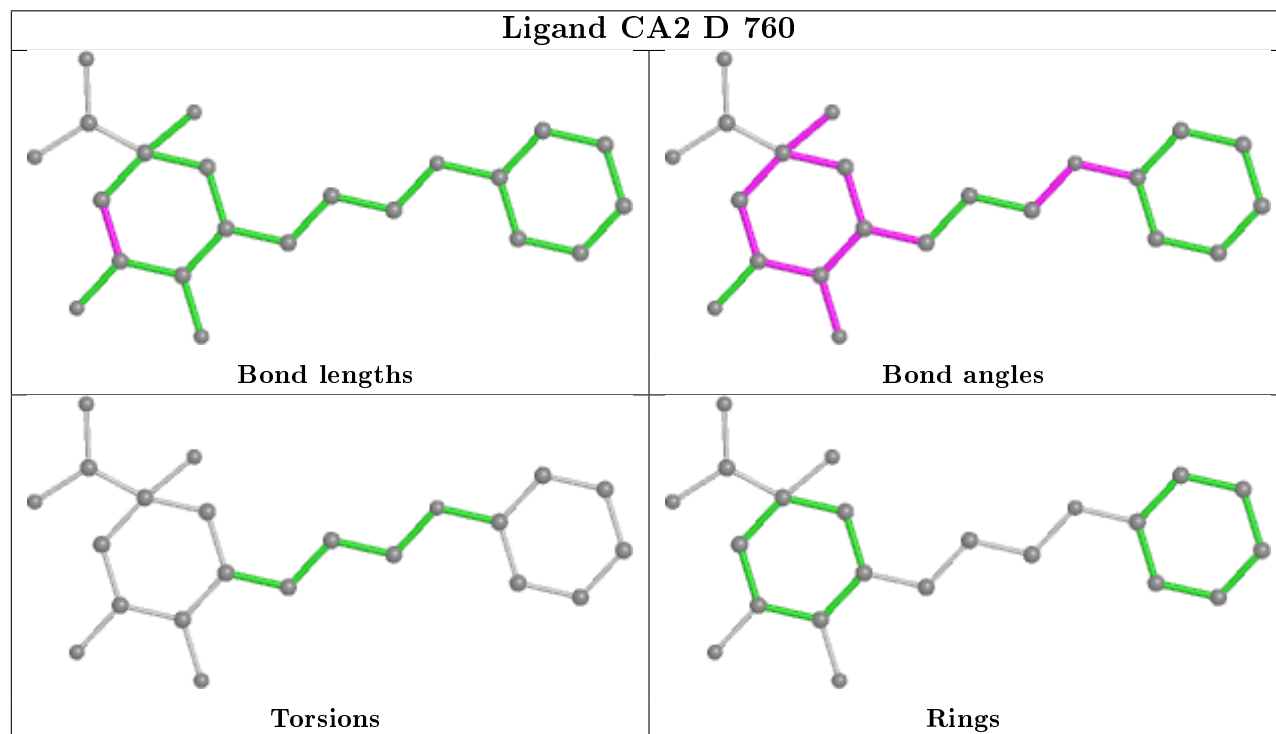
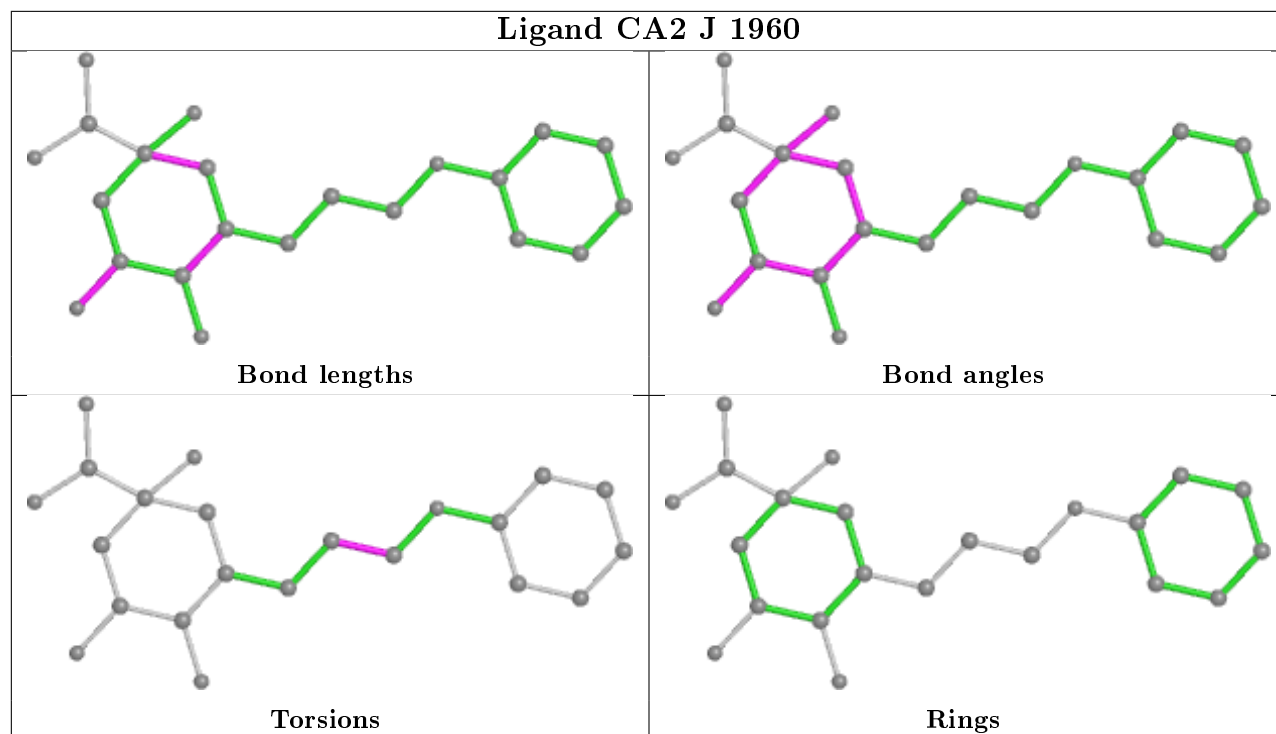
Bond angles

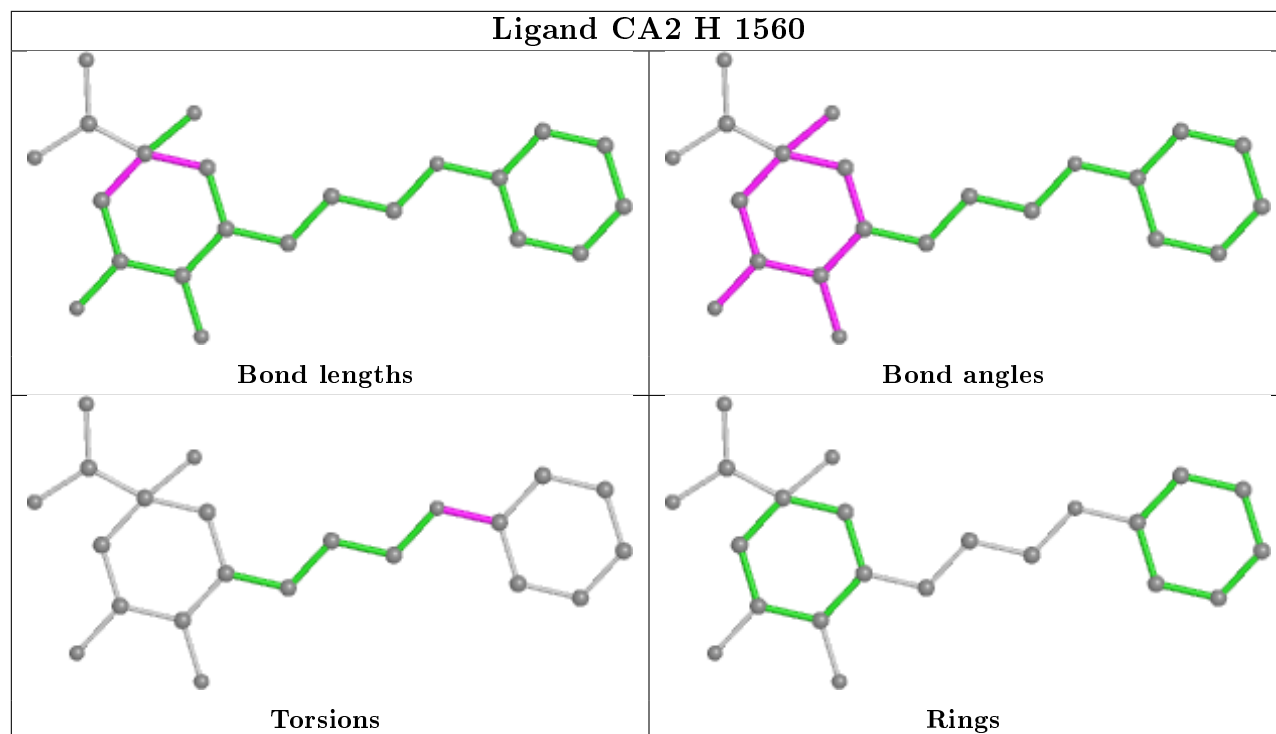


Torsions



Rings





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.