



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:37 AM UTC

PDB ID : 1N0H / pdb_00001n0h
Title : Crystal Structure of Yeast Acetohydroxyacid Synthase in Complex with a Sulfonylurea Herbicide, Chlorimuron Ethyl
Authors : Pang, S.S.; Guddat, L.W.; Duggleby, R.G.
Deposited on : 2002-10-14
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

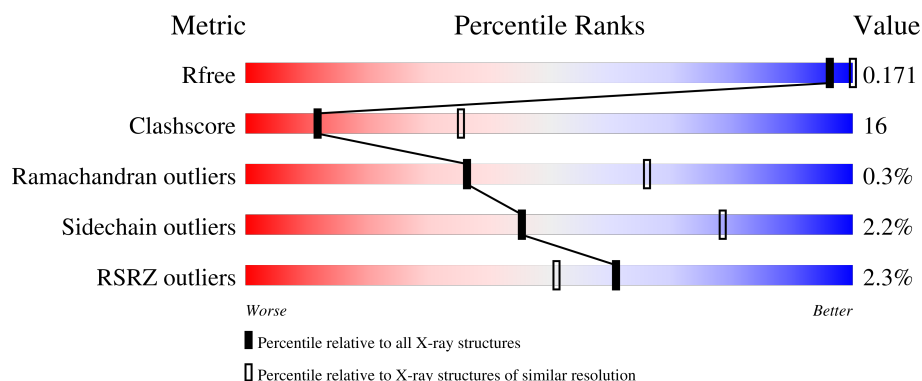
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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	677	% 66% 21% • 12%
1	B	677	3% 60% 26% • 12%

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
4	CIE	A	695	-	X	-	-
4	CIE	B	1695	-	X	-	-
6	AYD	A	700	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10196 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 Acetolactate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	599	Total	C	N	O	S	0	2	0
			4571	2894	791	864	22			
1	B	598	Total	C	N	O	S	0	2	0
			4563	2891	788	862	22			

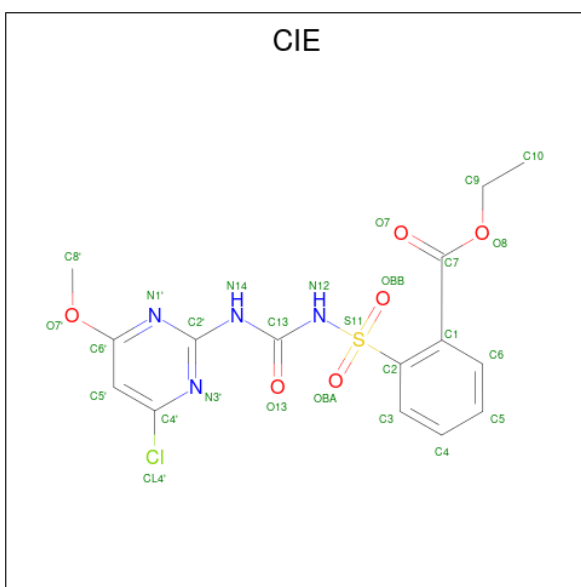
- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

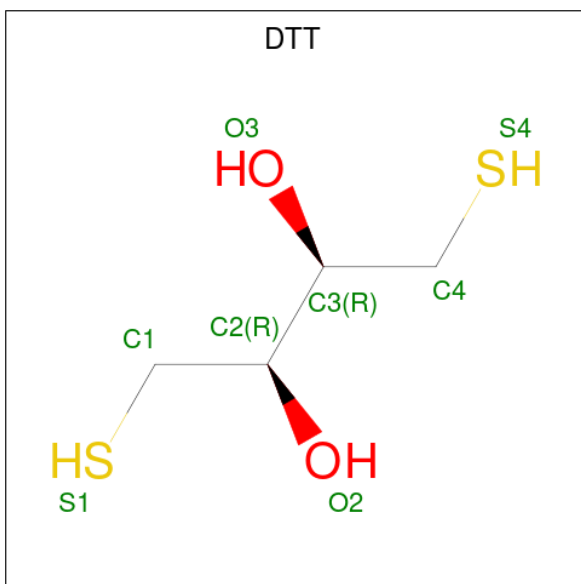
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2-[[[(4-CHLORO-6-METHOXY-2-PYRIMIDINYL)AMINO]CARBONYL]AMINO]SULFONYL]BENZOIC ACID ETHYL ESTER (CCD ID: CIE) (formula: C₁₅H₁₅ClN₄O₆S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0	0
			27	15	1	4	6	1		
4	B	1	Total	C	Cl	N	O	S	0	0
			27	15	1	4	6	1		

- Molecule 5 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: $C_4H_{10}O_2S_2$).



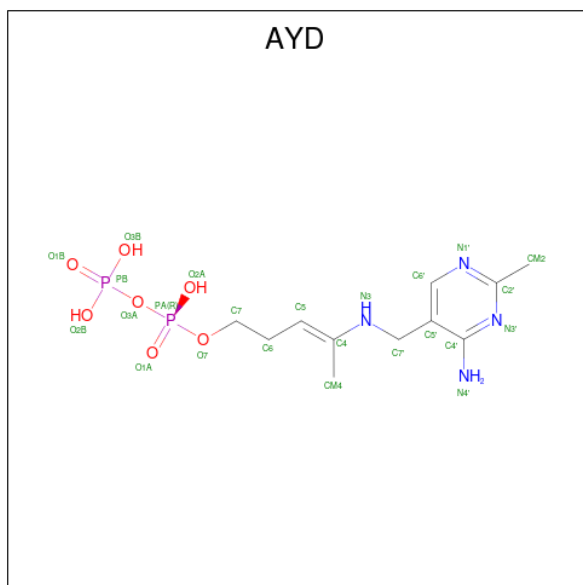
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			8	4	2	2		

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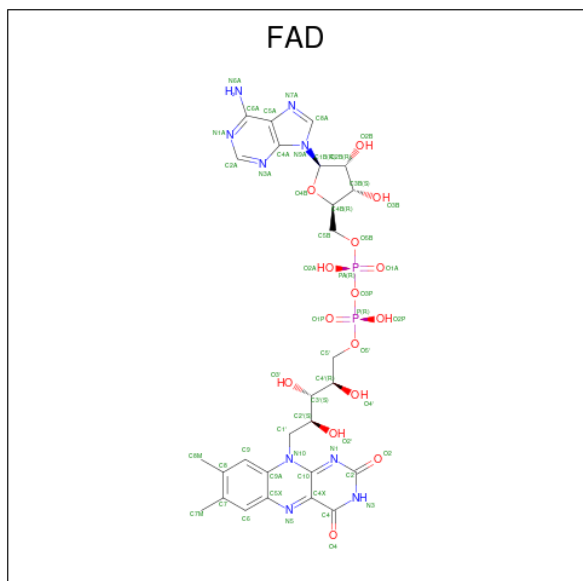
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 6 is 4-[[[(4'-AMINO-2'-METHYLPYRIMIDIN-5'-YL)METHYL]AMINO}PENT-3-ENYL DIPHOSPHATE (CCD ID: AYD) (formula: $C_{11}H_{20}N_4O_7P_2$).



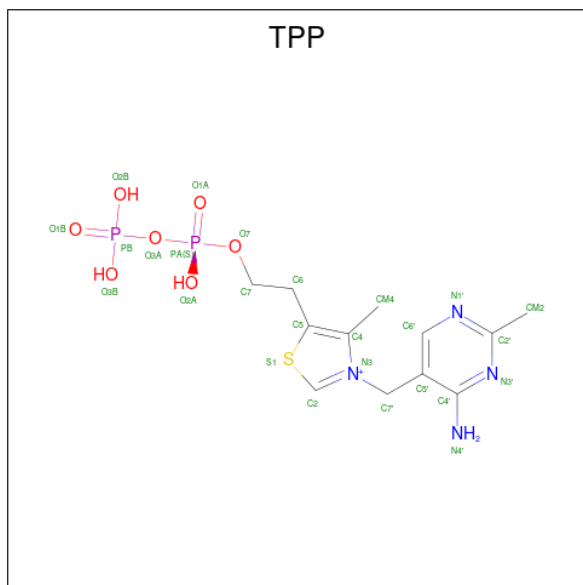
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0
			24	11	4	7	2	

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
7	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 8 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

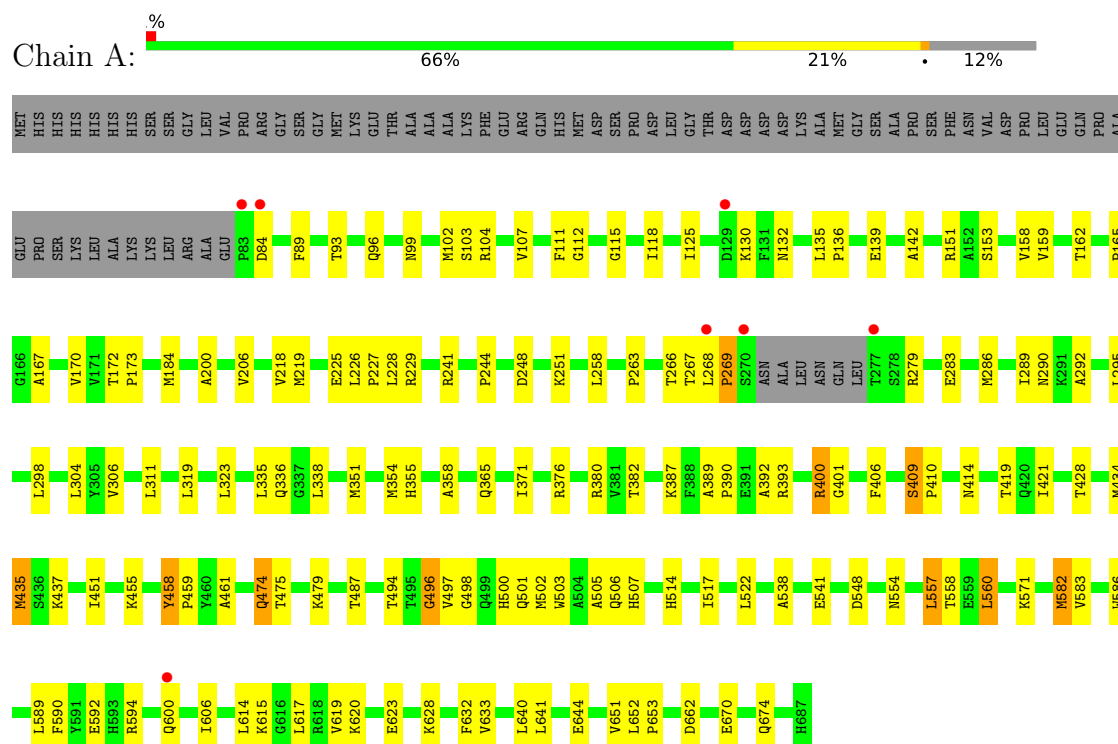
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	505	Total	O	0	0
			505	505		
9	B	327	Total	O	0	0
			327	327		

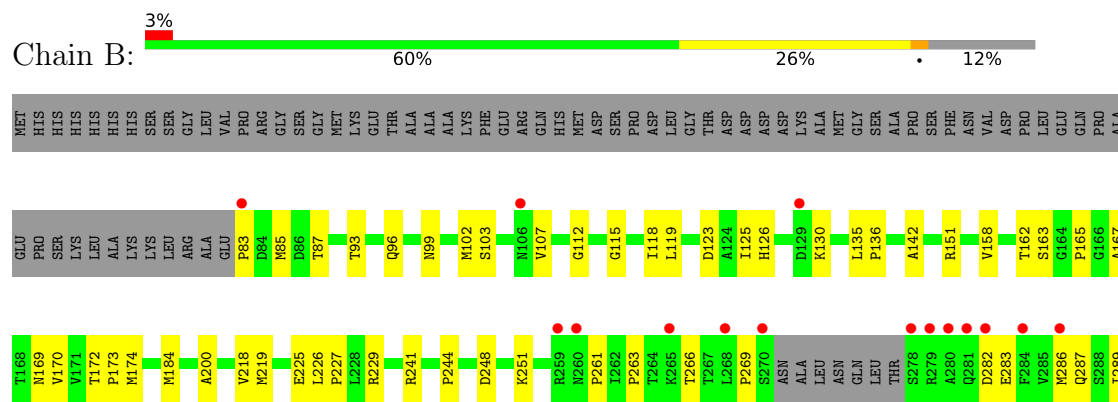
3 Residue-property plots [i](#)

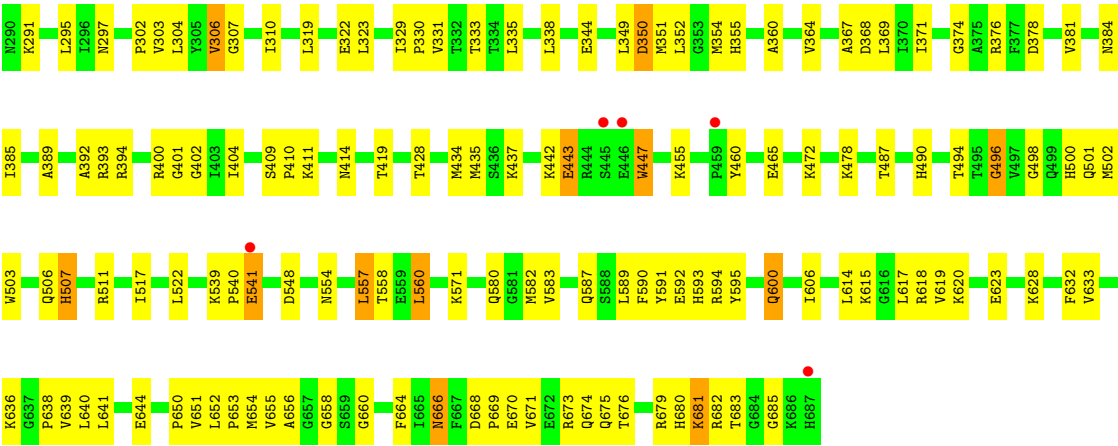
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Acetolactate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	153.98Å 153.98Å 178.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.80 48.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (48.70-2.80) 95.3 (48.70-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.163 , 0.205 0.170 , 0.171	Depositor DCC
R_{free} test set	5303 reflections (9.70%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10196	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CIE, MG, K, FAD, AYD, TPP, DTT

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	0.40	0/4676	0.92	9/6345 (0.1%)
1	B	0.37	0/4668	0.89	9/6334 (0.1%)
All	All	0.38	0/9344	0.90	18/12679 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	VAL	N-CA-C	6.42	117.54	108.36
1	B	507	HIS	N-CA-C	5.90	120.47	113.16
1	A	458	TYR	N-CA-C	5.89	119.69	108.97
1	A	507	HIS	N-CA-C	5.85	120.42	113.16
1	A	376	ARG	N-CA-C	5.83	119.71	112.59
1	A	241	ARG	N-CA-C	-5.64	101.40	109.24
1	B	241	ARG	N-CA-C	-5.60	101.45	109.24
1	A	409	SER	CA-C-N	5.51	125.18	119.56
1	A	409	SER	C-N-CA	5.51	125.18	119.56
1	B	385	ILE	N-CA-C	5.50	116.89	110.62
1	B	496	GLY	N-CA-C	-5.37	103.42	112.77
1	A	382	THR	N-CA-C	5.31	119.02	112.54
1	B	306	VAL	N-CA-C	5.31	116.62	108.71
1	B	592	GLU	N-CA-C	5.27	118.46	111.30
1	A	496	GLY	N-CA-C	-5.24	103.65	112.77
1	B	331	VAL	N-CA-C	5.21	115.35	107.75
1	B	368	ASP	N-CA-C	-5.06	106.96	113.23
1	B	660	GLY	N-CA-C	-5.05	104.71	112.85

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	4571	0	4557	136	0
1	B	4563	0	4552	164	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	14	4	0
4	B	27	0	14	5	0
5	A	8	0	9	2	0
5	B	8	0	9	3	0
6	A	24	0	17	3	0
7	A	53	0	31	3	0
7	B	53	0	31	3	0
8	B	26	0	16	8	0
9	A	505	0	0	9	0
9	B	327	0	0	14	0
All	All	10196	0	9250	294	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 16.

All (294) 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:B:498:GLY:HA2	1:B:582[A]:MET:HE3	1.46	0.98
1:B:498:GLY:HA2	1:B:582[A]:MET:CE	1.98	0.93
1:A:582[A]:MET:HE2	9:A:964:HOH:O	1.69	0.90
1:A:474:GLN:H	1:A:474:GLN:HE21	1.25	0.84
1:A:335:LEU:HA	1:A:351:MET:HE2	1.57	0.83
1:B:335:LEU:HA	1:B:351:MET:HE2	1.60	0.83
1:B:355:HIS:HB2	1:B:502:MET:HE2	1.66	0.78
9:A:1038:HOH:O	1:B:600:GLN:HB3	1.87	0.75
1:B:414:ASN:OD1	1:B:419:THR:HG22	1.87	0.74
1:B:619:VAL:HG22	1:B:628:LYS:HG3	1.70	0.74
1:B:591:TYR:O	1:B:594:ARG:HG3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:VAL:HG23	1:B:641:LEU:HD11	1.70	0.73
1:B:289:ILE:HG23	1:B:434:MET:HB2	1.71	0.72
1:A:474:GLN:H	1:A:474:GLN:NE2	1.86	0.72
1:A:619:VAL:HG22	1:A:628:LYS:HG3	1.72	0.72
1:A:497:VAL:HG12	1:A:582[B]:MET:HE1	1.70	0.72
1:A:286:MET:HE2	1:A:437:LYS:HE2	1.71	0.71
1:B:435:MET:HE3	1:B:435:MET:HA	1.72	0.71
1:B:295:LEU:HD11	1:B:401:GLY:HA2	1.73	0.70
1:A:498:GLY:HA2	1:A:582[B]:MET:HE3	1.73	0.70
1:B:354:MET:HA	1:B:655:VAL:HB	1.74	0.68
1:A:338:LEU:HD11	1:A:351:MET:HE3	1.76	0.68
1:A:600:GLN:HE21	1:B:135:LEU:HB3	1.58	0.66
1:B:355:HIS:HB2	1:B:502:MET:CE	2.26	0.65
1:B:226:LEU:HB3	1:B:227:PRO:HD3	1.79	0.65
1:B:286:MET:HE1	1:B:437:LYS:HZ2	1.62	0.64
1:A:619:VAL:HG23	1:A:641:LEU:HD11	1.79	0.64
1:B:410:PRO:HG2	1:B:411:LYS:HD2	1.80	0.64
1:A:226:LEU:HB3	1:A:227:PRO:HD3	1.78	0.64
1:B:286:MET:HE1	1:B:437:LYS:NZ	2.14	0.63
1:B:490:HIS:CE1	9:B:1259:HOH:O	2.52	0.62
1:A:289:ILE:HG23	1:A:434:MET:HB2	1.82	0.61
1:A:600:GLN:HG2	1:B:135:LEU:HD13	1.83	0.61
1:A:292:ALA:HB3	1:A:434:MET:HE2	1.83	0.61
1:B:668:ASP:HB3	1:B:671:VAL:HB	1.82	0.60
1:A:136:PRO:HG3	1:A:142:ALA:HB2	1.84	0.59
1:B:304:LEU:HD23	1:B:371:ILE:HB	1.84	0.59
1:B:381:VAL:HG22	7:B:1701:FAD:O2	2.03	0.59
1:A:414:ASN:ND2	1:A:419:THR:H	2.01	0.59
1:B:638:PRO:HD3	9:B:1082:HOH:O	2.03	0.58
1:B:539:LYS:HG3	9:B:1259:HOH:O	2.02	0.58
1:B:338:LEU:HD11	1:B:351:MET:HE3	1.85	0.58
1:B:582[A]:MET:CE	8:B:1702:TPP:S1	2.92	0.57
1:A:620:LYS:HE2	1:A:644:GLU:OE2	2.03	0.57
1:A:251:LYS:NZ	4:B:1695:CIE:H12	2.02	0.57
1:B:593:HIS:HD1	1:B:682:ARG:HH11	1.53	0.57
1:A:165:PRO:HD3	1:B:522:LEU:HG	1.86	0.56
1:A:582[B]:MET:HE2	7:A:701:FAD:C7M	2.36	0.56
1:B:669:PRO:O	1:B:673:ARG:HG3	2.04	0.56
1:B:442:LYS:HG2	1:B:443:GLU:HG3	1.86	0.56
1:A:338:LEU:HD11	1:A:351:MET:CE	2.35	0.56
1:A:351:MET:HE1	1:A:505:ALA:HB1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:MET:HE2	1:B:656:ALA:HB2	1.86	0.56
1:A:135:LEU:HD13	9:A:1038:HOH:O	2.04	0.56
4:A:695:CIE:H8'2	7:A:701:FAD:HM71	1.87	0.56
1:B:360:ALA:O	1:B:364:VAL:HG23	2.06	0.56
1:A:102:MET:CE	1:A:158:VAL:HG11	2.36	0.55
1:A:200:ALA:HB1	4:B:1695:CIE:H5	1.88	0.55
1:A:640:LEU:C	1:A:640:LEU:HD23	2.31	0.55
4:A:695:CIE:H5	1:B:200:ALA:HB1	1.89	0.55
1:B:580:GLN:HA	8:B:1702:TPP:H72	1.88	0.55
1:A:522:LEU:HG	1:B:165:PRO:HD3	1.88	0.55
5:A:698:DTT:S1	5:A:698:DTT:S4	3.05	0.55
1:B:102:MET:CE	1:B:158:VAL:HG11	2.36	0.55
1:B:172:THR:HB	1:B:173:PRO:HD3	1.89	0.55
1:B:619:VAL:CG2	1:B:641:LEU:HD11	2.35	0.55
1:A:151:ARG:HG3	1:A:517:ILE:HG23	1.88	0.55
1:B:620:LYS:HE2	1:B:644:GLU:OE2	2.07	0.55
1:A:319:LEU:HD12	1:A:428:THR:HG23	1.88	0.54
1:B:411:LYS:HD2	1:B:411:LYS:N	2.22	0.54
1:B:136:PRO:HG3	1:B:142:ALA:HB2	1.90	0.54
1:A:135:LEU:HD12	9:B:1041:HOH:O	2.07	0.54
1:A:172:THR:HB	1:A:173:PRO:HD3	1.90	0.54
1:B:371:ILE:HD12	1:B:371:ILE:N	2.24	0.53
1:A:623:GLU:CD	1:A:623:GLU:H	2.16	0.53
1:B:163:SER:HB2	9:B:987:HOH:O	2.08	0.53
1:B:434:MET:O	1:B:434:MET:HG2	2.08	0.53
1:A:172:THR:OG1	1:B:169:ASN:ND2	2.42	0.53
1:A:251:LYS:HZ3	4:B:1695:CIE:H12	1.54	0.53
1:B:306:VAL:HB	1:B:333:THR:HG22	1.88	0.53
1:A:170:VAL:C	1:A:173:PRO:HD2	2.33	0.53
1:A:474:GLN:HE21	1:A:474:GLN:N	1.99	0.53
1:B:589:LEU:HD23	1:B:590:PHE:CE1	2.44	0.53
1:B:170:VAL:C	1:B:173:PRO:HD2	2.34	0.53
1:B:295:LEU:HD11	1:B:401:GLY:CA	2.38	0.53
1:A:279:ARG:O	1:A:283:GLU:HB2	2.08	0.53
1:B:582[A]:MET:SD	4:B:1695:CIE:H5'	2.49	0.53
1:A:571:LYS:HB3	1:A:632:PHE:CZ	2.44	0.53
1:A:594:ARG:HD3	9:B:947:HOH:O	2.08	0.53
1:B:623:GLU:CD	1:B:623:GLU:H	2.16	0.53
1:B:302:PRO:O	1:B:330:PRO:HD2	2.09	0.52
1:B:478:LYS:HE2	1:B:507:HIS:ND1	2.24	0.52
1:B:322:GLU:OE2	1:B:435:MET:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:LEU:HD23	1:B:558:THR:N	2.24	0.52
5:B:1698:DTT:H2	9:B:1018:HOH:O	2.08	0.52
1:A:102:MET:HE3	1:A:107:VAL:HG11	1.91	0.52
5:B:1698:DTT:S1	5:B:1698:DTT:S4	3.08	0.52
1:A:323:LEU:HB2	1:A:435:MET:HE1	1.92	0.51
1:B:571:LYS:HB3	1:B:632:PHE:CZ	2.46	0.51
1:A:103:SER:HB2	1:A:130:LYS:HD3	1.92	0.51
1:A:319:LEU:HD12	1:A:428:THR:CG2	2.40	0.51
1:A:292:ALA:HB3	1:A:434:MET:CE	2.41	0.51
1:B:557:LEU:HD23	1:B:557:LEU:C	2.36	0.51
1:B:263:PRO:HB2	1:B:266:THR:HG23	1.92	0.51
1:B:455:LYS:HA	5:B:1698:DTT:S4	2.50	0.51
1:B:496:GLY:H	1:B:500:HIS:HE1	1.58	0.51
1:B:102:MET:HE3	1:B:107:VAL:HG11	1.93	0.50
1:A:583:VAL:HG21	6:A:700:AYD:HM43	1.93	0.50
1:A:496:GLY:H	1:A:500:HIS:HE1	1.59	0.50
1:B:102:MET:HE2	1:B:158:VAL:HG11	1.94	0.50
1:B:297:ASN:HA	9:B:1214:HOH:O	2.11	0.50
1:A:557:LEU:HD23	1:A:558:THR:N	2.26	0.50
1:A:589:LEU:HD23	1:A:590:PHE:CE1	2.46	0.50
1:B:307:GLY:O	1:B:310:ILE:HG22	2.11	0.50
1:B:319:LEU:HD12	1:B:428:THR:HG23	1.93	0.50
1:A:498:GLY:HA2	1:A:582[B]:MET:CE	2.39	0.50
1:A:311:LEU:O	1:A:514:HIS:HE1	1.92	0.50
1:A:99:ASN:ND2	1:A:125:ILE:HG22	2.27	0.50
1:A:497:VAL:O	6:A:700:AYD:H62	2.11	0.50
1:A:557:LEU:HD23	1:A:557:LEU:C	2.37	0.50
1:B:670:GLU:HA	1:B:673:ARG:NH1	2.26	0.50
1:A:652:LEU:HA	1:A:653:PRO:C	2.37	0.49
1:B:354:MET:O	1:B:654:MET:HA	2.12	0.49
1:A:497:VAL:CG1	1:A:582[B]:MET:HE1	2.42	0.49
1:B:653:PRO:HG2	9:B:1066:HOH:O	2.11	0.49
1:B:283:GLU:O	1:B:287:GLN:HG3	2.12	0.49
1:A:582[B]:MET:CE	6:A:700:AYD:H5	2.43	0.49
1:A:118:ILE:HG13	1:A:118:ILE:O	2.13	0.49
1:A:600:GLN:HG3	9:A:870:HOH:O	2.12	0.49
1:B:103:SER:HB2	1:B:130:LYS:HD3	1.95	0.48
1:B:389:ALA:HB1	1:B:392:ALA:HB3	1.95	0.48
1:B:554:ASN:HA	1:B:557:LEU:HD13	1.95	0.48
1:A:290:ASN:OD1	1:A:437:LYS:HE2	2.13	0.48
1:B:636:LYS:HA	9:B:1418:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:ASP:HB2	9:B:1409:HOH:O	2.13	0.48
1:A:554:ASN:HA	1:A:557:LEU:HD13	1.96	0.48
1:A:286:MET:HE2	1:A:437:LYS:CE	2.43	0.48
1:B:184:MET:O	1:B:244:PRO:HA	2.14	0.48
1:A:102:MET:HE2	1:A:158:VAL:HG11	1.96	0.47
1:B:83:PRO:HG2	1:B:85:MET:O	2.14	0.47
1:A:557:LEU:O	1:A:560:LEU:HB2	2.14	0.47
1:B:587:GLN:NE2	1:B:595:TYR:HA	2.28	0.47
1:B:640:LEU:C	1:B:640:LEU:HD23	2.39	0.47
1:B:394:ARG:HH12	1:B:400:ARG:NH2	2.12	0.47
1:A:228:LEU:HD13	1:A:266:THR:HG22	1.95	0.47
1:B:593:HIS:NE2	1:B:675:GLN:NE2	2.63	0.47
1:B:303:VAL:HG23	1:B:367:ALA:HB2	1.96	0.47
1:B:414:ASN:CG	1:B:419:THR:HG22	2.39	0.47
1:B:323:LEU:HA	1:B:435:MET:HE1	1.97	0.47
1:A:304:LEU:HD23	1:A:371:ILE:HB	1.96	0.47
1:B:582[A]:MET:HE3	8:B:1702:TPP:S1	2.54	0.47
1:A:93:THR:OG1	1:A:96:GLN:HG3	2.15	0.46
1:A:600:GLN:NE2	1:B:135:LEU:HD22	2.31	0.46
1:B:600:GLN:H	1:B:600:GLN:NE2	2.13	0.46
1:B:502:MET:O	1:B:506:GLN:HG3	2.15	0.46
8:B:1702:TPP:HN42	8:B:1702:TPP:H2	1.78	0.46
1:A:502:MET:O	1:A:506:GLN:HG3	2.15	0.46
1:B:349:LEU:O	1:B:350:ASP:CB	2.63	0.46
1:B:557:LEU:O	1:B:560:LEU:HB2	2.15	0.46
1:A:132:ASN:HB3	9:A:1551:HOH:O	2.15	0.46
1:B:118:ILE:HG13	1:B:118:ILE:O	2.15	0.46
1:B:498:GLY:HA2	1:B:582[A]:MET:HE2	1.93	0.46
1:A:355:HIS:HB2	1:A:502:MET:CE	2.45	0.46
1:B:335:LEU:HD12	1:B:351:MET:HE1	1.97	0.46
1:B:460:TYR:HB3	1:B:507:HIS:CE1	2.51	0.46
1:B:683:THR:C	1:B:685:GLY:H	2.24	0.46
1:A:295:LEU:HD12	1:A:421:ILE:CD1	2.46	0.46
1:A:455:LYS:HA	5:A:698:DTT:S4	2.56	0.46
1:B:472:LYS:HD2	9:B:1257:HOH:O	2.14	0.46
1:A:400:ARG:NH2	9:A:912:HOH:O	2.47	0.46
1:B:93:THR:OG1	1:B:96:GLN:HG3	2.16	0.46
1:B:291:LYS:HE2	9:B:1408:HOH:O	2.16	0.46
1:A:619:VAL:CG2	1:A:641:LEU:HD11	2.44	0.45
4:A:695:CIE:H12	1:B:251:LYS:HZ3	1.65	0.45
1:A:102:MET:HE1	1:A:158:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:PHE:HZ	1:A:434:MET:HE1	1.80	0.45
1:B:335:LEU:CA	1:B:351:MET:HE2	2.39	0.45
1:A:354:MET:HE1	1:A:380:ARG:NH1	2.31	0.45
1:B:487:THR:HG21	1:B:633:VAL:HG11	1.96	0.45
1:B:115:GLY:HA3	1:B:162:THR:CB	2.47	0.45
1:A:351:MET:CE	1:A:505:ALA:HB1	2.47	0.45
1:A:355:HIS:HB2	1:A:502:MET:HE2	1.98	0.45
1:A:494:THR:HG22	1:A:517:ILE:HB	1.99	0.45
1:B:151:ARG:HG3	1:B:517:ILE:HG23	1.97	0.45
8:B:1702:TPP:HN42	8:B:1702:TPP:C2	2.30	0.45
1:A:184:MET:O	1:A:244:PRO:HA	2.16	0.45
1:B:286:MET:CE	1:B:437:LYS:NZ	2.79	0.45
1:B:681:LYS:NZ	1:B:681:LYS:HB3	2.32	0.45
1:A:594:ARG:HH11	1:B:123:ASP:CG	2.24	0.45
1:B:225:GLU:HG2	1:B:229:ARG:HG2	1.97	0.45
1:A:225:GLU:HG2	1:A:229:ARG:HG2	1.99	0.45
1:B:115:GLY:HA3	1:B:162:THR:HB	1.99	0.45
1:B:494:THR:HG22	1:B:517:ILE:HB	1.99	0.45
1:B:392:ALA:O	1:B:402:GLY:HA2	2.17	0.44
1:B:496:GLY:N	1:B:500:HIS:HE1	2.15	0.44
1:B:615:LYS:HE2	1:B:617:LEU:HD21	1.99	0.44
1:B:670:GLU:O	1:B:674:GLN:HG3	2.18	0.44
1:A:153:SER:HB3	1:A:538:ALA:HB1	2.00	0.44
1:B:335:LEU:CD1	1:B:351:MET:HE1	2.47	0.44
1:B:503:TRP:CE2	1:B:651:VAL:HG22	2.52	0.44
1:A:358:ALA:HB3	1:A:458:TYR:CB	2.48	0.44
1:B:447:TRP:HE3	1:B:447:TRP:HA	1.82	0.44
1:B:465:GLU:HG3	1:B:472:LYS:HG2	1.98	0.44
1:B:593:HIS:CE1	1:B:675:GLN:NE2	2.86	0.44
1:A:219:MET:HA	1:A:248:ASP:HB3	2.00	0.44
1:B:498:GLY:O	1:B:501:GLN:HB3	2.18	0.44
1:B:540:PRO:HB2	1:B:541:GLU:OE2	2.17	0.44
1:B:355:HIS:CB	1:B:502:MET:HE2	2.43	0.44
1:A:406:PHE:HZ	1:A:434:MET:CE	2.31	0.44
1:A:498:GLY:O	1:A:501:GLN:HB3	2.17	0.44
1:B:389:ALA:O	1:B:393:ARG:HG3	2.18	0.44
1:A:115:GLY:HA3	1:A:162:THR:HB	2.00	0.44
1:A:167:ALA:O	1:A:170:VAL:HG22	2.17	0.44
1:A:409:SER:HA	1:A:410:PRO:HD3	1.85	0.43
1:B:102:MET:HE1	1:B:158:VAL:HG11	2.00	0.43
1:B:219:MET:HA	1:B:248:ASP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1695:CIE:H8'2	7:B:1701:FAD:HM71	2.00	0.43
1:A:139:GLU:OE2	8:B:1702:TPP:N1'	2.51	0.43
1:A:414:ASN:HD21	1:A:419:THR:H	1.65	0.43
1:B:411:LYS:HD2	1:B:411:LYS:H	1.83	0.43
1:B:447:TRP:HA	1:B:447:TRP:CE3	2.52	0.43
1:B:666:ASN:HD22	1:B:666:ASN:HA	1.62	0.43
1:A:393:ARG:HD2	9:A:1559:HOH:O	2.19	0.43
1:B:650:PRO:HG3	9:B:1206:HOH:O	2.18	0.43
1:B:676:THR:HG22	1:B:680:HIS:CD2	2.54	0.43
1:A:84:ASP:O	1:A:263:PRO:HA	2.19	0.43
1:A:387:LYS:O	1:A:390:PRO:HD3	2.19	0.43
1:A:496:GLY:N	1:A:500:HIS:HE1	2.17	0.43
1:B:384:ASN:HD22	1:B:658:GLY:C	2.27	0.43
1:A:451:ILE:O	1:A:455:LYS:HG3	2.19	0.43
1:A:594:ARG:HB3	1:B:126:HIS:ND1	2.34	0.43
1:B:369:LEU:HD11	1:B:404:ILE:HG13	2.00	0.43
1:A:365:GLN:HG3	1:A:662:ASP:HB3	2.01	0.42
1:B:580:GLN:CA	8:B:1702:TPP:H72	2.49	0.42
1:A:102:MET:HE3	1:A:107:VAL:HG21	2.01	0.42
1:A:586[B]:TRP:CD1	1:B:119:LEU:HD12	2.55	0.42
1:B:87:THR:HG22	1:B:261:PRO:HB3	2.01	0.42
1:B:303:VAL:CG2	1:B:367:ALA:HB2	2.48	0.42
1:B:652:LEU:HA	1:B:653:PRO:C	2.44	0.42
1:A:115:GLY:HA3	1:A:162:THR:CB	2.48	0.42
1:A:206:VAL:HG21	9:A:732:HOH:O	2.18	0.42
1:A:459:PRO:O	1:A:461:ALA:N	2.50	0.42
1:B:102:MET:HE3	1:B:107:VAL:HG21	2.00	0.42
1:B:218:VAL:HG22	1:B:219:MET:N	2.34	0.42
1:B:307:GLY:HA3	1:B:374:GLY:O	2.18	0.42
1:A:135:LEU:HD22	9:A:1038:HOH:O	2.19	0.42
1:A:295:LEU:HD12	1:A:421:ILE:HD12	2.01	0.42
1:A:268:LEU:HA	1:A:269:PRO:HD3	1.93	0.42
1:A:311:LEU:O	1:A:514:HIS:CE1	2.72	0.42
1:A:336:GLN:HA	1:A:336:GLN:OE1	2.20	0.42
1:B:99:ASN:ND2	1:B:125:ILE:HG22	2.35	0.42
1:B:170:VAL:HG23	1:B:174:MET:HE2	2.01	0.42
1:B:352:LEU:HG	1:B:381:VAL:HG13	2.01	0.42
1:A:487:THR:HG21	1:A:633:VAL:HG11	2.02	0.42
1:A:290:ASN:OD1	1:A:437:LYS:CE	2.68	0.41
1:B:394:ARG:HH12	1:B:400:ARG:HH21	1.67	0.41
1:A:218:VAL:HG22	1:A:219:MET:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:TRP:CE2	1:A:651:VAL:HG22	2.54	0.41
1:A:594:ARG:HD2	1:B:123:ASP:OD2	2.19	0.41
1:A:600:GLN:NE2	1:B:136:PRO:O	2.47	0.41
1:B:394:ARG:HB3	1:B:394:ARG:CZ	2.50	0.41
1:A:497:VAL:HG12	1:A:582[B]:MET:CE	2.44	0.41
4:A:695:CIE:H12	1:B:251:LYS:NZ	2.18	0.41
1:A:475:THR:O	1:A:479:LYS:HG3	2.21	0.41
1:A:615:LYS:HE2	1:A:617:LEU:HD21	2.02	0.41
1:B:167:ALA:O	1:B:170:VAL:HG22	2.21	0.41
1:B:606:ILE:HD13	1:B:618:ARG:NH2	2.35	0.41
1:A:498:GLY:HA2	1:A:582[B]:MET:HB2	2.03	0.41
1:A:112:GLY:O	1:A:136:PRO:HD2	2.21	0.41
1:A:670:GLU:HG2	1:A:674:GLN:NE2	2.36	0.41
1:B:329:ILE:HA	1:B:330:PRO:HD3	1.88	0.41
1:A:89:PHE:C	1:A:258:LEU:HD23	2.46	0.41
1:A:358:ALA:HB3	1:A:458:TYR:HB3	2.03	0.41
1:A:389:ALA:HB1	1:A:392:ALA:HB3	2.03	0.41
1:A:594:ARG:NH1	1:B:123:ASP:OD1	2.54	0.41
1:B:112:GLY:O	1:B:136:PRO:HD2	2.20	0.41
1:B:668:ASP:CG	1:B:671:VAL:HG23	2.45	0.41
1:A:104:ARG:NH1	1:A:267:THR:O	2.54	0.40
1:A:111:PHE:O	1:A:159:VAL:HA	2.21	0.40
1:A:295:LEU:HD22	1:A:401:GLY:HA2	2.03	0.40
1:A:600:GLN:NE2	1:B:135:LEU:HB3	2.32	0.40
1:B:344:GLU:HG3	1:B:511:ARG:CZ	2.51	0.40
1:B:354:MET:HB2	1:B:655:VAL:O	2.21	0.40
1:B:676:THR:HG23	1:B:679:ARG:NH2	2.36	0.40
1:A:606:ILE:N	1:A:606:ILE:HD12	2.35	0.40
1:B:571:LYS:HD2	1:B:639:VAL:CG1	2.51	0.40
1:A:298:LEU:HD21	1:A:400:ARG:HA	2.04	0.40
1:B:376:ARG:HB3	7:B:1701:FAD:O3B	2.22	0.40
1:B:409:SER:HA	1:B:410:PRO:HD2	1.96	0.40
1:A:286:MET:HE3	1:A:289:ILE:HB	2.03	0.40
1:A:582[B]:MET:HE2	7:A:701:FAD:HM72	2.03	0.40
1:B:655:VAL:HG22	1:B:664:PHE:HB3	2.03	0.40
1:B:583:VAL:HG23	8:B:1702:TPP:H61	2.04	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	597/677 (88%)	580 (97%)	16 (3%)	1 (0%)	43	72
1	B	596/677 (88%)	575 (96%)	19 (3%)	2 (0%)	36	66
All	All	1193/1354 (88%)	1155 (97%)	35 (3%)	3 (0%)	36	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	350	ASP
1	B	269	PRO
1	A	269	PRO

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	490/556 (88%)	479 (98%)	11 (2%)	45	78
1	B	489/556 (88%)	478 (98%)	11 (2%)	45	78
All	All	979/1112 (88%)	957 (98%)	22 (2%)	45	78

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	400	ARG
1	A	435	MET
1	A	474	GLN

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Mol	Chain	Res	Type
1	A	541	GLU
1	A	548	ASP
1	A	557	LEU
1	A	560	LEU
1	A	582[A]	MET
1	A	582[B]	MET
1	A	592	GLU
1	A	614	LEU
1	B	282	ASP
1	B	443	GLU
1	B	447	TRP
1	B	541	GLU
1	B	548	ASP
1	B	557	LEU
1	B	560	LEU
1	B	600	GLN
1	B	614	LEU
1	B	666	ASN
1	B	681	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	105	GLN
1	A	106	ASN
1	A	132	ASN
1	A	169	ASN
1	A	231	ASN
1	A	287	GLN
1	A	312	ASN
1	A	414	ASN
1	A	474	GLN
1	A	500	HIS
1	A	554	ASN
1	A	587	GLN
1	A	602	ASN
1	A	666	ASN
1	A	674	GLN
1	A	687	HIS
1	B	99	ASN
1	B	105	GLN

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Mol	Chain	Res	Type
1	B	106	ASN
1	B	132	ASN
1	B	169	ASN
1	B	312	ASN
1	B	366	ASN
1	B	452	ASN
1	B	500	HIS
1	B	565	GLN
1	B	587	GLN
1	B	600	GLN
1	B	602	ASN
1	B	666	ASN
1	B	675	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	CIE	A	695	-	28,28,28	4.58	17 (60%)	38,39,39	4.41	15 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FAD	A	701	-	58,58,58	2.19	20 (34%)	85,89,89	1.16	6 (7%)
5	DTT	A	698	1	7,7,7	1.30	1 (14%)	4,8,8	5.43	4 (100%)
6	AYD	A	700	3	22,24,24	3.70	15 (68%)	31,34,34	3.21	10 (32%)
8	TPP	B	1702	3	26,27,27	3.13	13 (50%)	38,40,40	2.43	12 (31%)
4	CIE	B	1695	-	28,28,28	4.54	16 (57%)	38,39,39	4.44	16 (42%)
7	FAD	B	1701	-	58,58,58	2.27	21 (36%)	85,89,89	1.13	4 (4%)
5	DTT	B	1698	1	7,7,7	1.31	1 (14%)	4,8,8	5.46	3 (75%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIE	A	695	-	-	8/24/24/24	0/2/2/2
7	FAD	A	701	-	-	2/34/50/50	0/6/6/6
5	DTT	A	698	1	-	2/8/8/8	-
6	AYD	A	700	3	-	7/19/19/19	0/1/1/1
8	TPP	B	1702	3	-	2/17/17/17	0/2/2/2
4	CIE	B	1695	-	-	9/24/24/24	0/2/2/2
7	FAD	B	1701	-	-	2/34/50/50	0/6/6/6
5	DTT	B	1698	1	-	2/8/8/8	-

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	695	CIE	OBA-S11	14.97	1.60	1.43
4	B	1695	CIE	OBA-S11	14.43	1.60	1.43
6	A	700	AYD	C4'-N3'	8.16	1.45	1.35
4	B	1695	CIE	C1-C2	7.79	1.48	1.40
8	B	1702	TPP	C4'-N3'	7.22	1.44	1.35
4	A	695	CIE	C3-C2	6.81	1.47	1.39
4	A	695	CIE	C1-C2	6.64	1.47	1.40
4	B	1695	CIE	C3-C2	6.52	1.46	1.39
4	A	695	CIE	OBB-S11	6.43	1.51	1.43
4	B	1695	CIE	OBB-S11	6.42	1.51	1.43
4	A	695	CIE	C5'-C6'	6.15	1.48	1.38
4	A	695	CIE	C6-C1	5.93	1.48	1.39
4	B	1695	CIE	C6-C1	5.93	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1701	FAD	C9A-C5X	5.90	1.50	1.41
4	B	1695	CIE	C5'-C6'	5.69	1.47	1.38
6	A	700	AYD	C6'-C5'	5.67	1.48	1.37
7	A	701	FAD	C9A-C5X	5.64	1.50	1.41
6	A	700	AYD	C5'-C4'	5.60	1.52	1.42
4	A	695	CIE	C2'-N14	-5.56	1.31	1.38
8	B	1702	TPP	C5-C4	5.47	1.46	1.35
8	B	1702	TPP	C6'-C5'	5.35	1.48	1.37
7	B	1701	FAD	C9-C8	5.27	1.46	1.39
6	A	700	AYD	C6'-N1'	5.17	1.45	1.34
6	A	700	AYD	C2'-N1'	5.15	1.42	1.34
4	B	1695	CIE	C5'-C4'	5.11	1.46	1.38
8	B	1702	TPP	C2'-N1'	5.06	1.42	1.34
8	B	1702	TPP	C6'-N1'	5.04	1.44	1.34
7	B	1701	FAD	C9-C9A	5.02	1.47	1.39
7	B	1701	FAD	C6-C7	4.87	1.46	1.39
7	A	701	FAD	C6-C7	4.82	1.46	1.39
8	B	1702	TPP	C5'-C4'	4.78	1.50	1.42
4	A	695	CIE	C5'-C4'	4.76	1.45	1.38
7	A	701	FAD	C9-C8	4.74	1.46	1.39
6	A	700	AYD	C7'-N3	4.72	1.55	1.46
7	A	701	FAD	C9-C9A	4.63	1.47	1.39
7	A	701	FAD	C8-C7	4.42	1.51	1.40
4	B	1695	CIE	O8-C7	4.34	1.44	1.33
7	B	1701	FAD	C8-C7	4.29	1.51	1.40
4	A	695	CIE	C5-C6	4.18	1.46	1.38
4	B	1695	CIE	C2'-N14	-4.17	1.33	1.38
4	B	1695	CIE	C5-C6	4.04	1.45	1.38
4	B	1695	CIE	S11-N12	4.00	1.73	1.64
4	A	695	CIE	O8-C7	4.00	1.43	1.33
7	B	1701	FAD	C5A-C4A	3.95	1.46	1.39
6	A	700	AYD	O7-C7	3.92	1.60	1.44
4	A	695	CIE	C4-C3	3.86	1.45	1.38
4	B	1695	CIE	C4'-N3'	3.83	1.41	1.33
4	B	1695	CIE	C4-C3	3.77	1.45	1.38
8	B	1702	TPP	O7-C7	3.76	1.59	1.44
6	A	700	AYD	PA-O2A	-3.75	1.38	1.55
7	A	701	FAD	C5A-C4A	3.74	1.45	1.39
4	A	695	CIE	S11-N12	3.54	1.72	1.64
7	B	1701	FAD	C4X-N5	3.50	1.38	1.30
7	A	701	FAD	C4X-N5	3.49	1.38	1.30
7	B	1701	FAD	P-O3P	-3.46	1.55	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	700	AYD	C4-N3	3.42	1.43	1.33
4	A	695	CIE	C4'-N3'	3.41	1.40	1.33
7	A	701	FAD	P-O3P	-3.33	1.55	1.59
7	B	1701	FAD	C6-C5X	3.27	1.44	1.40
7	A	701	FAD	C6-C5X	3.25	1.44	1.40
7	B	1701	FAD	C10-N1	3.22	1.39	1.33
4	A	695	CIE	C5-C4	3.21	1.45	1.38
4	B	1695	CIE	C5-C4	3.14	1.45	1.38
7	A	701	FAD	C10-N1	3.12	1.39	1.33
7	A	701	FAD	C7M-C7	3.12	1.56	1.51
7	B	1701	FAD	C4A-N3A	3.03	1.40	1.34
7	B	1701	FAD	C2A-N1A	2.99	1.39	1.33
7	A	701	FAD	C4A-N3A	2.99	1.40	1.34
6	A	700	AYD	PB-O2B	-2.96	1.43	1.54
7	A	701	FAD	C2A-N1A	2.92	1.39	1.33
6	A	700	AYD	C2'-N3'	2.87	1.39	1.34
7	B	1701	FAD	C10-N10	2.77	1.43	1.37
8	B	1702	TPP	PA-O2A	-2.72	1.42	1.55
8	B	1702	TPP	PB-O2B	-2.71	1.44	1.54
7	B	1701	FAD	C9A-N10	2.70	1.45	1.41
7	B	1701	FAD	O4'-C4'	2.66	1.48	1.43
6	A	700	AYD	C6-C7	2.63	1.58	1.51
8	B	1702	TPP	CM4-C4	2.53	1.54	1.49
6	A	700	AYD	PA-O3A	-2.52	1.56	1.59
4	A	695	CIE	C13-N12	-2.50	1.33	1.39
7	A	701	FAD	O4'-C4'	2.50	1.48	1.43
5	A	698	DTT	C1-S1	2.47	1.86	1.81
8	B	1702	TPP	C2-S1	2.47	1.76	1.69
6	A	700	AYD	PA-O1A	-2.47	1.42	1.50
4	B	1695	CIE	C2-S11	2.45	1.81	1.77
7	A	701	FAD	C2A-N3A	2.45	1.38	1.33
7	B	1701	FAD	C2A-N3A	2.42	1.38	1.33
7	A	701	FAD	C10-N10	2.32	1.42	1.37
7	A	701	FAD	C9A-N10	2.28	1.45	1.41
7	B	1701	FAD	C8A-N9A	2.24	1.41	1.37
5	B	1698	DTT	C1-S1	2.24	1.86	1.81
6	A	700	AYD	PA-O7	-2.24	1.50	1.59
7	A	701	FAD	C8A-N9A	2.22	1.41	1.37
7	B	1701	FAD	C7M-C7	2.21	1.55	1.51
4	B	1695	CIE	C13-N12	-2.17	1.34	1.39
7	A	701	FAD	C4-N3	2.15	1.42	1.38
8	B	1702	TPP	PA-O7	-2.14	1.51	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1701	FAD	C5'-C4'	-2.14	1.48	1.51
7	A	701	FAD	C1'-C2'	2.12	1.55	1.52
4	A	695	CIE	C13-N14	-2.12	1.32	1.37
7	B	1701	FAD	C1'-C2'	2.08	1.55	1.52
4	A	695	CIE	C2-S11	2.04	1.80	1.77
7	B	1701	FAD	C4-N3	2.03	1.42	1.38
8	B	1702	TPP	C5-S1	2.03	1.78	1.72

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1695	CIE	C8'-O7'-C6'	19.52	146.40	117.33
4	A	695	CIE	C8'-O7'-C6'	19.03	145.66	117.33
4	A	695	CIE	C2'-N14-C13	10.82	141.48	130.34
6	A	700	AYD	O7-C7-C6	10.76	148.48	108.98
4	B	1695	CIE	C2'-N14-C13	10.07	140.70	130.34
5	B	1698	DTT	C3-C4-S4	9.61	141.29	114.43
5	A	698	DTT	C3-C4-S4	9.45	140.83	114.43
6	A	700	AYD	C7-C6-C5	8.40	143.76	112.54
4	B	1695	CIE	C3-C2-S11	-7.29	107.04	117.51
4	A	695	CIE	C3-C2-S11	-6.81	107.73	117.51
4	A	695	CIE	C2-C1-C7	-6.72	115.28	124.25
8	B	1702	TPP	O7-C7-C6	6.32	134.03	108.63
8	B	1702	TPP	C7-C6-C5	6.20	132.19	112.73
4	B	1695	CIE	C2-C1-C7	-6.02	116.21	124.25
8	B	1702	TPP	CM2-C2'-N1'	5.91	123.49	117.20
4	B	1695	CIE	C2'-N1'-C6'	5.11	120.85	115.00
6	A	700	AYD	CM2-C2'-N1'	5.01	122.53	117.20
4	B	1695	CIE	O8-C7-O7	-5.01	113.65	123.67
4	A	695	CIE	O8-C7-O7	-4.95	113.77	123.67
4	A	695	CIE	OBB-S11-OBA	4.94	125.52	119.52
4	B	1695	CIE	OBB-S11-OBA	4.84	125.40	119.52
4	A	695	CIE	C2'-N1'-C6'	4.66	120.33	115.00
6	A	700	AYD	PA-O7-C7	4.66	143.43	121.26
4	A	695	CIE	C6-C1-C7	4.55	127.86	118.66
8	B	1702	TPP	PA-O7-C7	4.36	142.01	121.26
8	B	1702	TPP	C6'-N1'-C2'	4.28	123.11	116.07
4	B	1695	CIE	C6-C1-C7	4.15	127.06	118.66
5	B	1698	DTT	O3-C3-C2	-3.93	101.33	109.57
6	A	700	AYD	C6'-N1'-C2'	3.87	122.43	116.07
6	A	700	AYD	C5'-C7'-N3	3.84	120.89	113.15
5	A	698	DTT	O3-C3-C2	-3.79	101.61	109.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1702	TPP	N1'-C2'-N3'	-3.74	119.31	125.53
4	B	1695	CIE	O8-C7-C1	-3.73	104.92	112.24
4	A	695	CIE	C4'-N3'-C2'	3.69	118.08	114.83
6	A	700	AYD	C7'-N3-C4	-3.53	118.63	125.23
4	A	695	CIE	C5'-C4'-N3'	-3.44	121.57	125.47
4	B	1695	CIE	C5'-C4'-N3'	-3.36	121.66	125.47
4	A	695	CIE	O8-C7-C1	-3.34	105.68	112.24
6	A	700	AYD	N1'-C2'-N3'	-3.29	120.06	125.53
4	B	1695	CIE	C4'-N3'-C2'	3.23	117.67	114.83
5	A	698	DTT	C2-C1-S1	3.15	123.24	114.43
4	B	1695	CIE	N12-C13-N14	3.02	119.68	114.87
4	A	695	CIE	OBB-S11-N12	-2.95	98.33	106.77
8	B	1702	TPP	C7'-N3-C2	-2.90	117.44	123.48
4	B	1695	CIE	OBB-S11-N12	-2.87	98.54	106.77
8	B	1702	TPP	C2-S1-C5	-2.86	89.32	91.22
7	B	1701	FAD	C9-C9A-N10	2.82	125.65	121.85
8	B	1702	TPP	C5'-C6'-N1'	-2.78	119.31	123.83
8	B	1702	TPP	C2'-N3'-C4'	2.75	122.33	118.10
5	B	1698	DTT	C2-C1-S1	2.73	122.06	114.43
7	A	701	FAD	C9-C9A-N10	2.66	125.43	121.85
7	A	701	FAD	O2-C2-N1	-2.66	117.39	121.80
6	A	700	AYD	C2'-N3'-C4'	2.56	122.04	118.10
7	A	701	FAD	C5A-N7A-C8A	2.55	107.46	103.45
7	A	701	FAD	C4A-C5A-N7A	-2.54	107.68	110.58
7	B	1701	FAD	O2-C2-N1	-2.46	117.71	121.80
7	B	1701	FAD	C4A-C5A-N7A	-2.44	107.79	110.58
6	A	700	AYD	C5'-C6'-N1'	-2.43	119.87	123.83
7	B	1701	FAD	C5A-N7A-C8A	2.41	107.24	103.45
4	B	1695	CIE	N14-C2'-N3'	2.33	123.20	116.44
4	A	695	CIE	N12-C13-N14	2.30	118.52	114.87
4	B	1695	CIE	C5'-C6'-N1'	-2.13	121.67	124.16
7	A	701	FAD	C5'-C4'-C3'	-2.12	108.22	112.22
4	A	695	CIE	N14-C2'-N3'	2.08	122.49	116.44
5	A	698	DTT	O2-C2-C3	-2.03	105.31	109.57
8	B	1702	TPP	O3A-PA-O1A	-2.03	104.61	110.70
4	A	695	CIE	C5'-C6'-N1'	-2.02	121.80	124.16
4	B	1695	CIE	CL4'-C4'-N3'	2.02	119.74	115.45
8	B	1702	TPP	C7'-C5'-C4'	2.02	126.05	122.36
7	A	701	FAD	C4X-C10-N10	2.01	119.36	116.48

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1695	CIE	C1-C2-S11-OBA
5	A	698	DTT	S1-C1-C2-C3
5	B	1698	DTT	S1-C1-C2-C3
6	A	700	AYD	C4'-C5'-C7'-N3
6	A	700	AYD	C5-C4-N3-C7'
6	A	700	AYD	CM4-C4-N3-C7'
6	A	700	AYD	C4-C5-C6-C7
6	A	700	AYD	C6-C7-O7-PA
4	B	1695	CIE	O7-C7-O8-C9
4	A	695	CIE	O7-C7-O8-C9
4	A	695	CIE	C1-C2-S11-OBA
4	A	695	CIE	C3-C2-S11-N12
4	B	1695	CIE	C3-C2-S11-N12
4	A	695	CIE	C1-C2-S11-OB
4	B	1695	CIE	C1-C2-S11-OB
4	A	695	CIE	C1-C2-S11-N12
4	B	1695	CIE	C1-C2-S11-N12
6	A	700	AYD	C5-C6-C7-O7
8	B	1702	TPP	S1-C5-C6-C7
6	A	700	AYD	PB-O3A-PA-O7
5	A	698	DTT	S1-C1-C2-O2
5	B	1698	DTT	S1-C1-C2-O2
4	B	1695	CIE	C3-C2-S11-OBA
4	A	695	CIE	C3-C2-S11-OBA
4	B	1695	CIE	C3-C2-S11-OB
8	B	1702	TPP	C4'-C5'-C7'-N3
4	A	695	CIE	C3-C2-S11-OB
4	A	695	CIE	N12-C13-N14-C2'
4	B	1695	CIE	N12-C13-N14-C2'
7	A	701	FAD	C2B-C1B-N9A-C8A
7	B	1701	FAD	C2B-C1B-N9A-C8A
4	B	1695	CIE	O13-C13-N14-C2'
7	A	701	FAD	O4B-C4B-C5B-O5B
7	B	1701	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

8 monomers are involved in 29 short contacts:

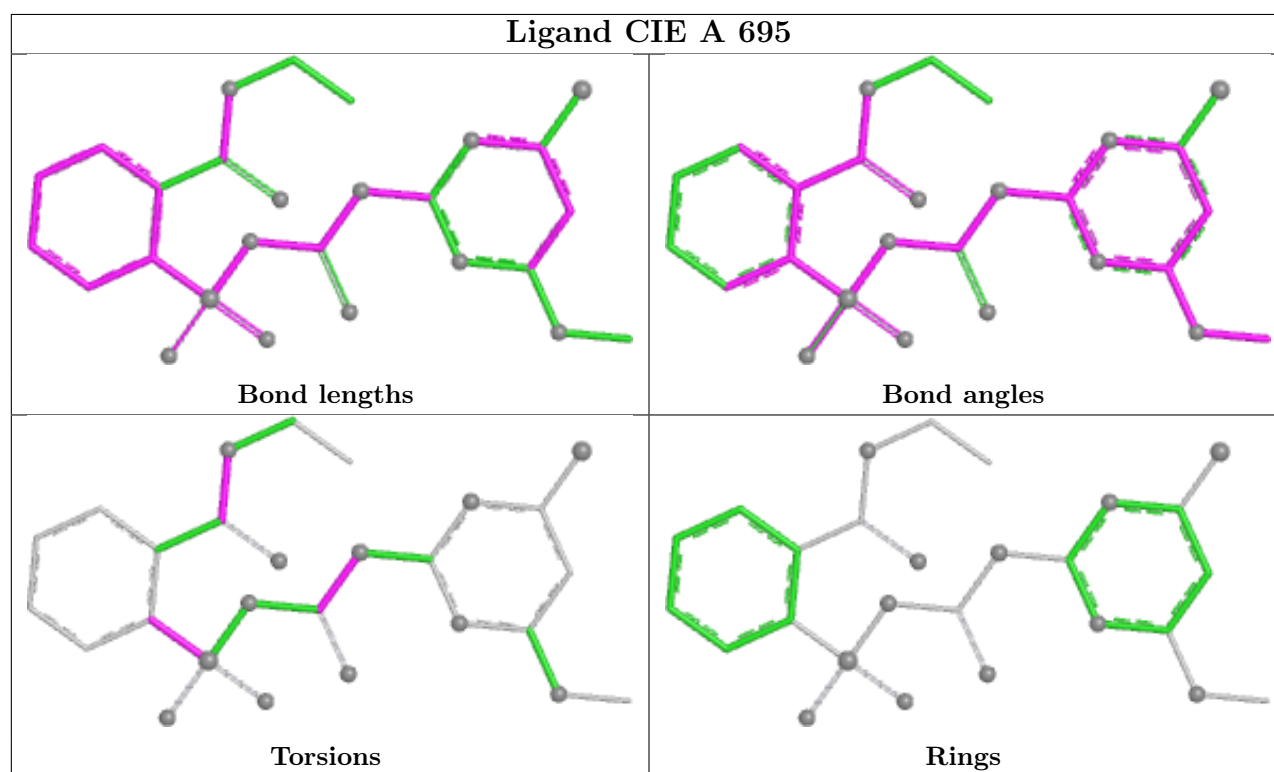
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	695	CIE	4	0
7	A	701	FAD	3	0
5	A	698	DTT	2	0
6	A	700	AYD	3	0

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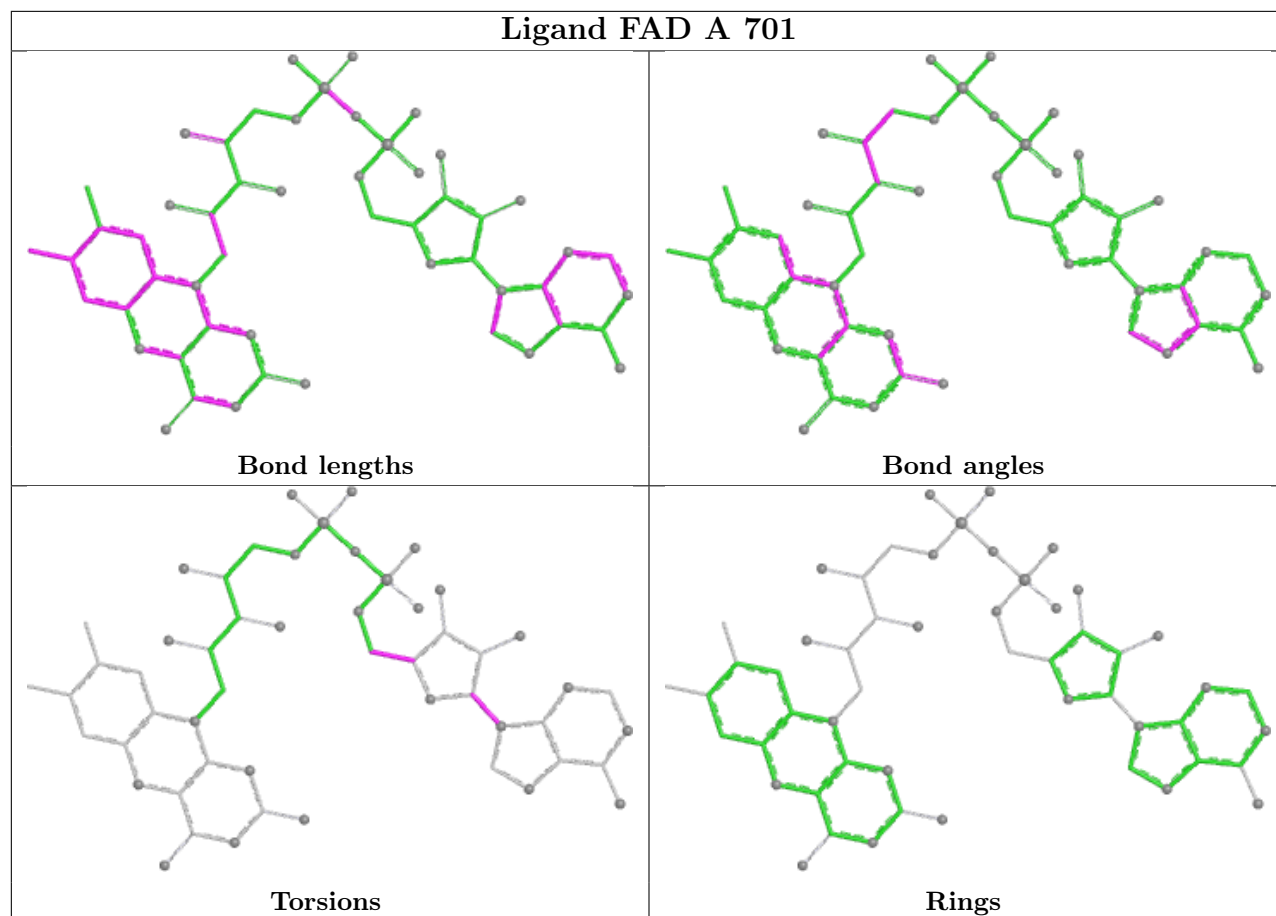
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1702	TPP	8	0
4	B	1695	CIE	5	0
7	B	1701	FAD	3	0
5	B	1698	DTT	3	0

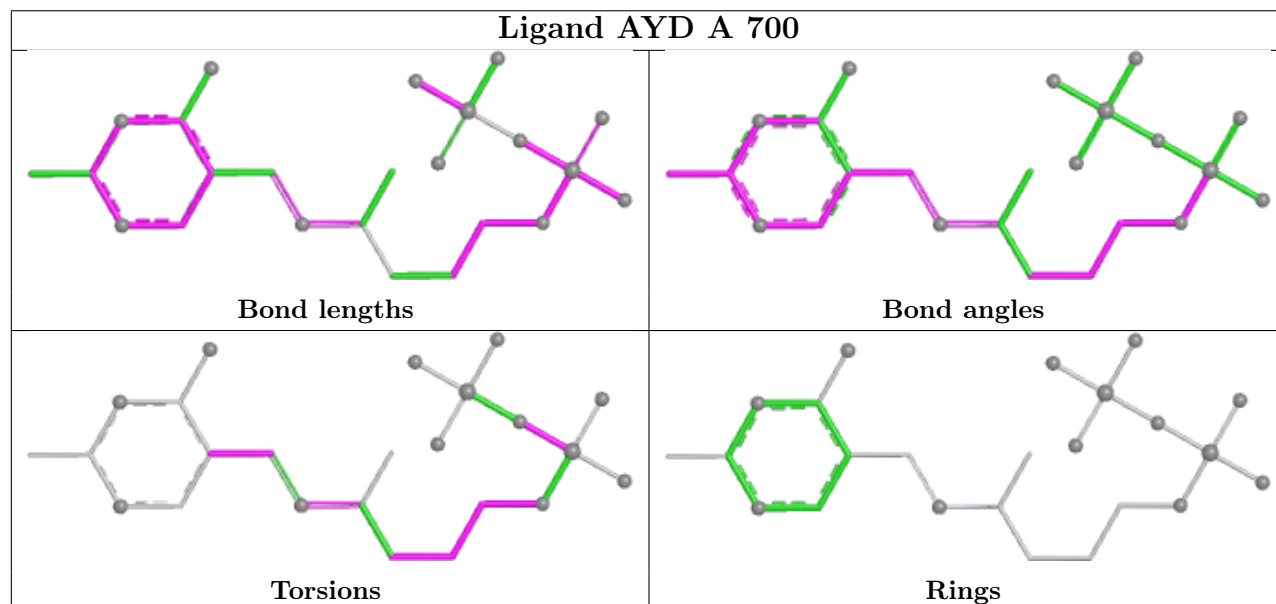
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



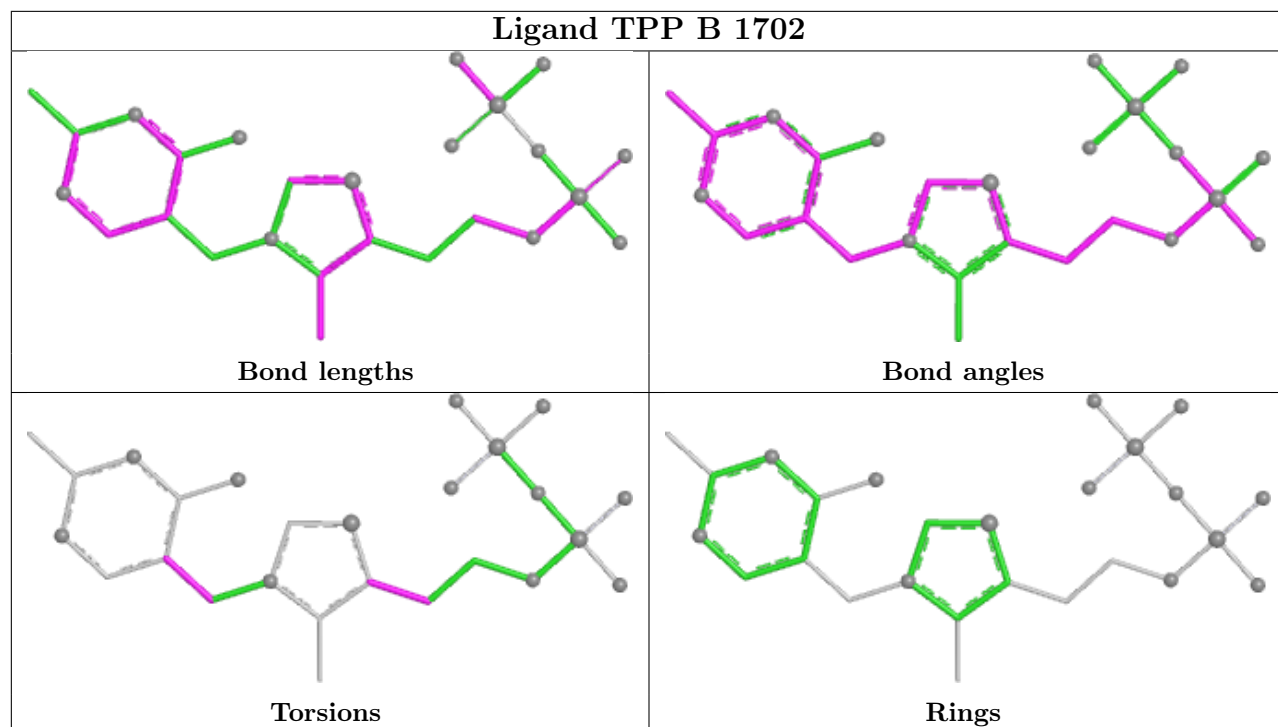
Ligand FAD A 701



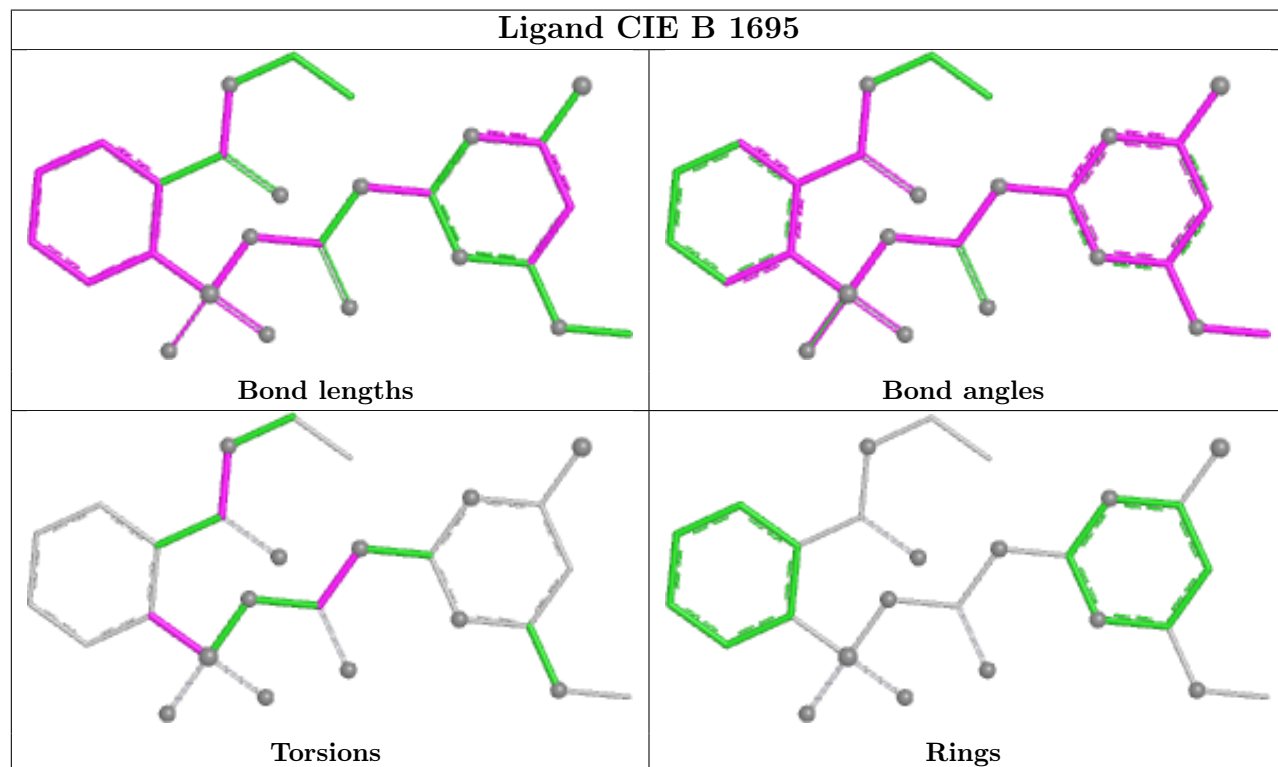
Ligand AYD A 700

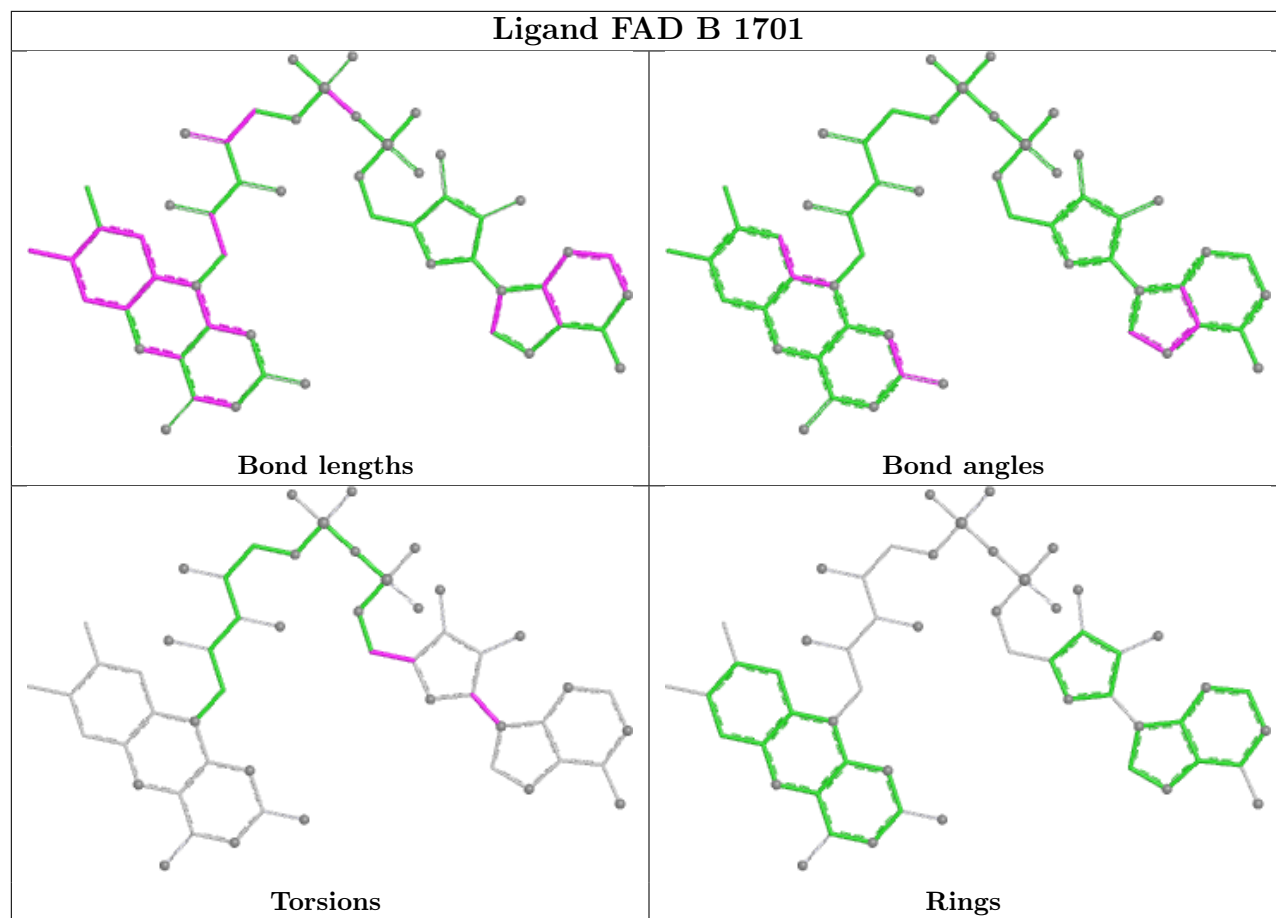


Ligand TPP B 1702



Ligand CIE B 1695





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	599/677 (88%)	-0.57	7 (1%) 76 68	7, 20, 42, 85	2 (0%)
1	B	598/677 (88%)	-0.02	20 (3%) 49 39	14, 35, 70, 101	2 (0%)
All	All	1197/1354 (88%)	-0.29	27 (2%) 61 51	7, 25, 64, 101	4 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	278	SER	5.4
1	A	83	PRO	4.7
1	B	83	PRO	4.3
1	B	260	ASN	4.1
1	B	280	ALA	3.6
1	A	270	SER	3.4
1	B	445	SER	3.3
1	A	277	THR	3.2
1	B	270	SER	3.2
1	B	279	ARG	3.0
1	B	259	ARG	3.0
1	B	459	PRO	2.8
1	A	268	LEU	2.8
1	B	129	ASP	2.7
1	B	265	LYS	2.6
1	B	282	ASP	2.5
1	A	600	GLN	2.4
1	B	268	LEU	2.4
1	A	84	ASP	2.3
1	B	106	ASN	2.2
1	B	541	GLU	2.2
1	A	129	ASP	2.2
1	B	281	GLN	2.1
1	B	284	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	446	GLU	2.1
1	B	687	HIS	2.0
1	B	286	MET	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

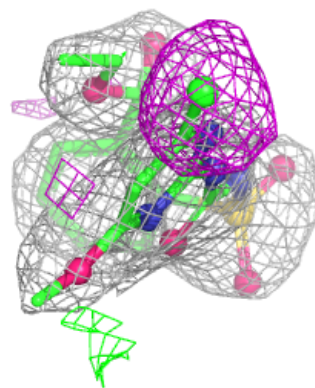
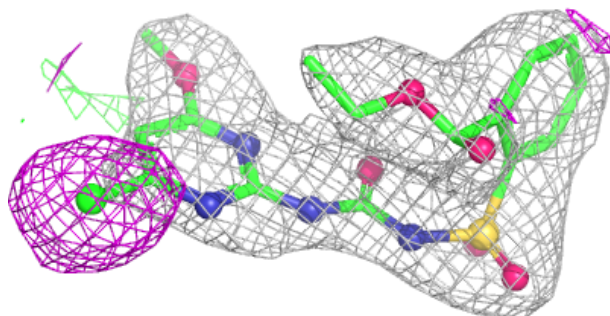
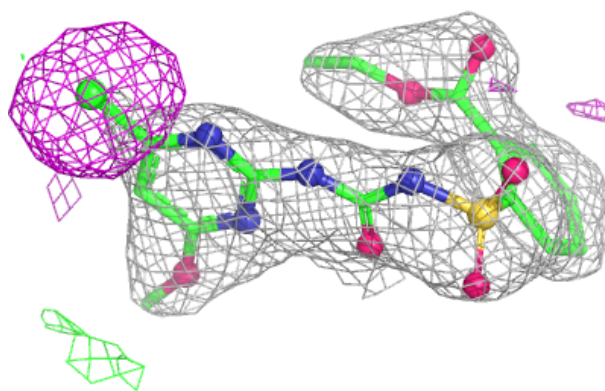
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DTT	B	1698	8/8	0.82	0.25	76,86,89,93	5
5	DTT	A	698	8/8	0.87	0.25	48,57,59,65	2
4	CIE	B	1695	27/27	0.88	0.13	41,46,51,51	0
4	CIE	A	695	27/27	0.89	0.11	19,24,27,31	0
8	TPP	B	1702	26/26	0.96	0.11	32,39,46,46	2
7	FAD	B	1701	53/53	0.97	0.08	29,32,40,41	0
6	AYD	A	700	24/24	0.97	0.10	16,41,47,47	0
2	K	B	1696	1/1	0.98	0.04	42,42,42,42	0
2	K	A	696	1/1	0.98	0.03	18,18,18,18	0
3	MG	B	1699	1/1	0.99	0.03	25,25,25,25	0
7	FAD	A	701	53/53	0.99	0.05	5,11,14,15	0
3	MG	A	699	1/1	1.00	0.03	2,2,2,2	0

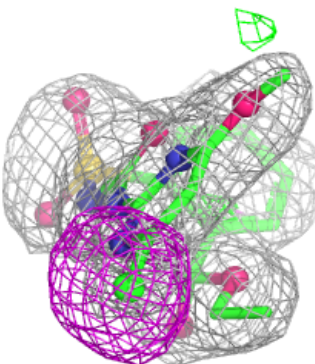
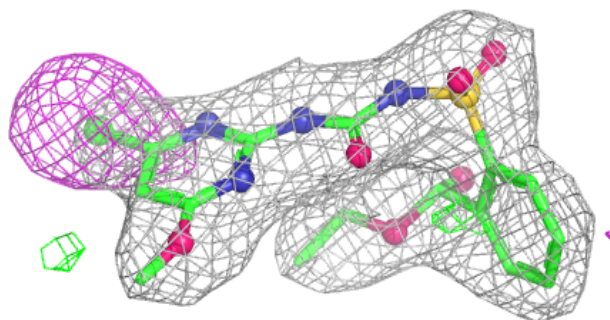
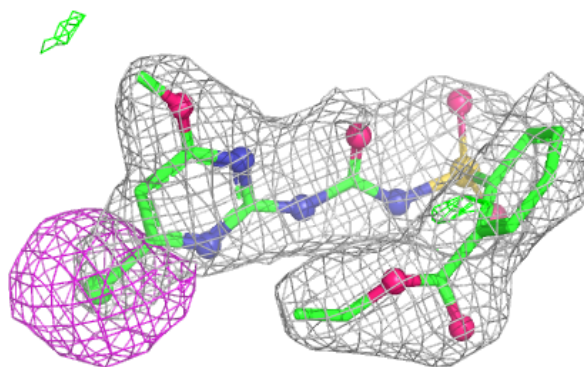
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CIE B 1695:

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

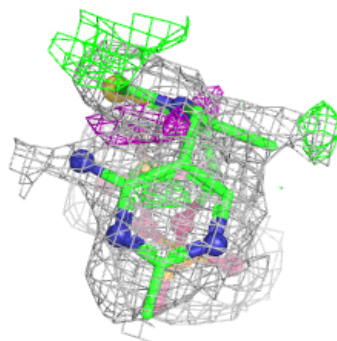
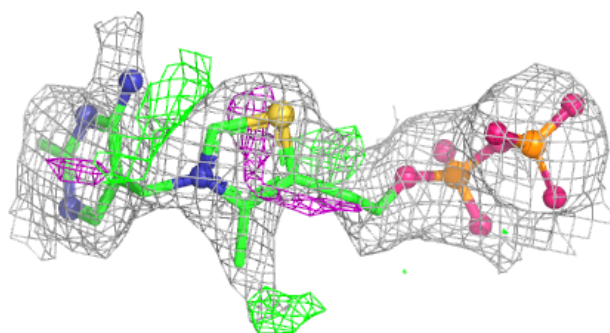
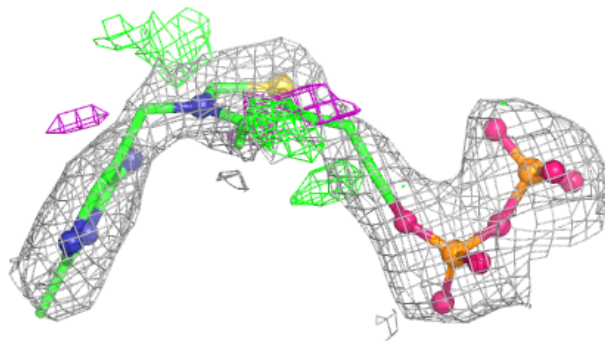
**Electron density around CIE A 695:**

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

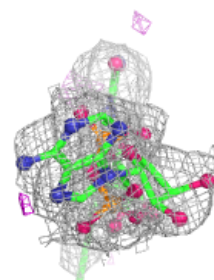
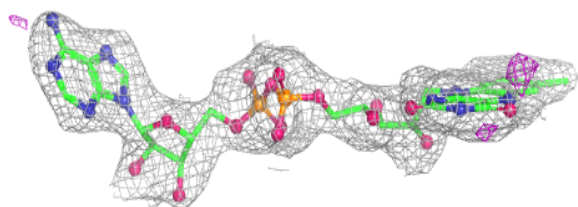
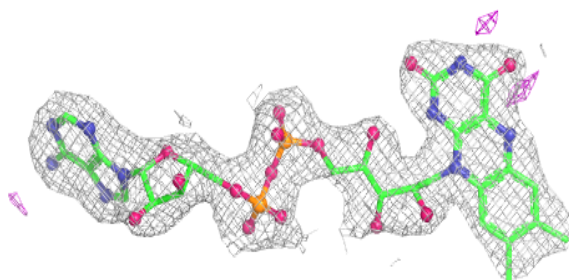


Electron density around TPP B 1702:

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

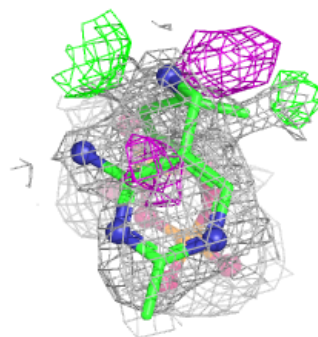
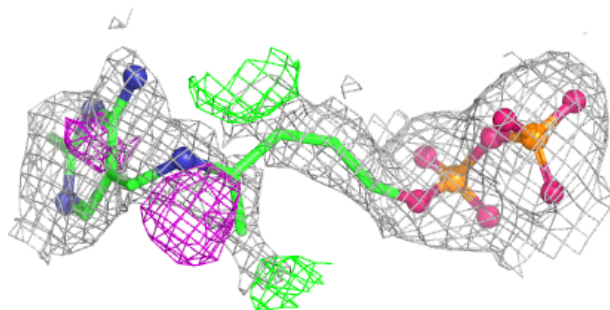
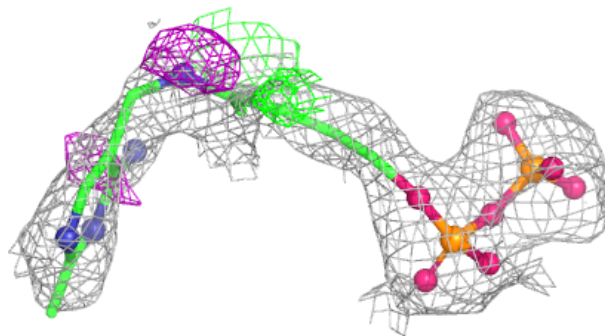
**Electron density around FAD B 1701:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

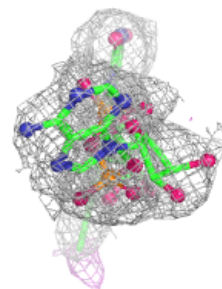
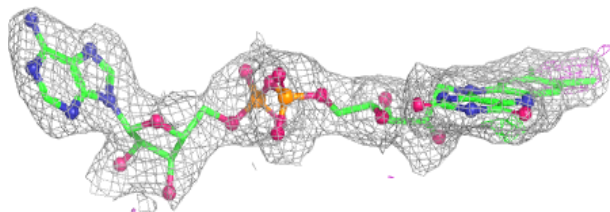
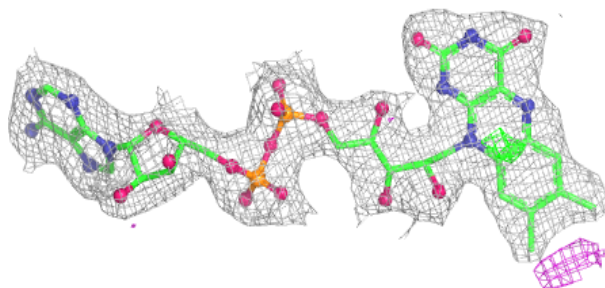


Electron density around AYD A 700:

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

**Electron density around FAD A 701:**

$2mF_o-DF_c$ (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.