



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:58 AM UTC

PDB ID : 6H3O / pdb_00006h3o
Title : Alcohol oxidase from Phanerochaete chrysosporium mutant F101S
Authors : Nguyen, Q.-T.; Romero, E.; Dijkman, W.P.; de Vasconcellos, S.P.; Binda, C.;
Mattevi, A.; Fraaije, M.W.
Deposited on : 2018-07-19
Resolution : 2.50 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

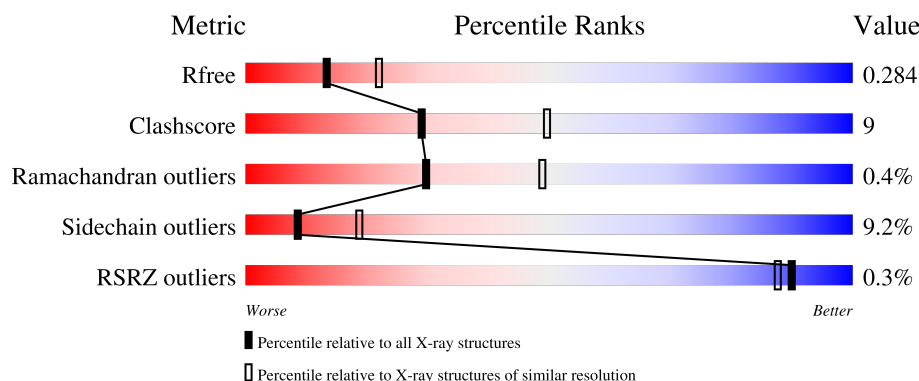
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	651	76% 20% .
1	B	651	77% 20% ..
1	C	651	77% 20% .
1	D	651	76% 20% .
1	E	651	76% 21% ..

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Mol	Chain	Length	Quality of chain
1	F	651	76% 19%
1	G	651	% 74% 22%
1	H	651	75% 21%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 41785 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.

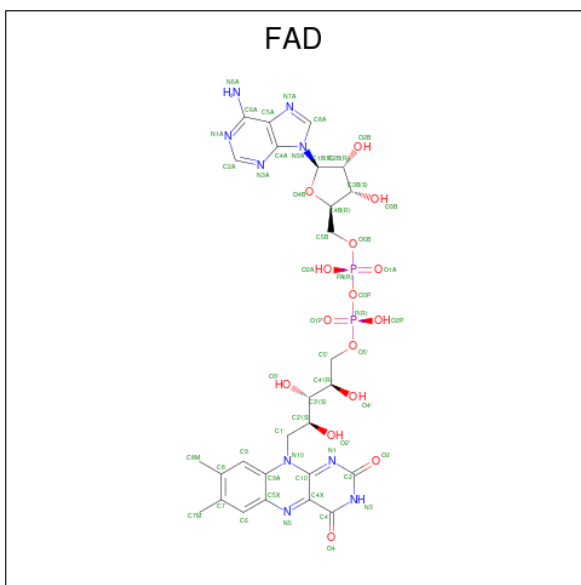
- Molecule 1 is a protein called Alcohol oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	1	0
			5095	3200	904	966	25			
1	B	647	Total	C	N	O	S	0	0	0
			5067	3184	896	962	25			
1	C	648	Total	C	N	O	S	0	0	0
			5078	3190	900	963	25			
1	D	649	Total	C	N	O	S	0	0	0
			5088	3196	903	964	25			
1	E	648	Total	C	N	O	S	0	0	0
			5078	3190	900	963	25			
1	F	650	Total	C	N	O	S	0	0	0
			5092	3198	904	965	25			
1	G	648	Total	C	N	O	S	0	0	0
			5078	3190	900	963	25			
1	H	648	Total	C	N	O	S	0	0	0
			5078	3190	900	963	25			

There are 8 discrepancies between the modelled and reference sequences:

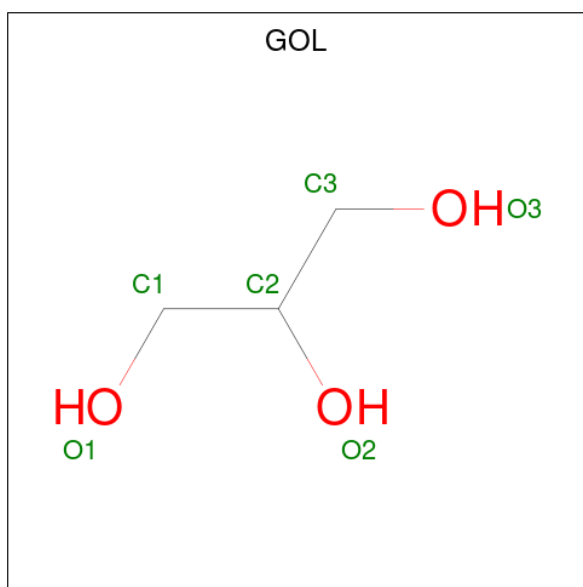
Chain	Residue	Modelled	Actual	Comment	Reference
A	101	SER	PHE	engineered mutation	UNP T2M2J4
B	101	SER	PHE	engineered mutation	UNP T2M2J4
C	101	SER	PHE	engineered mutation	UNP T2M2J4
D	101	SER	PHE	engineered mutation	UNP T2M2J4
E	101	SER	PHE	engineered mutation	UNP T2M2J4
F	101	SER	PHE	engineered mutation	UNP T2M2J4
G	101	SER	PHE	engineered mutation	UNP T2M2J4
H	101	SER	PHE	engineered mutation	UNP T2M2J4

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	E	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	F	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	G	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	H	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		

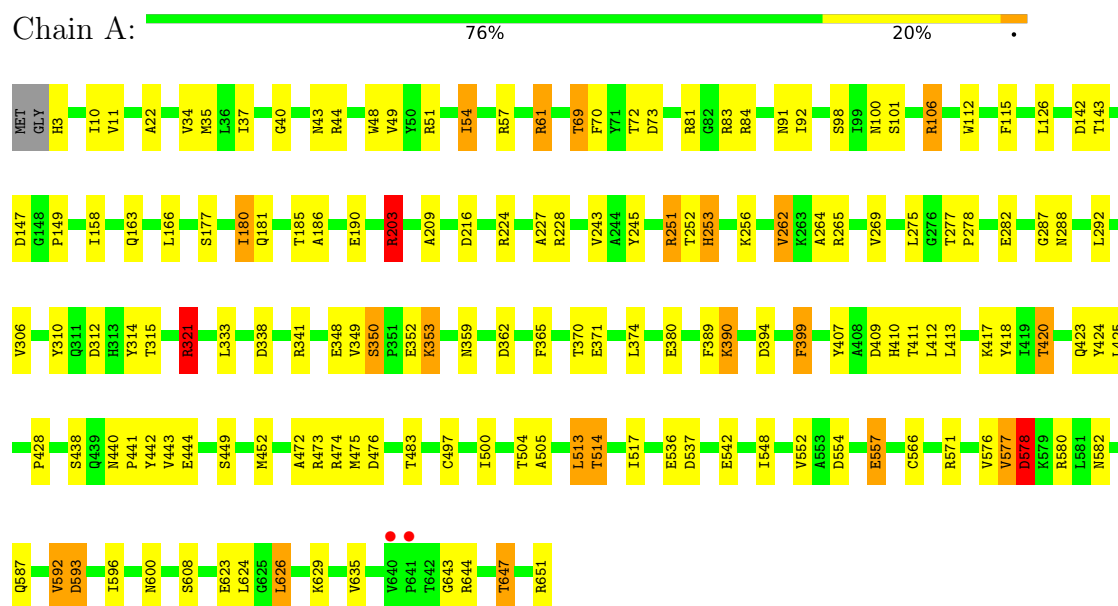
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total	O	0	0
			75	75		
4	B	112	Total	O	0	0
			112	112		
4	C	95	Total	O	0	0
			95	95		
4	D	111	Total	O	0	0
			111	111		
4	E	49	Total	O	0	0
			49	49		
4	F	78	Total	O	0	0
			78	78		
4	G	72	Total	O	0	0
			72	72		
4	H	103	Total	O	0	0
			103	103		

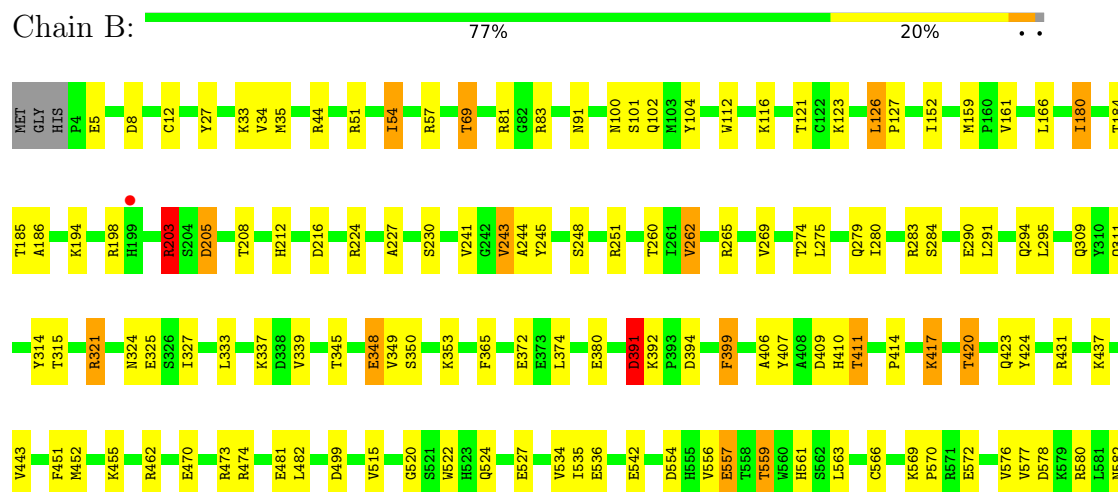
3 Residue-property plots

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: Alcohol oxidase



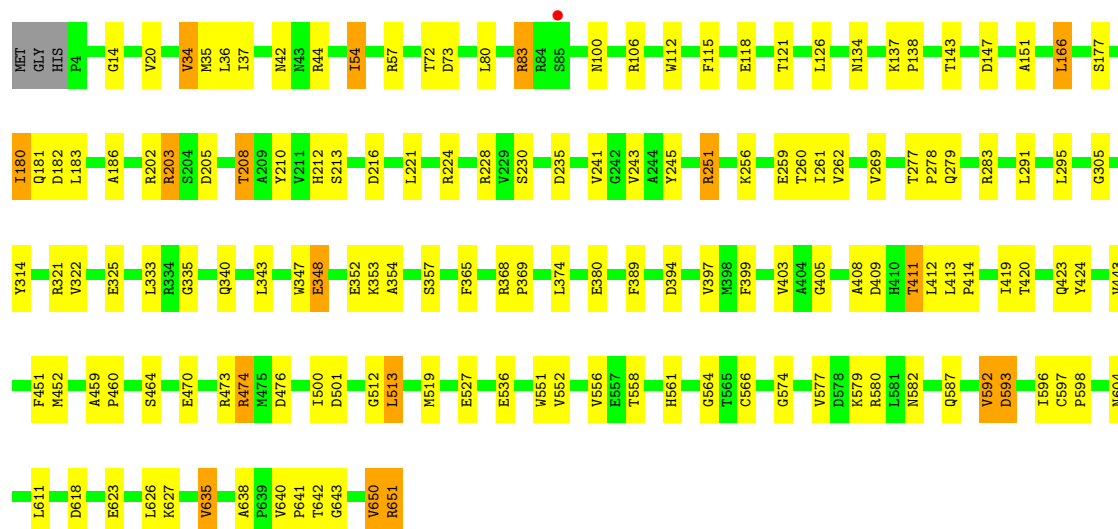
• Molecule 1: Alcohol oxidase





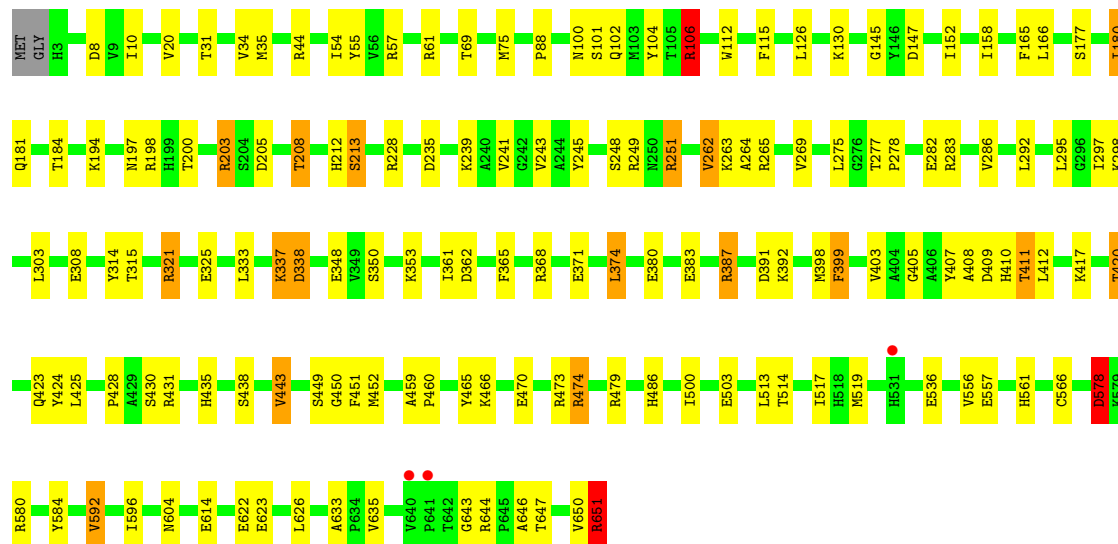
• Molecule 1: Alcohol oxidase

Chain C: 77% 20%



• Molecule 1: Alcohol oxidase

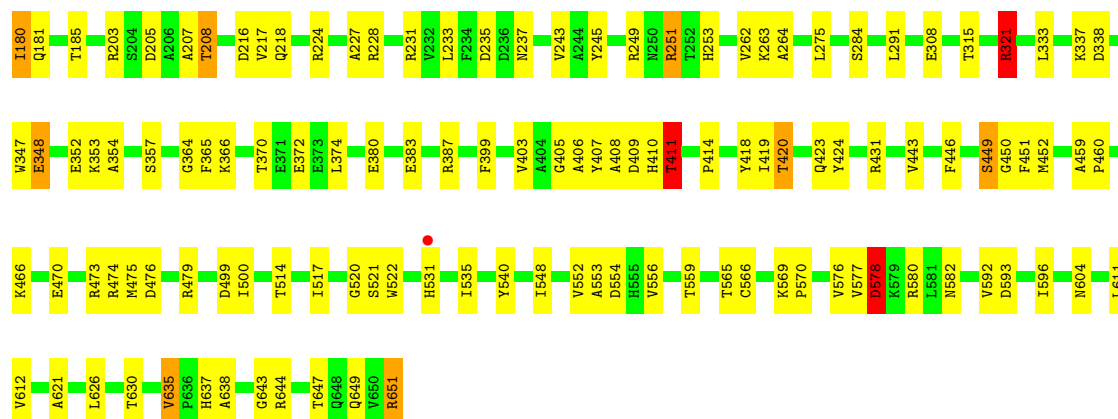
Chain D: 76% 20%



• Molecule 1: Alcohol oxidase

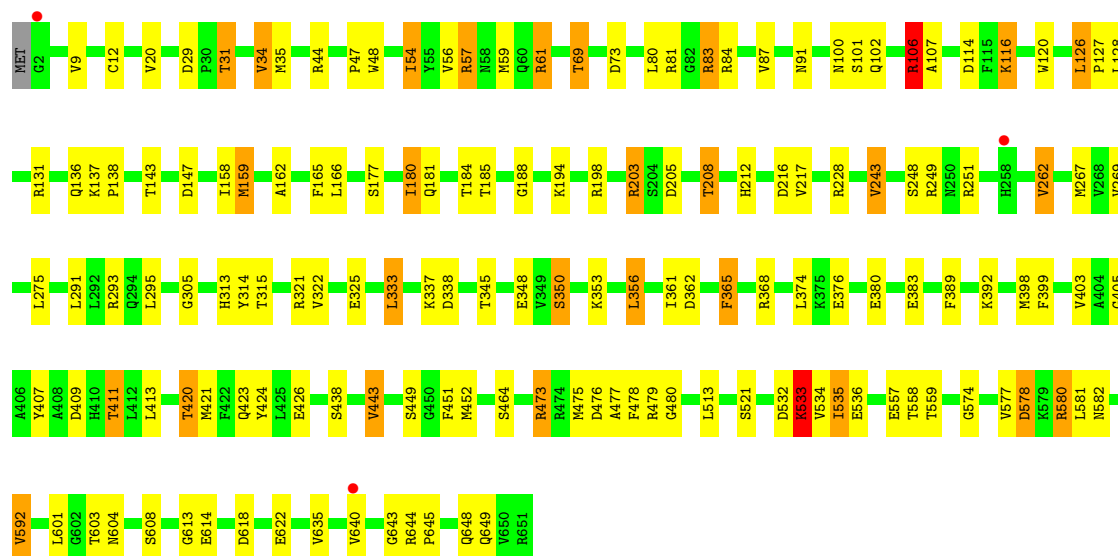
Chain E: 76% 21%





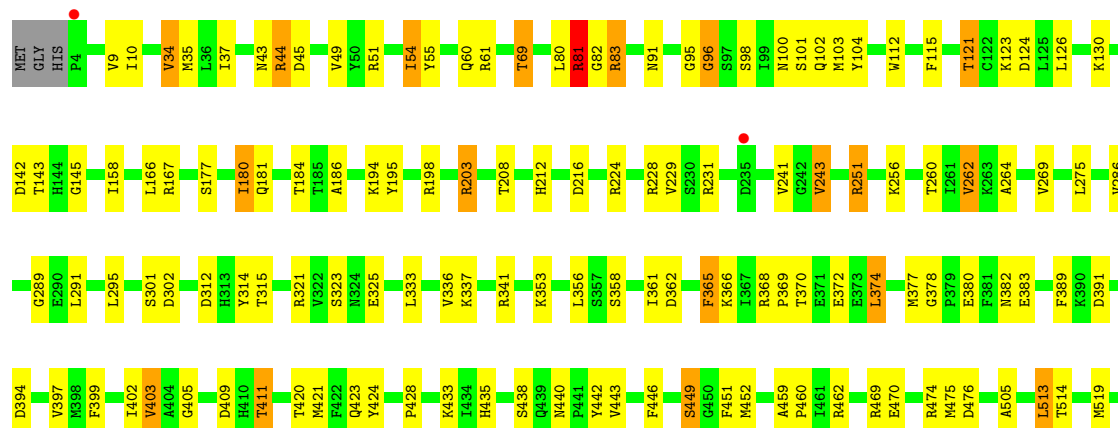
• Molecule 1: Alcohol oxidase

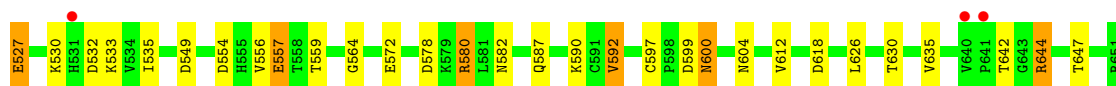
Chain F: 76% 19% •



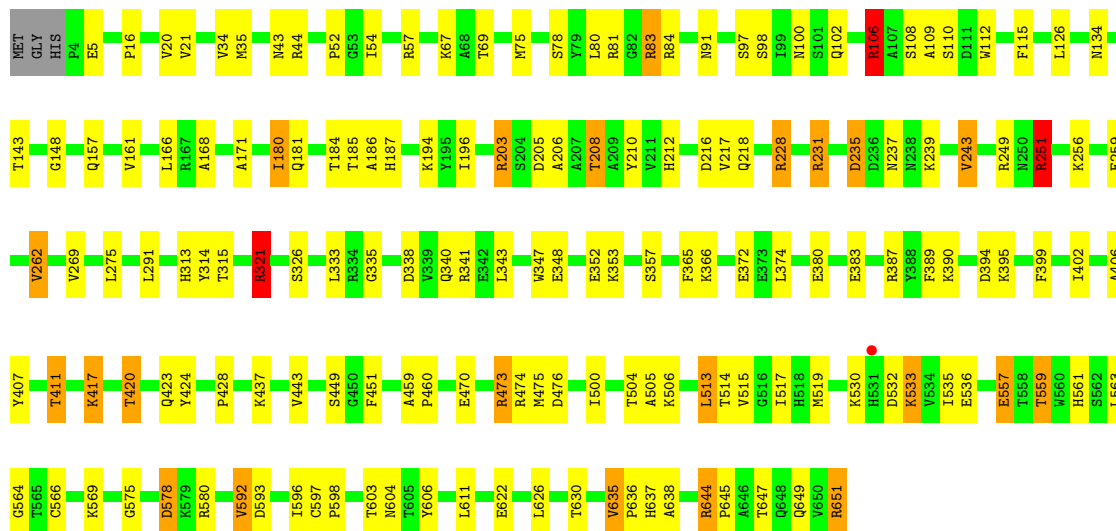
• Molecule 1: Alcohol oxidase

Chain G: 74% 22% •





• Molecule 1: Alcohol oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.07Å 203.55Å 116.01Å 90.00° 104.64° 90.00°	Depositor
Resolution (Å)	49.19 – 2.50 49.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.19-2.50) 98.4 (49.19-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.210 , 0.286 0.214 , 0.284	Depositor DCC
R_{free} test set	8397 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	41785	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: GOL, FAD

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	0.68	0/5220	1.02	3/7088 (0.0%)
1	B	0.67	0/5191	1.01	3/7048 (0.0%)
1	C	0.67	0/5202	1.01	0/7062
1	D	0.70	0/5213	1.04	2/7078 (0.0%)
1	E	0.67	0/5202	1.03	1/7062 (0.0%)
1	F	0.68	0/5217	1.03	1/7083 (0.0%)
1	G	0.67	0/5202	1.04	2/7062 (0.0%)
1	H	0.67	0/5202	1.02	0/7062
All	All	0.68	0/41649	1.02	12/56545 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	5
1	D	0	5
1	E	0	7
1	F	0	9
1	G	0	11
1	H	0	11
All	All	0	57

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	578	ASP	CB-CA-C	-5.76	98.96	110.42
1	G	527	GLU	CB-CA-C	5.59	116.91	108.86
1	B	365	PHE	CA-CB-CG	5.39	119.19	113.80
1	E	411	THR	CB-CA-C	5.35	119.64	110.01
1	A	577	VAL	CA-C-N	5.34	131.75	121.54
1	A	577	VAL	C-N-CA	5.34	131.75	121.54
1	G	365	PHE	CA-CB-CG	5.23	119.03	113.80
1	A	578	ASP	CA-CB-CG	5.14	117.74	112.60
1	F	365	PHE	CA-CB-CG	5.09	118.89	113.80
1	B	578	ASP	CA-CB-CG	5.09	117.69	112.60
1	D	338	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	391	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	ARG	Sidechain
1	A	224	ARG	Sidechain
1	A	265	ARG	Sidechain
1	A	321	ARG	Sidechain
1	A	571	ARG	Sidechain
1	B	203	ARG	Sidechain
1	B	321	ARG	Sidechain
1	B	431	ARG	Sidechain
1	B	462	ARG	Sidechain
1	C	203	ARG	Sidechain
1	C	224	ARG	Sidechain
1	C	228	ARG	Sidechain
1	C	474	ARG	Sidechain
1	C	83	ARG	Sidechain
1	D	106	ARG	Sidechain
1	D	228	ARG	Sidechain
1	D	321	ARG	Sidechain
1	D	368	ARG	Sidechain
1	D	651	ARG	Sidechain
1	E	106	ARG	Sidechain
1	E	224	ARG	Sidechain
1	E	321	ARG	Sidechain
1	E	44	ARG	Sidechain
1	E	479	ARG	Sidechain
1	E	61	ARG	Sidechain
1	E	644	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	106	ARG	Sidechain
1	F	203	ARG	Sidechain
1	F	249	ARG	Sidechain
1	F	293	ARG	Sidechain
1	F	321	ARG	Sidechain
1	F	479	ARG	Sidechain
1	F	580	ARG	Sidechain
1	F	81	ARG	Sidechain
1	F	83	ARG	Sidechain
1	G	167	ARG	Sidechain
1	G	228	ARG	Sidechain
1	G	231	ARG	Sidechain
1	G	321	ARG	Sidechain
1	G	341	ARG	Sidechain
1	G	469	ARG	Sidechain
1	G	580	ARG	Sidechain
1	G	61	ARG	Sidechain
1	G	644	ARG	Sidechain
1	G	81	ARG	Sidechain
1	G	83	ARG	Sidechain
1	H	106	ARG	Sidechain
1	H	228	ARG	Sidechain
1	H	231	ARG	Sidechain
1	H	251	ARG	Sidechain
1	H	321	ARG	Sidechain
1	H	341	ARG	Sidechain
1	H	473	ARG	Sidechain
1	H	644	ARG	Sidechain
1	H	81	ARG	Sidechain
1	H	83	ARG	Sidechain
1	H	84	ARG	Sidechain

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	5095	0	4969	102	0
1	B	5067	0	4944	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5078	0	4957	96	0
1	D	5088	0	4963	99	0
1	E	5078	0	4957	85	0
1	F	5092	0	4966	99	0
1	G	5078	0	4957	99	0
1	H	5078	0	4957	104	0
2	A	53	0	31	2	0
2	B	53	0	31	4	0
2	C	53	0	31	2	0
2	D	53	0	31	3	0
2	E	53	0	31	2	0
2	F	53	0	31	4	0
2	G	53	0	31	3	0
2	H	53	0	31	3	0
3	B	6	0	8	0	0
3	H	6	0	8	0	0
4	A	75	0	0	3	0
4	B	112	0	0	2	0
4	C	95	0	0	1	0
4	D	111	0	0	5	0
4	E	49	0	0	2	0
4	F	78	0	0	2	0
4	G	72	0	0	4	0
4	H	103	0	0	4	0
All	All	41785	0	39934	701	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 9.

All (701) 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:D:410:HIS:ND1	1:H:514:THR:HG21	1.83	0.94
1:F:100:ASN:O	1:F:203:ARG:NH2	2.06	0.89
1:A:228:ARG:NH1	1:A:441:PRO:O	2.05	0.88
1:A:106:ARG:NH1	1:A:181:GLN:O	2.11	0.83
1:G:51:ARG:O	1:G:54:ILE:HD13	1.79	0.83
1:D:104:TYR:OH	1:D:106:ARG:HD2	1.83	0.79
1:H:228:ARG:NH2	4:H:801:HOH:O	2.16	0.78
1:B:473:ARG:NH2	1:B:536:GLU:O	2.17	0.78
1:C:470:GLU:OE1	1:C:474:ARG:NH2	2.16	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:ARG:NH1	1:E:554:ASP:OD2	2.18	0.76
1:F:61:ARG:HG2	1:F:61:ARG:HH11	1.50	0.76
1:F:177:SER:HB3	1:F:180:ILE:HD13	1.67	0.75
1:B:407:TYR:H	1:B:420:THR:HG21	1.51	0.75
1:B:216:ASP:OD2	1:D:647:THR:HG22	1.87	0.74
1:F:61:ARG:HH11	1:F:61:ARG:CG	2.00	0.74
1:A:440:ASN:HD22	1:A:443:VAL:HG13	1.53	0.73
1:D:473:ARG:NH2	1:D:536:GLU:O	2.20	0.73
1:F:368:ARG:NH2	1:F:389:PHE:O	2.19	0.73
1:D:580:ARG:NH1	1:D:623:GLU:OE2	2.21	0.72
1:F:578:ASP:HB3	1:F:580:ARG:H	1.55	0.72
1:D:100:ASN:O	1:D:203:ARG:NH2	2.21	0.72
4:D:870:HOH:O	1:H:514:THR:HG22	1.89	0.71
1:H:100:ASN:HB2	2:H:701:FAD:N5	2.05	0.71
1:D:35:MET:HE1	1:D:262:VAL:HG11	1.73	0.70
1:H:100:ASN:O	1:H:203:ARG:NH2	2.25	0.70
1:D:407:TYR:H	1:D:420:THR:HG21	1.56	0.69
1:D:180:ILE:HG22	1:D:181:GLN:NE2	2.08	0.69
1:B:269:VAL:HG13	1:B:592:VAL:HG13	1.75	0.69
1:A:438:SER:HB3	1:A:443:VAL:HG21	1.74	0.68
1:C:566:CYS:O	1:C:596:ILE:HA	1.93	0.68
1:B:104:TYR:CE1	1:B:152:ILE:HD13	2.28	0.68
1:F:48:TRP:HE3	1:F:54:ILE:HG13	1.57	0.68
1:C:564:GLY:HA2	1:C:597:CYS:O	1.94	0.68
1:F:106:ARG:NH1	1:F:181:GLN:O	2.26	0.68
1:H:566:CYS:O	1:H:596:ILE:HA	1.94	0.68
1:D:8:ASP:OD1	1:D:265:ARG:NH1	2.23	0.68
1:B:100:ASN:O	1:B:203:ARG:NH2	2.27	0.67
1:E:106:ARG:NH2	1:E:143:THR:O	2.24	0.67
1:D:409:ASP:OD2	4:D:801:HOH:O	2.13	0.67
1:E:470:GLU:HB3	1:E:474:ARG:HH21	1.60	0.67
1:A:557:GLU:OE2	1:E:521:SER:OG	2.13	0.66
1:A:566:CYS:HA	1:A:576:VAL:HG21	1.77	0.66
1:F:48:TRP:CE3	1:F:54:ILE:HG13	2.31	0.66
1:F:399:PHE:CD1	1:F:424:TYR:CD2	2.84	0.66
1:B:410:HIS:ND1	1:G:514:THR:HG21	2.10	0.65
1:G:100:ASN:HB2	2:G:701:FAD:C5X	2.26	0.65
1:B:470:GLU:OE1	1:B:474:ARG:NH2	2.29	0.65
1:A:399:PHE:CD1	1:A:424:TYR:CD2	2.84	0.65
1:E:476:ASP:OD1	1:G:251:ARG:NH1	2.30	0.65
1:A:353:LYS:HE3	1:C:202:ARG:HH12	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:ASN:HB2	2:G:701:FAD:N5	2.12	0.64
1:G:440:ASN:HD21	1:G:442:TYR:HB2	1.62	0.64
1:A:647:THR:HG22	1:C:216:ASP:OD2	1.98	0.64
1:D:405:GLY:O	1:D:420:THR:HG22	1.97	0.64
1:G:409:ASP:OD1	1:G:411:THR:HB	1.97	0.64
1:D:452:MET:HE3	1:D:556:VAL:HG21	1.78	0.64
1:F:399:PHE:CG	1:F:424:TYR:CE2	2.86	0.64
1:G:81:ARG:NH1	1:G:554:ASP:OD2	2.31	0.64
1:A:399:PHE:CG	1:A:424:TYR:CE2	2.86	0.64
1:E:405:GLY:O	1:E:420:THR:HG22	1.97	0.63
1:G:535:ILE:HD12	1:H:251:ARG:HG2	1.81	0.63
1:C:409:ASP:OD1	1:C:411:THR:HB	1.98	0.63
1:C:399:PHE:CG	1:C:424:TYR:CE2	2.87	0.63
1:B:321:ARG:NH2	1:G:411:THR:O	2.31	0.63
1:G:513:LEU:N	1:G:513:LEU:HD23	2.14	0.63
1:C:230:SER:O	1:C:283:ARG:HD2	1.99	0.63
1:A:44:ARG:NH1	1:B:648:GLN:HE22	1.96	0.62
1:H:407:TYR:H	1:H:420:THR:HG21	1.64	0.62
1:E:370:THR:HG22	1:E:372:GLU:H	1.64	0.62
1:C:399:PHE:CD2	1:C:424:TYR:CE2	2.88	0.62
1:F:473:ARG:NH2	1:F:536:GLU:O	2.32	0.62
1:H:635:VAL:HG13	1:H:638:ALA:HB3	1.82	0.62
1:A:514[B]:THR:HG23	1:A:517:ILE:HD12	1.81	0.62
1:F:102:GLN:HG3	1:F:203:ARG:HH21	1.64	0.62
1:A:407:TYR:H	1:A:420:THR:HG21	1.65	0.62
1:A:147:ASP:HB3	1:A:643:GLY:HA2	1.82	0.62
1:A:580:ARG:NH1	1:A:623:GLU:OE2	2.33	0.62
1:E:407:TYR:H	1:E:420:THR:HG21	1.65	0.62
1:H:561:HIS:CE1	1:H:604:ASN:HA	2.35	0.62
1:E:635:VAL:HG13	1:E:638:ALA:HB3	1.81	0.61
1:H:352:GLU:OE2	1:H:651:ARG:HD2	2.00	0.61
1:D:398:MET:SD	1:D:425:LEU:HA	2.41	0.61
1:F:208:THR:HA	1:F:212:HIS:HB2	1.83	0.61
1:F:580:ARG:HH22	1:F:622:GLU:CD	2.09	0.61
1:A:474:ARG:NH2	1:A:537:ASP:OD1	2.34	0.61
1:H:80:LEU:O	1:H:83:ARG:HG2	2.01	0.61
1:A:44:ARG:HH11	1:B:648:GLN:HE22	1.48	0.60
1:G:647:THR:HG23	4:H:809:HOH:O	2.01	0.60
1:A:269:VAL:CG1	1:A:592:VAL:HG13	2.31	0.60
1:B:559:THR:O	1:B:561:HIS:CD2	2.55	0.60
1:E:140:ASN:HB2	1:E:178:ASP:OD2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:VAL:HG23	1:E:218:GLN:HG3	1.84	0.60
1:F:578:ASP:OD2	1:F:582:ASN:HB2	2.02	0.60
1:B:69:THR:HG22	1:B:91:ASN:HB2	1.84	0.60
1:B:51:ARG:O	1:B:54:ILE:HD13	2.02	0.59
1:C:368:ARG:NH2	1:C:389:PHE:O	2.35	0.59
1:F:205:ASP:OD1	1:F:208:THR:HG23	2.02	0.59
1:C:474:ARG:HD3	1:D:251:ARG:O	2.02	0.59
1:G:203:ARG:NH1	4:G:804:HOH:O	2.35	0.59
1:E:205:ASP:OD1	1:E:208:THR:HG23	2.02	0.59
1:G:399:PHE:CG	1:G:424:TYR:CE2	2.91	0.59
1:A:100:ASN:O	1:A:203:ARG:NH2	2.35	0.59
1:C:399:PHE:CD2	1:C:424:TYR:CD2	2.91	0.59
1:D:104:TYR:CE1	1:D:152:ILE:HD13	2.37	0.59
1:E:113:ASP:OD1	1:E:121:THR:HG23	2.03	0.59
1:E:347:TRP:CD1	1:E:357:SER:HG	2.21	0.58
1:E:577:VAL:HA	1:E:582:ASN:O	2.03	0.58
1:G:452:MET:HE3	1:G:556:VAL:HG21	1.84	0.58
1:B:580:ARG:NH1	1:B:623:GLU:OE2	2.36	0.58
1:F:228:ARG:NH2	4:F:801:HOH:O	2.37	0.58
1:B:407:TYR:H	1:B:420:THR:CG2	2.16	0.58
1:F:147:ASP:HB3	1:F:643:GLY:HA2	1.86	0.58
1:E:61:ARG:HH11	1:E:61:ARG:HB2	1.68	0.58
1:F:407:TYR:H	1:F:420:THR:HG21	1.68	0.58
1:C:512:GLY:HA2	1:F:333:LEU:O	2.04	0.57
1:E:132:LEU:HD12	1:E:132:LEU:C	2.30	0.57
1:C:408:ALA:HB3	1:C:413:LEU:HD11	1.86	0.57
1:H:180:ILE:CD1	1:H:185:THR:HG21	2.34	0.57
1:B:83:ARG:NH2	1:B:556:VAL:O	2.35	0.57
1:G:121:THR:HB	1:G:124:ASP:OD1	2.05	0.57
1:G:459:ALA:N	1:G:460:PRO:HD2	2.20	0.57
1:F:100:ASN:HB2	2:F:701:FAD:C5X	2.35	0.56
1:E:403:VAL:HB	1:E:420:THR:HG23	1.85	0.56
1:F:106:ARG:NH2	1:F:143:THR:O	2.38	0.56
1:A:251:ARG:O	1:B:474:ARG:HD3	2.06	0.56
1:B:203:ARG:NH1	4:B:807:HOH:O	2.38	0.56
1:C:100:ASN:N	1:C:203:ARG:NH2	2.53	0.56
1:G:208:THR:HA	1:G:212:HIS:HB2	1.87	0.56
1:B:227:ALA:HB1	1:B:245:TYR:CD1	2.40	0.56
1:H:314:TYR:O	1:H:424:TYR:HA	2.05	0.56
1:H:470:GLU:OE1	1:H:474:ARG:NH2	2.37	0.56
1:F:158:ILE:HG23	1:F:362:ASP:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:MET:HE2	1:A:37:ILE:HD11	1.88	0.56
1:C:322:VAL:HG11	1:C:419:ILE:HG23	1.86	0.56
1:B:309:GLN:O	1:B:311:GLN:HG3	2.05	0.56
1:E:249:ARG:NH1	1:F:476:ASP:OD2	2.39	0.56
1:E:452:MET:HE3	1:E:556:VAL:HG21	1.88	0.56
1:C:580:ARG:HH12	1:C:623:GLU:HG3	1.72	0.55
1:A:483:THR:HG22	1:A:497:CYS:HB2	1.87	0.55
1:D:578:ASP:HB3	1:D:580:ARG:H	1.71	0.55
1:E:44:ARG:NH2	1:E:216:ASP:OD1	2.30	0.55
1:C:470:GLU:HB3	1:C:474:ARG:HH21	1.72	0.55
1:B:280:ILE:O	1:B:284:SER:OG	2.07	0.55
1:E:231:ARG:HH11	1:E:231:ARG:HG3	1.70	0.55
1:A:472:ALA:HA	1:A:475:MET:HE3	1.88	0.55
1:E:10:ILE:HD12	1:E:264:ALA:HB2	1.87	0.55
1:H:100:ASN:HB2	2:H:701:FAD:C5X	2.34	0.55
1:A:35:MET:HE1	1:A:262:VAL:HG11	1.89	0.55
1:A:10:ILE:HD11	1:A:262:VAL:HG22	1.88	0.55
1:F:399:PHE:CD1	1:F:424:TYR:CE2	2.95	0.55
1:C:596:ILE:C	1:C:596:ILE:HD12	2.32	0.55
1:D:503:GLU:OE2	1:D:503:GLU:HA	2.07	0.55
1:F:59:MET:HE3	2:F:701:FAD:HM71	1.88	0.55
1:A:514[B]:THR:HG21	1:E:408:ALA:O	2.08	0.54
1:D:315:THR:HA	1:D:423:GLN:O	2.07	0.54
1:D:409:ASP:OD1	1:D:411:THR:HB	2.07	0.54
1:E:54:ILE:O	1:E:57:ARG:HG2	2.07	0.54
1:F:159:MET:HE2	1:F:159:MET:HA	1.89	0.54
1:G:35:MET:HE2	1:G:37:ILE:HD11	1.88	0.54
1:C:347:TRP:HA	1:C:354:ALA:CB	2.37	0.54
1:C:577:VAL:HA	1:C:582:ASN:O	2.08	0.54
1:D:308:GLU:OE2	1:D:435:HIS:NE2	2.40	0.54
1:C:277:THR:HB	1:C:278:PRO:HD3	1.89	0.54
1:B:33:LYS:HD2	1:B:265:ARG:HH22	1.73	0.54
1:A:399:PHE:CD1	1:A:424:TYR:CE2	2.96	0.54
1:C:347:TRP:CD1	1:C:357:SER:HG	2.25	0.54
1:G:592:VAL:HG23	1:G:612:VAL:HG12	1.90	0.54
1:H:313:HIS:O	1:H:559:THR:HG23	2.07	0.54
1:A:227:ALA:HB1	1:A:245:TYR:CD1	2.42	0.54
1:B:409:ASP:OD1	1:B:411:THR:HB	2.08	0.54
1:H:20:VAL:HG22	1:H:210:TYR:CE2	2.43	0.54
1:E:251:ARG:HG3	1:F:535:ILE:HG13	1.90	0.54
1:E:399:PHE:CG	1:E:424:TYR:CE2	2.95	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:419:ILE:HD13	1:E:475:MET:HE1	1.90	0.54
1:A:353:LYS:HE3	1:C:202:ARG:NH1	2.22	0.54
1:E:578:ASP:HB3	1:E:580:ARG:H	1.73	0.54
1:G:411:THR:HG21	4:G:841:HOH:O	2.08	0.54
1:A:180:ILE:HG22	1:A:181:GLN:NE2	2.22	0.53
1:D:177:SER:HB3	1:D:180:ILE:CD1	2.38	0.53
1:B:391:ASP:O	1:B:392:LYS:HD2	2.08	0.53
1:B:577:VAL:HA	1:B:582:ASN:O	2.08	0.53
1:F:54:ILE:HG12	1:F:54:ILE:O	2.07	0.53
1:G:368:ARG:NH2	1:G:389:PHE:O	2.40	0.53
1:B:186:ALA:HB2	1:B:394:ASP:C	2.32	0.53
1:A:49:VAL:O	1:A:203:ARG:HD2	2.09	0.53
1:A:314:TYR:O	1:A:424:TYR:HA	2.09	0.53
1:B:314:TYR:CD2	1:B:452:MET:CE	2.92	0.53
1:A:149:PRO:HB2	1:A:209:ALA:HB1	1.91	0.53
1:C:177:SER:HB3	1:C:180:ILE:CD1	2.38	0.53
1:G:158:ILE:HG23	1:G:362:ASP:HB3	1.91	0.53
1:B:348:GLU:O	1:D:651:ARG:NH2	2.42	0.53
1:F:29:ASP:OD1	1:F:31:THR:HB	2.09	0.53
1:H:108:SER:O	1:H:109:ALA:C	2.52	0.53
1:F:20:VAL:HG11	1:F:614:GLU:N	2.24	0.53
1:E:514:THR:HA	1:E:517:ILE:HD12	1.90	0.53
1:F:180:ILE:HD11	1:F:188:GLY:HA3	1.91	0.53
1:F:356:LEU:HB2	4:F:828:HOH:O	2.09	0.53
1:H:67:LYS:HE3	4:H:826:HOH:O	2.09	0.53
1:A:112:TRP:O	1:A:115:PHE:HB2	2.08	0.53
1:C:452:MET:HE3	1:C:556:VAL:HG21	1.90	0.53
1:D:321:ARG:NH1	1:D:500:ILE:HD12	2.24	0.53
1:F:421:MET:HE1	1:F:475:MET:CE	2.39	0.53
1:C:423:GLN:OE1	1:C:464:SER:OG	2.21	0.52
1:H:580:ARG:HH22	1:H:622:GLU:CD	2.17	0.52
1:E:112:TRP:CZ2	1:E:611:LEU:HD23	2.43	0.52
1:H:249:ARG:HB3	1:H:251:ARG:HD3	1.91	0.52
1:A:228:ARG:HG2	1:A:228:ARG:HH11	1.73	0.52
1:H:106:ARG:HH12	1:H:143:THR:HG22	1.73	0.52
1:A:100:ASN:HB2	2:A:701:FAD:N5	2.24	0.52
1:D:213:SER:HB2	1:D:633:ALA:HB3	1.92	0.52
1:B:290:GLU:OE1	1:B:294:GLN:NE2	2.37	0.52
1:C:459:ALA:N	1:C:460:PRO:HD2	2.24	0.52
1:H:106:ARG:NH2	1:H:143:THR:O	2.42	0.52
1:E:180:ILE:HG13	1:E:185:THR:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:217:VAL:HG23	1:H:218:GLN:HG3	1.91	0.52
1:A:180:ILE:HG13	1:A:185:THR:HG21	1.92	0.52
1:F:128:LEU:HD22	1:F:131:ARG:CZ	2.39	0.52
1:G:532:ASP:O	1:G:533:LYS:C	2.52	0.52
1:A:177:SER:HB3	1:A:180:ILE:CD1	2.39	0.52
1:H:205:ASP:OD1	1:H:208:THR:HG23	2.09	0.52
1:H:580:ARG:HH22	1:H:622:GLU:HG3	1.75	0.52
1:C:269:VAL:CG1	1:C:592:VAL:CG1	2.88	0.52
1:A:473:ARG:NH2	1:A:536:GLU:O	2.42	0.51
1:A:577:VAL:HA	1:A:582:ASN:O	2.11	0.51
1:G:95:GLY:O	1:G:96:GLY:C	2.54	0.51
1:A:61:ARG:HD2	1:A:70:PHE:CG	2.45	0.51
1:F:9:VAL:HG22	1:F:267:MET:HB3	1.93	0.51
1:B:279:GLN:O	1:B:283:ARG:HG2	2.11	0.51
1:D:198:ARG:NH2	1:D:646:ALA:O	2.42	0.51
1:A:314:TYR:CD2	1:A:452:MET:HE1	2.46	0.51
1:B:580:ARG:HH12	1:B:623:GLU:HG3	1.76	0.51
1:F:604:ASN:HB3	2:F:701:FAD:C2	2.41	0.51
1:D:286:VAL:HG13	1:D:303:LEU:HD12	1.92	0.51
1:G:476:ASP:OD2	1:H:249:ARG:NH1	2.44	0.51
1:F:269:VAL:HG13	1:F:592:VAL:HG13	1.93	0.51
1:G:402:ILE:HD12	1:G:475:MET:HE1	1.93	0.51
1:B:69:THR:CG2	1:B:91:ASN:HB2	2.41	0.51
1:F:69:THR:HG23	1:F:91:ASN:HB2	1.93	0.51
1:F:314:TYR:CD2	1:F:452:MET:CE	2.93	0.51
1:B:27:TYR:CE1	1:B:633:ALA:HB2	2.46	0.51
1:E:180:ILE:HG23	1:E:366:LYS:HE3	1.93	0.51
1:H:44:ARG:HH22	1:H:216:ASP:CG	2.19	0.51
1:A:315:THR:HA	1:A:423:GLN:O	2.11	0.51
1:A:44:ARG:NH1	1:B:648:GLN:NE2	2.59	0.50
1:E:227:ALA:HB1	1:E:245:TYR:CD1	2.46	0.50
1:G:604:ASN:HB3	2:G:701:FAD:C2	2.42	0.50
1:D:282:GLU:OE1	1:D:435:HIS:ND1	2.38	0.50
1:F:80:LEU:O	1:F:83:ARG:HG2	2.11	0.50
1:H:347:TRP:CD1	1:H:357:SER:HG	2.29	0.50
1:H:235:ASP:OD2	1:H:239:LYS:HB3	2.11	0.50
1:B:348:GLU:HG3	1:D:350:SER:OG	2.11	0.50
1:H:110:SER:OG	1:H:395:LYS:HE2	2.12	0.50
1:E:100:ASN:O	1:E:203:ARG:NH2	2.44	0.50
1:A:48:TRP:HA	1:A:54:ILE:HD12	1.93	0.50
1:C:180:ILE:HG22	1:C:181:GLN:NE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:TYR:CD1	1:D:245:TYR:C	2.90	0.50
1:G:44:ARG:HH22	1:G:216:ASP:CG	2.19	0.50
1:E:520:GLY:HA3	1:E:522:TRP:NE1	2.27	0.50
1:G:435:HIS:O	1:G:446:PHE:N	2.45	0.50
1:C:552:VAL:O	1:C:556:VAL:HB	2.12	0.49
1:G:369:PRO:CD	1:G:397:VAL:HG21	2.42	0.49
1:C:20:VAL:HG22	1:C:210:TYR:CZ	2.47	0.49
1:B:580:ARG:HH22	1:B:622:GLU:HG3	1.77	0.49
1:C:305:GLY:HA3	1:C:574:GLY:O	2.12	0.49
1:C:347:TRP:HA	1:C:354:ALA:HB2	1.95	0.49
1:D:580:ARG:HH22	1:D:622:GLU:CG	2.25	0.49
1:B:180:ILE:CD1	1:B:185:THR:HG21	2.42	0.49
1:C:321:ARG:NH2	1:C:414:PRO:HB2	2.27	0.49
1:C:635:VAL:HG22	1:C:638:ALA:HB3	1.94	0.49
1:D:104:TYR:CZ	1:D:106:ARG:HD2	2.47	0.49
1:A:51:ARG:HB2	1:A:54:ILE:HD13	1.95	0.49
1:C:118:GLU:OE1	1:C:579:LYS:NZ	2.31	0.49
1:D:282:GLU:O	1:D:292:LEU:CD2	2.61	0.49
1:E:637:HIS:CE1	1:F:648:GLN:HG3	2.47	0.49
1:D:604:ASN:HB3	2:D:701:FAD:C2	2.42	0.49
1:F:162:ALA:O	1:F:165:PHE:HB3	2.12	0.49
1:F:315:THR:HA	1:F:423:GLN:O	2.13	0.49
1:H:564:GLY:HA2	1:H:597:CYS:O	2.13	0.49
1:A:51:ARG:NH2	4:A:801:HOH:O	2.18	0.49
1:C:20:VAL:HG22	1:C:210:TYR:CE2	2.48	0.49
1:D:10:ILE:HD12	1:D:264:ALA:HB2	1.95	0.49
1:E:466:LYS:HG2	1:E:540:TYR:CZ	2.47	0.49
1:F:398:MET:HE2	1:F:464:SER:CB	2.43	0.49
1:A:251:ARG:HG2	1:B:535:ILE:HD12	1.94	0.49
1:B:399:PHE:CG	1:B:424:TYR:CE2	3.00	0.49
1:B:644:ARG:HB2	1:B:644:ARG:HH11	1.77	0.49
1:C:208:THR:HA	1:C:212:HIS:HB2	1.94	0.49
1:F:314:TYR:O	1:F:424:TYR:HA	2.13	0.49
1:A:440:ASN:ND2	1:A:443:VAL:HG13	2.25	0.48
1:D:514:THR:HA	1:D:517:ILE:HD12	1.95	0.48
1:E:474:ARG:HD3	1:G:251:ARG:O	2.13	0.48
1:A:100:ASN:HB2	2:A:701:FAD:C4X	2.44	0.48
1:F:102:GLN:O	1:F:194:LYS:HA	2.12	0.48
1:F:532:ASP:O	1:F:533:LYS:C	2.57	0.48
1:G:557:GLU:HG3	4:G:801:HOH:O	2.12	0.48
1:C:580:ARG:NH1	1:C:623:GLU:HG3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:THR:HA	1:D:212:HIS:HB2	1.95	0.48
1:D:314:TYR:O	1:D:424:TYR:HA	2.13	0.48
1:G:449:SER:OG	1:G:451:PHE:CD1	2.67	0.48
1:A:389:PHE:O	1:A:390:LYS:C	2.55	0.48
1:G:100:ASN:O	1:G:203:ARG:NH2	2.45	0.48
1:H:35:MET:HE1	1:H:262:VAL:HG11	1.95	0.48
1:H:580:ARG:NH2	1:H:622:GLU:OE1	2.47	0.48
1:A:548:ILE:O	1:A:552:VAL:HG23	2.14	0.48
1:C:100:ASN:HB2	2:C:701:FAD:N5	2.29	0.48
1:C:476:ASP:OD1	1:D:251:ARG:NH1	2.47	0.48
1:C:561:HIS:CE1	1:C:604:ASN:HA	2.49	0.48
1:F:61:ARG:HG2	1:F:61:ARG:NH1	2.24	0.48
1:G:269:VAL:HG13	1:G:592:VAL:CG1	2.44	0.48
1:B:314:TYR:CE1	1:B:451:PHE:CD1	3.01	0.48
1:G:180:ILE:HG23	1:G:366:LYS:HD2	1.95	0.48
1:G:369:PRO:HB2	1:G:374:LEU:HD22	1.96	0.48
1:B:324:ASN:O	1:B:417:LYS:NZ	2.46	0.48
1:D:269:VAL:HG13	1:D:592:VAL:HG13	1.96	0.48
1:F:47:PRO:HG3	1:H:157:GLN:OE1	2.12	0.48
1:H:580:ARG:HH22	1:H:622:GLU:CG	2.27	0.48
1:C:519:MET:SD	1:F:557:GLU:HG2	2.53	0.48
1:D:35:MET:CE	1:D:262:VAL:HG21	2.44	0.48
1:B:557:GLU:HG2	1:G:519:MET:SD	2.54	0.47
1:D:102:GLN:HG3	1:D:203:ARG:NH2	2.29	0.47
1:E:321:ARG:HD2	1:E:499:ASP:OD1	2.14	0.47
1:F:100:ASN:HB2	2:F:701:FAD:N5	2.29	0.47
1:H:399:PHE:CD1	1:H:424:TYR:CE2	3.02	0.47
1:A:310:TYR:OH	1:A:312:ASP:OD2	2.19	0.47
1:A:314:TYR:CD2	1:A:452:MET:CE	2.97	0.47
1:G:229:VAL:HG13	1:G:243:VAL:HG13	1.96	0.47
1:G:470:GLU:HB3	1:G:474:ARG:HH21	1.78	0.47
1:H:321:ARG:HG2	1:H:321:ARG:HH11	1.79	0.47
1:H:402:ILE:HD12	1:H:475:MET:HE1	1.97	0.47
1:A:190:GLU:HB2	4:A:836:HOH:O	2.13	0.47
1:A:252:THR:O	1:A:253:HIS:C	2.57	0.47
1:E:352:GLU:OE2	1:E:651:ARG:HD2	2.15	0.47
1:H:407:TYR:H	1:H:420:THR:CG2	2.25	0.47
1:A:407:TYR:H	1:A:420:THR:CG2	2.26	0.47
1:C:314:TYR:CE1	1:C:451:PHE:CD1	3.02	0.47
1:F:177:SER:HB3	1:F:180:ILE:CD1	2.42	0.47
1:H:161:VAL:HG13	4:H:865:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ARG:NH2	1:A:143:THR:O	2.48	0.47
1:A:514[A]:THR:OG1	1:E:409:ASP:HA	2.14	0.47
1:A:35:MET:CE	1:A:37:ILE:HD11	2.44	0.47
1:B:269:VAL:CG1	1:B:592:VAL:HG13	2.42	0.47
1:C:186:ALA:HB2	1:C:394:ASP:C	2.40	0.47
1:E:83:ARG:NH1	1:E:553:ALA:O	2.48	0.47
1:F:217:VAL:HA	1:H:645:PRO:HB2	1.96	0.47
1:F:361:ILE:HG12	1:F:403:VAL:HG22	1.96	0.47
1:H:532:ASP:O	1:H:533:LYS:C	2.56	0.47
1:B:230:SER:O	1:B:283:ARG:HD2	2.15	0.47
1:H:16:PRO:O	1:H:20:VAL:HG23	2.15	0.47
1:A:72:THR:O	1:A:73:ASP:C	2.56	0.47
1:B:8:ASP:OD1	1:B:265:ARG:NH1	2.47	0.47
1:A:163:GLN:HE22	1:C:42:ASN:HB3	1.80	0.47
1:E:466:LYS:HG2	1:E:540:TYR:CE1	2.50	0.47
1:G:314:TYR:CD2	1:G:452:MET:HE2	2.50	0.47
1:H:20:VAL:HG22	1:H:210:TYR:CZ	2.50	0.47
1:H:168:ALA:O	1:H:171:ALA:HB3	2.15	0.47
1:A:500:ILE:HD11	1:A:504:THR:HG22	1.96	0.46
1:C:205:ASP:OD2	1:C:208:THR:HG23	2.15	0.46
1:C:414:PRO:HA	1:F:413:LEU:O	2.15	0.46
1:D:100:ASN:HB2	2:D:701:FAD:C5X	2.44	0.46
1:E:621:ALA:O	1:E:626:LEU:N	2.39	0.46
1:H:449:SER:HB3	1:H:451:PHE:CD1	2.50	0.46
1:G:80:LEU:O	1:G:83:ARG:HG2	2.16	0.46
1:G:564:GLY:HA2	1:G:597:CYS:O	2.15	0.46
1:H:578:ASP:HB3	1:H:580:ARG:H	1.80	0.46
1:B:414:PRO:HG2	1:B:482:LEU:HD11	1.95	0.46
1:C:369:PRO:CD	1:C:397:VAL:HG21	2.45	0.46
1:D:479:ARG:NH2	4:D:803:HOH:O	2.30	0.46
1:C:54:ILE:O	1:C:57:ARG:CG	2.63	0.46
1:D:580:ARG:HH12	1:D:623:GLU:HG3	1.80	0.46
1:G:35:MET:HE1	1:G:262:VAL:HG11	1.97	0.46
1:G:130:LYS:O	1:G:145:GLY:HA3	2.16	0.46
1:A:11:VAL:HG21	1:A:22:ALA:HB2	1.97	0.46
1:D:203:ARG:NH1	4:D:808:HOH:O	2.48	0.46
1:E:205:ASP:CG	1:E:208:THR:HG23	2.41	0.46
1:F:35:MET:HE1	1:F:262:VAL:HG11	1.98	0.46
1:H:269:VAL:CG1	1:H:592:VAL:CG1	2.94	0.46
1:C:100:ASN:HB2	2:C:701:FAD:C5X	2.45	0.46
1:G:112:TRP:O	1:G:115:PHE:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:187:HIS:HA	1:H:366:LYS:O	2.15	0.46
1:C:321:ARG:NH2	1:F:411:THR:O	2.48	0.46
1:G:369:PRO:HD3	1:G:397:VAL:HG21	1.98	0.46
1:G:370:THR:HG22	1:G:372:GLU:H	1.81	0.46
1:A:48:TRP:HA	1:A:54:ILE:CD1	2.46	0.46
1:A:410:HIS:HA	1:A:413:LEU:HD12	1.97	0.46
1:D:100:ASN:HB2	2:D:701:FAD:N5	2.30	0.46
1:D:410:HIS:H	1:H:514:THR:HG23	1.81	0.46
1:F:9:VAL:O	1:F:34:VAL:HA	2.16	0.46
1:G:269:VAL:HG13	1:G:592:VAL:HG12	1.98	0.46
1:H:326:SER:O	1:H:417:LYS:HE2	2.15	0.46
1:B:274:THR:OG1	1:B:563:LEU:HA	2.16	0.46
1:C:314:TYR:CD2	1:C:452:MET:CE	2.99	0.46
1:D:459:ALA:N	1:D:460:PRO:HD2	2.32	0.46
1:D:557:GLU:HG2	1:H:519:MET:SD	2.55	0.46
1:B:101:SER:HB2	2:B:701:FAD:O4	2.16	0.45
1:B:399:PHE:CD1	1:B:424:TYR:CD2	3.04	0.45
1:C:14:GLY:HA2	1:C:36:LEU:HD11	1.97	0.45
1:D:314:TYR:CE1	1:D:451:PHE:CD1	3.04	0.45
1:E:548:ILE:O	1:E:552:VAL:HG23	2.15	0.45
1:E:552:VAL:O	1:E:556:VAL:HB	2.15	0.45
1:F:409:ASP:OD1	1:F:411:THR:HB	2.16	0.45
1:D:282:GLU:O	1:D:292:LEU:HD21	2.16	0.45
1:D:399:PHE:CD1	1:D:424:TYR:CD2	3.05	0.45
1:D:399:PHE:CD1	1:D:424:TYR:CE2	3.05	0.45
1:F:216:ASP:HB2	1:H:647:THR:HG22	1.98	0.45
1:G:180:ILE:HG22	1:G:181:GLN:NE2	2.31	0.45
1:A:278:PRO:HB2	4:A:844:HOH:O	2.16	0.45
1:B:33:LYS:HD2	1:B:265:ARG:NH2	2.32	0.45
1:B:35:MET:HE2	1:B:262:VAL:HG11	1.97	0.45
1:C:112:TRP:CZ2	1:C:611:LEU:HD23	2.51	0.45
1:C:269:VAL:HG13	1:C:592:VAL:HG12	1.99	0.45
1:H:235:ASP:HB3	1:H:237:ASN:H	1.82	0.45
1:B:102:GLN:O	1:B:194:LYS:HA	2.17	0.45
1:D:566:CYS:O	1:D:596:ILE:HA	2.16	0.45
1:G:599:ASP:OD1	1:G:600:ASN:N	2.39	0.45
1:H:112:TRP:O	1:H:115:PHE:HB2	2.16	0.45
1:H:506:LYS:HA	1:H:515:VAL:HG11	1.98	0.45
1:A:40:GLY:HA3	1:A:92:ILE:HA	1.98	0.45
1:A:505:ALA:HB1	1:E:411:THR:HG21	1.97	0.45
1:C:72:THR:O	1:C:73:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:SER:HB2	2:E:701:FAD:O4	2.17	0.45
1:G:286:VAL:HG13	1:G:301:SER:HB3	1.99	0.45
1:H:604:ASN:HB3	2:H:701:FAD:C2	2.46	0.45
1:A:101:SER:O	1:A:359:ASN:ND2	2.40	0.45
1:D:580:ARG:NH1	1:D:623:GLU:HG3	2.32	0.45
1:E:348:GLU:HG3	1:F:350:SER:OG	2.17	0.45
1:E:354:ALA:HB1	4:E:808:HOH:O	2.17	0.45
1:E:370:THR:HG22	1:E:372:GLU:N	2.31	0.45
1:C:80:LEU:O	1:C:83:ARG:HG2	2.17	0.45
1:C:182:ASP:O	1:C:183:LEU:HB2	2.17	0.45
1:E:446:PHE:CD1	1:E:446:PHE:C	2.95	0.45
1:F:69:THR:CG2	1:F:91:ASN:HB2	2.47	0.45
1:B:569:LYS:HB2	1:B:570:PRO:CD	2.47	0.45
1:C:405:GLY:O	1:C:420:THR:HG22	2.17	0.45
1:C:473:ARG:NH2	1:C:536:GLU:O	2.50	0.45
1:C:513:LEU:HD13	1:F:57:ARG:HB3	1.99	0.45
1:F:136:GLN:O	1:F:198:ARG:NH1	2.50	0.45
1:C:137:LYS:HB2	1:C:138:PRO:HD2	1.98	0.44
1:E:473:ARG:HD3	4:E:813:HOH:O	2.17	0.44
1:F:314:TYR:CD2	1:F:452:MET:HE3	2.53	0.44
1:F:313:HIS:CD2	1:F:426:GLU:O	2.70	0.44
1:H:43:ASN:ND2	1:H:98:SER:OG	2.42	0.44
1:B:208:THR:HA	1:B:212:HIS:HB2	1.98	0.44
1:C:35:MET:HE2	1:C:37:ILE:HD11	1.98	0.44
1:D:102:GLN:O	1:D:194:LYS:HA	2.18	0.44
1:E:135:TYR:CZ	1:E:144:HIS:CD2	3.05	0.44
1:E:165:PHE:CZ	1:E:364:GLY:HA2	2.53	0.44
1:H:243:VAL:HG12	1:H:262:VAL:HG13	2.00	0.44
1:D:391:ASP:O	1:D:392:LYS:HD2	2.17	0.44
1:A:578:ASP:HB3	1:A:580:ARG:H	1.83	0.44
1:D:55:TYR:CD2	1:D:101:SER:HA	2.53	0.44
1:D:408:ALA:O	1:H:514:THR:OG1	2.36	0.44
1:E:604:ASN:HB3	2:E:701:FAD:C2	2.48	0.44
1:G:9:VAL:HB	1:G:34:VAL:HB	2.00	0.44
1:A:43:ASN:ND2	1:A:98:SER:OG	2.42	0.44
1:B:12:CYS:SG	1:B:243:VAL:HG21	2.58	0.44
1:B:557:GLU:CG	1:G:519:MET:SD	3.06	0.44
1:F:102:GLN:CG	1:F:203:ARG:HH21	2.30	0.44
1:C:147:ASP:HA	1:C:641:PRO:HB2	2.00	0.44
1:F:87:VAL:HG22	1:F:558:THR:HB	1.99	0.44
1:B:180:ILE:HD12	1:B:185:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:ASP:HB2	1:D:239:LYS:HB3	1.99	0.44
1:F:314:TYR:HD2	1:F:452:MET:CE	2.31	0.44
1:G:411:THR:CG2	4:G:841:HOH:O	2.66	0.44
1:G:580:ARG:O	1:G:590:LYS:NZ	2.49	0.44
1:C:470:GLU:CB	1:C:474:ARG:HH21	2.29	0.44
1:F:251:ARG:HG2	1:H:535:ILE:HD12	1.99	0.44
1:H:459:ALA:N	1:H:460:PRO:HD2	2.33	0.44
1:A:54:ILE:O	1:A:57:ARG:HG2	2.18	0.43
1:A:352:GLU:HG2	1:A:353:LYS:HG2	2.00	0.43
1:C:34:VAL:HG22	1:C:221:LEU:CD1	2.48	0.43
1:C:513:LEU:CD2	1:C:513:LEU:N	2.82	0.43
1:D:147:ASP:HB3	1:D:643:GLY:HA2	1.98	0.43
1:D:165:PHE:CD1	1:D:165:PHE:C	2.96	0.43
1:F:120:TRP:CZ2	1:F:581:LEU:HD21	2.52	0.43
1:F:405:GLY:O	1:F:420:THR:HG22	2.18	0.43
1:G:462:ARG:NH1	1:G:549:ASP:OD1	2.51	0.43
1:H:97:SER:HB2	1:H:606:TYR:CZ	2.53	0.43
1:D:102:GLN:CG	1:D:203:ARG:NH2	2.82	0.43
1:E:321:ARG:HD3	1:E:500:ILE:HB	1.99	0.43
1:E:466:LYS:O	1:E:470:GLU:HG2	2.18	0.43
1:F:114:ASP:O	1:F:116:LYS:HG2	2.18	0.43
1:G:102:GLN:O	1:G:194:LYS:HA	2.19	0.43
1:A:514[A]:THR:HG21	1:E:410:HIS:HB2	2.00	0.43
1:C:147:ASP:HB3	1:C:643:GLY:HA2	2.01	0.43
1:D:158:ILE:HG23	1:D:362:ASP:HB3	2.00	0.43
1:F:421:MET:HE1	1:F:475:MET:HE3	2.00	0.43
1:F:478:PHE:CZ	1:F:480:GLY:HA2	2.53	0.43
1:G:399:PHE:CD1	1:G:424:TYR:CD2	3.06	0.43
1:A:73:ASP:O	1:A:84:ARG:HD2	2.18	0.43
1:B:315:THR:HA	1:B:423:GLN:O	2.19	0.43
1:D:112:TRP:O	1:D:115:PHE:HB2	2.18	0.43
1:D:314:TYR:CD2	1:D:452:MET:HE2	2.53	0.43
1:H:569:LYS:O	1:H:575:GLY:HA3	2.17	0.43
1:D:403:VAL:HB	1:D:420:THR:HG23	2.00	0.43
1:D:438:SER:HB3	1:D:443:VAL:HG21	1.99	0.43
1:E:235:ASP:HB3	1:E:237:ASN:H	1.84	0.43
1:F:73:ASP:O	1:F:84:ARG:HD2	2.18	0.43
1:F:107:ALA:HB2	1:F:603:THR:HG21	1.99	0.43
1:F:251:ARG:NH1	1:H:476:ASP:OD1	2.50	0.43
1:G:103:MET:O	1:G:195:TYR:HE2	2.02	0.43
1:G:315:THR:HA	1:G:423:GLN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:440:ASN:ND2	1:G:442:TYR:H	2.16	0.43
1:H:514:THR:HA	1:H:517:ILE:HD12	2.01	0.43
1:B:126:LEU:N	1:B:127:PRO:CD	2.82	0.43
1:C:279:GLN:O	1:C:283:ARG:HG2	2.18	0.43
1:D:205:ASP:OD2	1:D:208:THR:CG2	2.66	0.43
1:F:126:LEU:N	1:F:127:PRO:CD	2.81	0.43
1:G:43:ASN:ND2	1:G:98:SER:OG	2.50	0.43
1:H:313:HIS:C	1:H:559:THR:HG23	2.43	0.43
1:H:406:ALA:HA	1:H:420:THR:HG22	2.01	0.43
1:A:69:THR:CG2	1:A:91:ASN:HB2	2.49	0.43
1:A:476:ASP:OD1	1:C:251:ARG:NH1	2.52	0.43
1:D:411:THR:HG21	1:H:505:ALA:CB	2.49	0.43
1:E:69:THR:CG2	1:E:91:ASN:HB2	2.49	0.43
1:G:647:THR:HG22	1:H:216:ASP:OD2	2.18	0.43
1:H:106:ARG:NH1	1:H:181:GLN:O	2.52	0.43
1:A:350:SER:OG	1:C:348:GLU:HG3	2.19	0.43
1:B:100:ASN:HB2	2:B:701:FAD:C4X	2.48	0.43
1:B:244:ALA:HA	1:B:260:THR:O	2.18	0.43
1:C:115:PHE:CZ	1:C:598:PRO:HD2	2.54	0.43
1:C:205:ASP:CG	1:C:208:THR:HG23	2.44	0.43
1:C:470:GLU:HB3	1:C:474:ARG:NH2	2.33	0.43
1:C:473:ARG:HD2	4:C:836:HOH:O	2.18	0.43
1:D:465:TYR:OH	1:D:486:HIS:ND1	2.43	0.43
1:F:269:VAL:CG1	1:F:592:VAL:HG13	2.49	0.43
1:G:49:VAL:O	1:G:203:ARG:HD2	2.19	0.43
1:G:312:ASP:O	1:G:428:PRO:HG2	2.19	0.43
1:H:112:TRP:CZ2	1:H:611:LEU:HD23	2.53	0.43
1:B:205:ASP:OD2	1:B:208:THR:HG23	2.19	0.43
1:B:481:GLU:O	1:B:499:ASP:HA	2.18	0.43
1:D:130:LYS:O	1:D:145:GLY:HA3	2.19	0.43
1:D:277:THR:HB	1:D:278:PRO:HD3	1.99	0.43
1:D:321:ARG:NH2	1:H:411:THR:O	2.50	0.43
1:E:69:THR:HG22	1:E:91:ASN:HB2	2.01	0.43
1:E:566:CYS:HA	1:E:576:VAL:HG21	2.01	0.43
1:H:335:GLY:HA2	1:H:340:GLN:NE2	2.34	0.43
1:A:277:THR:N	1:A:278:PRO:CD	2.81	0.43
1:D:411:THR:HG22	1:D:412:LEU:CD2	2.49	0.43
1:D:430:SER:OG	1:D:450:GLY:O	2.37	0.43
1:E:205:ASP:OD2	1:E:207:ALA:HB3	2.19	0.43
1:F:322:VAL:HA	1:F:477:ALA:O	2.19	0.43
1:D:337:LYS:H	1:D:337:LYS:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:596:ILE:HD12	1:D:596:ILE:C	2.43	0.42
1:E:147:ASP:HB3	1:E:643:GLY:HA2	2.00	0.42
1:E:593:ASP:O	1:E:596:ILE:HG13	2.19	0.42
1:E:593:ASP:O	1:E:612:VAL:HG11	2.18	0.42
1:G:578:ASP:HB2	1:G:582:ASN:HB2	2.01	0.42
1:H:231:ARG:NH2	1:H:259:GLU:OE1	2.49	0.42
1:C:580:ARG:NH1	1:C:623:GLU:CG	2.82	0.42
1:D:283:ARG:HA	1:D:297:ILE:HD13	2.01	0.42
1:D:383:GLU:OE2	1:D:387:ARG:HD3	2.20	0.42
1:F:128:LEU:HD22	1:F:131:ARG:NH2	2.35	0.42
1:G:55:TYR:CD2	1:G:101:SER:HA	2.54	0.42
1:H:100:ASN:N	1:H:203:ARG:NH2	2.66	0.42
1:A:440:ASN:HD21	1:A:442:TYR:HB2	1.83	0.42
1:C:403:VAL:HB	1:C:420:THR:CG2	2.48	0.42
1:D:314:TYR:CE2	1:D:428:PRO:HB3	2.53	0.42
1:E:449:SER:HB3	1:E:451:PHE:CD1	2.54	0.42
1:G:399:PHE:CD2	1:G:424:TYR:CE2	3.08	0.42
1:B:100:ASN:HB2	2:B:701:FAD:N5	2.35	0.42
1:F:20:VAL:HG11	1:F:613:GLY:C	2.44	0.42
1:H:194:LYS:CB	1:H:196:ILE:HD12	2.49	0.42
1:H:315:THR:HA	1:H:423:GLN:O	2.20	0.42
1:B:515:VAL:O	1:G:60:GLN:NE2	2.48	0.42
1:E:134:ASN:HB2	1:E:148:GLY:O	2.19	0.42
1:G:449:SER:OG	1:G:451:PHE:CG	2.72	0.42
1:C:513:LEU:HD13	1:F:57:ARG:HG2	2.00	0.42
1:C:650:VAL:O	1:C:651:ARG:C	2.63	0.42
1:E:217:VAL:HA	1:F:645:PRO:HB2	2.02	0.42
1:G:80:LEU:O	1:G:81:ARG:C	2.63	0.42
1:A:287:GLY:O	1:A:288:ASN:C	2.63	0.42
1:C:500:ILE:HG12	1:C:501:ASP:O	2.20	0.42
1:D:69:THR:O	1:D:88:PRO:HA	2.20	0.42
1:D:277:THR:N	1:D:278:PRO:CD	2.82	0.42
1:D:431:ARG:HG2	1:D:431:ARG:HH11	1.85	0.42
1:G:44:ARG:O	1:G:45:ASP:C	2.62	0.42
1:H:115:PHE:CZ	1:H:598:PRO:HD2	2.54	0.42
1:A:158:ILE:HG23	1:A:362:ASP:HB3	2.01	0.42
1:A:269:VAL:HG13	1:A:592:VAL:CG1	2.49	0.42
1:B:161:VAL:HG13	4:B:860:HOH:O	2.18	0.42
1:C:314:TYR:CD2	1:C:452:MET:HE2	2.55	0.42
1:H:313:HIS:HE1	1:H:603:THR:O	2.02	0.42
1:A:349:VAL:HG22	1:B:349:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514[B]:THR:CG2	1:E:408:ALA:O	2.68	0.42
1:B:470:GLU:HB3	1:B:474:ARG:HH21	1.84	0.42
1:D:519:MET:SD	1:H:557:GLU:HG2	2.60	0.42
1:E:431:ARG:O	1:E:450:GLY:HA3	2.19	0.42
1:F:305:GLY:HA3	1:F:574:GLY:O	2.19	0.42
1:G:104:TYR:HA	1:G:195:TYR:CE2	2.54	0.42
1:G:130:LYS:HE2	1:G:142:ASP:O	2.19	0.42
1:G:428:PRO:HD2	1:G:600:ASN:ND2	2.35	0.42
1:A:163:GLN:NE2	1:C:42:ASN:HB3	2.35	0.42
1:A:228:ARG:NH1	1:A:228:ARG:HG2	2.34	0.42
1:A:425:LEU:HD23	1:A:428:PRO:HB3	2.02	0.42
1:B:81:ARG:HD3	1:B:554:ASP:OD1	2.19	0.42
1:D:57:ARG:HA	1:H:513:LEU:O	2.20	0.42
1:D:205:ASP:CG	1:D:208:THR:HG23	2.45	0.42
1:E:406:ALA:HB2	1:E:418:TYR:HB2	2.02	0.42
1:G:10:ILE:HD12	1:G:264:ALA:HB2	2.02	0.42
1:G:69:THR:CG2	1:G:91:ASN:HB2	2.49	0.42
1:G:421:MET:HE1	1:G:475:MET:CE	2.50	0.42
1:H:636:PRO:O	1:H:637:HIS:HB2	2.19	0.42
1:A:624:LEU:HB2	1:A:626:LEU:HD22	2.01	0.41
1:B:112:TRP:CZ2	1:B:611:LEU:HD23	2.55	0.41
1:B:411:THR:HG21	1:G:505:ALA:CB	2.49	0.41
1:B:566:CYS:HA	1:B:576:VAL:HG21	2.02	0.41
1:D:269:VAL:CG1	1:D:592:VAL:HG13	2.50	0.41
1:G:44:ARG:NH2	1:G:216:ASP:OD1	2.47	0.41
1:G:69:THR:HG23	1:G:91:ASN:HB2	2.02	0.41
1:A:44:ARG:HH22	1:A:216:ASP:CG	2.28	0.41
1:G:80:LEU:O	1:G:82:GLY:N	2.53	0.41
1:G:177:SER:HB3	1:G:180:ILE:CD1	2.50	0.41
1:G:470:GLU:OE1	1:G:474:ARG:NH2	2.53	0.41
1:H:208:THR:HA	1:H:212:HIS:HB2	2.02	0.41
1:C:54:ILE:O	1:C:57:ARG:HG2	2.20	0.41
1:C:166:LEU:HD12	1:C:166:LEU:HA	1.88	0.41
1:C:335:GLY:HA2	1:C:340:GLN:NE2	2.35	0.41
1:C:592:VAL:O	1:C:593:ASP:HB3	2.20	0.41
1:D:374:LEU:HD13	1:D:374:LEU:HA	1.92	0.41
1:H:313:HIS:O	1:H:559:THR:CG2	2.68	0.41
1:A:81:ARG:HD3	1:A:554:ASP:OD1	2.20	0.41
1:A:409:ASP:HA	1:E:514:THR:HB	2.02	0.41
1:B:57:ARG:HB3	1:G:513:LEU:HB3	2.01	0.41
1:C:177:SER:HB3	1:C:180:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:LEU:HD21	1:D:584:TYR:HB2	2.02	0.41
1:H:321:ARG:HH11	1:H:321:ARG:CG	2.33	0.41
1:A:43:ASN:HB2	1:A:49:VAL:HG21	2.03	0.41
1:C:352:GLU:HG2	1:C:353:LYS:HG3	2.03	0.41
1:E:459:ALA:N	1:E:460:PRO:HD2	2.36	0.41
1:F:398:MET:HE2	1:F:464:SER:HB2	2.02	0.41
1:G:513:LEU:N	1:G:513:LEU:CD2	2.83	0.41
1:H:473:ARG:NH2	1:H:536:GLU:O	2.53	0.41
1:H:593:ASP:OD1	1:H:593:ASP:C	2.63	0.41
1:B:159:MET:SD	1:B:327:ILE:HG22	2.60	0.41
1:B:348:GLU:CG	1:D:350:SER:OG	2.69	0.41
1:D:197:ASN:HB3	1:D:200:THR:OG1	2.20	0.41
1:D:561:HIS:O	4:D:802:HOH:O	2.22	0.41
1:E:83:ARG:NH2	1:E:556:VAL:O	2.34	0.41
1:F:12:CYS:SG	1:F:243:VAL:HG21	2.61	0.41
1:F:162:ALA:HB2	1:F:362:ASP:HB2	2.03	0.41
1:H:115:PHE:CE1	1:H:598:PRO:HD2	2.56	0.41
1:H:399:PHE:CD1	1:H:399:PHE:C	2.97	0.41
1:A:177:SER:HB3	1:A:180:ILE:HD13	2.02	0.41
1:A:513:LEU:HD23	1:A:513:LEU:N	2.36	0.41
1:B:520:GLY:HA3	1:B:522:TRP:NE1	2.35	0.41
1:C:369:PRO:HD2	1:C:397:VAL:HG21	2.03	0.41
1:D:20:VAL:HG11	1:D:614:GLU:N	2.35	0.41
1:F:438:SER:HB3	1:F:443:VAL:HG21	2.02	0.41
1:G:289:GLY:HA3	1:G:302:ASP:OD2	2.20	0.41
1:H:91:ASN:O	1:H:91:ASN:CG	2.63	0.41
2:B:701:FAD:O2A	2:B:701:FAD:O4'	2.34	0.41
1:C:34:VAL:HG22	1:C:221:LEU:HD13	2.02	0.41
1:D:466:LYS:O	1:D:470:GLU:HG2	2.20	0.41
1:E:308:GLU:O	1:E:565:THR:HA	2.21	0.41
1:F:449:SER:HB3	1:F:451:PHE:CD1	2.56	0.41
1:G:269:VAL:CG1	1:G:592:VAL:CG1	2.99	0.41
1:G:356:LEU:C	1:G:358:SER:H	2.28	0.41
1:A:282:GLU:O	1:A:292:LEU:CD2	2.69	0.41
1:C:106:ARG:NH2	1:C:143:THR:O	2.46	0.41
1:E:10:ILE:HD11	1:E:262:VAL:HG22	2.03	0.41
1:E:253:HIS:ND1	1:F:536:GLU:HA	2.35	0.41
1:E:569:LYS:HB2	1:E:570:PRO:HD2	2.01	0.41
1:G:184:THR:O	1:G:184:THR:HG22	2.20	0.41
1:G:459:ALA:N	1:G:460:PRO:CD	2.82	0.41
1:H:16:PRO:HA	1:H:206:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:208:THR:O	1:H:636:PRO:HD2	2.20	0.41
1:H:389:PHE:O	1:H:390:LYS:C	2.63	0.41
1:A:142:ASP:OD1	1:A:142:ASP:C	2.64	0.41
1:B:121:THR:HG22	1:B:123:LYS:H	1.86	0.41
1:B:121:THR:HG22	1:B:123:LYS:N	2.36	0.41
1:B:406:ALA:HA	1:B:420:THR:HG22	2.03	0.41
1:H:52:PRO:HB3	1:H:102:GLN:OE1	2.21	0.41
1:H:500:ILE:HD11	1:H:504:THR:HG22	2.03	0.41
1:A:10:ILE:HD12	1:A:264:ALA:HB2	2.03	0.40
1:A:186:ALA:HB2	1:A:394:ASP:C	2.46	0.40
1:D:513:LEU:O	1:H:57:ARG:HA	2.22	0.40
1:F:399:PHE:CD1	1:F:399:PHE:C	2.99	0.40
1:F:577:VAL:HA	1:F:582:ASN:O	2.21	0.40
1:H:186:ALA:HB2	1:H:394:ASP:C	2.46	0.40
1:C:134:ASN:HB3	1:C:151:ALA:HA	2.02	0.40
1:F:137:LYS:HB2	1:F:138:PRO:HD2	2.03	0.40
1:G:403:VAL:CG2	1:G:420:THR:HG23	2.50	0.40
1:H:134:ASN:HB2	1:H:148:GLY:O	2.22	0.40
1:H:314:TYR:CE2	1:H:428:PRO:HB3	2.56	0.40
1:A:321:ARG:HG2	1:A:418:TYR:CE1	2.56	0.40
1:A:593:ASP:OD1	1:A:593:ASP:C	2.63	0.40
1:C:269:VAL:CG1	1:C:592:VAL:HG12	2.52	0.40
1:G:186:ALA:HB2	1:G:394:ASP:C	2.46	0.40
1:G:378:GLY:O	1:G:382:ASN:ND2	2.40	0.40
1:E:55:TYR:O	1:E:56:VAL:C	2.65	0.40
1:E:315:THR:HA	1:E:423:GLN:O	2.22	0.40
1:F:618:ASP:O	1:F:622:GLU:HG2	2.21	0.40
1:G:405:GLY:O	1:G:420:THR:HG22	2.22	0.40
1:G:474:ARG:HD3	1:H:251:ARG:O	2.21	0.40
1:C:245:TYR:O	1:C:259:GLU:HA	2.21	0.40
1:D:407:TYR:H	1:D:420:THR:CG2	2.30	0.40
1:D:470:GLU:OE1	1:D:474:ARG:NH2	2.54	0.40
1:E:106:ARG:HB2	1:E:181:GLN:HB3	2.03	0.40
1:F:313:HIS:NE2	1:F:426:GLU:O	2.54	0.40
1:G:336:VAL:O	1:G:337:LYS:C	2.65	0.40
1:H:106:ARG:HH12	1:H:143:THR:CG2	2.34	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	648/651 (100%)	607 (94%)	36 (6%)	5 (1%)	16	31
1	B	645/651 (99%)	604 (94%)	40 (6%)	1 (0%)	43	63
1	C	646/651 (99%)	605 (94%)	38 (6%)	3 (0%)	24	43
1	D	647/651 (99%)	617 (95%)	29 (4%)	1 (0%)	43	63
1	E	646/651 (99%)	614 (95%)	29 (4%)	3 (0%)	24	43
1	F	648/651 (100%)	607 (94%)	39 (6%)	2 (0%)	36	55
1	G	646/651 (99%)	608 (94%)	35 (5%)	3 (0%)	24	43
1	H	646/651 (99%)	599 (93%)	45 (7%)	2 (0%)	36	55
All	All	5172/5208 (99%)	4861 (94%)	291 (6%)	20 (0%)	30	49

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	578	ASP
1	G	81	ARG
1	A	253	HIS
1	C	593	ASP
1	D	578	ASP
1	E	578	ASP
1	A	593	ASP
1	G	96	GLY
1	A	449	SER
1	B	198	ARG
1	F	533	LYS
1	F	578	ASP
1	G	323	SER
1	H	235	ASP
1	A	306	VAL
1	C	235	ASP
1	C	558	THR

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Mol	Chain	Res	Type
1	E	414	PRO
1	E	92	ILE
1	H	21	VAL

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	548/548 (100%)	496 (90%)	52 (10%)	8	17
1	B	545/548 (100%)	490 (90%)	55 (10%)	7	15
1	C	546/548 (100%)	505 (92%)	41 (8%)	12	26
1	D	547/548 (100%)	498 (91%)	49 (9%)	9	19
1	E	546/548 (100%)	500 (92%)	46 (8%)	10	22
1	F	547/548 (100%)	491 (90%)	56 (10%)	7	15
1	G	546/548 (100%)	493 (90%)	53 (10%)	8	17
1	H	546/548 (100%)	496 (91%)	50 (9%)	8	19
All	All	4371/4384 (100%)	3969 (91%)	402 (9%)	8	19

All (402) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	34	VAL
1	A	54	ILE
1	A	61	ARG
1	A	69	THR
1	A	83	ARG
1	A	106	ARG
1	A	126	LEU
1	A	166	LEU
1	A	180	ILE
1	A	203	ARG
1	A	243	VAL

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Mol	Chain	Res	Type
1	A	251	ARG
1	A	256	LYS
1	A	262	VAL
1	A	275	LEU
1	A	321	ARG
1	A	333	LEU
1	A	338	ASP
1	A	341	ARG
1	A	348	GLU
1	A	350	SER
1	A	353	LYS
1	A	365	PHE
1	A	370	THR
1	A	371	GLU
1	A	374	LEU
1	A	380	GLU
1	A	390	LYS
1	A	399	PHE
1	A	411	THR
1	A	412	LEU
1	A	417	LYS
1	A	420	THR
1	A	444	GLU
1	A	513	LEU
1	A	514[A]	THR
1	A	514[B]	THR
1	A	542	GLU
1	A	557	GLU
1	A	578	ASP
1	A	587	GLN
1	A	592	VAL
1	A	596	ILE
1	A	600	ASN
1	A	608	SER
1	A	626	LEU
1	A	629	LYS
1	A	635	VAL
1	A	644	ARG
1	A	647	THR
1	A	651	ARG
1	B	5	GLU
1	B	34	VAL

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Mol	Chain	Res	Type
1	B	44	ARG
1	B	54	ILE
1	B	69	THR
1	B	116	LYS
1	B	126	LEU
1	B	166	LEU
1	B	180	ILE
1	B	184	THR
1	B	203	ARG
1	B	205	ASP
1	B	224	ARG
1	B	241	VAL
1	B	243	VAL
1	B	248	SER
1	B	251	ARG
1	B	262	VAL
1	B	275	LEU
1	B	291	LEU
1	B	295	LEU
1	B	325	GLU
1	B	333	LEU
1	B	337	LYS
1	B	339	VAL
1	B	345	THR
1	B	348	GLU
1	B	350	SER
1	B	353	LYS
1	B	372	GLU
1	B	374	LEU
1	B	380	GLU
1	B	391	ASP
1	B	399	PHE
1	B	411	THR
1	B	417	LYS
1	B	420	THR
1	B	437	LYS
1	B	443	VAL
1	B	455	LYS
1	B	524	GLN
1	B	527	GLU
1	B	534	VAL
1	B	542	GLU

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Mol	Chain	Res	Type
1	B	557	GLU
1	B	559	THR
1	B	572	GLU
1	B	587	GLN
1	B	592	VAL
1	B	608	SER
1	B	626	LEU
1	B	635	VAL
1	B	640	VAL
1	B	644	ARG
1	B	650	VAL
1	C	34	VAL
1	C	44	ARG
1	C	54	ILE
1	C	121	THR
1	C	126	LEU
1	C	166	LEU
1	C	180	ILE
1	C	208	THR
1	C	213	SER
1	C	241	VAL
1	C	243	VAL
1	C	251	ARG
1	C	256	LYS
1	C	260	THR
1	C	261	ILE
1	C	262	VAL
1	C	291	LEU
1	C	295	LEU
1	C	325	GLU
1	C	333	LEU
1	C	343	LEU
1	C	348	GLU
1	C	365	PHE
1	C	374	LEU
1	C	380	GLU
1	C	411	THR
1	C	412	LEU
1	C	443	VAL
1	C	513	LEU
1	C	527	GLU
1	C	551	TRP

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Mol	Chain	Res	Type
1	C	587	GLN
1	C	592	VAL
1	C	618	ASP
1	C	626	LEU
1	C	627	LYS
1	C	635	VAL
1	C	640	VAL
1	C	642	THR
1	C	650	VAL
1	C	651	ARG
1	D	31	THR
1	D	34	VAL
1	D	44	ARG
1	D	54	ILE
1	D	61	ARG
1	D	75	MET
1	D	106	ARG
1	D	126	LEU
1	D	166	LEU
1	D	180	ILE
1	D	184	THR
1	D	203	ARG
1	D	208	THR
1	D	213	SER
1	D	241	VAL
1	D	243	VAL
1	D	248	SER
1	D	249	ARG
1	D	251	ARG
1	D	262	VAL
1	D	263	LYS
1	D	275	LEU
1	D	295	LEU
1	D	298	LYS
1	D	325	GLU
1	D	333	LEU
1	D	337	LYS
1	D	338	ASP
1	D	348	GLU
1	D	353	LYS
1	D	361	ILE
1	D	365	PHE

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Mol	Chain	Res	Type
1	D	371	GLU
1	D	374	LEU
1	D	380	GLU
1	D	387	ARG
1	D	399	PHE
1	D	411	THR
1	D	417	LYS
1	D	420	THR
1	D	443	VAL
1	D	449	SER
1	D	474	ARG
1	D	592	VAL
1	D	626	LEU
1	D	635	VAL
1	D	644	ARG
1	D	650	VAL
1	D	651	ARG
1	E	5	GLU
1	E	34	VAL
1	E	44	ARG
1	E	54	ILE
1	E	61	ARG
1	E	69	THR
1	E	75	MET
1	E	106	ARG
1	E	126	LEU
1	E	147	ASP
1	E	166	LEU
1	E	180	ILE
1	E	208	THR
1	E	228	ARG
1	E	233	LEU
1	E	243	VAL
1	E	251	ARG
1	E	263	LYS
1	E	275	LEU
1	E	284	SER
1	E	291	LEU
1	E	321	ARG
1	E	333	LEU
1	E	337	LYS
1	E	338	ASP

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Mol	Chain	Res	Type
1	E	348	GLU
1	E	353	LYS
1	E	365	PHE
1	E	374	LEU
1	E	380	GLU
1	E	383	GLU
1	E	387	ARG
1	E	411	THR
1	E	420	THR
1	E	443	VAL
1	E	449	SER
1	E	531	HIS
1	E	535	ILE
1	E	559	THR
1	E	578	ASP
1	E	592	VAL
1	E	630	THR
1	E	635	VAL
1	E	647	THR
1	E	649	GLN
1	E	651	ARG
1	F	31	THR
1	F	34	VAL
1	F	44	ARG
1	F	54	ILE
1	F	56	VAL
1	F	57	ARG
1	F	61	ARG
1	F	69	THR
1	F	101	SER
1	F	106	ARG
1	F	116	LYS
1	F	126	LEU
1	F	159	MET
1	F	166	LEU
1	F	180	ILE
1	F	184	THR
1	F	185	THR
1	F	208	THR
1	F	243	VAL
1	F	248	SER
1	F	262	VAL

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Mol	Chain	Res	Type
1	F	275	LEU
1	F	291	LEU
1	F	295	LEU
1	F	325	GLU
1	F	333	LEU
1	F	337	LYS
1	F	338	ASP
1	F	345	THR
1	F	348	GLU
1	F	350	SER
1	F	353	LYS
1	F	356	LEU
1	F	365	PHE
1	F	374	LEU
1	F	376	GLU
1	F	380	GLU
1	F	383	GLU
1	F	392	LYS
1	F	411	THR
1	F	420	THR
1	F	443	VAL
1	F	473	ARG
1	F	513	LEU
1	F	521	SER
1	F	533	LYS
1	F	534	VAL
1	F	535	ILE
1	F	559	THR
1	F	592	VAL
1	F	601	LEU
1	F	608	SER
1	F	635	VAL
1	F	640	VAL
1	F	644	ARG
1	F	649	GLN
1	G	34	VAL
1	G	44	ARG
1	G	54	ILE
1	G	69	THR
1	G	121	THR
1	G	123	LYS
1	G	126	LEU

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Mol	Chain	Res	Type
1	G	143	THR
1	G	166	LEU
1	G	180	ILE
1	G	198	ARG
1	G	203	ARG
1	G	224	ARG
1	G	241	VAL
1	G	243	VAL
1	G	251	ARG
1	G	256	LYS
1	G	260	THR
1	G	262	VAL
1	G	275	LEU
1	G	291	LEU
1	G	295	LEU
1	G	325	GLU
1	G	333	LEU
1	G	353	LYS
1	G	361	ILE
1	G	365	PHE
1	G	374	LEU
1	G	377	MET
1	G	380	GLU
1	G	383	GLU
1	G	391	ASP
1	G	403	VAL
1	G	411	THR
1	G	433	LYS
1	G	438	SER
1	G	443	VAL
1	G	449	SER
1	G	513	LEU
1	G	527	GLU
1	G	530	LYS
1	G	557	GLU
1	G	559	THR
1	G	572	GLU
1	G	587	GLN
1	G	592	VAL
1	G	600	ASN
1	G	618	ASP
1	G	626	LEU

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Mol	Chain	Res	Type
1	G	630	THR
1	G	635	VAL
1	G	642	THR
1	G	644	ARG
1	H	5	GLU
1	H	34	VAL
1	H	54	ILE
1	H	69	THR
1	H	75	MET
1	H	78	SER
1	H	106	ARG
1	H	126	LEU
1	H	166	LEU
1	H	180	ILE
1	H	184	THR
1	H	203	ARG
1	H	208	THR
1	H	243	VAL
1	H	251	ARG
1	H	256	LYS
1	H	262	VAL
1	H	275	LEU
1	H	291	LEU
1	H	321	ARG
1	H	333	LEU
1	H	338	ASP
1	H	343	LEU
1	H	348	GLU
1	H	353	LYS
1	H	365	PHE
1	H	372	GLU
1	H	374	LEU
1	H	380	GLU
1	H	383	GLU
1	H	387	ARG
1	H	411	THR
1	H	417	LYS
1	H	420	THR
1	H	437	LYS
1	H	443	VAL
1	H	513	LEU
1	H	530	LYS

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Mol	Chain	Res	Type
1	H	533	LYS
1	H	557	GLU
1	H	559	THR
1	H	563	LEU
1	H	578	ASP
1	H	592	VAL
1	H	626	LEU
1	H	630	THR
1	H	635	VAL
1	H	644	ARG
1	H	649	GLN
1	H	651	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	157	GLN
1	A	288	ASN
1	A	309	GLN
1	A	324	ASN
1	A	440	ASN
1	A	507	GLN
1	A	524	GLN
1	B	60	GLN
1	B	157	GLN
1	B	218	GLN
1	B	226	ASN
1	B	250	ASN
1	B	279	GLN
1	B	309	GLN
1	B	311	GLN
1	B	386	ASN
1	B	423	GLN
1	B	524	GLN
1	C	157	GLN
1	C	218	GLN
1	C	294	GLN
1	C	311	GLN
1	C	340	GLN
1	D	218	GLN
1	D	309	GLN

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Mol	Chain	Res	Type
1	D	649	GLN
1	E	134	ASN
1	E	157	GLN
1	E	218	GLN
1	E	250	ASN
1	E	294	GLN
1	E	524	GLN
1	E	531	HIS
1	F	136	GLN
1	F	157	GLN
1	G	324	ASN
1	G	440	ASN
1	G	573	GLN
1	G	600	ASN
1	H	91	ASN
1	H	212	HIS
1	H	279	GLN
1	H	288	ASN
1	H	311	GLN
1	H	340	GLN
1	H	531	HIS
1	H	649	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](#)

10 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
2	FAD	B	701	-	58,58,58	1.50	11 (18%)	85,89,89	1.74	19 (22%)
2	FAD	D	701	-	58,58,58	1.41	7 (12%)	85,89,89	1.86	24 (28%)
2	FAD	A	701	-	58,58,58	1.54	9 (15%)	85,89,89	1.66	19 (22%)
2	FAD	C	701	-	58,58,58	1.46	8 (13%)	85,89,89	1.66	18 (21%)
3	GOL	H	702	-	5,5,5	0.57	0	5,5,5	0.45	0
3	GOL	B	702	-	5,5,5	0.69	0	5,5,5	0.74	0
2	FAD	E	701	-	58,58,58	1.51	9 (15%)	85,89,89	1.64	18 (21%)
2	FAD	G	701	-	58,58,58	1.38	7 (12%)	85,89,89	1.76	21 (24%)
2	FAD	H	701	-	58,58,58	1.46	9 (15%)	85,89,89	1.76	16 (18%)
2	FAD	F	701	-	58,58,58	1.49	9 (15%)	85,89,89	1.67	21 (24%)

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	FAD	B	701	-	-	6/34/50/50	0/6/6/6
2	FAD	D	701	-	-	6/34/50/50	0/6/6/6
2	FAD	A	701	-	-	7/34/50/50	0/6/6/6
2	FAD	C	701	-	-	5/34/50/50	0/6/6/6
3	GOL	H	702	-	-	2/4/4/4	-
3	GOL	B	702	-	-	3/4/4/4	-
2	FAD	E	701	-	-	5/34/50/50	0/6/6/6
2	FAD	G	701	-	-	6/34/50/50	0/6/6/6
2	FAD	H	701	-	-	2/34/50/50	0/6/6/6
2	FAD	F	701	-	-	6/34/50/50	0/6/6/6

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	FAD	C9A-C5X	5.84	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FAD	C9A-C5X	5.82	1.50	1.41
2	D	701	FAD	C9A-C5X	5.54	1.50	1.41
2	E	701	FAD	C9A-C5X	5.47	1.50	1.41
2	F	701	FAD	C9A-C5X	5.47	1.50	1.41
2	G	701	FAD	C9A-C5X	5.30	1.49	1.41
2	H	701	FAD	C9A-C5X	5.24	1.49	1.41
2	A	701	FAD	C9A-C5X	5.19	1.49	1.41
2	E	701	FAD	C5A-C4A	4.71	1.47	1.39
2	B	701	FAD	C5A-C4A	4.54	1.47	1.39
2	C	701	FAD	C5A-C4A	4.47	1.47	1.39
2	H	701	FAD	C5A-C4A	4.26	1.46	1.39
2	F	701	FAD	C5A-C4A	4.19	1.46	1.39
2	A	701	FAD	C5A-C4A	4.19	1.46	1.39
2	G	701	FAD	C5A-C4A	3.95	1.46	1.39
2	D	701	FAD	C5A-C4A	3.92	1.46	1.39
2	A	701	FAD	P-O3P	3.86	1.63	1.59
2	A	701	FAD	C8-C7	3.60	1.49	1.40
2	G	701	FAD	C8-C7	3.45	1.49	1.40
2	B	701	FAD	C8-C7	3.44	1.49	1.40
2	H	701	FAD	C8-C7	3.39	1.49	1.40
2	F	701	FAD	C8-C7	3.34	1.49	1.40
2	E	701	FAD	C8-C7	3.34	1.49	1.40
2	C	701	FAD	C8-C7	3.20	1.48	1.40
2	H	701	FAD	C5A-C6A	2.99	1.49	1.41
2	D	701	FAD	C4A-N9A	-2.98	1.31	1.37
2	D	701	FAD	C8-C7	2.97	1.48	1.40
2	F	701	FAD	C4A-N9A	-2.86	1.31	1.37
2	C	701	FAD	C8A-N7A	2.81	1.37	1.31
2	A	701	FAD	PA-O3P	2.68	1.62	1.59
2	G	701	FAD	C4A-N9A	-2.65	1.32	1.37
2	D	701	FAD	C5A-N7A	-2.58	1.34	1.39
2	A	701	FAD	C5A-C6A	2.54	1.48	1.41
2	G	701	FAD	C5A-N7A	-2.54	1.34	1.39
2	A	701	FAD	C4A-N9A	-2.53	1.32	1.37
2	E	701	FAD	C5A-C6A	2.52	1.48	1.41
2	B	701	FAD	C5A-C6A	2.52	1.48	1.41
2	C	701	FAD	C5A-C6A	2.51	1.48	1.41
2	A	701	FAD	C8A-N7A	2.49	1.36	1.31
2	C	701	FAD	C4A-N9A	-2.49	1.32	1.37
2	B	701	FAD	C5A-N7A	-2.47	1.34	1.39
2	F	701	FAD	C5A-N7A	-2.47	1.34	1.39
2	D	701	FAD	C5A-C6A	2.39	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	701	FAD	C5A-C6A	2.38	1.47	1.41
2	H	701	FAD	C4X-N5	2.37	1.35	1.30
2	E	701	FAD	C5X-N5	-2.33	1.35	1.39
2	F	701	FAD	C5A-C6A	2.33	1.47	1.41
2	C	701	FAD	C4X-N5	2.31	1.35	1.30
2	E	701	FAD	C8A-N7A	2.31	1.36	1.31
2	E	701	FAD	C4X-N5	2.30	1.35	1.30
2	D	701	FAD	C8A-N7A	2.27	1.36	1.31
2	H	701	FAD	C8A-N7A	2.24	1.36	1.31
2	E	701	FAD	C5A-N7A	-2.24	1.35	1.39
2	H	701	FAD	C5A-N7A	-2.23	1.35	1.39
2	A	701	FAD	C4X-N5	2.23	1.35	1.30
2	F	701	FAD	C4X-N5	2.20	1.35	1.30
2	F	701	FAD	PA-O3P	2.19	1.61	1.59
2	G	701	FAD	C4X-N5	2.19	1.35	1.30
2	B	701	FAD	C4A-N9A	-2.19	1.33	1.37
2	B	701	FAD	PA-O3P	2.19	1.61	1.59
2	B	701	FAD	C8A-N9A	-2.13	1.33	1.37
2	H	701	FAD	C4A-N9A	-2.11	1.33	1.37
2	B	701	FAD	C8A-N7A	2.11	1.35	1.31
2	E	701	FAD	C10-N10	2.09	1.41	1.37
2	F	701	FAD	P-O3P	2.09	1.61	1.59
2	H	701	FAD	C8A-N9A	-2.08	1.34	1.37
2	B	701	FAD	C4X-N5	2.07	1.35	1.30
2	B	701	FAD	P-O3P	2.05	1.61	1.59
2	C	701	FAD	C5A-N7A	-2.01	1.35	1.39

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	701	FAD	C5A-C4A-N3A	-6.17	118.23	126.72
2	B	701	FAD	C5A-C4A-N3A	-5.71	118.86	126.72
2	E	701	FAD	C5A-C4A-N3A	-5.46	119.20	126.72
2	D	701	FAD	C4A-N9A-C8A	4.81	110.79	105.74
2	G	701	FAD	C5A-C4A-N3A	-4.79	120.12	126.72
2	H	701	FAD	C4A-C5A-N7A	-4.79	105.11	110.58
2	E	701	FAD	N3A-C4A-N9A	4.76	135.27	127.17
2	B	701	FAD	N3A-C4A-N9A	4.75	135.25	127.17
2	A	701	FAD	N3A-C2A-N1A	-4.73	121.42	128.58
2	G	701	FAD	C9A-C5X-N5	-4.70	117.47	122.45
2	C	701	FAD	C5A-C4A-N3A	-4.67	120.28	126.72
2	A	701	FAD	C5A-C4A-N3A	-4.60	120.38	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	701	FAD	N3A-C4A-N9A	4.46	134.75	127.17
2	G	701	FAD	N3A-C2A-N1A	-4.42	121.89	128.58
2	C	701	FAD	C9A-C5X-N5	-4.40	117.79	122.45
2	F	701	FAD	C4A-N9A-C8A	4.37	110.33	105.74
2	E	701	FAD	N3A-C2A-N1A	-4.35	122.00	128.58
2	G	701	FAD	C4'-C3'-C2'	-4.30	106.42	113.57
2	D	701	FAD	N3A-C2A-N1A	-4.20	122.22	128.58
2	F	701	FAD	C5A-C4A-N3A	-4.20	120.94	126.72
2	G	701	FAD	N3A-C4A-N9A	4.17	134.26	127.17
2	D	701	FAD	C5A-C4A-N3A	-4.14	121.02	126.72
2	H	701	FAD	C2A-N3A-C4A	4.10	121.84	111.83
2	C	701	FAD	C4-C4X-N5	4.07	123.83	118.21
2	H	701	FAD	C9A-C5X-N5	-4.06	118.15	122.45
2	C	701	FAD	N3A-C2A-N1A	-4.03	122.49	128.58
2	F	701	FAD	N3A-C4A-N9A	4.00	133.97	127.17
2	C	701	FAD	N3A-C4A-N9A	3.96	133.90	127.17
2	A	701	FAD	C2A-N3A-C4A	3.94	121.44	111.83
2	E	701	FAD	C2A-N3A-C4A	3.92	121.40	111.83
2	D	701	FAD	O4B-C1B-N9A	-3.87	100.65	108.09
2	G	701	FAD	C2A-N3A-C4A	3.85	121.23	111.83
2	C	701	FAD	C4A-N9A-C8A	3.81	109.73	105.74
2	F	701	FAD	N3A-C2A-N1A	-3.77	122.88	128.58
2	B	701	FAD	C4A-C5A-N7A	-3.75	106.29	110.58
2	D	701	FAD	O3B-C3B-C4B	-3.75	100.32	111.08
2	H	701	FAD	N3A-C2A-N1A	-3.74	122.92	128.58
2	D	701	FAD	N3A-C4A-N9A	3.71	133.48	127.17
2	G	701	FAD	C4A-N9A-C8A	3.70	109.62	105.74
2	C	701	FAD	C2A-N3A-C4A	3.66	120.78	111.83
2	G	701	FAD	C4-C4X-N5	3.66	123.26	118.21
2	D	701	FAD	C9A-C5X-N5	-3.63	118.60	122.45
2	D	701	FAD	C4-C4X-N5	3.60	123.18	118.21
2	B	701	FAD	C2A-N3A-C4A	3.59	120.60	111.83
2	B	701	FAD	C9A-N10-C10	-3.55	115.33	120.75
2	F	701	FAD	C9A-C5X-N5	-3.55	118.68	122.45
2	D	701	FAD	N9A-C8A-N7A	-3.54	108.91	113.94
2	B	701	FAD	C4A-N9A-C8A	3.52	109.43	105.74
2	F	701	FAD	C4-C4X-N5	3.51	123.06	118.21
2	H	701	FAD	C5A-N7A-C8A	3.49	108.93	103.45
2	A	701	FAD	N3A-C4A-N9A	3.42	132.99	127.17
2	B	701	FAD	N3A-C2A-N1A	-3.39	123.45	128.58
2	A	701	FAD	C4A-C5A-N7A	-3.37	106.73	110.58
2	D	701	FAD	C2A-N3A-C4A	3.36	120.03	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	701	FAD	C4-C4X-N5	3.35	122.84	118.21
2	D	701	FAD	O3P-PA-O1A	-3.30	100.78	110.70
2	B	701	FAD	O2-C2-N1	-3.28	116.34	121.80
2	D	701	FAD	C4A-C5A-N7A	-3.27	106.85	110.58
2	F	701	FAD	C2A-N3A-C4A	3.21	119.67	111.83
2	H	701	FAD	C4A-N9A-C8A	3.20	109.10	105.74
2	B	701	FAD	O4-C4-C4X	-3.18	118.14	126.53
2	A	701	FAD	C4-C4X-N5	3.18	122.60	118.21
2	E	701	FAD	C4A-N9A-C8A	3.16	109.05	105.74
2	E	701	FAD	O2A-PA-O3P	3.14	115.75	107.27
2	A	701	FAD	C4A-N9A-C8A	3.13	109.02	105.74
2	A	701	FAD	C6A-C5A-N7A	3.02	137.91	132.09
2	D	701	FAD	O2-C2-N1	-2.98	116.86	121.80
2	B	701	FAD	C9A-C5X-N5	-2.97	119.30	122.45
2	B	701	FAD	C4-N3-C2	-2.92	120.45	125.64
2	H	701	FAD	N9A-C8A-N7A	-2.89	109.83	113.94
2	D	701	FAD	C5A-N7A-C8A	2.87	107.97	103.45
2	G	701	FAD	C4A-C5A-N7A	-2.87	107.30	110.58
2	E	701	FAD	C4A-C5A-N7A	-2.86	107.32	110.58
2	F	701	FAD	C4A-C5A-N7A	-2.86	107.32	110.58
2	B	701	FAD	C5A-N7A-C8A	2.85	107.93	103.45
2	E	701	FAD	C4-C4X-N5	2.81	122.10	118.21
2	C	701	FAD	C4A-C5A-N7A	-2.81	107.37	110.58
2	D	701	FAD	C4A-N9A-C1B	-2.78	120.14	126.63
2	F	701	FAD	N9A-C8A-N7A	-2.76	110.03	113.94
2	F	701	FAD	O2-C2-N1	-2.75	117.23	121.80
2	A	701	FAD	C4'-C3'-C2'	-2.65	109.15	113.57
2	A	701	FAD	O4-C4-C4X	-2.62	119.61	126.53
2	D	701	FAD	C2A-N1A-C6A	2.62	123.03	118.73
2	D	701	FAD	C5X-N5-C4X	2.60	122.30	118.09
2	G	701	FAD	N9A-C8A-N7A	-2.60	110.25	113.94
2	C	701	FAD	C10-N1-C2	2.59	122.45	116.85
2	F	701	FAD	C4A-N9A-C1B	-2.58	120.61	126.63
2	A	701	FAD	C2A-N1A-C6A	2.57	122.96	118.73
2	C	701	FAD	N9A-C8A-N7A	-2.57	110.29	113.94
2	H	701	FAD	C6A-C5A-N7A	2.54	137.00	132.09
2	A	701	FAD	N9A-C8A-N7A	-2.54	110.33	113.94
2	H	701	FAD	C10-N1-C2	2.53	122.32	116.85
2	B	701	FAD	N9A-C8A-N7A	-2.49	110.40	113.94
2	B	701	FAD	C4X-C4-N3	2.49	119.58	113.25
2	B	701	FAD	C4-C4X-N5	2.48	121.64	118.21
2	D	701	FAD	C6A-C5A-N7A	2.48	136.86	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	701	FAD	C2A-N1A-C6A	2.47	122.78	118.73
2	A	701	FAD	C9A-C5X-N5	-2.46	119.84	122.45
2	B	701	FAD	C2B-C3B-C4B	2.44	107.33	102.61
2	E	701	FAD	C2A-N1A-C6A	2.44	122.74	118.73
2	D	701	FAD	C10-N1-C2	2.44	122.13	116.85
2	A	701	FAD	C5A-N7A-C8A	2.44	107.28	103.45
2	C	701	FAD	C4X-C4-N3	2.43	119.44	113.25
2	E	701	FAD	C5A-N7A-C8A	2.42	107.26	103.45
2	G	701	FAD	O4-C4-C4X	-2.42	120.14	126.53
2	F	701	FAD	C5A-N7A-C8A	2.41	107.23	103.45
2	D	701	FAD	C2B-C3B-C4B	2.40	107.25	102.61
2	D	701	FAD	O2A-PA-O3P	2.39	113.74	107.27
2	G	701	FAD	O2-C2-N1	-2.39	117.83	121.80
2	G	701	FAD	C5A-N7A-C8A	2.38	107.19	103.45
2	E	701	FAD	C4X-C10-N1	-2.38	118.76	124.59
2	H	701	FAD	O4-C4-C4X	-2.38	120.26	126.53
2	H	701	FAD	C4X-C4-N3	2.37	119.28	113.25
2	G	701	FAD	C4X-C4-N3	2.37	119.28	113.25
2	F	701	FAD	C10-N1-C2	2.36	121.96	116.85
2	A	701	FAD	C4A-N9A-C1B	-2.36	121.12	126.63
2	G	701	FAD	C6A-C5A-N7A	2.34	136.61	132.09
2	G	701	FAD	C10-N1-C2	2.31	121.84	116.85
2	F	701	FAD	C4X-C10-N10	2.29	119.76	116.48
2	E	701	FAD	C10-N1-C2	2.29	121.80	116.85
2	C	701	FAD	C6A-C5A-N7A	2.28	136.48	132.09
2	C	701	FAD	C2A-N1A-C6A	2.28	122.47	118.73
2	D	701	FAD	O4-C4-C4X	-2.28	120.53	126.53
2	G	701	FAD	C2A-N1A-C6A	2.25	122.43	118.73
2	H	701	FAD	O2A-PA-O3P	2.24	113.34	107.27
2	H	701	FAD	C4X-C10-N1	-2.24	119.11	124.59
2	D	701	FAD	C10-C4X-N5	-2.24	120.24	124.81
2	G	701	FAD	C4-N3-C2	-2.22	121.70	125.64
2	C	701	FAD	O2-C2-N1	-2.21	118.13	121.80
2	A	701	FAD	C4X-C4-N3	2.20	118.85	113.25
2	F	701	FAD	N6A-C6A-N1A	2.20	123.27	118.38
2	B	701	FAD	C4X-C10-N1	-2.20	119.21	124.59
2	B	701	FAD	C2B-C1B-N9A	2.19	118.75	113.30
2	E	701	FAD	C4'-C3'-C2'	-2.19	109.93	113.57
2	E	701	FAD	N9A-C8A-N7A	-2.19	110.83	113.94
2	C	701	FAD	O4-C4-C4X	-2.18	120.78	126.53
2	A	701	FAD	O2A-PA-O3P	2.17	113.14	107.27
2	E	701	FAD	O4-C4-C4X	-2.17	120.81	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	701	FAD	C4X-C10-N1	-2.17	119.28	124.59
2	G	701	FAD	O2A-PA-O3P	2.15	113.09	107.27
2	C	701	FAD	C4A-N9A-C1B	-2.15	121.61	126.63
2	E	701	FAD	C6A-C5A-N7A	2.15	136.23	132.09
2	F	701	FAD	C6A-C5A-N7A	2.13	136.21	132.09
2	C	701	FAD	C5A-N7A-C8A	2.12	106.79	103.45
2	B	701	FAD	C10-N1-C2	2.10	121.40	116.85
2	F	701	FAD	C10-C4X-N5	-2.09	120.55	124.81
2	A	701	FAD	C10-N1-C2	2.09	121.36	116.85
2	F	701	FAD	C6-C5X-N5	-2.08	115.00	118.44
2	E	701	FAD	C4X-C4-N3	2.07	118.51	113.25
2	F	701	FAD	C4X-C10-N1	-2.06	119.53	124.59
2	G	701	FAD	C10-C4X-N5	-2.05	120.63	124.81
2	A	701	FAD	O2-C2-N1	-2.04	118.41	121.80
2	C	701	FAD	C4X-C10-N10	2.04	119.40	116.48
2	E	701	FAD	C4-N3-C2	-2.03	122.05	125.64
2	F	701	FAD	O4-C4-C4X	-2.03	121.19	126.53
2	D	701	FAD	O4B-C4B-C5B	2.01	115.77	109.33

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FAD	C5B-O5B-PA-O1A
2	A	701	FAD	N10-C1'-C2'-O2'
2	B	701	FAD	N10-C1'-C2'-O2'
2	C	701	FAD	N10-C1'-C2'-O2'
2	D	701	FAD	N10-C1'-C2'-O2'
2	D	701	FAD	N10-C1'-C2'-C3'
2	E	701	FAD	N10-C1'-C2'-O2'
2	F	701	FAD	N10-C1'-C2'-O2'
2	F	701	FAD	N10-C1'-C2'-C3'
2	G	701	FAD	N10-C1'-C2'-O2'
2	G	701	FAD	N10-C1'-C2'-C3'
3	B	702	GOL	O1-C1-C2-C3
3	H	702	GOL	C1-C2-C3-O3
3	B	702	GOL	O1-C1-C2-O2
3	H	702	GOL	O2-C2-C3-O3
2	F	701	FAD	PA-O3P-P-O1P
2	G	701	FAD	PA-O3P-P-O1P
2	A	701	FAD	PA-O3P-P-O5'
2	B	701	FAD	PA-O3P-P-O5'

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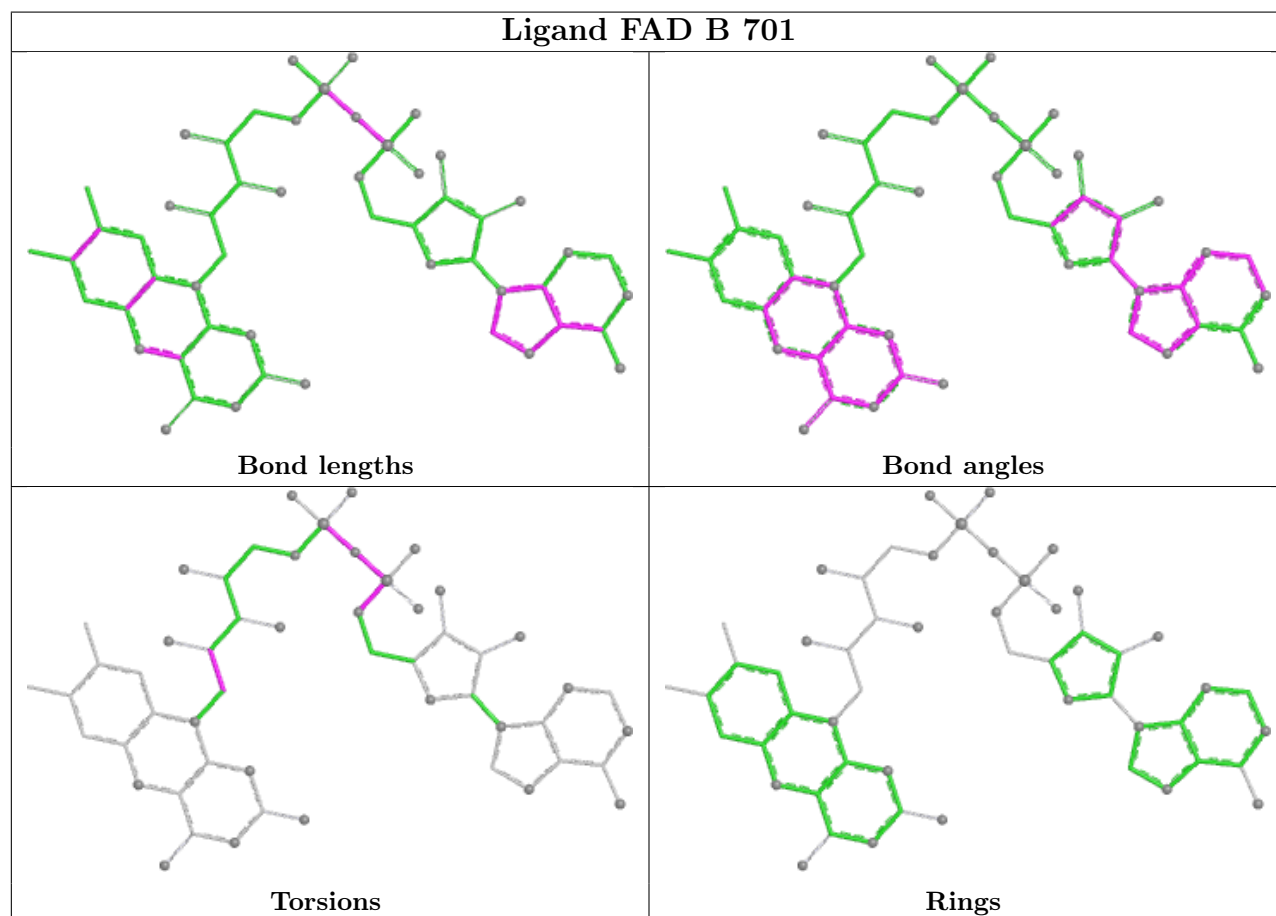
Mol	Chain	Res	Type	Atoms
2	C	701	FAD	PA-O3P-P-O5'
2	D	701	FAD	PA-O3P-P-O5'
2	E	701	FAD	PA-O3P-P-O5'
2	H	701	FAD	PA-O3P-P-O5'
2	B	701	FAD	PA-O3P-P-O1P
2	F	701	FAD	P-O3P-PA-O1A
3	B	702	GOL	O2-C2-C3-O3
2	A	701	FAD	N10-C1'-C2'-C3'
2	A	701	FAD	C5'-O5'-P-O1P
2	B	701	FAD	C5B-O5B-PA-O1A
2	D	701	FAD	C5'-O5'-P-O1P
2	A	701	FAD	P-O3P-PA-O2A
2	B	701	FAD	P-O3P-PA-O2A
2	C	701	FAD	P-O3P-PA-O2A
2	E	701	FAD	P-O3P-PA-O2A
2	E	701	FAD	PA-O3P-P-O1P
2	G	701	FAD	P-O3P-PA-O2A
2	H	701	FAD	P-O3P-PA-O1A
2	F	701	FAD	PA-O3P-P-O5'
2	G	701	FAD	PA-O3P-P-O5'
2	A	701	FAD	P-O3P-PA-O1A
2	C	701	FAD	PA-O3P-P-O1P
2	D	701	FAD	P-O3P-PA-O2A
2	F	701	FAD	P-O3P-PA-O2A
2	G	701	FAD	P-O3P-PA-O1A
2	B	701	FAD	P-O3P-PA-O1A
2	C	701	FAD	P-O3P-PA-O1A
2	D	701	FAD	P-O3P-PA-O1A
2	E	701	FAD	P-O3P-PA-O1A

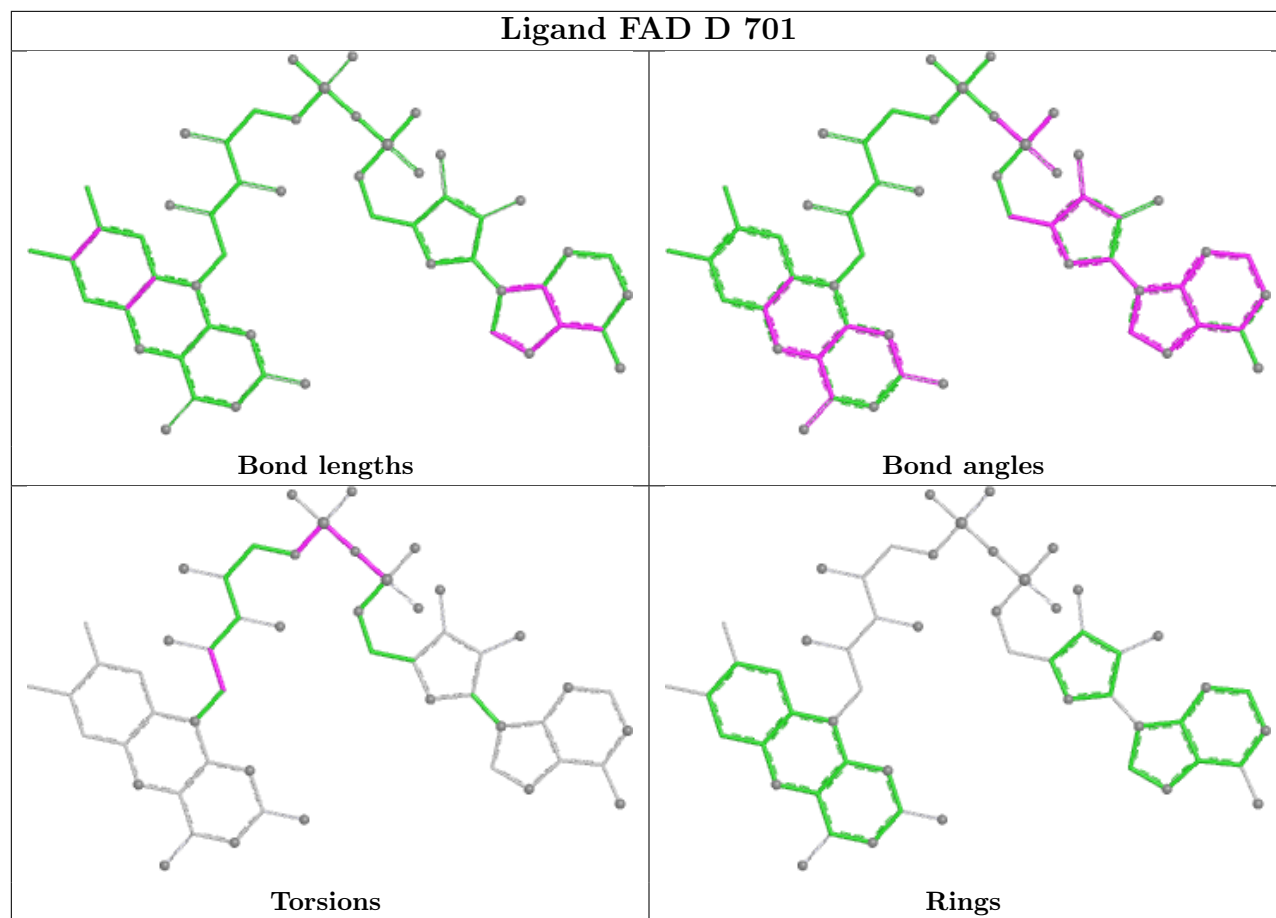
There are no ring outliers.

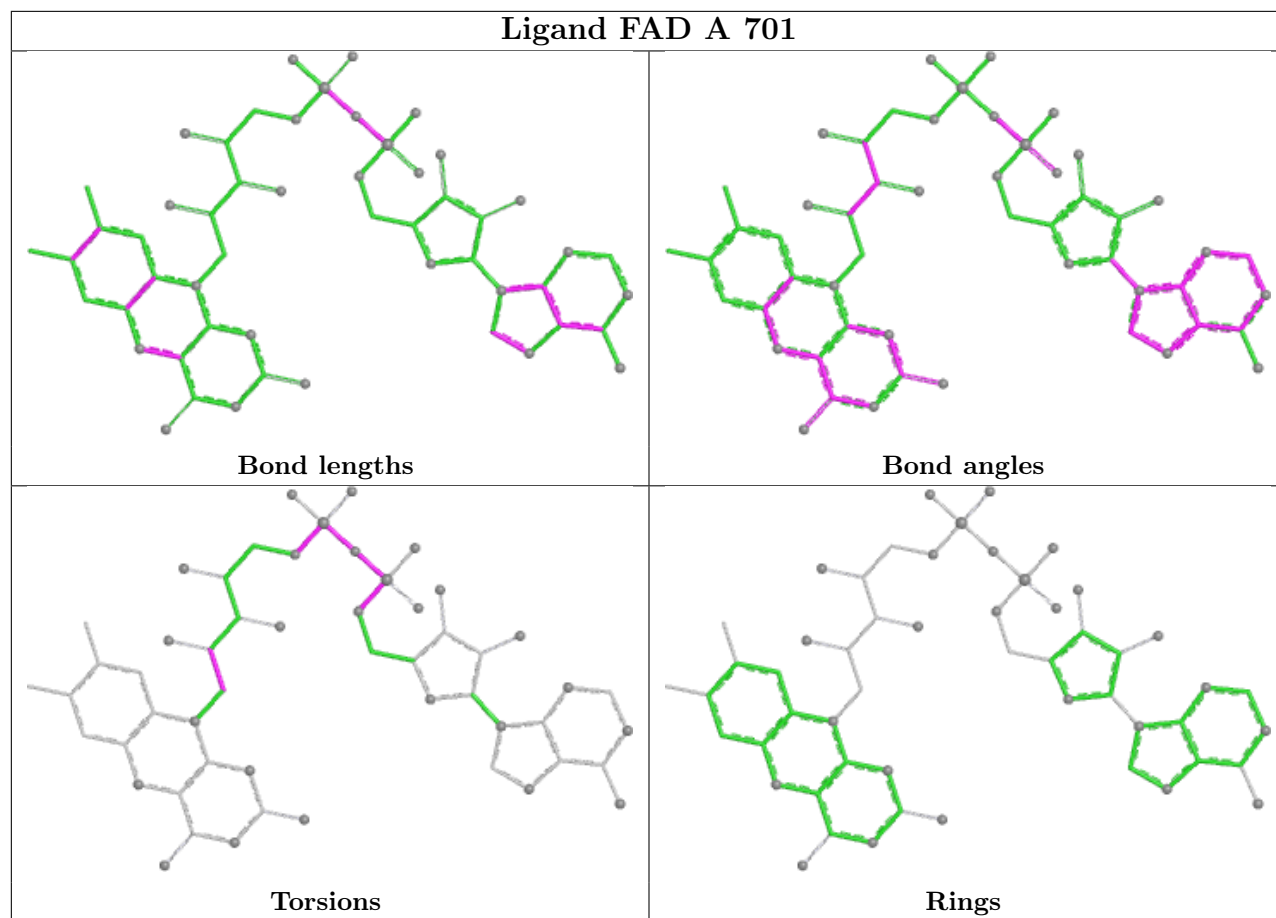
8 monomers are involved in 23 short contacts:

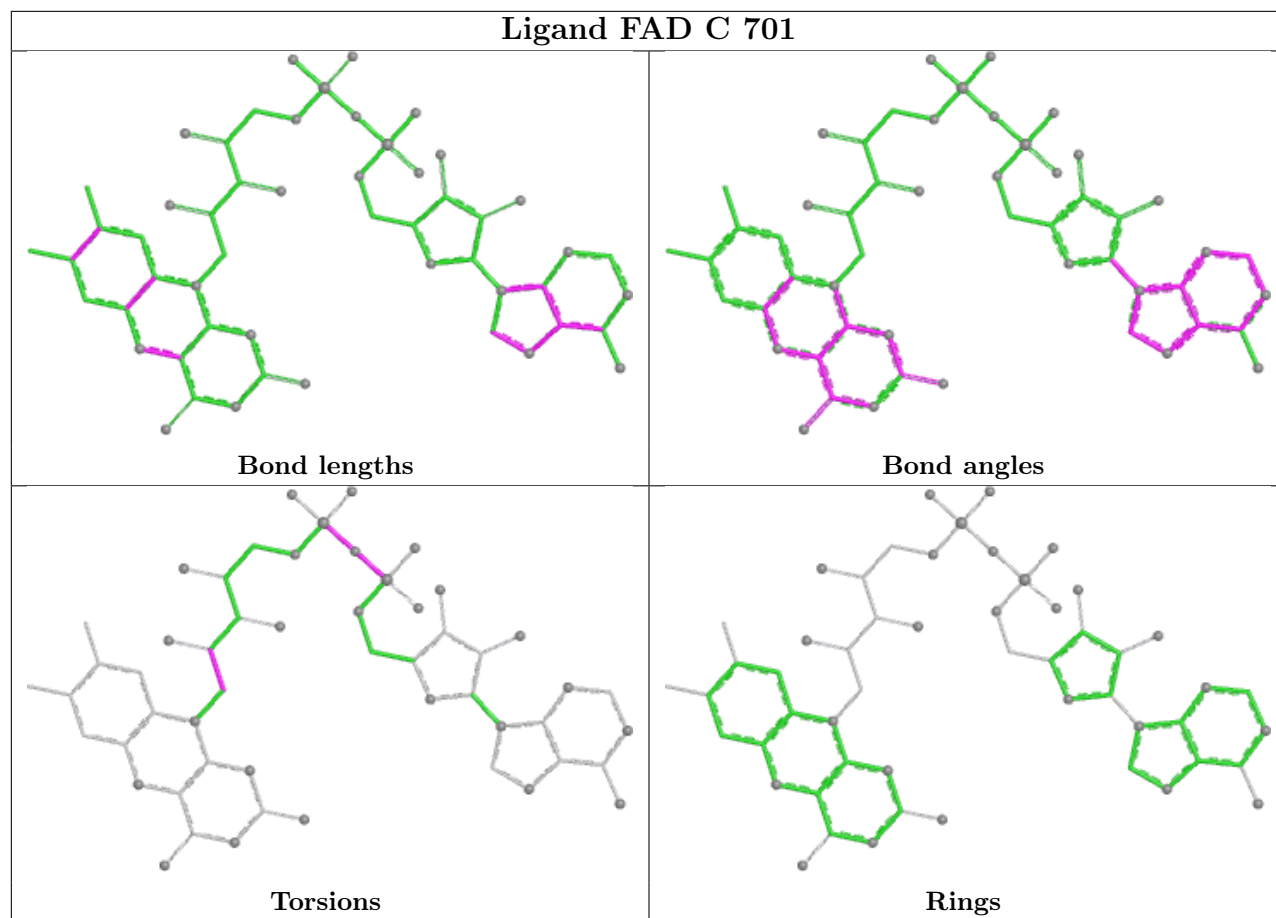
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	FAD	4	0
2	D	701	FAD	3	0
2	A	701	FAD	2	0
2	C	701	FAD	2	0
2	E	701	FAD	2	0
2	G	701	FAD	3	0
2	H	701	FAD	3	0
2	F	701	FAD	4	0

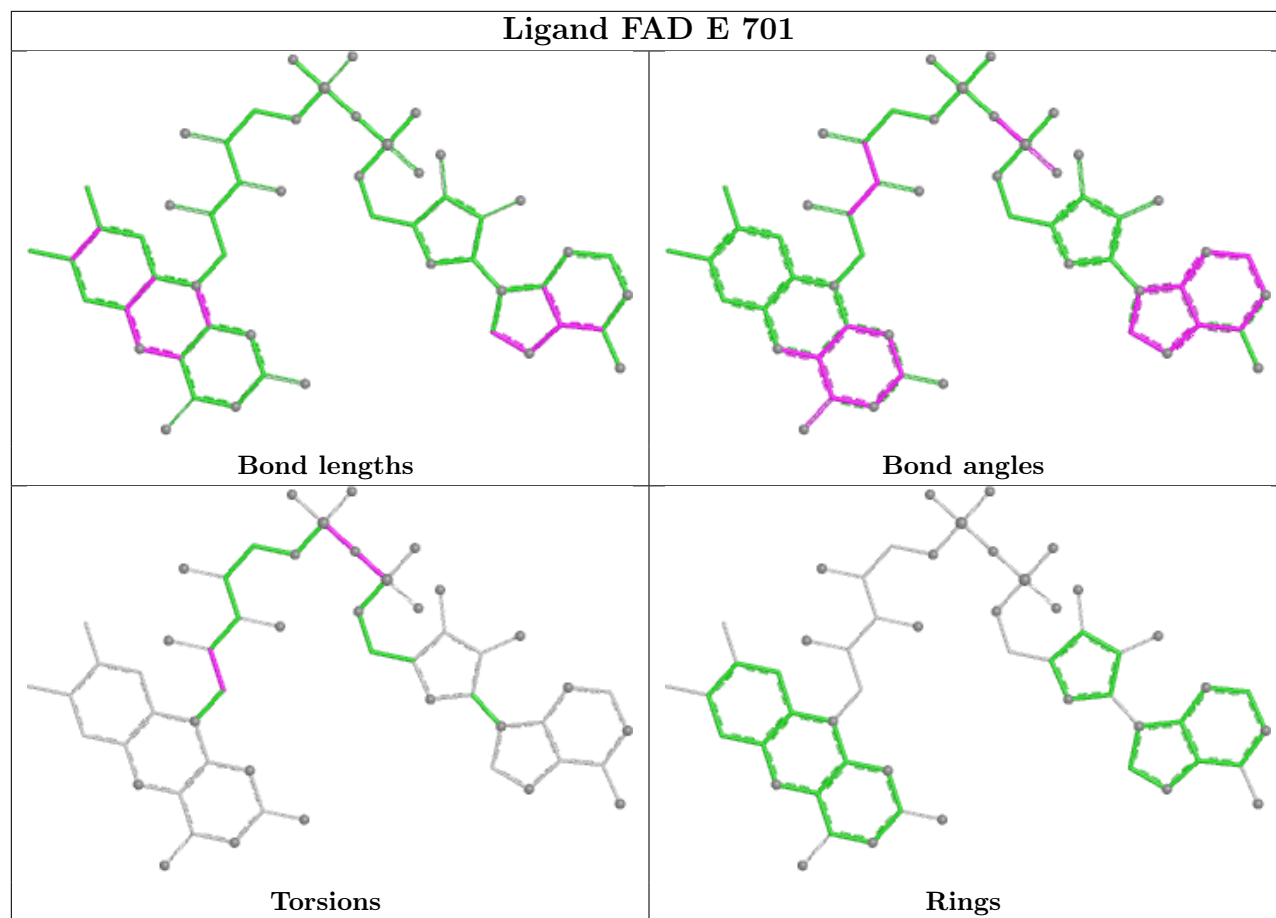
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

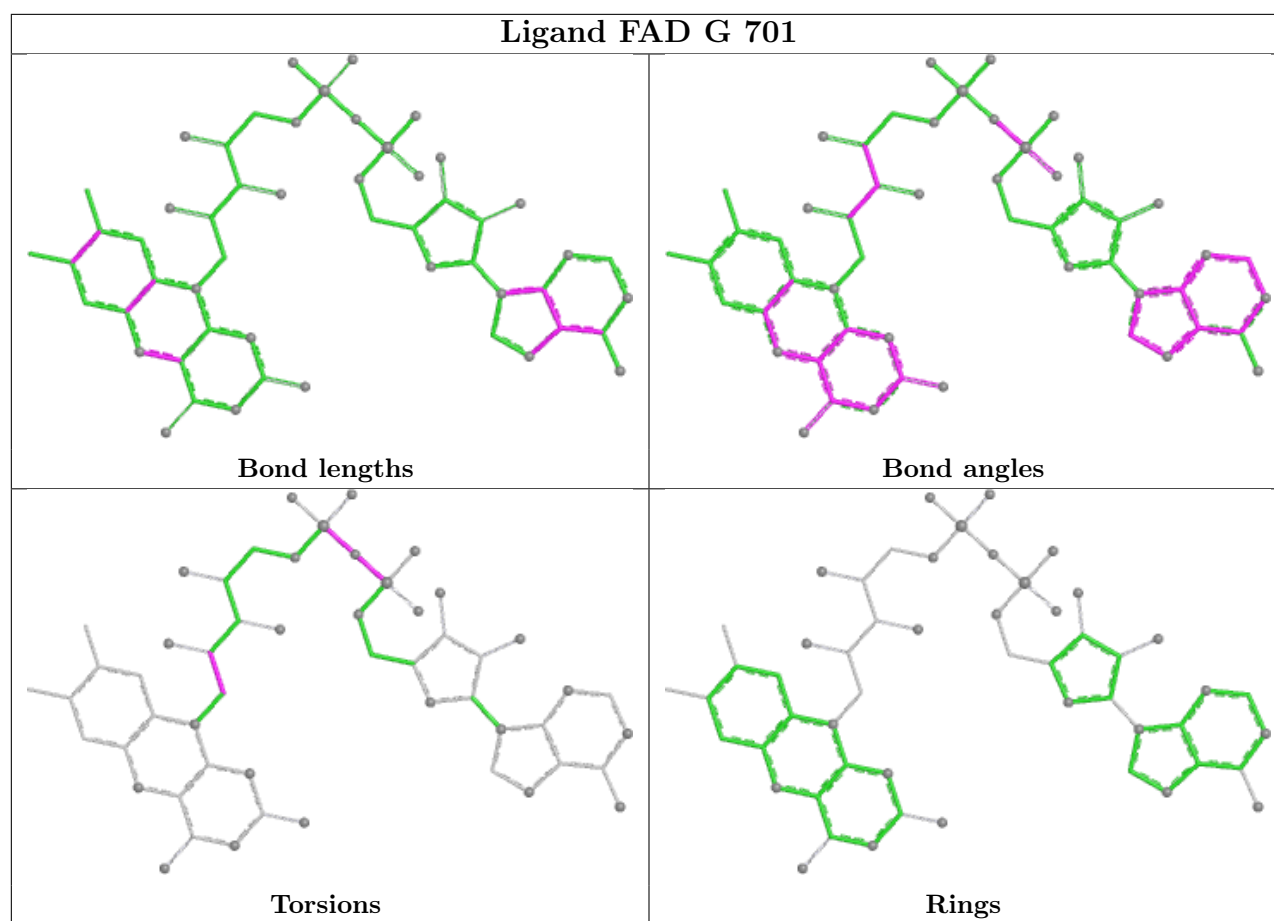


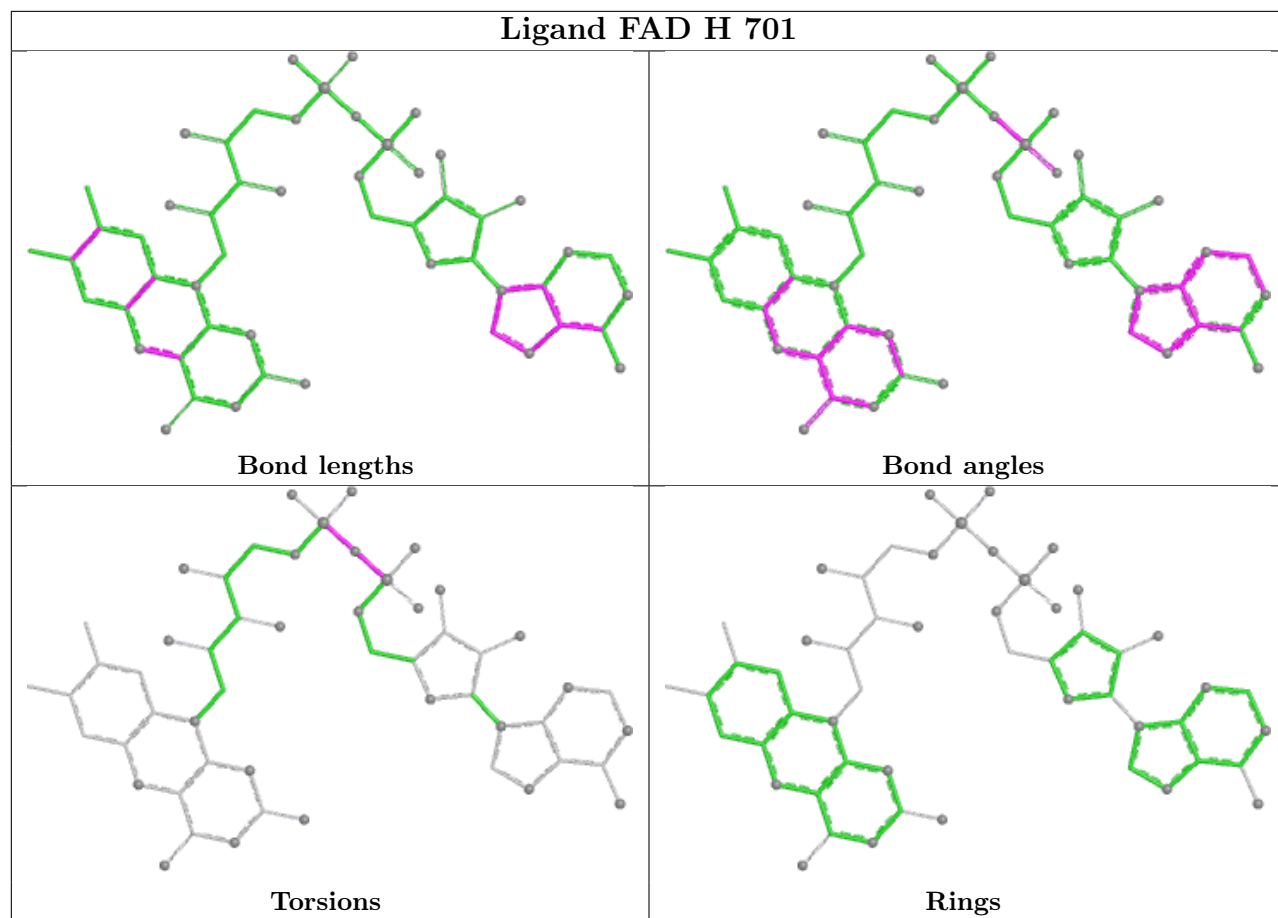


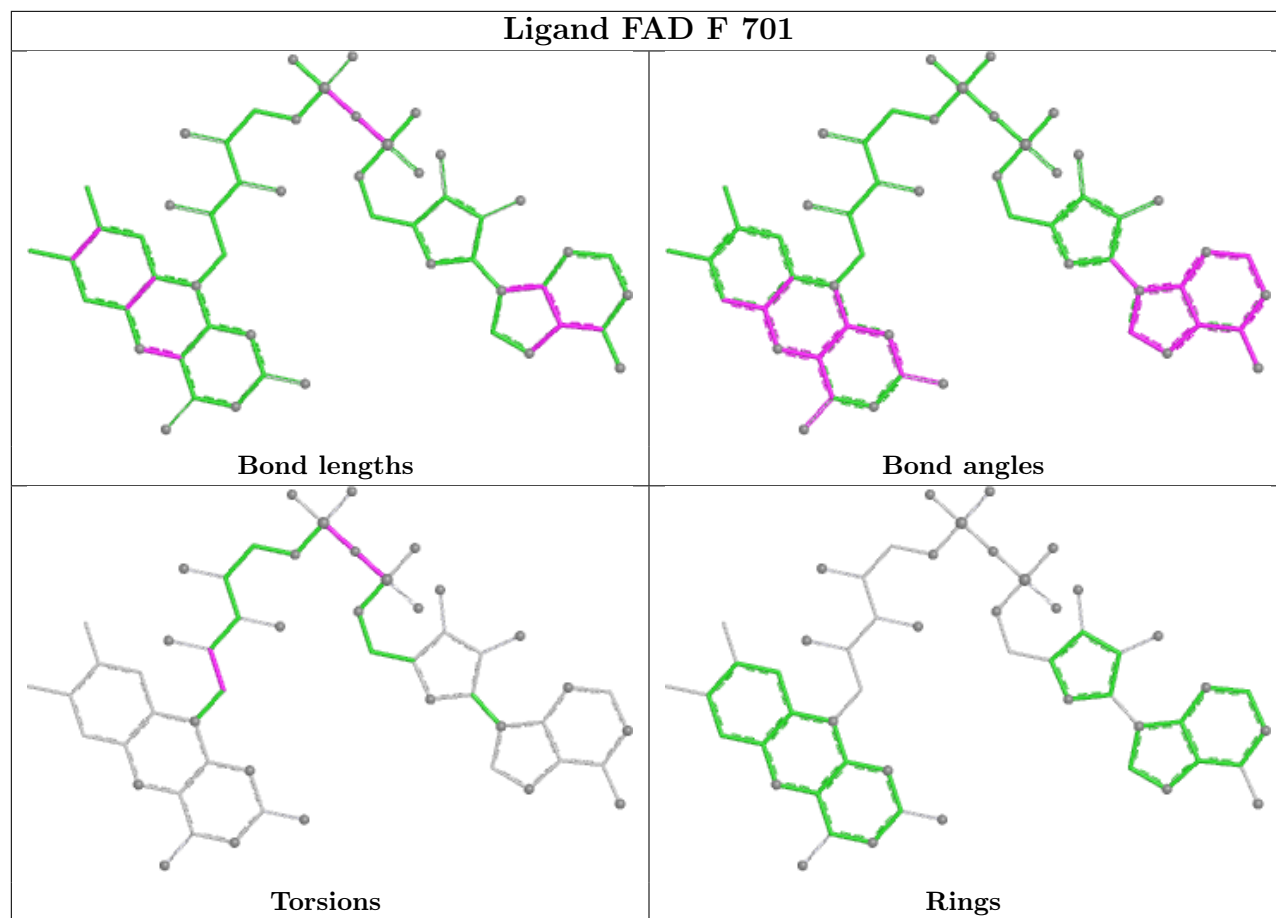












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	649/651 (99%)	-0.02	2 (0%) 90 87	16, 33, 49, 73	1 (0%)
1	B	647/651 (99%)	-0.11	2 (0%) 90 87	21, 30, 47, 61	0
1	C	648/651 (99%)	-0.04	1 (0%) 91 89	21, 33, 48, 60	0
1	D	649/651 (99%)	-0.09	3 (0%) 87 85	20, 30, 45, 67	0
1	E	648/651 (99%)	0.07	1 (0%) 91 89	22, 36, 52, 68	0
1	F	650/651 (99%)	-0.09	3 (0%) 87 85	22, 32, 49, 73	0
1	G	648/651 (99%)	-0.02	5 (0%) 82 80	20, 33, 51, 66	0
1	H	648/651 (99%)	-0.07	1 (0%) 91 89	20, 32, 48, 72	0
All	All	5187/5208 (99%)	-0.05	18 (0%) 90 87	16, 32, 49, 73	1 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	641	PRO	3.8
1	A	640	VAL	3.6
1	B	640	VAL	3.6
1	D	640	VAL	3.5
1	G	531	HIS	3.0
1	F	2	GLY	3.0
1	H	531	HIS	2.9
1	G	641	PRO	2.8
1	B	199	HIS	2.5
1	G	640	VAL	2.3
1	G	4	PRO	2.3
1	F	640	VAL	2.2
1	D	531	HIS	2.2
1	G	235	ASP	2.1
1	C	85	SER	2.0
1	F	258	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	641	PRO	2.0
1	E	531	HIS	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](#)

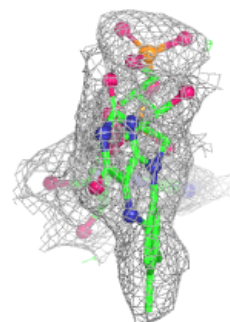
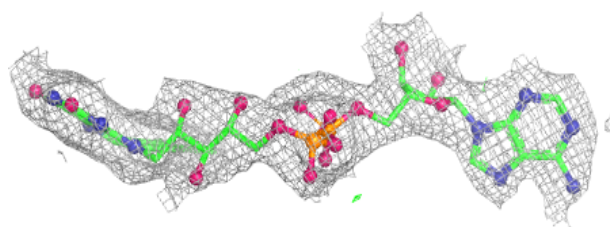
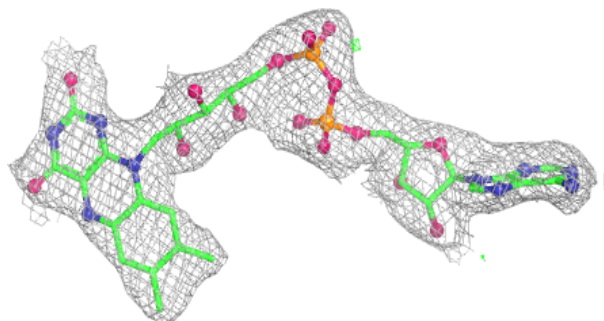
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	GOL	B	702	6/6	0.83	0.10	30,31,32,32	0
3	GOL	H	702	6/6	0.83	0.12	30,30,32,32	0
2	FAD	C	701	53/53	0.94	0.08	29,34,45,46	0
2	FAD	E	701	53/53	0.94	0.08	30,37,40,42	0
2	FAD	H	701	53/53	0.95	0.07	29,31,36,37	0
2	FAD	A	701	53/53	0.95	0.07	23,28,32,35	0
2	FAD	G	701	53/53	0.95	0.07	28,32,37,38	0
2	FAD	D	701	53/53	0.96	0.07	18,22,30,33	0
2	FAD	F	701	53/53	0.96	0.06	23,26,31,32	0
2	FAD	B	701	53/53	0.97	0.06	21,26,29,32	0

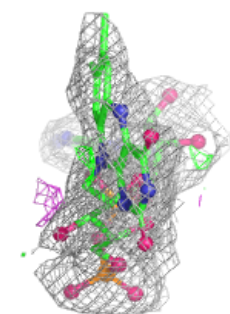
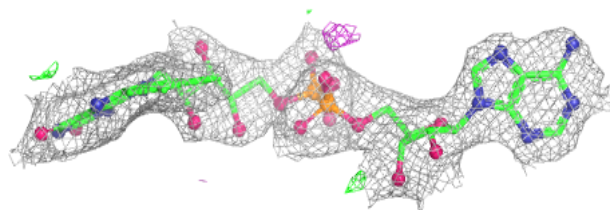
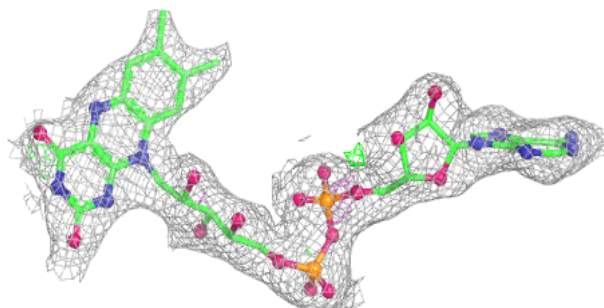
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD C 701:

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

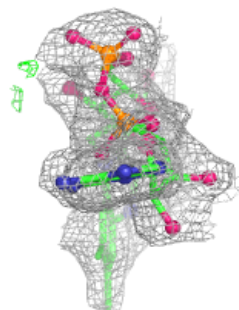
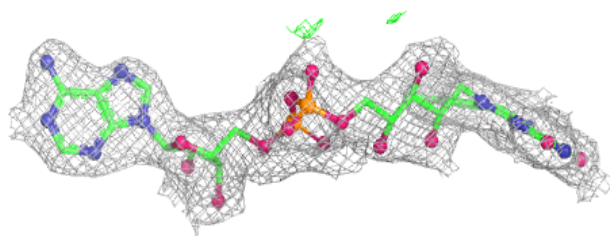
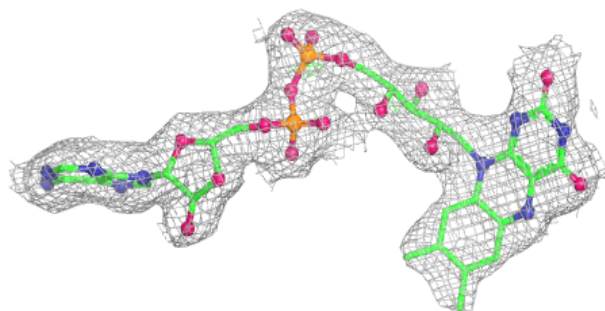
**Electron density around FAD E 701:**

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

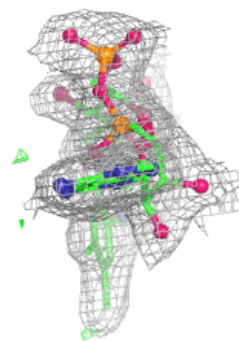
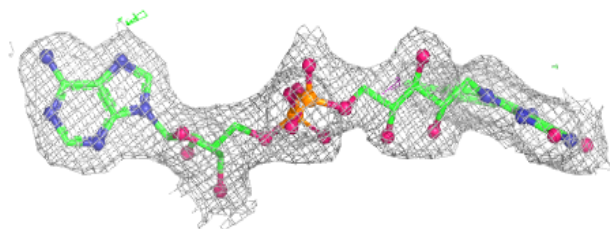
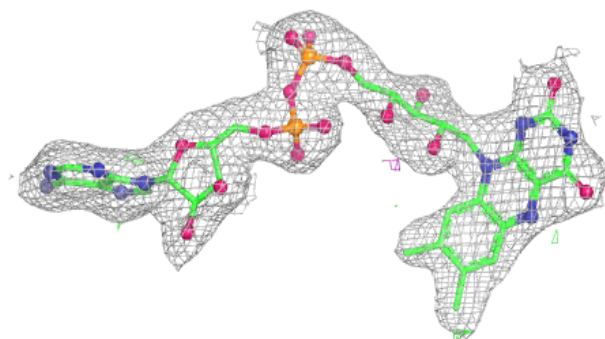


Electron density around FAD H 701:

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

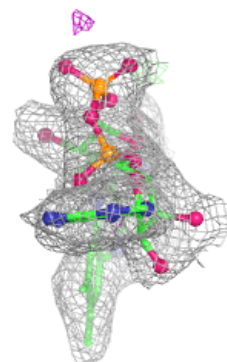
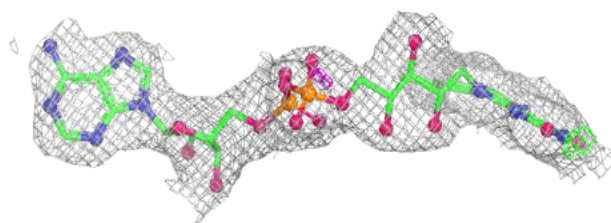
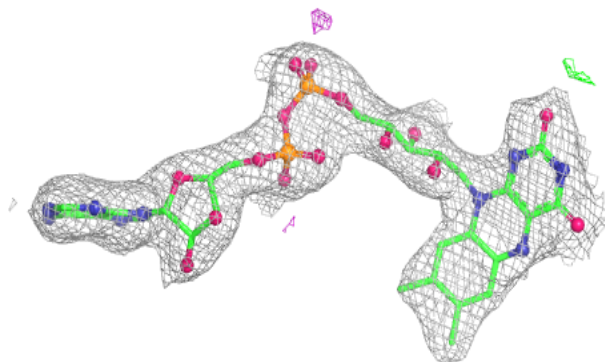
**Electron density around FAD A 701:**

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

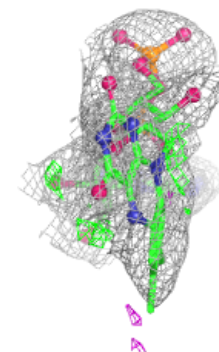
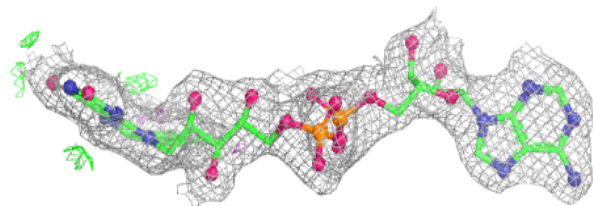
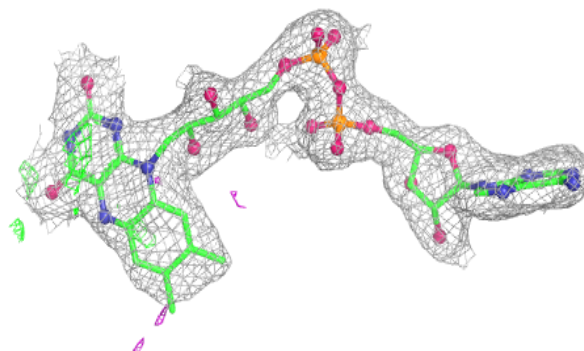


Electron density around FAD G 701:

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

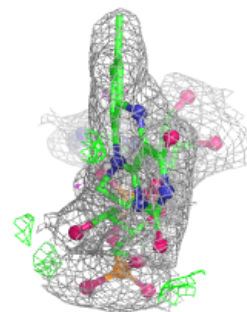
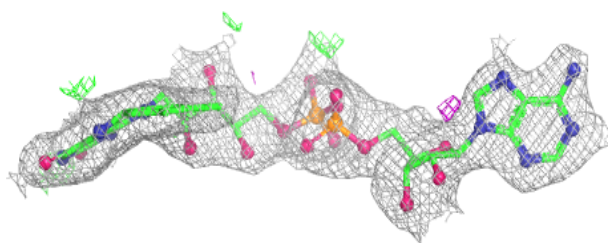
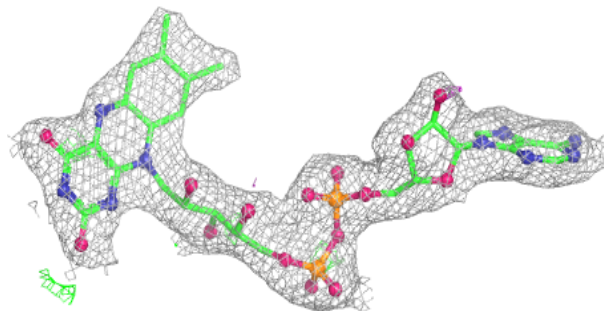
**Electron density around FAD D 701:**

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

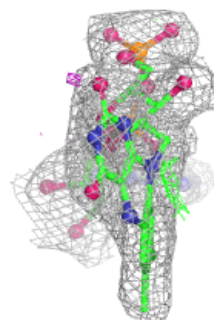
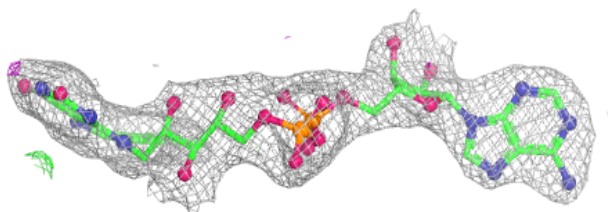
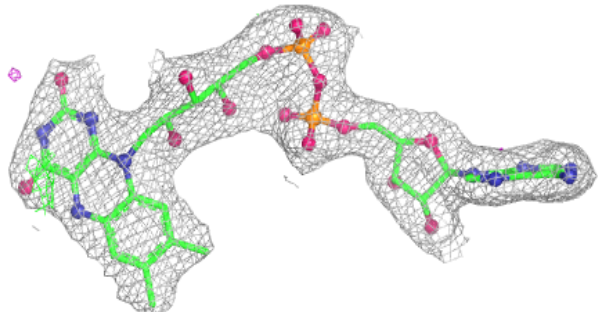


Electron density around FAD F 701:

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

**Electron density around FAD B 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.