



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:17 AM UTC

PDB ID : 8X0O / pdb_00008x0o
Title : Crystal structure of Tyrosine decarboxylase H203F mutant in complex with the cofactor PLP and Tyrosine
Authors : Wang, H.; Yu, J.; Yao, M.
Deposited on : 2023-11-05
Resolution : 3.35 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:

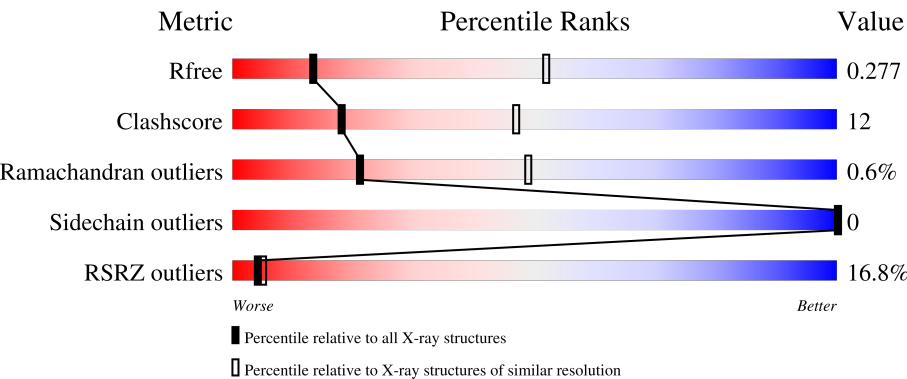
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

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

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	531	2% 75% 15% • 9%
1	B	531	2% 74% 17% • 9%
1	C	531	2% 71% 19% • 9%
1	D	531	% 76% 15% • 9%
1	E	531	45% 54% 36% 10%

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Mol	Chain	Length	Quality of chain
1	F	531	40% 52% 37% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22960 atoms, of which 22 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.

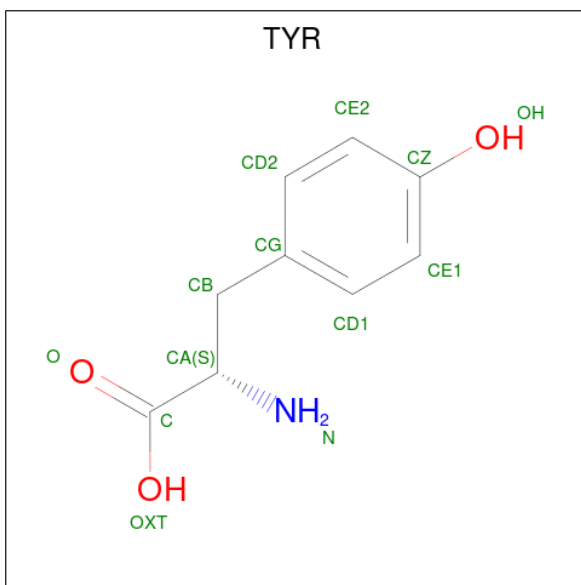
- Molecule 1 is a protein called Tyrosine/DOPA decarboxylase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	P	S	0	0	0
			3841	2467	641	708	1	24			
1	B	483	Total	C	N	O	P	S	0	0	0
			3824	2457	637	705	1	24			
1	C	485	Total	C	N	O	P	S	0	0	0
			3841	2467	641	708	1	24			
1	D	483	Total	C	N	O	P	S	0	0	0
			3824	2457	637	705	1	24			
1	E	479	Total	C	N	O	P	S	0	0	0
			3803	2445	633	700	1	24			
1	F	474	Total	C	N	O	P	S	0	0	0
			3755	2417	625	688	1	24			

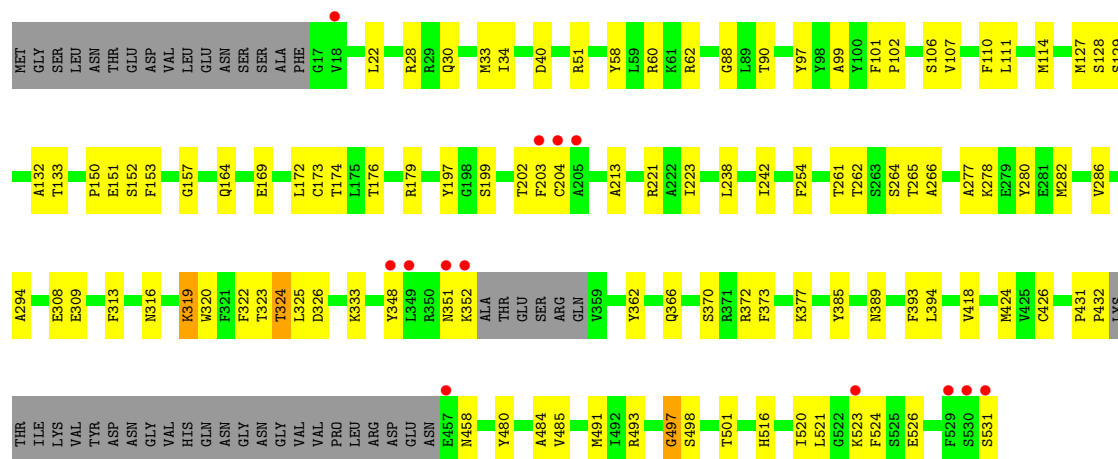
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	PHE	HIS	engineered mutation	UNP P54769
B	203	PHE	HIS	engineered mutation	UNP P54769
C	203	PHE	HIS	engineered mutation	UNP P54769
D	203	PHE	HIS	engineered mutation	UNP P54769
E	203	PHE	HIS	engineered mutation	UNP P54769
F	203	PHE	HIS	engineered mutation	UNP P54769

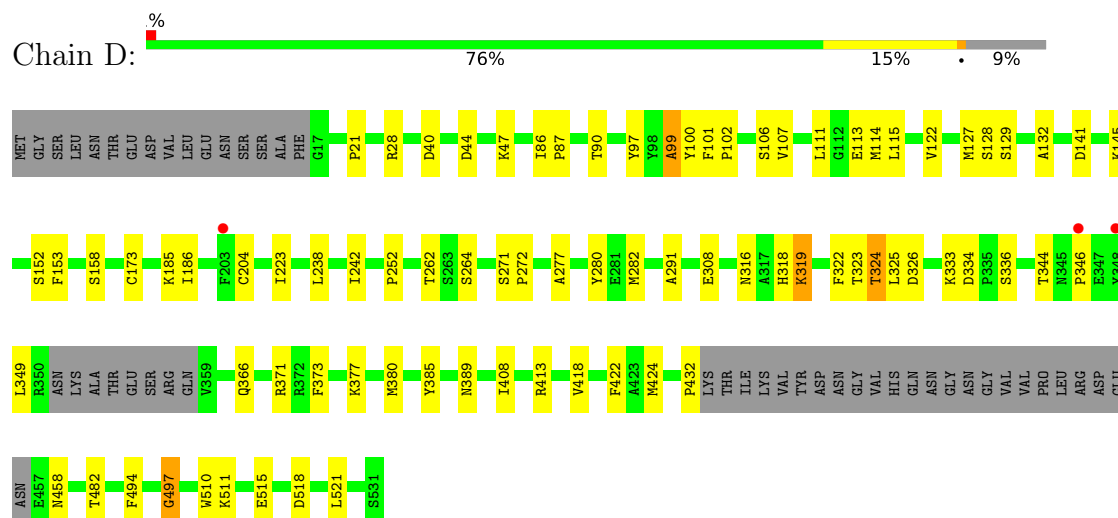
- Molecule 2 is TYROSINE (CCD ID: TYR) (formula: $C_9H_{11}NO_3$) (labeled as "Ligand of Interest" by depositor).



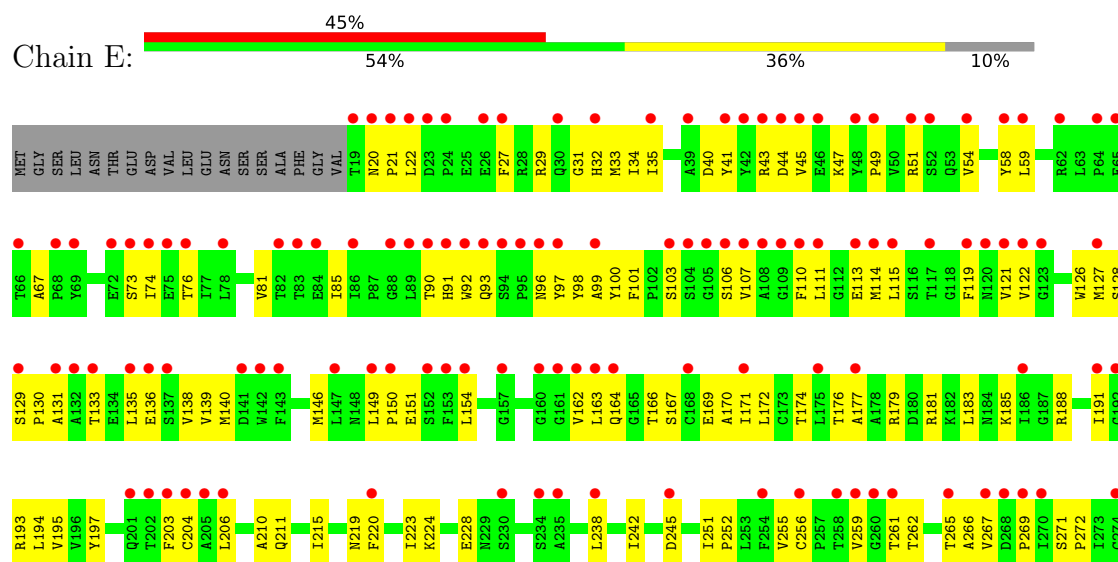
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			24	9	11	1	3		
2	B	1	Total	C	H	N	O	0	0
			24	9	11	1	3		
2	C	1	Total	C	N	O		0	0
			12	9	1	2			
2	D	1	Total	C	N	O		0	0
			12	9	1	2			

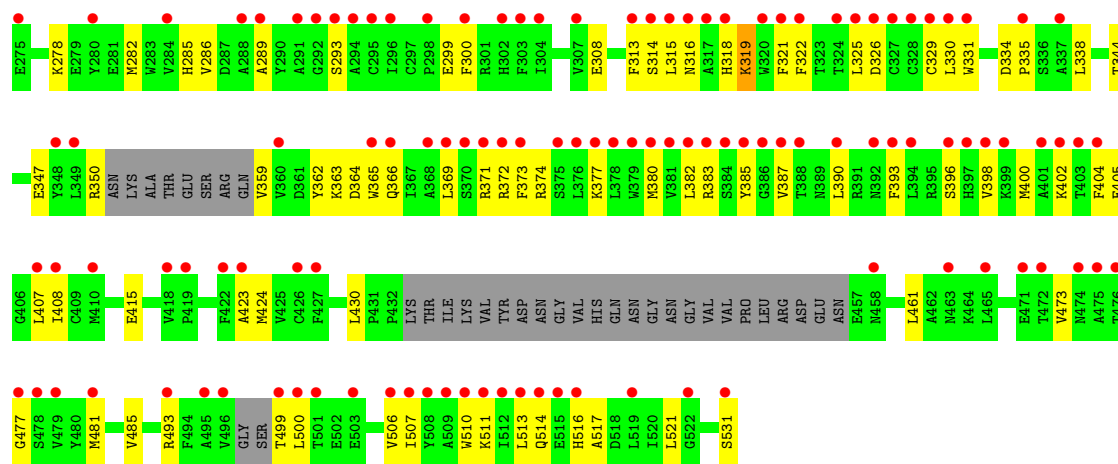


• Molecule 1: Tyrosine/DOPA decarboxylase 2

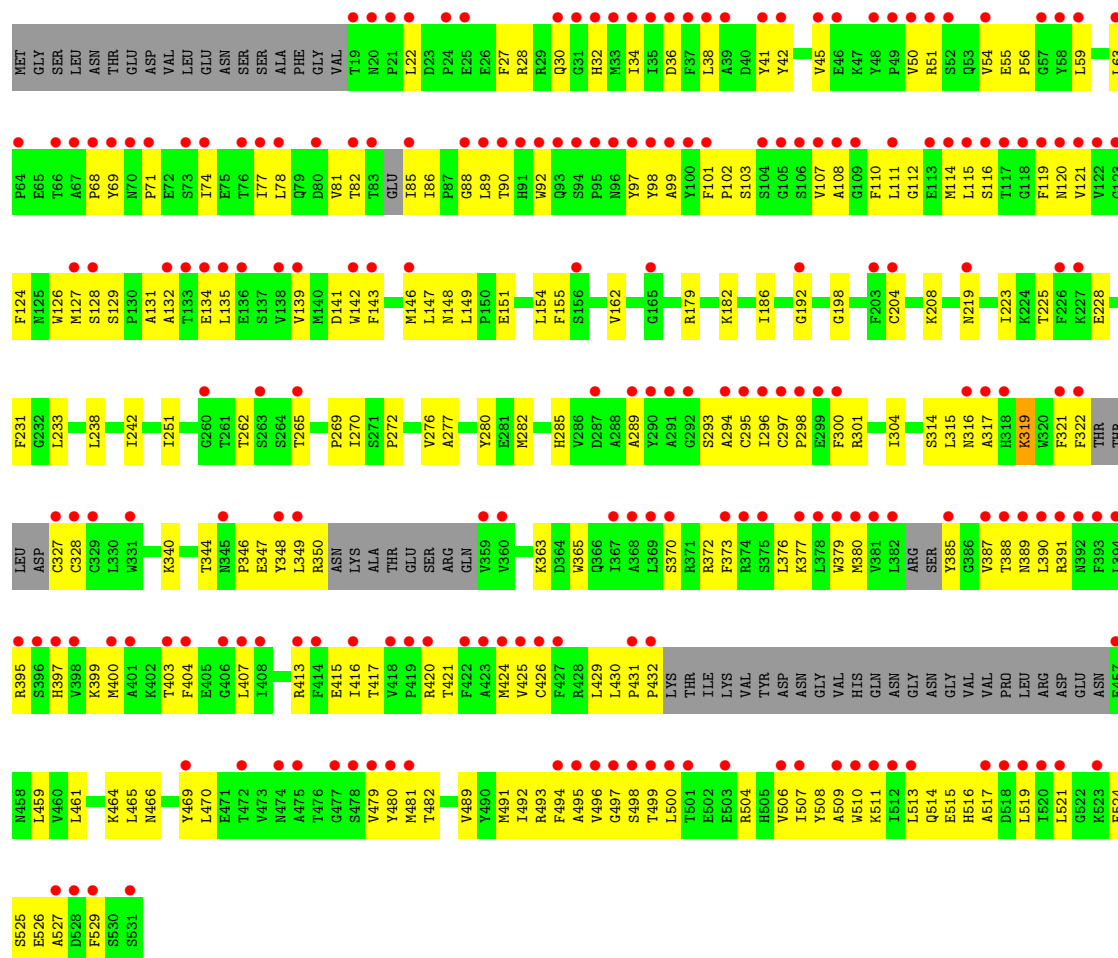
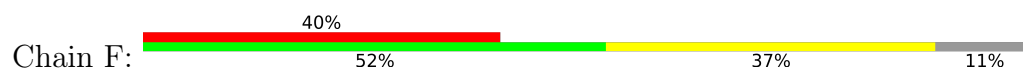


• Molecule 1: Tyrosine/DOPA decarboxylase 2





● Molecule 1: Tyrosine/DOPA decarboxylase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	218.55Å 118.50Å 181.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.41 – 3.35 48.41 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.41-3.35) 99.9 (48.41-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.16_3549, PHENIX 1.16_3549	Depositor
R, R_{free}	0.234 , 0.279 0.233 , 0.277	Depositor DCC
R_{free} test set	3433 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	22960	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8880e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LLP

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	0.07	0/3910	0.27	0/5308
1	B	0.07	0/3893	0.27	0/5286
1	C	0.08	0/3910	0.26	0/5308
1	D	0.07	0/3893	0.25	0/5286
1	E	0.08	0/3871	0.27	0/5255
1	F	0.08	0/3821	0.31	0/5183
All	All	0.08	0/23298	0.27	0/31626

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3841	0	3785	65	0
1	B	3824	0	3766	64	0
1	C	3841	0	3785	78	0
1	D	3824	0	3766	62	0
1	E	3803	0	3745	167	0
1	F	3755	0	3692	192	0
2	A	13	11	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	13	11	8	1	0
2	C	12	0	8	3	0
2	D	12	0	8	2	0
All	All	22938	22	22571	557	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 12.

All (557) 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:E:113:GLU:HG3	1:E:377:LYS:HE2	1.53	0.90
1:E:481:MET:HE1	1:E:513:LEU:HD21	1.51	0.90
1:F:108:ALA:HB1	1:F:380:MET:HB3	1.54	0.89
1:C:277:ALA:HA	1:C:282:MET:HE3	1.54	0.87
1:F:81:VAL:HG13	1:F:85:ILE:HB	1.59	0.85
1:A:344:THR:HG21	1:B:204:CYS:HB3	1.58	0.83
1:B:323:THR:O	1:B:324:THR:OG1	1.97	0.81
1:F:280:TYR:HB2	1:F:282:MET:HE2	1.62	0.81
1:E:511:LYS:HA	1:E:514:GLN:HG2	1.64	0.80
1:B:277:ALA:HA	1:B:282:MET:HE3	1.64	0.78
1:F:415:GLU:HB2	1:F:430:LEU:HD11	1.66	0.76
1:C:485:VAL:HB	1:E:531:SER:HA	1.68	0.75
1:F:413:ARG:HH21	1:F:517:ALA:HB3	1.49	0.75
1:C:30:GLN:HA	1:C:33:MET:HE3	1.68	0.74
1:C:280:TYR:HB2	1:C:282:MET:HE2	1.69	0.74
1:A:481:MET:HE3	1:A:494:PHE:HD1	1.52	0.74
1:D:277:ALA:HA	1:D:282:MET:HE3	1.68	0.74
1:D:323:THR:O	1:D:324:THR:HG22	1.88	0.74
1:E:127:MET:HE2	1:F:51:ARG:HH21	1.52	0.74
1:F:277:ALA:HA	1:F:282:MET:HE3	1.70	0.74
1:A:323:THR:O	1:A:324:THR:HB	1.89	0.72
1:C:262:THR:HG1	2:C:601:TYR:N	1.86	0.72
1:A:280:TYR:HB2	1:A:282:MET:HE2	1.72	0.71
1:F:417:THR:HG21	1:F:491:MET:HB2	1.73	0.71
1:F:417:THR:OG1	1:F:426:CYS:HB2	1.88	0.71
1:D:264:SER:HB2	1:D:418:VAL:HG21	1.72	0.71
1:F:521:LEU:HA	1:F:524:PHE:HB2	1.73	0.71
1:C:242:ILE:HD13	1:C:282:MET:HE1	1.72	0.71
1:F:285:HIS:HE2	1:F:314:SER:HG	1.36	0.71
1:C:323:THR:O	1:C:324:THR:OG1	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ALA:HA	1:A:282:MET:HE3	1.73	0.70
1:C:204:CYS:HB3	1:D:344:THR:HG21	1.73	0.70
1:F:111:LEU:O	1:F:115:LEU:HD12	1.92	0.69
1:D:316:ASN:HD22	1:D:319:LLP:HE2	1.58	0.69
1:A:413:ARG:NH1	1:A:518:ASP:OD1	2.23	0.69
1:E:151:GLU:HA	1:E:154:LEU:HG	1.74	0.69
1:E:344:THR:HG21	1:F:204:CYS:HB3	1.73	0.68
1:E:122:VAL:N	1:F:92:TRP:HZ2	1.92	0.68
1:E:289:ALA:HA	1:E:316:ASN:H	1.58	0.67
1:F:289:ALA:HA	1:F:315:LEU:HA	1.77	0.67
1:E:107:VAL:HA	1:E:110:PHE:HB3	1.75	0.67
1:D:102:PRO:HG3	1:D:497:GLY:HA3	1.74	0.67
1:E:122:VAL:H	1:F:92:TRP:HZ2	1.43	0.67
1:A:242:ILE:HD13	1:A:282:MET:HE1	1.77	0.66
1:E:44:ASP:HB2	1:E:47:LYS:HD3	1.77	0.66
1:E:424:MET:SD	1:E:493:ARG:NH1	2.68	0.66
1:B:280:TYR:HB2	1:B:282:MET:HE2	1.76	0.66
1:E:67:ALA:HB2	1:F:142:TRP:HB3	1.78	0.66
1:E:128:SER:HB3	1:F:92:TRP:HH2	1.60	0.65
1:A:346:PRO:HG2	1:A:349:LEU:HD12	1.78	0.65
1:E:261:THR:HG22	1:E:266:ALA:H	1.62	0.65
1:C:264:SER:HB2	1:C:418:VAL:HG21	1.77	0.65
1:D:280:TYR:HB2	1:D:282:MET:HE2	1.77	0.65
1:E:293:SER:HB3	1:E:321:PHE:HD1	1.62	0.65
1:C:97:TYR:CZ	1:C:99:ALA:HB3	2.31	0.65
1:D:325:LEU:HG	1:D:326:ASP:HB3	1.78	0.65
1:E:101:PHE:HE2	1:E:262:THR:HA	1.62	0.65
1:F:242:ILE:HD13	1:F:282:MET:HE1	1.77	0.64
1:E:398:VAL:HG22	1:E:423:ALA:HB2	1.78	0.64
1:A:113:GLU:HG2	1:A:377:LYS:HD3	1.81	0.64
1:F:420:ARG:HG3	1:F:425:VAL:HB	1.79	0.64
1:C:101:PHE:HE2	1:C:262:THR:HA	1.64	0.63
1:E:166:THR:HG23	1:E:169:GLU:H	1.63	0.63
1:E:265:THR:HB	1:E:424:MET:HE2	1.80	0.63
1:F:429:LEU:HD11	1:F:521:LEU:HD11	1.79	0.63
1:A:179:ARG:NH1	1:A:213:ALA:O	2.31	0.63
1:C:531:SER:HA	1:E:485:VAL:HB	1.80	0.63
1:E:170:ALA:HB1	1:E:330:LEU:HD22	1.79	0.63
1:B:264:SER:HB2	1:B:418:VAL:HG21	1.80	0.63
1:C:128:SER:O	1:D:90:THR:HB	1.99	0.63
1:E:34:ILE:HD13	1:F:111:LEU:HD13	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:PHE:CE2	1:E:262:THR:HA	2.34	0.62
1:F:51:ARG:HD3	1:F:480:TYR:CE1	2.35	0.62
1:E:383:ARG:HG2	1:F:68:PRO:HG3	1.82	0.62
1:F:131:ALA:O	1:F:135:LEU:HD12	1.99	0.62
1:A:40:ASP:OD1	1:B:28:ARG:NH2	2.33	0.62
1:A:200:ASP:OD2	1:A:224:LYS:HD3	2.00	0.61
1:D:326:ASP:O	1:D:377:LYS:NZ	2.27	0.61
1:E:31:GLY:HA2	1:F:111:LEU:HD11	1.81	0.61
1:E:81:VAL:HA	1:E:85:ILE:HD13	1.83	0.61
1:E:97:TYR:CE1	1:E:99:ALA:HB3	2.35	0.61
1:E:128:SER:HB3	1:F:92:TRP:CH2	2.36	0.61
1:E:41:TYR:O	1:E:45:VAL:HG13	2.01	0.61
1:C:60:ARG:NH2	1:D:141:ASP:OD2	2.34	0.61
1:E:197:TYR:HB2	1:E:255:VAL:HG12	1.82	0.61
1:C:523:LYS:O	1:C:523:LYS:HD3	2.01	0.60
1:E:41:TYR:HH	1:E:91:HIS:HD1	1.48	0.60
1:E:96:ASN:HA	1:E:98:TYR:CZ	2.36	0.60
1:F:143:PHE:HE1	1:F:296:ILE:HD11	1.65	0.60
1:E:176:THR:HG22	1:E:179:ARG:HH21	1.66	0.60
1:A:35:ILE:HD11	1:A:114:MET:HE1	1.84	0.60
1:C:526:GLU:HB3	1:E:224:LYS:HE2	1.84	0.60
1:F:92:TRP:CD1	1:F:103:SER:HB3	2.37	0.60
1:F:102:PRO:HG3	1:F:497:GLY:HA3	1.83	0.60
1:C:114:MET:HG2	1:D:114:MET:SD	2.42	0.59
1:E:92:TRP:HB3	1:E:103:SER:HB3	1.84	0.59
1:F:400:MET:HE3	1:F:506:VAL:HG21	1.84	0.59
1:B:323:THR:C	1:B:324:THR:HG1	2.06	0.59
1:F:74:ILE:HA	1:F:77:ILE:HG22	1.84	0.59
1:E:191:ILE:HD12	1:E:194:LEU:HD12	1.84	0.59
1:F:81:VAL:HG12	1:F:86:ILE:HG13	1.84	0.59
1:A:481:MET:HE3	1:A:494:PHE:CD1	2.36	0.59
1:F:74:ILE:O	1:F:78:LEU:HG	2.03	0.59
1:F:399:LYS:O	1:F:403:THR:HG23	2.03	0.59
1:B:481:MET:HE1	1:B:513:LEU:HD21	1.83	0.59
1:E:286:VAL:HB	1:E:313:PHE:HD1	1.67	0.59
1:A:146:MET:HE3	1:A:387:VAL:HG22	1.84	0.59
1:E:111:LEU:HD11	1:F:30:GLN:HB3	1.85	0.59
1:F:50:VAL:HG21	1:F:479:VAL:C	2.28	0.59
1:B:203:PHE:CD1	1:B:262:THR:HG21	2.38	0.58
1:E:135:LEU:O	1:E:139:VAL:HG22	2.03	0.58
1:A:136:GLU:OE1	1:A:371:ARG:NH2	2.25	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ARG:NH2	1:D:40:ASP:OD1	2.36	0.58
1:E:54:VAL:HG13	1:E:58:TYR:CD2	2.38	0.58
1:F:192:GLY:O	1:F:219:ASN:ND2	2.36	0.58
1:E:107:VAL:HG21	1:F:27:PHE:HA	1.86	0.58
1:E:40:ASP:OD1	1:E:43:ARG:NH1	2.33	0.58
1:C:484:ALA:HB2	1:C:493:ARG:HD2	1.86	0.57
1:C:426:CYS:HB3	1:C:491:MET:HE3	1.85	0.57
1:A:30:GLN:HA	1:A:33:MET:HE3	1.85	0.57
1:D:106:SER:HB3	1:D:322:PHE:HB3	1.85	0.57
1:F:265:THR:O	1:F:421:THR:OG1	2.21	0.57
1:D:408:ILE:HD13	1:D:510:TRP:HZ3	1.69	0.57
1:F:126:TRP:NE1	1:F:134:GLU:OE2	2.37	0.57
1:E:166:THR:HG23	1:E:169:GLU:HB2	1.85	0.57
1:E:211:GLN:O	1:F:179:ARG:NH2	2.31	0.57
1:C:106:SER:HB3	1:C:322:PHE:HB3	1.87	0.56
1:F:51:ARG:HD3	1:F:480:TYR:CZ	2.40	0.56
1:F:388:THR:HA	1:F:391:ARG:HG3	1.86	0.56
1:B:99:ALA:HB1	1:B:482:THR:HG23	1.87	0.56
1:C:326:ASP:O	1:C:377:LYS:NZ	2.37	0.56
1:E:366:GLN:HE22	1:E:371:ARG:HG3	1.70	0.56
1:F:74:ILE:O	1:F:77:ILE:HG22	2.06	0.56
1:F:88:GLY:O	1:F:89:LEU:HD23	2.05	0.56
1:F:293:SER:HB3	1:F:321:PHE:CD1	2.41	0.56
1:C:372:ARG:HG2	1:D:325:LEU:HD23	1.87	0.56
1:E:204:CYS:HB2	1:F:344:THR:HG21	1.88	0.56
1:B:296:ILE:HG22	1:B:391:ARG:HG2	1.87	0.56
1:B:385:TYR:O	1:B:389:ASN:HB2	2.05	0.56
1:D:308:GLU:O	1:D:333:LYS:NZ	2.26	0.56
1:F:162:VAL:HB	1:F:365:TRP:CE3	2.40	0.56
1:A:424:MET:SD	1:A:493:ARG:NH2	2.79	0.56
1:E:278:LYS:HD2	1:E:278:LYS:O	2.06	0.55
1:F:151:GLU:HA	1:F:154:LEU:HG	1.88	0.55
1:F:319:LLP:NZ	1:F:319:LLP:O3	2.39	0.55
1:F:420:ARG:HG2	1:F:424:MET:O	2.07	0.55
1:E:415:GLU:HB2	1:E:430:LEU:HD11	1.88	0.55
1:F:98:TYR:OH	1:F:506:VAL:HA	2.06	0.55
1:F:141:ASP:OD2	1:F:155:PHE:HB2	2.06	0.55
1:A:34:ILE:HG13	1:B:111:LEU:HD22	1.89	0.55
1:C:34:ILE:HG13	1:D:111:LEU:HD22	1.88	0.55
1:E:107:VAL:O	1:E:111:LEU:HG	2.06	0.55
1:D:101:PHE:CE2	1:D:262:THR:HA	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:LEU:HD12	1:E:315:LEU:O	2.06	0.55
1:A:174:THR:HG22	1:A:254:PHE:HE2	1.70	0.55
1:F:510:TRP:CD1	1:F:511:LYS:HZ3	2.25	0.55
1:F:385:TYR:C	1:F:389:ASN:HD21	2.15	0.55
1:B:325:LEU:HG	1:B:326:ASP:HB3	1.89	0.54
1:E:404:PHE:CE1	1:E:408:ILE:HD11	2.42	0.54
1:C:521:LEU:HA	1:C:524:PHE:HB2	1.88	0.54
1:D:346:PRO:HG2	1:D:349:LEU:HD12	1.89	0.54
1:F:99:ALA:HB1	1:F:482:THR:HG23	1.88	0.54
1:F:110:PHE:HD2	1:F:111:LEU:HG	1.71	0.54
1:C:348:TYR:O	1:C:351:ASN:ND2	2.39	0.54
1:D:318:HIS:CD2	1:D:325:LEU:HD12	2.42	0.54
1:F:297:CYS:HA	1:F:391:ARG:HH11	1.73	0.54
1:C:40:ASP:OD1	1:D:28:ARG:NH2	2.30	0.54
1:E:166:THR:OG1	1:E:319:LLP:OP2	2.24	0.54
1:F:101:PHE:HE1	1:F:424:MET:HE3	1.73	0.54
1:B:106:SER:HB3	1:B:322:PHE:HB3	1.90	0.54
1:C:101:PHE:CE2	1:C:262:THR:HA	2.42	0.54
1:E:206:LEU:HG	1:E:220:PHE:HE1	1.73	0.54
1:F:233:LEU:HD21	1:F:238:LEU:HB2	1.89	0.54
1:A:323:THR:O	1:A:324:THR:CB	2.55	0.53
1:B:127:MET:HE3	1:B:127:MET:HA	1.91	0.53
1:A:316:ASN:HD22	1:A:319:LLP:HE2	1.72	0.53
1:D:511:LYS:NZ	1:D:515:GLU:OE2	2.39	0.53
1:B:100:TYR:HB3	2:B:601:TYR:HB3	1.89	0.53
1:E:499:THR:HG23	1:F:22:LEU:HD23	1.88	0.53
1:E:259:VAL:HG13	1:E:267:VAL:HG13	1.91	0.53
1:E:49:PRO:HA	1:E:477:GLY:HA3	1.91	0.53
1:E:366:GLN:NE2	1:E:371:ARG:HG3	2.23	0.53
1:A:106:SER:HB3	1:A:322:PHE:HB3	1.91	0.53
1:E:34:ILE:HG21	1:F:111:LEU:HD22	1.91	0.53
1:F:322:PHE:CE1	1:F:499:THR:HG21	2.44	0.53
1:F:340:LYS:HE3	1:F:347:GLU:OE1	2.08	0.53
1:C:278:LYS:HE2	1:C:309:GLU:O	2.09	0.53
1:E:238:LEU:O	1:E:242:ILE:HG13	2.09	0.53
1:E:183:LEU:HB3	1:E:188:ARG:HG2	1.91	0.52
1:A:174:THR:HG22	1:A:254:PHE:CE2	2.44	0.52
1:D:271:SER:HB3	1:D:272:PRO:HD3	1.91	0.52
1:F:132:ALA:HA	1:F:373:PHE:CE1	2.44	0.52
1:A:264:SER:HB2	1:A:418:VAL:HG21	1.90	0.52
1:A:516:HIS:O	1:A:520:ILE:HG12	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:GLU:HG2	1:E:300:PHE:CD1	2.45	0.52
1:A:102:PRO:HG3	1:A:497:GLY:HA3	1.92	0.52
1:E:32:HIS:NE2	1:F:36:ASP:OD1	2.42	0.52
1:E:151:GLU:HG3	1:E:154:LEU:HB2	1.92	0.52
1:F:404:PHE:HD1	1:F:407:LEU:HD12	1.75	0.52
1:A:408:ILE:HG12	1:A:510:TRP:CZ3	2.44	0.52
1:B:172:LEU:O	1:B:176:THR:HG23	2.10	0.52
1:F:316:ASN:HA	1:F:328:CYS:HA	1.91	0.52
1:B:143:PHE:CE1	1:B:296:ILE:HD11	2.45	0.52
1:F:162:VAL:HB	1:F:365:TRP:HE3	1.75	0.52
1:F:348:TYR:CD1	1:F:349:LEU:HG	2.45	0.52
1:E:121:VAL:HG21	1:E:129:SER:HB2	1.92	0.52
1:E:122:VAL:N	1:F:92:TRP:CZ2	2.72	0.52
1:E:321:PHE:CZ	1:E:390:LEU:HD13	2.45	0.52
1:B:429:LEU:HD11	1:B:521:LEU:HD11	1.91	0.52
1:F:293:SER:HB3	1:F:321:PHE:CE1	2.45	0.52
1:C:242:ILE:CD1	1:C:282:MET:HE1	2.38	0.51
1:F:127:MET:HE3	1:F:127:MET:HA	1.92	0.51
1:A:308:GLU:O	1:A:333:LYS:NZ	2.33	0.51
1:E:299:GLU:HG2	1:E:300:PHE:HD1	1.75	0.51
1:F:289:ALA:HB1	1:F:316:ASN:ND2	2.25	0.51
1:A:429:LEU:N	1:A:466:ASN:OD1	2.35	0.51
1:F:346:PRO:O	1:F:350:ARG:HG3	2.11	0.51
1:A:99:ALA:HB1	1:A:482:THR:HG23	1.93	0.51
1:E:111:LEU:HB3	1:F:34:ILE:HG13	1.92	0.51
1:E:252:PRO:HB2	1:E:282:MET:SD	2.51	0.51
1:E:278:LYS:HD2	1:E:278:LYS:C	2.35	0.51
1:B:51:ARG:HD3	1:B:480:TYR:CE1	2.45	0.51
1:E:372:ARG:O	1:E:374:ARG:N	2.44	0.51
1:F:51:ARG:HA	1:F:90:THR:HG23	1.92	0.51
1:C:101:PHE:HB2	2:C:601:TYR:CD1	2.46	0.50
1:E:517:ALA:O	1:E:521:LEU:HB2	2.11	0.50
1:B:429:LEU:N	1:B:466:ASN:OD1	2.40	0.50
1:D:100:TYR:HB3	2:D:601:TYR:HA	1.93	0.50
1:A:261:THR:HG1	1:A:266:ALA:H	1.58	0.50
1:B:25:GLU:OE2	1:B:28:ARG:NH1	2.45	0.50
1:E:92:TRP:H	1:F:121:VAL:HG12	1.76	0.50
1:F:38:LEU:O	1:F:41:TYR:HB3	2.11	0.50
1:E:93:GLN:CD	1:E:93:GLN:H	2.20	0.50
1:E:171:ILE:HA	1:E:174:THR:HG22	1.94	0.50
1:A:242:ILE:CD1	1:A:282:MET:HE1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ILE:HD13	1:B:282:MET:HE1	1.93	0.50
1:E:203:PHE:CD1	1:E:262:THR:HG21	2.47	0.50
1:F:148:ASN:HB3	1:F:301:ARG:HH11	1.76	0.50
1:B:252:PRO:HB2	1:B:282:MET:SD	2.52	0.50
1:E:181:ARG:NH1	1:E:334:ASP:OD2	2.44	0.50
1:D:107:VAL:O	1:D:111:LEU:HG	2.12	0.49
1:E:22:LEU:HB2	1:F:500:LEU:HD11	1.92	0.49
1:E:223:ILE:HD13	1:E:238:LEU:HA	1.94	0.49
1:A:393:PHE:CZ	1:B:21:PRO:HG3	2.47	0.49
1:E:195:VAL:HG12	1:E:219:ASN:HB3	1.94	0.49
1:F:525:SER:C	1:F:527:ALA:H	2.21	0.49
1:A:204:CYS:HB3	1:B:344:THR:HG21	1.94	0.49
1:A:344:THR:CG2	1:B:204:CYS:HB3	2.35	0.49
1:B:143:PHE:HE1	1:B:296:ILE:HD11	1.77	0.49
1:B:508:TYR:CZ	1:B:512:ILE:HD11	2.47	0.49
1:D:141:ASP:O	1:D:145:LYS:HG3	2.12	0.49
1:F:298:PRO:HD3	1:F:391:ARG:HH12	1.76	0.49
1:B:316:ASN:HD22	1:B:319:LLP:HE2	1.78	0.49
1:D:366:GLN:OE1	1:D:371:ARG:HD2	2.12	0.49
1:E:34:ILE:CG2	1:F:111:LEU:HD22	2.43	0.49
1:C:458:ASN:OD1	1:C:458:ASN:N	2.45	0.49
1:E:271:SER:HB2	1:E:272:PRO:HD3	1.95	0.49
1:C:164:GLN:OE1	1:C:169:GLU:HG2	2.13	0.49
1:D:458:ASN:N	1:D:458:ASN:OD1	2.45	0.49
1:E:106:SER:OG	1:E:322:PHE:HB3	2.12	0.49
1:E:121:VAL:HG23	1:F:92:TRP:CZ2	2.47	0.49
1:D:86:ILE:N	1:D:87:PRO:HD2	2.28	0.49
1:E:135:LEU:HA	1:E:138:VAL:HG12	1.94	0.49
1:F:497:GLY:O	1:F:498:SER:HB3	2.12	0.49
1:D:334:ASP:OD1	1:D:336:SER:OG	2.30	0.49
1:F:147:LEU:HB2	1:F:149:LEU:HG	1.94	0.49
1:B:308:GLU:O	1:B:333:LYS:NZ	2.33	0.49
1:E:131:ALA:HB1	1:F:85:ILE:HD13	1.94	0.49
1:E:383:ARG:HB2	1:F:77:ILE:HD12	1.94	0.48
1:C:132:ALA:HA	1:C:373:PHE:CE1	2.48	0.48
1:F:82:THR:HA	1:F:86:ILE:HD12	1.95	0.48
1:F:400:MET:HE2	1:F:496:VAL:HG11	1.95	0.48
1:C:110:PHE:O	1:C:114:MET:HG3	2.13	0.48
1:E:133:THR:HG22	1:E:362:TYR:HD2	1.79	0.48
1:E:146:MET:HE1	1:E:382:LEU:HD22	1.94	0.48
1:E:383:ARG:CB	1:F:77:ILE:HD12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:THR:O	1:C:324:THR:CB	2.62	0.48
1:A:113:GLU:HG2	1:A:377:LYS:CD	2.42	0.48
1:F:101:PHE:CE1	1:F:424:MET:HE3	2.48	0.48
1:D:153:PHE:CE1	1:D:333:LYS:HG3	2.48	0.48
1:F:54:VAL:HG12	1:F:55:GLU:H	1.79	0.48
1:F:322:PHE:HE1	1:F:499:THR:HG21	1.79	0.48
1:A:294:ALA:HB2	1:A:320:TRP:CZ3	2.49	0.48
1:E:193:ARG:HB2	1:E:251:ILE:HD12	1.95	0.48
1:C:516:HIS:O	1:C:520:ILE:HG12	2.14	0.48
1:D:113:GLU:HB2	1:D:377:LYS:HD3	1.94	0.48
1:F:269:PRO:HB2	1:F:272:PRO:HD2	1.96	0.48
1:C:197:TYR:CE1	1:C:221:ARG:HG3	2.49	0.48
1:B:322:PHE:HZ	1:B:393:PHE:HB3	1.78	0.48
1:A:319:LLP:OP3	1:B:370:SER:OG	2.29	0.47
1:B:468:VAL:O	1:B:472:THR:HG23	2.14	0.47
1:E:289:ALA:HA	1:E:315:LEU:HA	1.95	0.47
1:F:404:PHE:HE1	1:F:510:TRP:CZ3	2.32	0.47
1:A:216:ASN:OD1	1:A:218:LYS:HD2	2.15	0.47
1:A:102:PRO:CG	1:A:497:GLY:HA3	2.44	0.47
1:A:114:MET:HG3	1:B:110:PHE:HZ	1.79	0.47
1:A:239:ARG:NH2	1:A:279:GLU:OE1	2.37	0.47
1:E:73:SER:OG	1:E:76:THR:HG22	2.14	0.47
1:E:197:TYR:OH	1:E:245:ASP:OD2	2.29	0.47
1:E:335:PRO:HB3	1:E:365:TRP:CH2	2.50	0.47
1:F:59:LEU:CD2	1:F:63:LEU:HD21	2.44	0.47
1:F:119:PHE:O	1:F:121:VAL:HG13	2.13	0.47
1:C:370:SER:OG	1:D:319:LLP:OP3	2.30	0.47
1:D:152:SER:HA	1:D:158:SER:HB3	1.96	0.47
1:F:459:LEU:HD11	1:F:489:VAL:HA	1.97	0.47
1:C:203:PHE:CD1	1:C:262:THR:HG21	2.49	0.47
1:D:242:ILE:HD13	1:D:282:MET:HE1	1.96	0.47
1:F:142:TRP:O	1:F:146:MET:HG3	2.15	0.47
1:F:385:TYR:HB3	1:F:390:LEU:HD21	1.96	0.47
1:D:97:TYR:CZ	1:D:99:ALA:HB3	2.50	0.47
1:D:122:VAL:O	1:D:128:SER:HB3	2.14	0.47
1:E:20:ASN:ND2	1:E:21:PRO:HD2	2.30	0.47
1:F:385:TYR:O	1:F:389:ASN:ND2	2.46	0.47
1:F:404:PHE:HA	1:F:407:LEU:HD12	1.96	0.47
1:F:420:ARG:CZ	1:F:420:ARG:HB3	2.45	0.47
1:F:511:LYS:HA	1:F:514:GLN:HB3	1.96	0.47
1:D:242:ILE:CD1	1:D:282:MET:HE1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:LEU:HD23	1:E:150:PRO:HD2	1.97	0.46
1:D:115:LEU:HD12	1:D:380:MET:HE2	1.98	0.46
1:E:402:LYS:HA	1:E:405:GLU:HB3	1.96	0.46
1:F:198:GLY:O	1:F:223:ILE:HG12	2.16	0.46
1:E:407:LEU:HD13	1:E:510:TRP:CD1	2.50	0.46
1:F:415:GLU:HB3	1:F:430:LEU:HD21	1.97	0.46
1:E:326:ASP:CG	1:E:374:ARG:HH12	2.23	0.46
1:A:114:MET:HG3	1:B:110:PHE:CZ	2.49	0.46
1:C:151:GLU:HG2	1:C:157:GLY:HA3	1.96	0.46
1:D:346:PRO:HG2	1:D:349:LEU:CD1	2.46	0.46
1:E:127:MET:HE3	1:F:51:ARG:HB3	1.97	0.46
1:E:172:LEU:O	1:E:176:THR:HG23	2.16	0.46
1:A:372:ARG:HG2	1:B:325:LEU:HD23	1.97	0.46
1:B:111:LEU:HB2	1:B:380:MET:HE3	1.97	0.46
1:B:265:THR:HG23	1:B:424:MET:HE2	1.98	0.46
1:E:81:VAL:HG22	1:F:379:TRP:HZ3	1.79	0.46
1:E:206:LEU:HD22	1:E:256:CYS:HB3	1.97	0.46
1:A:44:ASP:O	1:A:47:LYS:HG2	2.16	0.46
1:C:102:PRO:CG	1:C:497:GLY:HA3	2.46	0.46
1:C:385:TYR:O	1:C:389:ASN:HB2	2.16	0.46
1:C:432:PRO:HD2	1:C:524:PHE:CE2	2.51	0.46
1:E:41:TYR:OH	1:E:91:HIS:ND1	2.40	0.46
1:A:199:SER:H	1:A:202:THR:CG2	2.29	0.46
1:A:199:SER:H	1:A:202:THR:HG23	1.80	0.46
1:E:129:SER:HA	1:F:89:LEU:HA	1.96	0.46
1:E:135:LEU:HD22	1:F:85:ILE:HD11	1.98	0.46
1:A:90:THR:HB	1:B:128:SER:O	2.16	0.46
1:B:286:VAL:HB	1:B:313:PHE:HD1	1.81	0.46
1:C:199:SER:H	1:C:202:THR:HG23	1.80	0.46
1:C:325:LEU:HA	1:C:326:ASP:HA	1.52	0.46
1:E:285:HIS:NE2	1:E:314:SER:OG	2.47	0.46
1:E:289:ALA:HA	1:E:316:ASN:N	2.30	0.46
1:D:413:ARG:HD2	1:D:521:LEU:HD12	1.97	0.45
1:E:115:LEU:O	1:E:119:PHE:N	2.38	0.45
1:F:51:ARG:HG2	1:F:480:TYR:CD2	2.50	0.45
1:F:143:PHE:CE1	1:F:296:ILE:HD11	2.47	0.45
1:F:289:ALA:HB1	1:F:316:ASN:HD21	1.81	0.45
1:E:31:GLY:O	1:E:35:ILE:HG12	2.16	0.45
1:F:270:ILE:HD12	1:F:304:ILE:HA	1.98	0.45
1:E:136:GLU:OE2	1:E:163:LEU:N	2.47	0.45
1:D:185:LYS:HG3	1:D:186:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:MET:HB3	1:E:506:VAL:HG21	1.97	0.45
1:F:429:LEU:HD12	1:F:465:LEU:HD21	1.98	0.45
1:E:325:LEU:HD11	1:F:370:SER:OG	2.17	0.45
1:E:177:ALA:HB2	1:E:338:LEU:HD23	1.98	0.45
1:C:107:VAL:O	1:C:111:LEU:HG	2.17	0.45
1:E:181:ARG:O	1:E:185:LYS:HG3	2.17	0.45
1:A:324:THR:HG22	1:A:377:LYS:CD	2.47	0.45
1:D:99:ALA:HB1	1:D:482:THR:HG23	1.99	0.45
1:A:324:THR:HG22	1:A:377:LYS:HD3	1.99	0.45
1:B:146:MET:HB3	1:B:296:ILE:HG13	1.99	0.45
1:B:326:ASP:O	1:B:377:LYS:NZ	2.32	0.45
1:C:127:MET:HE3	1:C:127:MET:HA	1.98	0.45
1:D:325:LEU:HA	1:D:326:ASP:HA	1.50	0.45
1:E:228:GLU:OE1	1:E:228:GLU:N	2.47	0.45
1:C:179:ARG:NH1	1:C:213:ALA:O	2.45	0.44
1:C:316:ASN:HD22	1:C:319:LLP:HE2	1.80	0.44
1:C:352:LYS:HA	1:C:352:LYS:HD2	1.81	0.44
1:E:315:LEU:HD12	1:E:315:LEU:C	2.41	0.44
1:C:265:THR:HB	1:C:424:MET:HE2	1.98	0.44
1:F:98:TYR:HB2	1:F:481:MET:HG2	1.97	0.44
1:B:107:VAL:O	1:B:111:LEU:HG	2.17	0.44
1:B:322:PHE:CZ	1:B:393:PHE:HB3	2.51	0.44
1:F:98:TYR:HA	1:F:495:ALA:O	2.16	0.44
1:C:418:VAL:HG22	1:C:426:CYS:HB2	1.99	0.44
1:C:498:SER:HB3	1:C:501:THR:OG1	2.17	0.44
1:D:127:MET:HA	1:D:127:MET:HE3	1.99	0.44
1:F:519:LEU:C	1:F:519:LEU:HD23	2.42	0.44
1:B:402:LYS:HE2	1:B:420:ARG:NH2	2.33	0.44
1:D:291:ALA:HB1	1:D:422:PHE:CZ	2.52	0.44
1:F:504:ARG:HA	1:F:507:ILE:HD12	2.00	0.44
1:B:332:VAL:HG11	1:B:338:LEU:HD11	1.99	0.44
1:B:399:LYS:HA	1:B:399:LYS:HD2	1.67	0.44
1:D:291:ALA:HB1	1:D:422:PHE:CE1	2.53	0.44
1:E:380:MET:HB2	1:E:380:MET:HE3	1.76	0.44
1:F:417:THR:HG21	1:F:491:MET:CB	2.46	0.44
1:F:464:LYS:HG3	1:F:529:PHE:HB3	1.99	0.44
1:C:133:THR:HG23	1:C:362:TYR:CD2	2.53	0.44
1:D:223:ILE:HD13	1:D:238:LEU:HA	2.00	0.44
1:E:92:TRP:HE1	1:F:128:SER:HB3	1.82	0.44
1:F:297:CYS:HA	1:F:391:ARG:NH1	2.33	0.44
1:A:135:LEU:O	1:A:139:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:O	1:A:176:THR:HG23	2.17	0.44
1:B:207:GLN:O	1:B:211:GLN:HG3	2.17	0.44
1:C:152:SER:HB2	1:C:333:LYS:HD3	1.99	0.44
1:D:385:TYR:O	1:D:389:ASN:HB2	2.18	0.44
1:F:97:TYR:CZ	1:F:99:ALA:HB3	2.53	0.44
1:F:102:PRO:CG	1:F:497:GLY:HA3	2.48	0.44
1:A:319:LLP:HG3	2:A:601:TYR:CZ	2.53	0.43
1:D:132:ALA:HA	1:D:373:PHE:CE1	2.53	0.43
1:E:127:MET:CE	1:F:51:ARG:HH21	2.28	0.43
1:E:369:LEU:HD21	1:F:208:LYS:HD3	2.00	0.43
1:A:97:TYR:CZ	1:A:99:ALA:HB3	2.52	0.43
1:E:164:GLN:HB3	1:E:366:GLN:OE1	2.18	0.43
1:F:28:ARG:HG3	1:F:32:HIS:CD2	2.53	0.43
1:C:294:ALA:HB2	1:C:320:TRP:CZ3	2.53	0.43
1:D:252:PRO:HB2	1:D:282:MET:SD	2.59	0.43
1:E:29:ARG:HD2	1:E:33:MET:HE2	2.00	0.43
1:E:106:SER:HB2	1:E:322:PHE:O	2.18	0.43
1:E:114:MET:HB2	1:F:114:MET:CE	2.48	0.43
1:F:115:LEU:O	1:F:119:PHE:N	2.31	0.43
1:F:296:ILE:HD12	1:F:321:PHE:HZ	1.82	0.43
1:C:173:CYS:SG	1:C:366:GLN:HA	2.58	0.43
1:E:27:PHE:HA	1:F:107:VAL:HG21	2.00	0.43
1:B:271:SER:HB3	1:B:272:PRO:HD3	2.00	0.43
1:C:286:VAL:HB	1:C:313:PHE:HD1	1.83	0.43
1:F:81:VAL:CG1	1:F:85:ILE:HB	2.38	0.43
1:F:373:PHE:CE1	1:F:376:LEU:HG	2.53	0.43
1:C:101:PHE:HB2	2:C:601:TYR:CE1	2.54	0.43
1:E:325:LEU:O	1:F:372:ARG:HD3	2.18	0.43
1:F:416:ILE:O	1:F:416:ILE:HG13	2.17	0.43
1:A:55:GLU:OE1	1:A:55:GLU:N	2.42	0.43
1:C:90:THR:HB	1:D:128:SER:O	2.19	0.43
1:D:100:TYR:HB3	2:D:601:TYR:N	2.33	0.43
1:E:315:LEU:HG	1:E:331:TRP:CH2	2.53	0.43
1:E:385:TYR:O	1:F:71:PRO:HB3	2.19	0.43
1:F:116:SER:OG	1:F:373:PHE:HB3	2.19	0.43
1:A:128:SER:O	1:B:90:THR:HB	2.19	0.43
1:A:301:ARG:NH1	1:A:304:ILE:HG13	2.34	0.43
1:C:51:ARG:HD3	1:C:480:TYR:CE1	2.53	0.43
1:E:224:LYS:HA	1:E:224:LYS:HD3	1.74	0.43
1:F:42:TYR:HA	1:F:45:VAL:HG23	2.01	0.43
1:F:272:PRO:O	1:F:276:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:481:MET:SD	1:F:513:LEU:HD21	2.58	0.43
1:C:150:PRO:HG2	1:C:153:PHE:HD2	1.83	0.43
1:F:295:CYS:O	1:F:301:ARG:HB3	2.19	0.43
1:F:461:LEU:HD21	1:F:526:GLU:HG2	1.99	0.43
1:E:126:TRP:CE2	1:E:130:PRO:HB3	2.54	0.42
1:F:413:ARG:NH2	1:F:514:GLN:O	2.46	0.42
1:A:398:VAL:HG22	1:A:423:ALA:HB2	2.01	0.42
1:C:308:GLU:CD	1:C:308:GLU:H	2.26	0.42
1:E:59:LEU:HG	1:F:134:GLU:CB	2.49	0.42
1:E:318:HIS:CG	1:E:325:LEU:HD12	2.54	0.42
1:F:50:VAL:CG2	1:F:480:TYR:HB2	2.50	0.42
1:E:92:TRP:CE3	1:E:103:SER:HB2	2.54	0.42
1:E:363:LYS:HG3	1:E:364:ASP:OD1	2.19	0.42
1:E:461:LEU:C	1:E:461:LEU:HD13	2.44	0.42
1:F:294:ALA:O	1:F:300:PHE:HD2	2.02	0.42
1:C:174:THR:HG22	1:C:254:PHE:CE1	2.55	0.42
1:C:323:THR:O	1:C:324:THR:HG23	2.19	0.42
1:D:413:ARG:NH1	1:D:518:ASP:OD1	2.44	0.42
1:E:74:ILE:HD12	1:E:74:ILE:N	2.35	0.42
1:E:325:LEU:HA	1:E:326:ASP:HA	1.52	0.42
1:E:255:VAL:HG13	1:E:282:MET:CE	2.50	0.42
1:F:391:ARG:O	1:F:395:ARG:NH1	2.53	0.42
1:F:429:LEU:N	1:F:466:ASN:OD1	2.48	0.42
1:F:479:VAL:HG11	1:F:509:ALA:HB1	2.00	0.42
1:C:322:PHE:CZ	1:C:393:PHE:HB3	2.55	0.42
1:E:269:PRO:HB2	1:E:272:PRO:HD2	2.02	0.42
1:E:318:HIS:CD2	1:E:325:LEU:HD12	2.55	0.42
1:F:269:PRO:HB2	1:F:272:PRO:HG2	2.01	0.42
1:F:317:ALA:N	1:F:327:CYS:O	2.45	0.42
1:A:322:PHE:CZ	1:A:393:PHE:HB3	2.55	0.42
1:A:408:ILE:HG23	1:A:414:PHE:CB	2.50	0.42
1:C:431:PRO:HA	1:C:432:PRO:HD3	1.87	0.42
1:D:44:ASP:O	1:D:47:LYS:HG2	2.19	0.42
1:E:51:ARG:HA	1:E:90:THR:HG23	2.02	0.42
1:E:387:VAL:HB	1:F:69:TYR:HA	2.01	0.42
1:E:393:PHE:O	1:E:396:SER:HB3	2.20	0.42
1:F:469:TYR:OH	1:F:513:LEU:HB3	2.19	0.42
1:C:58:TYR:OH	1:C:88:GLY:HA3	2.20	0.42
1:D:424:MET:HA	1:D:494:PHE:O	2.20	0.42
1:E:359:VAL:HG12	1:F:56:PRO:HB3	2.02	0.42
1:F:124:PHE:CE1	1:F:363:LYS:HE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:387:VAL:O	1:F:391:ARG:HG3	2.19	0.42
1:F:510:TRP:CD1	1:F:511:LYS:HG3	2.55	0.42
1:A:239:ARG:NH1	1:A:276:VAL:HG22	2.35	0.41
1:B:102:PRO:CG	1:B:497:GLY:HA3	2.50	0.41
1:C:523:LYS:O	1:C:524:PHE:C	2.63	0.41
1:D:432:PRO:HD3	1:D:521:LEU:HD22	2.02	0.41
1:E:210:ALA:HB1	1:E:215:ILE:HB	2.01	0.41
1:F:295:CYS:SG	1:F:301:ARG:HA	2.60	0.41
1:E:140:MET:HE1	1:E:329:CYS:HB3	2.01	0.41
1:F:182:LYS:O	1:F:186:ILE:HG12	2.20	0.41
1:F:251:ILE:O	1:F:251:ILE:HG23	2.20	0.41
1:F:373:PHE:CZ	1:F:376:LEU:HG	2.54	0.41
1:F:112:GLY:HA3	1:F:377:LYS:HA	2.02	0.41
1:F:135:LEU:O	1:F:139:VAL:HG13	2.20	0.41
1:F:119:PHE:O	1:F:120:ASN:C	2.63	0.41
1:B:132:ALA:HA	1:B:373:PHE:CE1	2.55	0.41
1:B:458:ASN:OD1	1:B:458:ASN:N	2.53	0.41
1:D:185:LYS:HE3	1:D:185:LYS:HB2	1.84	0.41
1:E:167:SER:O	1:E:171:ILE:HG13	2.19	0.41
1:E:347:GLU:HG2	1:E:350:ARG:NH1	2.35	0.41
1:F:28:ARG:HG3	1:F:32:HIS:HD2	1.85	0.41
1:F:470:LEU:CD2	1:F:492:ILE:HD13	2.50	0.41
1:B:29:ARG:NH1	1:B:33:MET:HE1	2.35	0.41
1:C:102:PRO:HG3	1:C:497:GLY:HA3	2.02	0.41
1:B:299:GLU:HG2	1:B:300:PHE:CD1	2.55	0.41
1:C:223:ILE:HD13	1:C:238:LEU:HA	2.02	0.41
1:C:261:THR:HG1	1:C:266:ALA:H	1.67	0.41
1:E:22:LEU:HD23	1:E:22:LEU:HA	1.87	0.41
1:E:90:THR:CG2	1:E:97:TYR:HE2	2.34	0.41
1:E:407:LEU:HD11	1:E:507:ILE:HD13	2.03	0.41
1:E:473:VAL:HG22	1:E:516:HIS:CG	2.55	0.41
1:F:54:VAL:HG12	1:F:55:GLU:N	2.35	0.41
1:F:403:THR:O	1:F:407:LEU:HG	2.20	0.41
1:F:482:THR:OG1	1:F:493:ARG:NH1	2.54	0.41
1:F:110:PHE:CD2	1:F:111:LEU:HG	2.53	0.41
1:F:431:PRO:HA	1:F:432:PRO:HD3	1.93	0.41
1:A:22:LEU:HD12	1:A:22:LEU:HA	1.91	0.41
1:A:58:TYR:OH	1:A:88:GLY:HA3	2.20	0.41
1:B:162:VAL:HB	1:B:365:TRP:CE3	2.56	0.41
1:B:325:LEU:HA	1:B:326:ASP:HA	1.55	0.41
1:C:294:ALA:HA	1:C:394:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:VAL:HG23	1:E:252:PRO:HA	2.03	0.41
1:F:101:PHE:CE2	1:F:262:THR:HA	2.56	0.41
1:F:225:THR:HB	1:F:231:PHE:HA	2.02	0.41
1:F:376:LEU:HD23	1:F:376:LEU:HA	1.81	0.41
1:F:397:HIS:CE1	1:F:499:THR:HG22	2.56	0.41
1:F:424:MET:HA	1:F:494:PHE:O	2.20	0.41
1:F:504:ARG:O	1:F:508:TYR:N	2.45	0.41
1:A:431:PRO:HA	1:A:432:PRO:HD3	1.98	0.41
1:B:173:CYS:SG	1:B:366:GLN:HA	2.61	0.41
1:B:274:CYS:O	1:B:278:LYS:HG2	2.20	0.41
1:C:62:ARG:HE	1:C:62:ARG:HB3	1.76	0.41
1:C:172:LEU:O	1:C:176:THR:HG23	2.20	0.41
1:E:32:HIS:O	1:F:32:HIS:HE1	2.04	0.41
1:E:59:LEU:HG	1:F:134:GLU:HB2	2.02	0.41
1:E:140:MET:HE2	1:E:162:VAL:O	2.21	0.41
1:F:413:ARG:O	1:F:429:LEU:HD22	2.21	0.41
1:B:82:THR:HA	1:B:86:ILE:HD12	2.03	0.40
1:B:361:ASP:OD1	1:B:363:LYS:HG2	2.22	0.40
1:E:90:THR:HB	1:F:128:SER:C	2.45	0.40
1:E:150:PRO:HG3	1:E:308:GLU:HG3	2.02	0.40
1:E:499:THR:HG22	1:E:500:LEU:HD23	2.03	0.40
1:F:228:GLU:H	1:F:228:GLU:HG3	1.72	0.40
1:B:261:THR:HG1	1:B:266:ALA:H	1.68	0.40
1:D:173:CYS:SG	1:D:366:GLN:HA	2.61	0.40
1:F:135:LEU:HD13	1:F:373:PHE:HZ	1.87	0.40
1:F:429:LEU:CD1	1:F:521:LEU:HD11	2.47	0.40
1:C:22:LEU:HD12	1:C:22:LEU:HA	1.89	0.40
1:E:166:THR:CG2	1:E:169:GLU:HB2	2.50	0.40
1:E:265:THR:O	1:E:265:THR:HG23	2.21	0.40
1:E:289:ALA:CA	1:E:316:ASN:H	2.28	0.40
1:F:397:HIS:HE1	1:F:499:THR:HG22	1.85	0.40
1:F:515:GLU:HG3	1:F:516:HIS:ND1	2.36	0.40
1:C:393:PHE:CZ	1:D:21:PRO:HG3	2.57	0.40
1:D:44:ASP:HB3	1:D:47:LYS:HE2	2.04	0.40
1:E:111:LEU:HD22	1:F:34:ILE:HG13	2.02	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	478/531 (90%)	463 (97%)	11 (2%)	4 (1%)	16	44
1	B	476/531 (90%)	457 (96%)	17 (4%)	2 (0%)	30	58
1	C	478/531 (90%)	459 (96%)	16 (3%)	3 (1%)	21	49
1	D	476/531 (90%)	455 (96%)	16 (3%)	5 (1%)	11	36
1	E	470/531 (88%)	440 (94%)	28 (6%)	2 (0%)	30	58
1	F	461/531 (87%)	426 (92%)	34 (7%)	1 (0%)	43	70
All	All	2839/3186 (89%)	2700 (95%)	122 (4%)	17 (1%)	21	49

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	THR
1	C	324	THR
1	D	324	THR
1	E	100	TYR
1	E	373	PHE
1	A	99	ALA
1	A	497	GLY
1	B	497	GLY
1	C	497	GLY
1	D	99	ALA
1	D	204	CYS
1	D	497	GLY
1	D	129	SER
1	B	129	SER
1	F	129	SER
1	C	129	SER
1	A	129	SER

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	415/455 (91%)	415 (100%)	0	100	100
1	B	413/455 (91%)	413 (100%)	0	100	100
1	C	415/455 (91%)	415 (100%)	0	100	100
1	D	413/455 (91%)	413 (100%)	0	100	100
1	E	411/455 (90%)	411 (100%)	0	100	100
1	F	404/455 (89%)	404 (100%)	0	100	100
All	All	2471/2730 (90%)	2471 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	96	ASN
1	A	316	ASN
1	A	483	HIS
1	C	93	GLN
1	D	316	ASN
1	E	20	ASN
1	E	458	ASN
1	E	514	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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$
1	LLP	D	319	1	23,24,25	2.52	6 (26%)	25,32,34	1.25	3 (12%)
1	LLP	B	319	1	23,24,25	2.51	6 (26%)	25,32,34	1.29	4 (16%)
1	LLP	F	319	1	23,24,25	2.52	6 (26%)	25,32,34	1.28	4 (16%)
1	LLP	A	319	1	23,24,25	2.49	6 (26%)	25,32,34	1.35	4 (16%)
1	LLP	E	319	1	23,24,25	2.51	6 (26%)	25,32,34	1.28	3 (12%)
1	LLP	C	319	1	23,24,25	2.51	6 (26%)	25,32,34	1.32	4 (16%)

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
1	LLP	D	319	1	-	4/16/17/19	0/1/1/1
1	LLP	B	319	1	-	4/16/17/19	0/1/1/1
1	LLP	F	319	1	-	5/16/17/19	0/1/1/1
1	LLP	A	319	1	-	4/16/17/19	0/1/1/1
1	LLP	E	319	1	-	8/16/17/19	0/1/1/1
1	LLP	C	319	1	-	3/16/17/19	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	319	LLP	C4-C4'	7.25	1.62	1.46
1	D	319	LLP	C4-C4'	7.25	1.62	1.46
1	F	319	LLP	C4-C4'	7.22	1.62	1.46
1	C	319	LLP	C4-C4'	7.14	1.61	1.46
1	B	319	LLP	C4-C4'	7.14	1.61	1.46
1	A	319	LLP	C4-C4'	7.07	1.61	1.46
1	E	319	LLP	C4'-NZ	5.00	1.43	1.27
1	F	319	LLP	C4'-NZ	4.99	1.43	1.27
1	D	319	LLP	C4'-NZ	4.98	1.43	1.27
1	B	319	LLP	C4'-NZ	4.97	1.43	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	319	LLP	C4'-NZ	4.92	1.43	1.27
1	A	319	LLP	C4'-NZ	4.88	1.43	1.27
1	C	319	LLP	C4-C5	-3.82	1.36	1.42
1	B	319	LLP	C4-C5	-3.81	1.36	1.42
1	F	319	LLP	C2'-C2	3.78	1.56	1.50
1	D	319	LLP	C4-C5	-3.77	1.36	1.42
1	D	319	LLP	C2'-C2	3.77	1.56	1.50
1	C	319	LLP	C2'-C2	3.76	1.56	1.50
1	B	319	LLP	C2'-C2	3.76	1.56	1.50
1	A	319	LLP	C2'-C2	3.76	1.56	1.50
1	E	319	LLP	C2'-C2	3.76	1.56	1.50
1	F	319	LLP	C4-C5	-3.76	1.36	1.42
1	A	319	LLP	C4-C5	-3.75	1.36	1.42
1	E	319	LLP	C4-C5	-3.55	1.37	1.42
1	A	319	LLP	C6-N1	3.17	1.40	1.34
1	F	319	LLP	C6-N1	3.16	1.40	1.34
1	C	319	LLP	C6-N1	3.16	1.40	1.34
1	B	319	LLP	C6-N1	3.14	1.40	1.34
1	D	319	LLP	C6-N1	3.13	1.40	1.34
1	E	319	LLP	C6-N1	3.12	1.40	1.34
1	A	319	LLP	C5'-C5	2.22	1.56	1.50
1	E	319	LLP	C5'-C5	2.21	1.56	1.50
1	F	319	LLP	C5'-C5	2.21	1.56	1.50
1	B	319	LLP	C5'-C5	2.18	1.56	1.50
1	C	319	LLP	C5'-C5	2.17	1.56	1.50
1	D	319	LLP	C5'-C5	2.15	1.56	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	319	LLP	C4-C4'-NZ	-3.61	107.38	124.04
1	C	319	LLP	C4-C4'-NZ	-3.31	108.76	124.04
1	F	319	LLP	C4-C4'-NZ	-3.31	108.79	124.04
1	D	319	LLP	C4-C4'-NZ	-3.19	109.30	124.04
1	A	319	LLP	C4-C4'-NZ	-3.19	109.34	124.04
1	B	319	LLP	C4-C4'-NZ	-3.17	109.41	124.04
1	A	319	LLP	CE-NZ-C4'	-3.15	108.63	118.72
1	C	319	LLP	CE-NZ-C4'	-2.89	109.46	118.72
1	B	319	LLP	CE-NZ-C4'	-2.87	109.54	118.72
1	F	319	LLP	CE-NZ-C4'	-2.65	110.22	118.72
1	D	319	LLP	CE-NZ-C4'	-2.63	110.29	118.72
1	C	319	LLP	C5-C6-N1	-2.40	119.93	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	319	LLP	C5-C6-N1	-2.39	119.94	123.83
1	A	319	LLP	C3-C4-C5	2.39	120.19	118.28
1	A	319	LLP	C5-C6-N1	-2.36	120.00	123.83
1	D	319	LLP	C5-C6-N1	-2.35	120.00	123.83
1	B	319	LLP	C3-C4-C5	2.26	120.09	118.28
1	F	319	LLP	C5-C6-N1	-2.26	120.15	123.83
1	C	319	LLP	C3-C4-C5	2.26	120.09	118.28
1	E	319	LLP	CE-NZ-C4'	-2.24	111.53	118.72
1	E	319	LLP	C5-C6-N1	-2.15	120.33	123.83
1	F	319	LLP	C3-C4-C5	2.02	119.90	118.28

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	319	LLP	C-CA-CB-CG
1	B	319	LLP	C4-C4'-NZ-CE
1	B	319	LLP	C-CA-CB-CG
1	C	319	LLP	C-CA-CB-CG
1	D	319	LLP	C4-C4'-NZ-CE
1	D	319	LLP	C-CA-CB-CG
1	E	319	LLP	C4-C5-C5'-OP4
1	E	319	LLP	C6-C5-C5'-OP4
1	E	319	LLP	O-C-CA-CB
1	E	319	LLP	CG-CD-CE-NZ
1	F	319	LLP	N-CA-CB-CG
1	F	319	LLP	C-CA-CB-CG
1	C	319	LLP	C4-C4'-NZ-CE
1	A	319	LLP	C4-C4'-NZ-CE
1	F	319	LLP	C4-C4'-NZ-CE
1	E	319	LLP	CA-CB-CG-CD
1	F	319	LLP	CE-CD-CG-CB
1	B	319	LLP	CD-CE-NZ-C4'
1	E	319	LLP	CD-CE-NZ-C4'
1	F	319	LLP	CD-CE-NZ-C4'
1	A	319	LLP	CD-CE-NZ-C4'
1	C	319	LLP	CD-CE-NZ-C4'
1	D	319	LLP	CD-CE-NZ-C4'
1	E	319	LLP	C3-C4-C4'-NZ
1	D	319	LLP	CG-CD-CE-NZ
1	A	319	LLP	C3-C4-C4'-NZ
1	B	319	LLP	C3-C4-C4'-NZ

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Mol	Chain	Res	Type	Atoms
1	E	319	LLP	C-CA-CB-CG

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	319	LLP	2	0
1	B	319	LLP	1	0
1	F	319	LLP	1	0
1	A	319	LLP	3	0
1	E	319	LLP	1	0
1	C	319	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	TYR	A	601	-	12,13,13	0.72	1 (8%)	13,17,17	0.75	1 (7%)
2	TYR	D	601	-	11,12,13	0.42	0	10,15,17	0.17	0
2	TYR	B	601	-	12,13,13	0.72	1 (8%)	13,17,17	0.76	1 (7%)
2	TYR	C	601	-	11,12,13	0.42	0	10,15,17	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TYR	A	601	-	-	2/8/8/8	0/1/1/1
2	TYR	D	601	-	-	3/5/6/8	0/1/1/1
2	TYR	B	601	-	-	2/8/8/8	0/1/1/1
2	TYR	C	601	-	-	5/5/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	TYR	OXT-C	-2.22	1.23	1.30
2	B	601	TYR	OXT-C	-2.18	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	TYR	OXT-C-O	-2.64	118.10	124.08
2	B	601	TYR	OXT-C-O	-2.62	118.14	124.08

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	TYR	O-C-CA-CB
2	C	601	TYR	C-CA-CB-CG
2	D	601	TYR	O-C-CA-CB
2	D	601	TYR	C-CA-CB-CG
2	C	601	TYR	N-CA-CB-CG
2	A	601	TYR	C-CA-CB-CG
2	D	601	TYR	N-CA-CB-CG
2	A	601	TYR	N-CA-CB-CG
2	B	601	TYR	N-CA-CB-CG
2	B	601	TYR	C-CA-CB-CG
2	C	601	TYR	CA-CB-CG-CD1
2	C	601	TYR	CA-CB-CG-CD2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

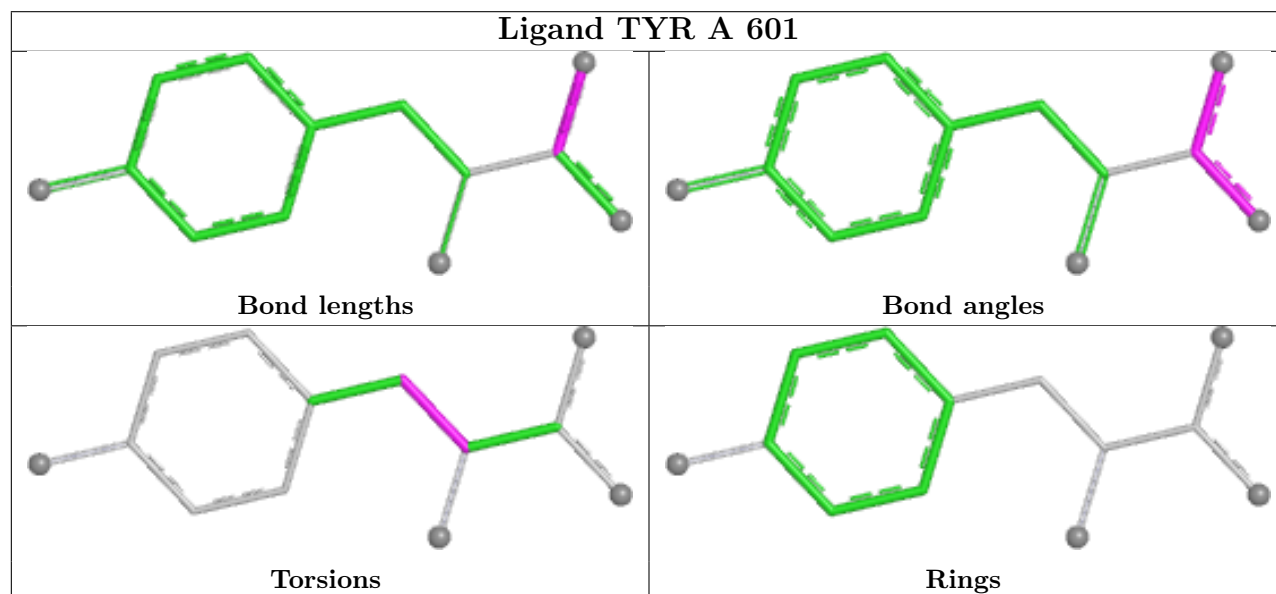
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	TYR	1	0
2	D	601	TYR	2	0
2	B	601	TYR	1	0

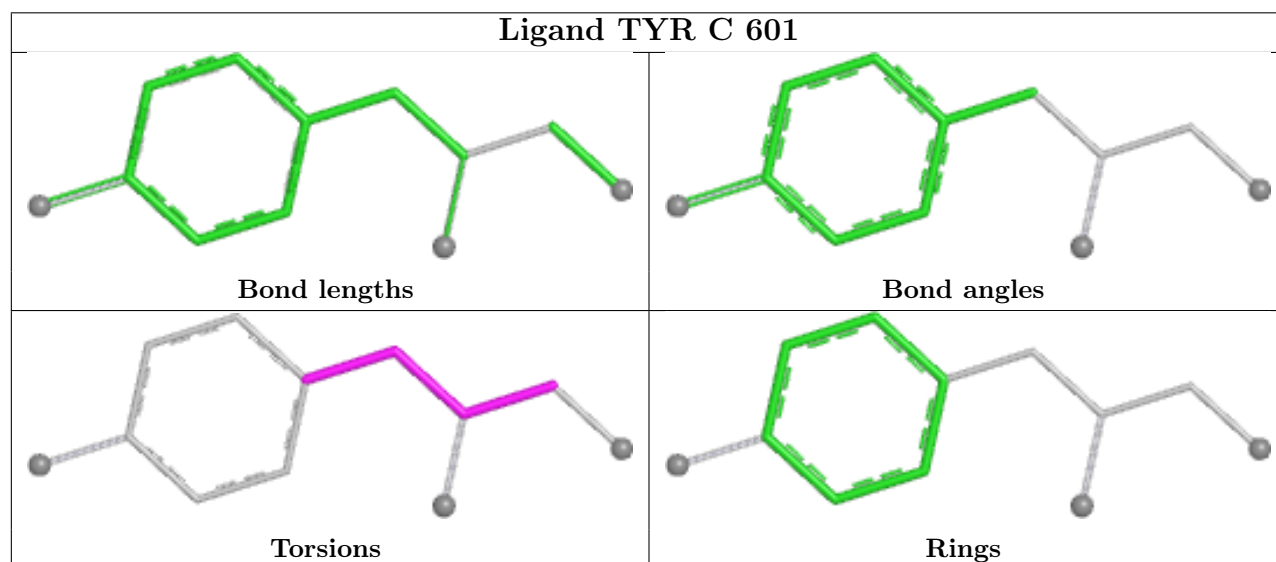
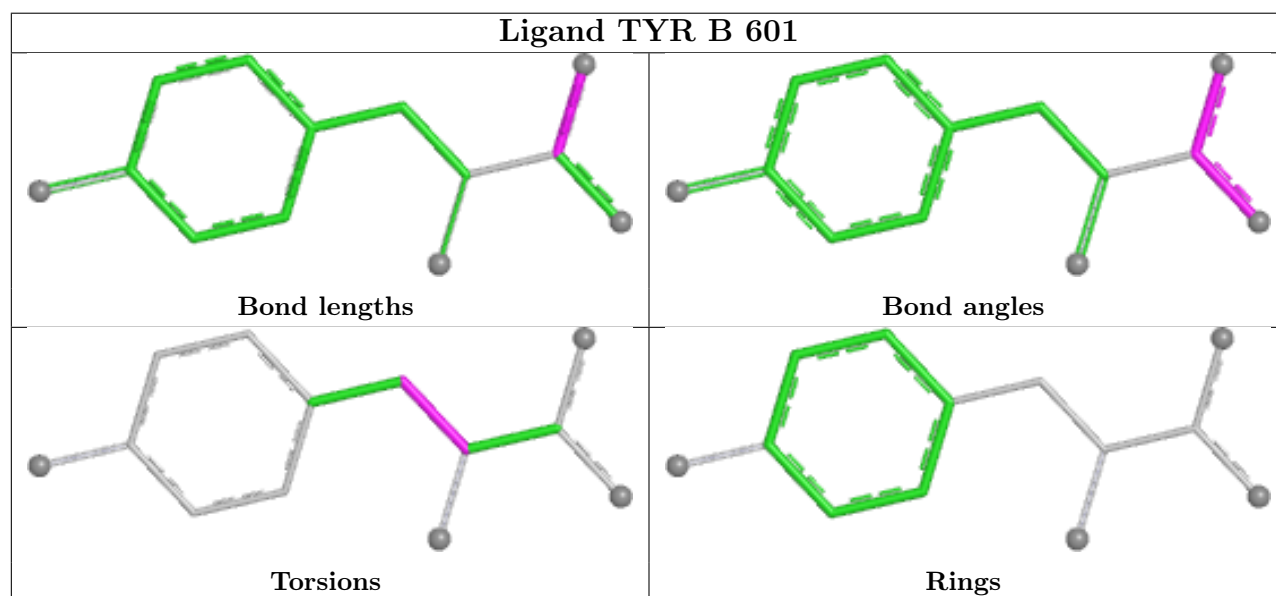
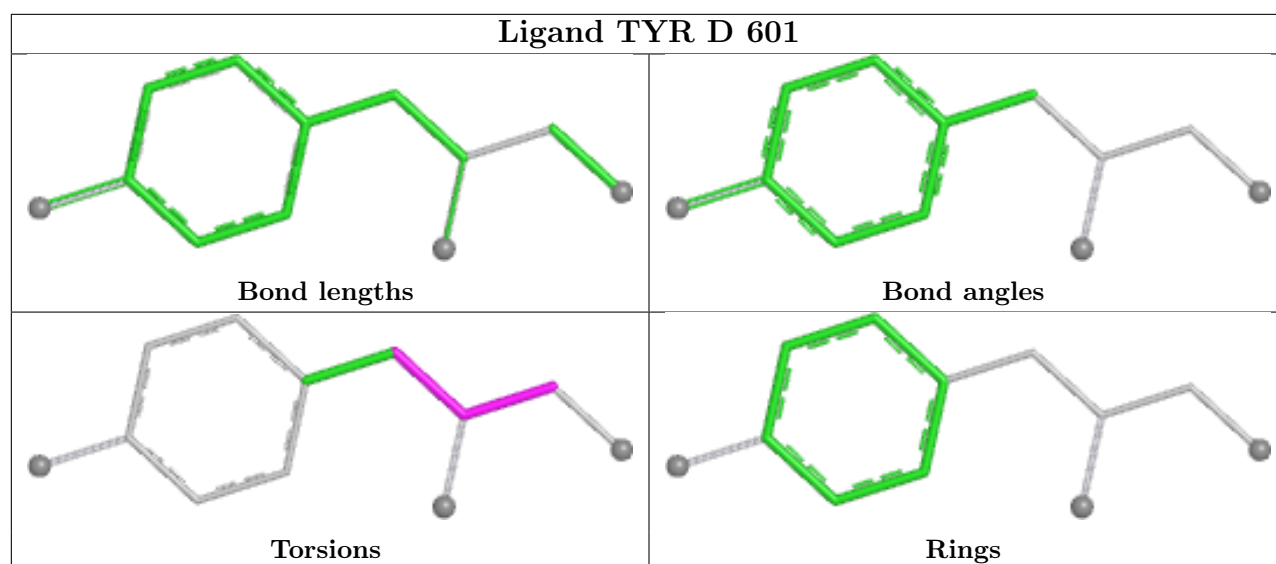
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	TYR	3	0

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.





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	484/531 (91%)	0.09	10 (2%) 63 47	8, 20, 45, 87	0
1	B	482/531 (90%)	-0.03	10 (2%) 63 47	5, 17, 38, 98	0
1	C	484/531 (91%)	0.13	13 (2%) 56 41	9, 21, 52, 97	0
1	D	482/531 (90%)	-0.00	3 (0%) 85 75	6, 17, 39, 85	0
1	E	478/531 (90%)	2.18	239 (50%) 0 0	42, 75, 95, 115	0
1	F	473/531 (89%)	2.04	210 (44%) 0 0	26, 71, 95, 108	0
All	All	2883/3186 (90%)	0.73	485 (16%) 4 5	5, 25, 89, 115	0

All (485) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	478	SER	8.8
1	E	96	ASN	7.4
1	F	379	TRP	6.6
1	F	132	ALA	6.5
1	E	122	VAL	6.5
1	F	387	VAL	6.4
1	F	120	ASN	6.1
1	E	500	LEU	6.1
1	F	498	SER	6.0
1	E	22	LEU	6.0
1	F	423	ALA	5.7
1	E	292	GLY	5.7
1	E	328	CYS	5.6
1	F	42	TYR	5.5
1	B	349	LEU	5.4
1	F	74	ILE	5.4
1	E	88	GLY	5.3
1	F	37	PHE	5.3
1	E	20	ASN	5.2

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Mol	Chain	Res	Type	RSRZ
1	F	318	HIS	5.2
1	E	121	VAL	5.2
1	E	394	LEU	5.1
1	F	348	TYR	5.1
1	E	163	LEU	5.1
1	E	168	CYS	5.1
1	F	380	MET	5.0
1	F	382	LEU	5.0
1	F	92	TRP	4.9
1	F	96	ASN	4.9
1	E	269	PRO	4.9
1	F	85	ILE	4.9
1	F	474	ASN	4.8
1	F	41	TYR	4.8
1	E	45	VAL	4.8
1	F	480	TYR	4.8
1	E	373	PHE	4.8
1	F	513	LEU	4.8
1	F	24	PRO	4.7
1	E	27	PHE	4.7
1	F	393	PHE	4.6
1	E	474	ASN	4.6
1	E	393	PHE	4.6
1	E	365	TRP	4.5
1	F	90	THR	4.5
1	F	478	SER	4.5
1	F	67	ALA	4.5
1	F	406	GLY	4.5
1	F	477	GLY	4.5
1	F	45	VAL	4.5
1	E	404	PHE	4.5
1	E	507	ILE	4.4
1	E	58	TYR	4.4
1	B	346	PRO	4.4
1	F	77	ILE	4.4
1	E	324	THR	4.3
1	F	66	THR	4.3
1	B	348	TYR	4.3
1	E	51	ARG	4.3
1	E	379	TRP	4.3
1	F	400	MET	4.3
1	F	499	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	49	PRO	4.2
1	F	291	ALA	4.2
1	F	59	LEU	4.2
1	F	529	PHE	4.1
1	E	316	ASN	4.1
1	F	327	CYS	4.1
1	A	348	TYR	4.1
1	F	48	TYR	4.1
1	F	370	SER	4.1
1	E	205	ALA	4.1
1	F	296	ILE	4.1
1	E	19	THR	4.0
1	F	381	VAL	4.0
1	E	384	SER	4.0
1	E	24	PRO	4.0
1	F	122	VAL	4.0
1	F	142	TRP	4.0
1	E	143	PHE	4.0
1	F	317	ALA	4.0
1	F	97	TYR	3.9
1	E	105	GLY	3.9
1	E	109	GLY	3.9
1	E	397	HIS	3.9
1	E	381	VAL	3.9
1	E	479	VAL	3.9
1	F	408	ILE	3.9
1	F	375	SER	3.9
1	E	72	GLU	3.8
1	F	133	THR	3.8
1	E	93	GLN	3.8
1	F	292	GLY	3.8
1	E	52	SER	3.8
1	E	377	LYS	3.8
1	F	64	PRO	3.8
1	F	20	ASN	3.8
1	E	506	VAL	3.8
1	E	511	LYS	3.8
1	F	396	SER	3.8
1	E	44	ASP	3.8
1	E	21	PRO	3.8
1	E	84	GLU	3.8
1	E	161	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	372	ARG	3.8
1	F	373	PHE	3.8
1	F	494	PHE	3.8
1	F	425	VAL	3.7
1	F	22	LEU	3.7
1	F	349	LEU	3.7
1	F	300	PHE	3.7
1	F	52	SER	3.7
1	F	203	PHE	3.7
1	E	117	THR	3.7
1	E	123	GLY	3.7
1	F	419	PRO	3.7
1	E	30	GLN	3.7
1	E	329	CYS	3.7
1	E	383	ARG	3.6
1	E	91	HIS	3.6
1	F	38	LEU	3.6
1	F	100	TYR	3.6
1	E	120	ASN	3.6
1	E	509	ALA	3.6
1	F	401	ALA	3.6
1	E	42	TYR	3.6
1	E	378	LEU	3.6
1	F	481	MET	3.6
1	E	106	SER	3.6
1	F	391	ARG	3.5
1	F	510	TRP	3.5
1	E	59	LEU	3.5
1	E	327	CYS	3.5
1	E	82	THR	3.5
1	E	203	PHE	3.5
1	E	382	LEU	3.5
1	E	73	SER	3.5
1	F	34	ILE	3.5
1	F	82	THR	3.5
1	F	106	SER	3.5
1	D	348	TYR	3.5
1	F	98	TYR	3.5
1	F	93	GLN	3.5
1	A	531	SER	3.5
1	F	503	GLU	3.4
1	F	115	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	119	PHE	3.4
1	E	501	THR	3.4
1	E	147	LEU	3.4
1	E	267	VAL	3.4
1	F	76	THR	3.4
1	E	104	SER	3.4
1	E	471	GLU	3.4
1	F	322	PHE	3.3
1	E	89	LEU	3.3
1	E	48	TYR	3.3
1	E	260	GLY	3.3
1	E	418	VAL	3.3
1	E	380	MET	3.3
1	E	74	ILE	3.3
1	F	321	PHE	3.3
1	F	457	GLU	3.3
1	E	114	MET	3.3
1	F	36	ASP	3.3
1	E	68	PRO	3.3
1	F	21	PRO	3.3
1	E	265	THR	3.3
1	F	395	ARG	3.3
1	E	407	LEU	3.3
1	F	33	MET	3.3
1	E	41	TYR	3.3
1	F	104	SER	3.3
1	E	204	CYS	3.3
1	F	298	PRO	3.3
1	E	83	THR	3.3
1	F	506	VAL	3.3
1	F	424	MET	3.2
1	A	352	LYS	3.2
1	E	514	GLN	3.2
1	F	496	VAL	3.2
1	E	142	TRP	3.2
1	E	463	ASN	3.2
1	E	493	ARG	3.2
1	E	508	TYR	3.2
1	F	138	VAL	3.2
1	F	394	LEU	3.2
1	E	97	TYR	3.2
1	E	403	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	517	ALA	3.2
1	C	351	ASN	3.2
1	E	422	PHE	3.2
1	F	143	PHE	3.2
1	F	404	PHE	3.2
1	E	481	MET	3.2
1	F	416	ILE	3.2
1	F	388	THR	3.2
1	D	203	PHE	3.1
1	F	389	ASN	3.1
1	F	51	ARG	3.1
1	E	369	LEU	3.1
1	F	369	LEU	3.1
1	F	426	CYS	3.1
1	E	110	PHE	3.1
1	F	398	VAL	3.1
1	F	422	PHE	3.1
1	F	432	PRO	3.1
1	E	293	SER	3.1
1	E	477	GLY	3.1
1	F	83	THR	3.1
1	F	501	THR	3.1
1	F	299	GLU	3.1
1	F	89	LEU	3.1
1	E	268	ASP	3.1
1	E	149	LEU	3.0
1	E	322	PHE	3.0
1	F	507	ILE	3.0
1	C	348	TYR	3.0
1	E	111	LEU	3.0
1	E	206	LEU	3.0
1	E	513	LEU	3.0
1	E	499	THR	3.0
1	E	103	SER	3.0
1	F	94	SER	3.0
1	F	95	PRO	3.0
1	F	63	LEU	3.0
1	E	132	ALA	3.0
1	F	32	HIS	3.0
1	F	295	CYS	3.0
1	F	50	VAL	3.0
1	F	121	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	317	ALA	3.0
1	F	523	LYS	3.0
1	F	30	GLN	3.0
1	F	31	GLY	3.0
1	E	90	THR	3.0
1	F	135	LEU	3.0
1	E	164	GLN	3.0
1	C	204	CYS	3.0
1	C	529	PHE	3.0
1	E	113	GLU	2.9
1	F	46	GLU	2.9
1	E	375	SER	2.9
1	F	88	GLY	2.9
1	F	479	VAL	2.9
1	B	203	PHE	2.9
1	E	270	ILE	2.9
1	E	304	ILE	2.9
1	E	515	GLU	2.9
1	F	377	LYS	2.9
1	F	69	TYR	2.9
1	E	387	VAL	2.9
1	E	402	LYS	2.9
1	F	403	THR	2.9
1	E	303	PHE	2.9
1	E	531	SER	2.9
1	F	116	SER	2.9
1	F	128	SER	2.9
1	F	413	ARG	2.9
1	F	500	LEU	2.9
1	F	518	ASP	2.9
1	E	39	ALA	2.9
1	F	528	ASP	2.9
1	E	503	GLU	2.9
1	E	326	ASP	2.8
1	F	287	ASP	2.8
1	F	19	THR	2.8
1	F	71	PRO	2.8
1	A	203	PHE	2.8
1	F	165	GLY	2.8
1	F	512	ILE	2.8
1	A	530	SER	2.8
1	E	259	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	378	LEU	2.8
1	E	256	CYS	2.8
1	E	401	ALA	2.8
1	F	108	ALA	2.8
1	F	109	GLY	2.8
1	F	329	CYS	2.8
1	F	495	ALA	2.8
1	E	95	PRO	2.8
1	E	133	THR	2.8
1	E	325	LEU	2.8
1	E	300	PHE	2.8
1	F	127	MET	2.8
1	F	385	TYR	2.8
1	E	294	ALA	2.8
1	F	117	THR	2.8
1	E	410	MET	2.7
1	E	516	HIS	2.7
1	E	423	ALA	2.7
1	F	294	ALA	2.7
1	E	129	SER	2.7
1	F	397	HIS	2.7
1	F	527	ALA	2.7
1	E	284	VAL	2.7
1	E	157	GLY	2.7
1	F	368	ALA	2.7
1	E	398	VAL	2.7
1	E	296	ILE	2.7
1	E	386	GLY	2.7
1	C	531	SER	2.7
1	E	108	ALA	2.7
1	E	289	ALA	2.7
1	E	115	LEU	2.7
1	E	238	LEU	2.7
1	F	54	VAL	2.7
1	E	335	PRO	2.7
1	F	101	PHE	2.7
1	F	472	THR	2.7
1	E	43	ARG	2.6
1	F	328	CYS	2.6
1	F	263	SER	2.6
1	E	141	ASP	2.6
1	E	298	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	368	ALA	2.6
1	E	314	SER	2.6
1	C	352	LYS	2.6
1	C	349	LEU	2.6
1	E	320	TRP	2.6
1	F	420	ARG	2.6
1	E	94	SER	2.6
1	E	191	ILE	2.6
1	F	427	PHE	2.6
1	E	136	GLU	2.6
1	E	330	LEU	2.6
1	E	162	VAL	2.6
1	F	35	ILE	2.6
1	E	119	PHE	2.6
1	E	371	ARG	2.6
1	E	313	PHE	2.5
1	F	192	GLY	2.5
1	E	78	LEU	2.5
1	F	345	ASN	2.5
1	F	374	ARG	2.5
1	E	46	GLU	2.5
1	E	495	ALA	2.5
1	F	99	ALA	2.5
1	F	289	ALA	2.5
1	E	331	TRP	2.5
1	E	396	SER	2.5
1	C	457	GLU	2.5
1	F	316	ASN	2.5
1	E	202	THR	2.5
1	F	414	PHE	2.5
1	E	295	CYS	2.5
1	E	522	GLY	2.5
1	C	205	ALA	2.5
1	A	458	ASN	2.5
1	E	388	THR	2.5
1	E	472	THR	2.5
1	F	431	PRO	2.5
1	F	227	LYS	2.5
1	F	407	LEU	2.5
1	F	469	TYR	2.5
1	F	511	LYS	2.5
1	F	57	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	359	VAL	2.5
1	F	156	SER	2.4
1	E	510	TRP	2.4
1	F	80	ASP	2.4
1	E	69	TYR	2.4
1	F	58	TYR	2.4
1	F	91	HIS	2.4
1	E	131	ALA	2.4
1	F	146	MET	2.4
1	E	220	PHE	2.4
1	F	111	LEU	2.4
1	F	519	LEU	2.4
1	E	64	PRO	2.4
1	E	291	ALA	2.4
1	F	475	ALA	2.4
1	E	201	GLN	2.4
1	C	203	PHE	2.4
1	F	390	LEU	2.4
1	F	265	THR	2.4
1	F	331	TRP	2.4
1	E	399	LYS	2.4
1	B	169	GLU	2.4
1	F	297	CYS	2.4
1	E	54	VAL	2.4
1	E	458	ASN	2.4
1	E	23	ASP	2.4
1	E	385	TYR	2.4
1	F	114	MET	2.4
1	E	135	LEU	2.4
1	F	25	GLU	2.4
1	F	73	SER	2.4
1	E	307	VAL	2.4
1	E	496	VAL	2.4
1	F	418	VAL	2.4
1	E	160	GLY	2.3
1	E	392	ASN	2.3
1	E	512	ILE	2.3
1	E	154	LEU	2.3
1	B	347	GLU	2.3
1	F	105	GLY	2.3
1	A	18	VAL	2.3
1	C	18	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	17	GLY	2.3
1	E	66	THR	2.3
1	E	99	ALA	2.3
1	E	337	ALA	2.3
1	E	370	SER	2.3
1	F	497	GLY	2.3
1	E	86	ILE	2.3
1	E	408	ILE	2.3
1	E	368	ALA	2.3
1	E	76	THR	2.3
1	E	65	GLU	2.3
1	E	35	ILE	2.3
1	E	150	PRO	2.3
1	F	68	PRO	2.3
1	F	78	LEU	2.3
1	E	137	SER	2.3
1	E	427	PHE	2.3
1	E	186	ILE	2.2
1	E	318	HIS	2.2
1	E	426	CYS	2.2
1	F	107	VAL	2.2
1	E	26	GLU	2.2
1	E	235	ALA	2.2
1	F	521	LEU	2.2
1	E	258	THR	2.2
1	C	530	SER	2.2
1	F	136	GLU	2.2
1	D	346	PRO	2.2
1	E	519	LEU	2.2
1	E	153	PHE	2.2
1	E	476	THR	2.2
1	E	230	SER	2.2
1	F	219	ASN	2.2
1	F	392	ASN	2.2
1	E	177	ALA	2.2
1	E	274	CYS	2.2
1	F	260	GLY	2.2
1	E	254	PHE	2.2
1	B	369	LEU	2.2
1	E	349	LEU	2.2
1	E	390	LEU	2.2
1	E	465	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	192	GLY	2.2
1	F	123	GLY	2.2
1	B	204	CYS	2.2
1	E	62	ARG	2.2
1	E	32	HIS	2.2
1	F	367	ILE	2.1
1	E	75	GLU	2.1
1	E	275	GLU	2.1
1	E	475	ALA	2.1
1	F	39	ALA	2.1
1	E	419	PRO	2.1
1	A	529	PHE	2.1
1	E	360	VAL	2.1
1	E	127	MET	2.1
1	F	360	VAL	2.1
1	F	509	ALA	2.1
1	F	118	GLY	2.1
1	E	234	SER	2.1
1	F	226	PHE	2.1
1	F	531	SER	2.1
1	C	523	LYS	2.1
1	E	152	SER	2.1
1	F	139	VAL	2.1
1	E	175	LEU	2.1
1	E	302	HIS	2.1
1	E	245	ASP	2.1
1	E	261	THR	2.1
1	E	280	TYR	2.1
1	E	288	ALA	2.1
1	E	366	GLN	2.1
1	E	321	PHE	2.1
1	E	171	ILE	2.0
1	E	315	LEU	2.0
1	F	204	CYS	2.0
1	E	49	PRO	2.0
1	E	107	VAL	2.0
1	A	234	SER	2.0
1	F	520	ILE	2.0
1	A	351	ASN	2.0
1	F	70	ASN	2.0
1	E	92	TRP	2.0
1	E	348	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	290	TYR	2.0
1	F	113	GLU	2.0
1	F	134	GLU	2.0
1	E	376	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	LLP	E	319	24/25	0.78	0.22	60,85,107,115	0
1	LLP	F	319	24/25	0.83	0.20	43,70,90,99	0
1	LLP	C	319	24/25	0.90	0.15	6,37,54,68	0
1	LLP	B	319	24/25	0.93	0.14	8,31,51,62	0
1	LLP	A	319	24/25	0.93	0.13	12,39,62,73	0
1	LLP	D	319	24/25	0.94	0.11	13,25,47,60	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

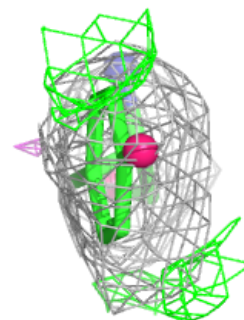
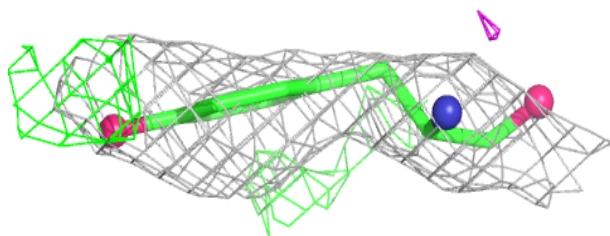
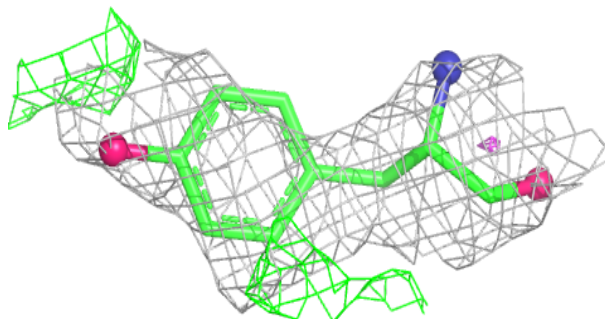
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TYR	D	601	12/13	0.77	0.27	29,41,56,56	0
2	TYR	C	601	12/13	0.85	0.19	26,32,44,49	0
2	TYR	A	601	13/13	0.86	0.23	22,47,66,66	0
2	TYR	B	601	13/13	0.90	0.18	19,37,46,57	0

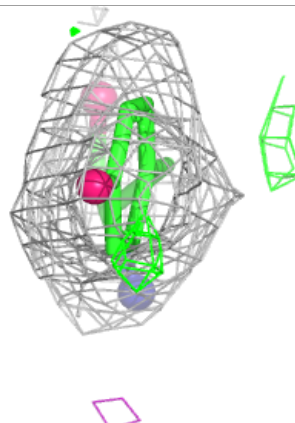
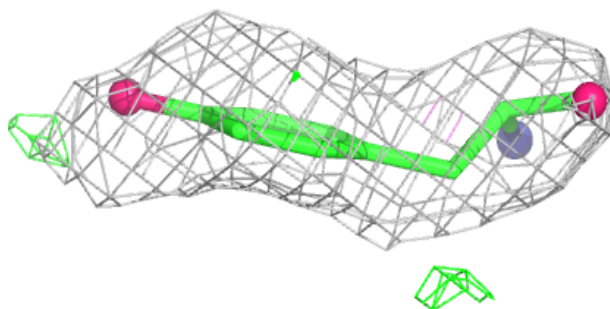
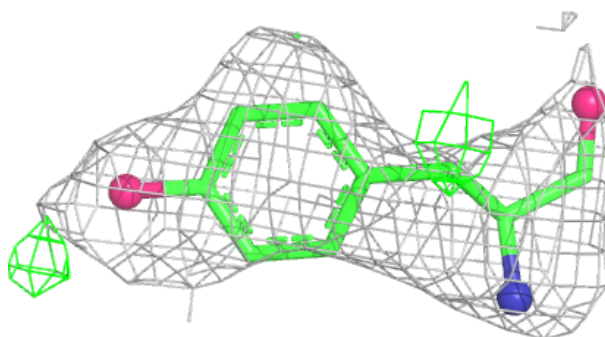
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TYR D 601:

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

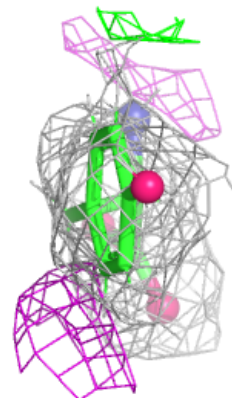
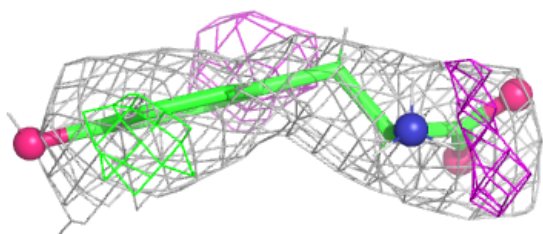
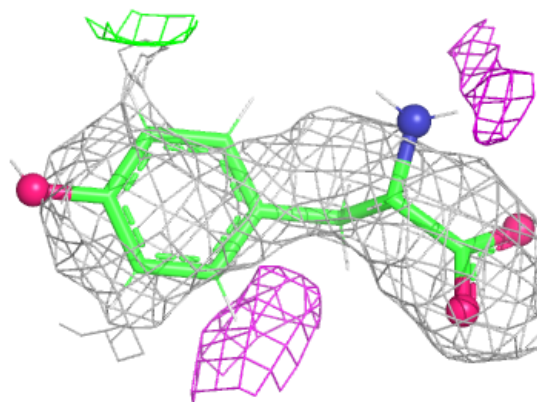
**Electron density around TYR C 601:**

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

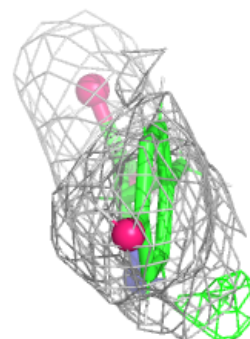
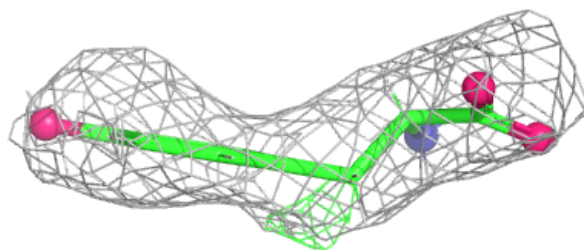
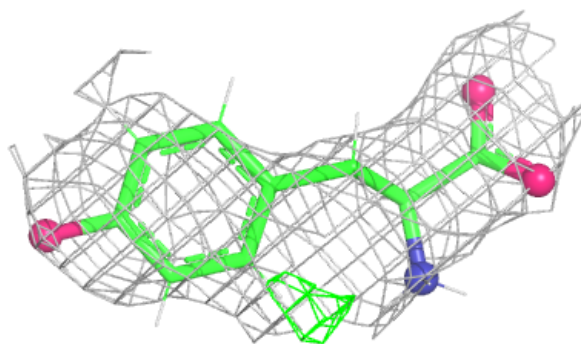


Electron density around TYR A 601:

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

**Electron density around TYR B 601:**

$2mF_o-DF_c$ (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.