



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:55 AM UTC

PDB ID : 5K1I / pdb_00005k1i
Title : PDE4 crystal structure in complex with small molecule inhibitor
Authors : Segarra, V.; Hernandez, B.; Ferrer-Miralles, N.; Korndorfer, I.; Aymami, J.
Deposited on : 2016-05-18
Resolution : 2.61 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

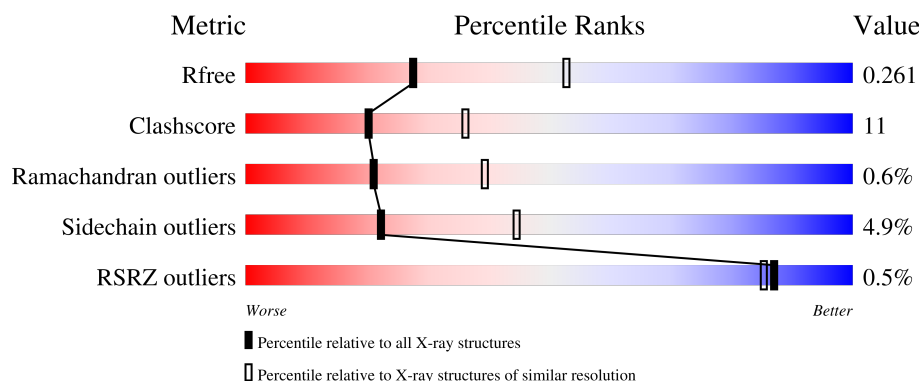
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	326	% 69% 27% ..
1	B	326	75% 23% .
1	C	326	75% 22% ..
1	D	326	77% 22% .
1	E	326	79% 19% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	326	% 66% 31%
1	G	326	% 75% 21%
1	H	326	% 75% 23%

2 Entry composition

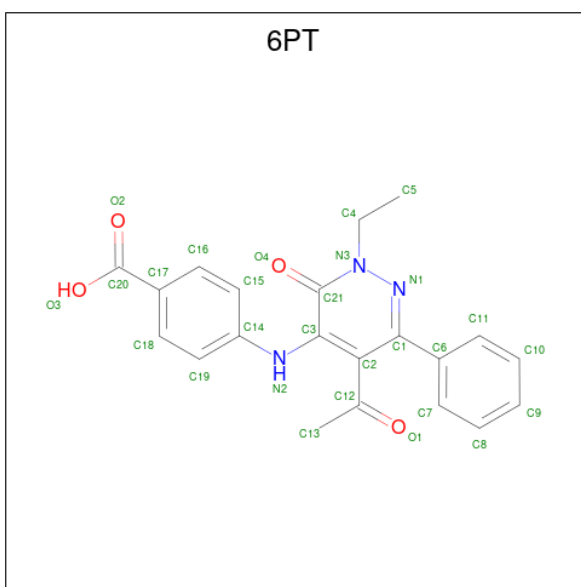
There are 5 unique types of molecules in this entry. The entry contains 21443 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2613	1655	446	498	14			
1	B	326	Total	C	N	O	S	0	0	0
			2637	1668	450	505	14			
1	C	321	Total	C	N	O	S	0	0	0
			2608	1652	445	497	14			
1	D	326	Total	C	N	O	S	0	0	0
			2638	1668	450	506	14			
1	E	321	Total	C	N	O	S	0	0	0
			2608	1652	445	497	14			
1	F	326	Total	C	N	O	S	0	0	0
			2638	1668	450	506	14			
1	G	322	Total	C	N	O	S	0	0	0
			2613	1655	446	498	14			
1	H	326	Total	C	N	O	S	0	0	0
			2638	1668	450	506	14			

- Molecule 2 is 4-[(5-acetyl-2-ethyl-3-oxo-6-phenyl-2,3-dihydropyridazin-4-yl)amino]benzoic acid (CCD ID: 6PT) (formula: C₂₁H₁₉N₃O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	21	3	4		
2	B	1	Total	C	N	O	0	0
			28	21	3	4		
2	C	1	Total	C	N	O	0	0
			28	21	3	4		
2	D	1	Total	C	N	O	0	0
			28	21	3	4		
2	E	1	Total	C	N	O	0	0
			28	21	3	4		
2	F	1	Total	C	N	O	0	0
			28	21	3	4		
2	G	1	Total	C	N	O	0	0
			28	21	3	4		
2	H	1	Total	C	N	O	0	0
			28	21	3	4		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0
3	G	1	Total 1	Zn 1	0	0
3	H	1	Total 1	Zn 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0
4	G	1	Total 1	Mg 1	0	0
4	H	1	Total 1	Mg 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total 18	O 18	0	0
5	B	35	Total 35	O 35	0	0
5	C	33	Total 33	O 33	0	0
5	D	21	Total 21	O 21	0	0
5	E	32	Total 32	O 32	0	0

Continued on next page...

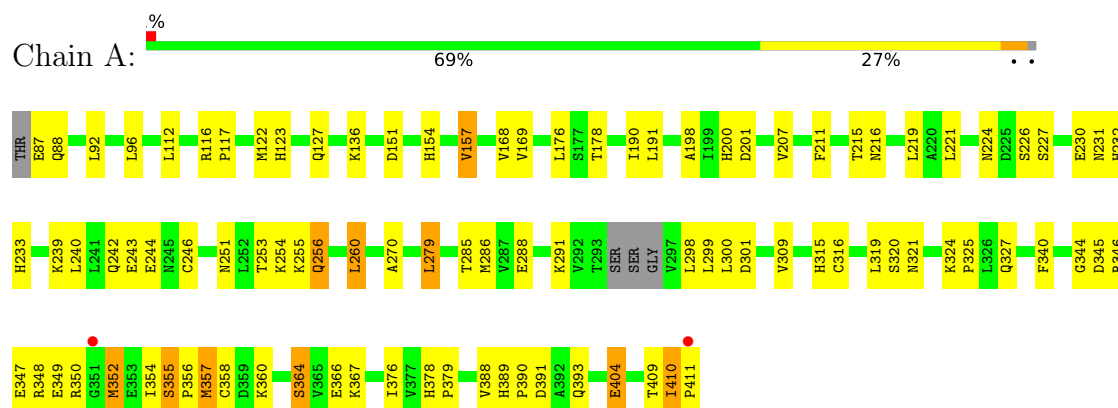
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	15	Total 15	O 15	0	0
5	G	33	Total 33	O 33	0	0
5	H	23	Total 23	O 23	0	0

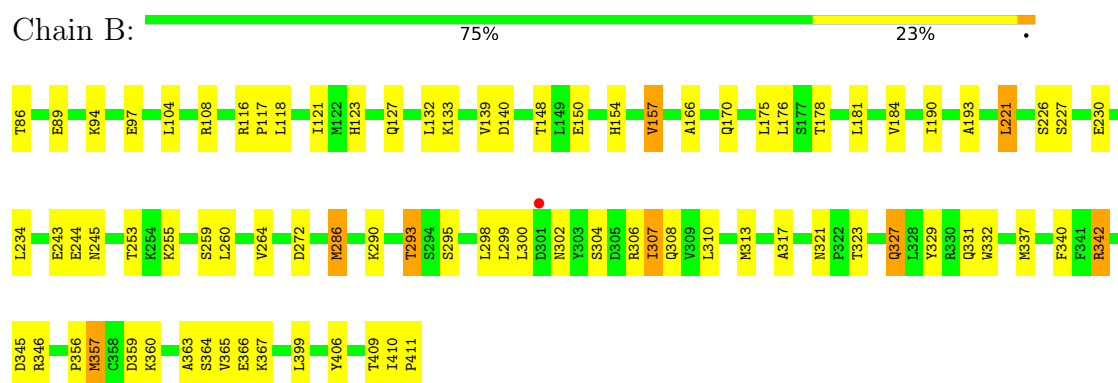
3 Residue-property plots

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.

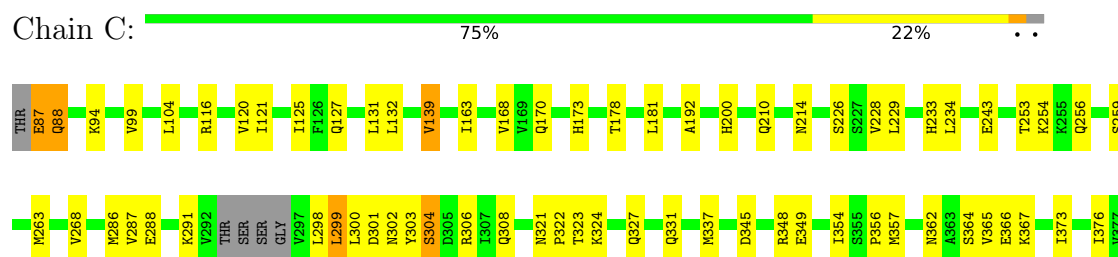
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

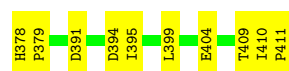


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



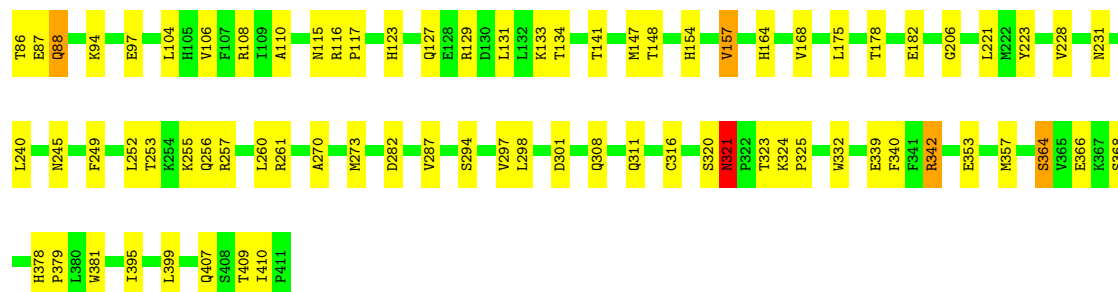
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D





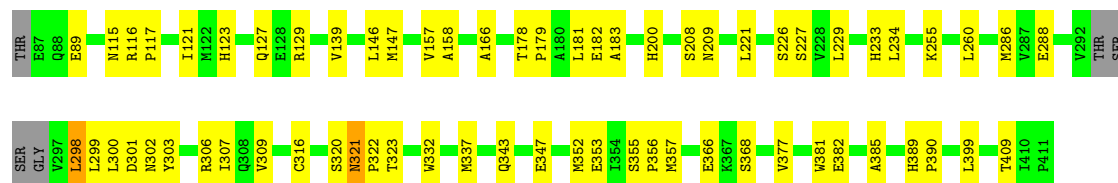
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain D: 77% 22% .



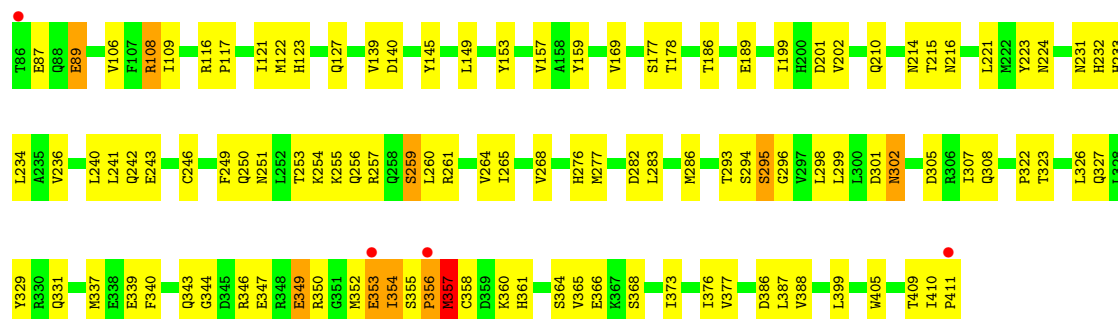
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain E: 79% 19% ..



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

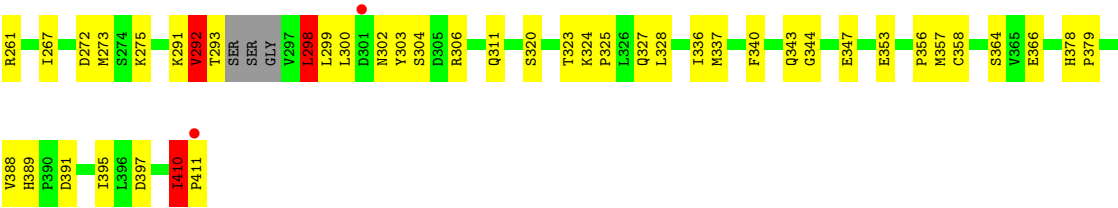
Chain F: 66% 31% .



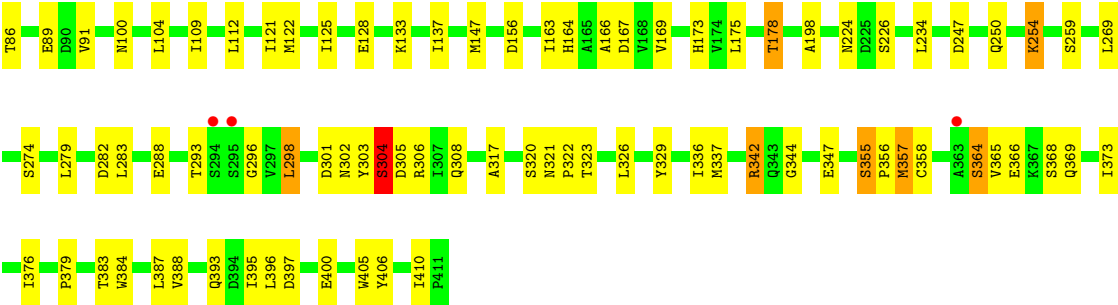
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain G: 75% 21% ...





● Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.44Å 78.35Å 161.76Å 91.01° 92.79° 90.08°	Depositor
Resolution (Å)	25.00 – 2.61 25.00 – 2.61	Depositor EDS
% Data completeness (in resolution range)	94.8 (25.00-2.61) 95.0 (25.00-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.191 , 0.258 0.197 , 0.261	Depositor DCC
R_{free} test set	4409 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.077 for h,-k,-l 0.069 for -h,k,-l 0.065 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21443	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 6PT

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	0.71	0/2666	0.96	3/3621 (0.1%)
1	B	0.77	0/2691	0.99	1/3656 (0.0%)
1	C	0.76	0/2661	1.01	4/3614 (0.1%)
1	D	0.77	0/2692	1.01	3/3658 (0.1%)
1	E	0.82	0/2661	1.02	1/3614 (0.0%)
1	F	0.70	0/2692	0.94	4/3658 (0.1%)
1	G	0.77	1/2666 (0.0%)	0.99	7/3621 (0.2%)
1	H	0.74	0/2692	0.98	6/3658 (0.2%)
All	All	0.76	1/21421 (0.0%)	0.99	29/29100 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	157	VAL	CA-CB	5.56	1.60	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	292	VAL	N-CA-C	7.03	118.26	107.78
1	C	376	ILE	CB-CA-C	-6.66	105.13	111.05
1	A	350	ARG	N-CA-C	-6.36	104.27	111.07
1	C	228	VAL	N-CA-C	6.17	116.65	110.23
1	G	88	GLN	N-CA-C	-6.04	104.69	111.28
1	H	137	ILE	CA-C-N	-5.99	113.77	119.76
1	H	137	ILE	C-N-CA	-5.99	113.77	119.76
1	H	355	SER	CA-C-N	-5.98	113.37	119.83
1	H	355	SER	C-N-CA	-5.98	113.37	119.83
1	F	89	GLU	N-CA-C	-5.89	104.94	111.36
1	G	410	ILE	N-CA-C	5.66	121.10	108.88
1	G	298	LEU	N-CA-C	5.59	118.13	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ILE	CB-CA-C	-5.51	107.03	111.71
1	H	269	LEU	N-CA-C	-5.47	105.42	111.71
1	G	397	ASP	N-CA-C	5.44	117.20	111.28
1	B	317	ALA	N-CA-C	-5.41	105.47	111.36
1	F	253	THR	N-CA-C	-5.40	102.90	110.35
1	A	321	ASN	N-CA-C	5.30	121.53	109.81
1	E	158	ALA	N-CA-C	5.28	117.72	111.33
1	G	320	SER	N-CA-C	5.23	119.82	113.38
1	C	131	LEU	N-CA-C	5.20	117.85	111.82
1	F	178	THR	CA-C-N	5.19	126.33	119.84
1	F	178	THR	C-N-CA	5.19	126.33	119.84
1	D	106	VAL	N-CA-C	5.16	115.88	110.62
1	D	321	ASN	CA-C-N	-5.15	114.41	120.12
1	D	321	ASN	C-N-CA	-5.15	114.41	120.12
1	H	410	ILE	CB-CA-C	-5.14	106.16	110.94
1	G	391	ASP	N-CA-C	5.07	117.54	111.71
1	C	163	ILE	N-CA-CB	5.01	116.42	110.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2613	0	2565	63	0
1	B	2637	0	2589	61	0
1	C	2608	0	2563	54	0
1	D	2638	0	2591	53	0
1	E	2608	0	2563	45	0
1	F	2638	0	2591	94	0
1	G	2613	0	2565	51	0
1	H	2638	0	2591	52	0
2	A	28	0	0	1	0
2	B	28	0	0	3	0
2	C	28	0	0	3	0
2	D	28	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	28	0	0	1	0
2	F	28	0	0	3	0
2	G	28	0	0	3	0
2	H	28	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	18	0	0	6	0
5	B	35	0	0	3	0
5	C	33	0	0	3	0
5	D	21	0	0	2	0
5	E	32	0	0	2	0
5	F	15	0	0	11	0
5	G	33	0	0	0	0
5	H	23	0	0	4	0
All	All	21443	0	20618	474	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (474) 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:F:301:ASP:HB3	5:F:1109:HOH:O	1.18	1.27
1:C:411:PRO:HB3	5:C:1125:HOH:O	1.35	1.26
1:F:358:CYS:HB3	5:F:1103:HOH:O	1.02	1.17
1:F:331:GLN:HB3	5:F:1104:HOH:O	1.40	1.16
1:F:108:ARG:CG	1:F:108:ARG:HH11	1.57	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:337:MET:HE2	5:H:1106:HOH:O	1.44	1.12
1:F:108:ARG:HH11	1:F:108:ARG:HG2	0.96	1.09
1:H:175:LEU:O	1:H:178:THR:HG22	1.49	1.09
1:A:357:MET:HE3	1:A:357:MET:HA	1.24	1.07
1:E:337:MET:HE3	5:E:1106:HOH:O	1.51	1.07
1:B:357:MET:HE3	1:B:357:MET:HA	1.38	1.04
1:B:293:THR:HG23	1:B:299:LEU:HD21	1.37	1.04
1:E:337:MET:CE	5:E:1106:HOH:O	2.03	1.04
1:A:358:CYS:HA	5:A:1107:HOH:O	1.60	1.01
1:H:86:THR:HB	1:H:89:GLU:OE1	1.61	1.00
1:F:108:ARG:HG2	1:F:108:ARG:NH1	1.72	0.99
1:G:175:LEU:O	1:G:178:THR:HG22	1.69	0.93
1:D:342:ARG:CG	1:D:342:ARG:HH11	1.82	0.90
1:A:357:MET:HA	1:A:357:MET:CE	2.01	0.90
1:D:253:THR:OG1	1:D:256:GLN:HG3	1.70	0.90
1:D:342:ARG:HH11	1:D:342:ARG:HG2	1.37	0.89
1:E:306:ARG:HG2	1:E:306:ARG:HH11	1.35	0.89
1:D:407:GLN:HA	1:D:410:ILE:HD12	1.54	0.88
1:C:87:GLU:HG3	1:C:88:GLN:N	1.89	0.86
1:B:356:PRO:O	1:B:357:MET:HB2	1.74	0.85
1:F:123:HIS:CE1	1:F:127:GLN:HE21	1.92	0.85
1:H:337:MET:CE	5:H:1106:HOH:O	2.09	0.83
1:B:340:PHE:HZ	2:B:1001:6PT:C13	1.92	0.82
1:G:356:PRO:O	1:G:357:MET:HB2	1.80	0.80
1:B:193:ALA:HB2	1:B:310:LEU:HD22	1.63	0.79
1:B:357:MET:HA	1:B:357:MET:CE	2.11	0.79
1:F:373:ILE:HA	1:F:377:VAL:HB	1.65	0.79
1:E:306:ARG:HG2	1:E:306:ARG:NH1	1.98	0.77
1:H:125:ILE:HD13	1:H:173:HIS:HB2	1.67	0.76
1:F:123:HIS:HE1	1:F:127:GLN:HE21	1.32	0.76
1:F:282:ASP:HB3	1:F:308:GLN:NE2	2.01	0.76
1:C:324:LYS:NZ	5:C:1101:HOH:O	2.17	0.75
1:E:234:LEU:HB3	1:F:224:ASN:OD1	1.86	0.75
1:C:378:HIS:HB3	1:C:379:PRO:HD3	1.68	0.74
1:B:410:ILE:O	5:B:1101:HOH:O	2.04	0.74
1:A:340:PHE:HB3	5:A:1107:HOH:O	1.86	0.74
1:C:356:PRO:O	1:C:357:MET:HB2	1.86	0.74
1:F:356:PRO:O	1:F:357:MET:HB2	1.86	0.74
1:D:342:ARG:HG2	1:D:342:ARG:NH1	2.00	0.73
1:D:116:ARG:N	1:D:117:PRO:CD	2.51	0.73
1:H:393:GLN:NE2	1:H:397:ASP:OD1	2.21	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:THR:HB	1:B:89:GLU:OE1	1.88	0.72
1:B:175:LEU:O	1:B:178:THR:HG22	1.90	0.72
1:F:87:GLU:O	1:F:87:GLU:HG2	1.88	0.72
1:E:298:LEU:HD13	1:E:300:LEU:HD11	1.72	0.72
1:F:108:ARG:CG	1:F:108:ARG:NH1	2.29	0.71
1:D:116:ARG:CZ	1:D:147:MET:HE2	2.21	0.71
1:G:104:LEU:HD11	1:G:109:ILE:HD11	1.74	0.70
1:D:94:LYS:O	1:D:97:GLU:HB2	1.93	0.69
1:B:340:PHE:CZ	2:B:1001:6PT:C13	2.75	0.69
1:A:345:ASP:OD1	1:A:360:LYS:HE2	1.93	0.69
1:F:327:GLN:O	1:F:331:GLN:HG3	1.93	0.68
1:G:323:THR:HB	1:G:395:ILE:HG23	1.75	0.68
1:A:123:HIS:CE1	1:A:127:GLN:HE21	2.12	0.68
1:B:364:SER:OG	1:B:367:LYS:HB2	1.94	0.68
1:G:116:ARG:NH2	1:G:147:MET:HE2	2.09	0.67
1:C:373:ILE:HG23	1:C:399:LEU:HD11	1.76	0.67
1:F:355:SER:HB2	1:F:358:CYS:SG	2.34	0.67
1:D:407:GLN:HA	1:D:410:ILE:CD1	2.25	0.67
1:C:132:LEU:CD2	1:C:139:VAL:HG23	2.24	0.66
1:G:366:GLU:OE2	1:G:366:GLU:N	2.25	0.66
1:G:298:LEU:HD13	1:G:300:LEU:HD21	1.77	0.65
1:G:94:LYS:O	1:G:97:GLU:HB2	1.96	0.65
1:H:121:ILE:HD12	1:H:166:ALA:HB1	1.78	0.65
1:C:345:ASP:O	1:C:349:GLU:HG2	1.96	0.65
1:B:366:GLU:HG2	1:B:409:THR:OG1	1.97	0.65
1:G:154:HIS:HB2	1:G:157:VAL:HG13	1.77	0.64
1:B:293:THR:CG2	1:B:299:LEU:HD21	2.23	0.64
1:C:178:THR:HG22	1:C:181:LEU:HD12	1.80	0.64
1:F:327:GLN:HB3	5:F:1115:HOH:O	1.97	0.64
1:C:104:LEU:HD22	1:C:170:GLN:HG3	1.79	0.64
1:D:175:LEU:O	1:D:178:THR:HG22	1.98	0.64
2:D:1001:6PT:C12	2:D:1001:6PT:C15	2.75	0.64
1:G:243:GLU:O	1:G:246:CYS:HB2	1.98	0.63
1:E:260:LEU:HD23	1:E:260:LEU:C	2.23	0.63
1:A:136:LYS:O	1:A:251:ASN:ND2	2.31	0.63
1:G:292:VAL:HG23	1:G:292:VAL:O	1.98	0.63
1:A:286:MET:HE1	1:A:309:VAL:HG23	1.81	0.62
1:C:286:MET:HE1	1:C:308:GLN:HB2	1.80	0.62
1:D:123:HIS:CE1	1:D:127:GLN:HE21	2.16	0.62
1:E:321:ASN:HB3	1:E:332:TRP:CD1	2.33	0.62
1:B:359:ASP:O	1:B:363:ALA:HB2	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:MET:HE1	1:E:309:VAL:HG23	1.81	0.62
1:F:357:MET:HE3	1:F:357:MET:HA	1.81	0.62
1:B:342:ARG:HH11	1:B:342:ARG:CG	2.13	0.62
1:F:326:LEU:HD21	1:F:405:TRP:CD2	2.35	0.62
1:H:298:LEU:HD11	1:H:387:LEU:HD11	1.80	0.62
1:C:366:GLU:HG2	1:C:409:THR:OG1	1.99	0.62
1:B:123:HIS:CE1	1:B:127:GLN:HE21	2.19	0.61
1:F:302:ASN:H	1:F:302:ASN:ND2	1.98	0.61
1:G:141:THR:OG1	1:G:245:ASN:ND2	2.33	0.61
1:D:366:GLU:HG2	1:D:409:THR:OG1	2.01	0.61
1:H:282:ASP:HB3	1:H:308:GLN:NE2	2.16	0.61
2:H:1001:6PT:C15	2:H:1001:6PT:C12	2.78	0.61
1:B:104:LEU:HD22	1:B:170:GLN:HG3	1.83	0.61
1:F:340:PHE:HZ	2:F:1001:6PT:C13	2.14	0.61
1:B:345:ASP:OD1	1:B:360:LYS:HE2	2.00	0.60
1:C:356:PRO:O	1:C:357:MET:CB	2.47	0.60
1:C:410:ILE:O	1:C:411:PRO:C	2.43	0.60
1:F:327:GLN:CB	5:F:1115:HOH:O	2.50	0.60
1:A:301:ASP:HB3	5:A:1113:HOH:O	1.99	0.60
1:F:277:MET:HG2	5:F:1105:HOH:O	2.01	0.60
1:B:356:PRO:O	1:B:357:MET:CB	2.47	0.60
1:D:116:ARG:N	1:D:117:PRO:HD2	2.16	0.60
1:B:260:LEU:O	1:B:264:VAL:HG23	2.01	0.59
1:D:321:ASN:HB3	1:D:332:TRP:CD1	2.37	0.59
1:A:357:MET:HE1	1:A:364:SER:H	1.67	0.59
2:A:1001:6PT:C12	2:A:1001:6PT:C15	2.81	0.59
1:B:123:HIS:HE1	1:B:127:GLN:HE21	1.50	0.59
1:H:322:PRO:HB3	1:H:329:TYR:CZ	2.38	0.59
1:H:125:ILE:HD13	1:H:173:HIS:CB	2.32	0.59
1:H:303:TYR:O	1:H:305:ASP:N	2.35	0.59
1:D:116:ARG:NH2	1:D:147:MET:HE2	2.18	0.59
1:F:366:GLU:HG2	1:F:409:THR:OG1	2.03	0.59
1:F:301:ASP:CB	5:F:1109:HOH:O	2.02	0.58
1:E:357:MET:SD	1:E:368:SER:OG	2.61	0.58
1:E:123:HIS:HE1	1:E:127:GLN:HE21	1.51	0.58
1:C:394:ASP:HB2	5:C:1117:HOH:O	2.02	0.58
1:A:404:GLU:O	1:A:404:GLU:HG3	2.04	0.58
2:C:1001:6PT:C15	2:C:1001:6PT:C12	2.82	0.58
1:E:356:PRO:O	1:E:357:MET:HB2	2.03	0.58
1:A:176:LEU:HD13	1:A:190:ILE:HG23	1.86	0.57
1:F:260:LEU:O	1:F:264:VAL:HG23	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:352:MET:O	1:F:354:ILE:N	2.37	0.57
1:E:286:MET:HE1	1:E:309:VAL:CG2	2.35	0.57
1:C:304:SER:O	1:C:308:GLN:HG3	2.05	0.57
1:G:410:ILE:O	1:G:411:PRO:O	2.22	0.57
1:C:178:THR:CG2	1:C:181:LEU:HD12	2.35	0.57
1:H:356:PRO:O	1:H:357:MET:HB2	2.04	0.57
1:C:378:HIS:HB3	1:C:379:PRO:CD	2.35	0.57
1:F:254:LYS:O	1:F:255:LYS:C	2.47	0.57
1:F:243:GLU:O	1:F:246:CYS:HB2	2.05	0.56
1:F:356:PRO:O	1:F:357:MET:CB	2.53	0.56
1:A:239:LYS:HB2	1:B:221:LEU:HD21	1.86	0.56
1:G:302:ASN:OD1	1:G:304:SER:HB3	2.05	0.56
1:H:321:ASN:N	1:H:322:PRO:CD	2.68	0.56
1:D:154:HIS:HB2	1:D:157:VAL:HG13	1.88	0.56
1:C:210:GLN:HE21	1:C:214:ASN:ND2	2.04	0.56
1:A:344:GLY:HA2	1:A:347:GLU:HB2	1.87	0.56
1:C:87:GLU:CG	1:C:88:GLN:N	2.68	0.56
1:H:342:ARG:HD3	5:H:1115:HOH:O	2.06	0.56
1:A:393:GLN:OE1	1:A:393:GLN:HA	2.06	0.55
1:F:282:ASP:HB3	1:F:308:GLN:HE22	1.69	0.55
1:G:336:ILE:HG23	1:G:337:MET:HE2	1.87	0.55
1:H:224:ASN:O	1:H:226:SER:HB2	2.06	0.55
1:D:141:THR:OG1	1:D:245:ASN:ND2	2.40	0.55
1:A:211:PHE:O	1:A:215:THR:HG23	2.07	0.55
1:A:285:THR:O	1:A:288:GLU:HB3	2.07	0.55
1:F:250:GLN:HA	1:F:257:ARG:HH12	1.71	0.55
1:B:94:LYS:O	1:B:97:GLU:HB2	2.07	0.55
1:F:87:GLU:O	1:F:87:GLU:CG	2.54	0.55
1:H:369:GLN:HG2	5:H:1106:HOH:O	2.06	0.55
1:D:182:GLU:OE2	1:D:182:GLU:HA	2.06	0.54
1:F:199:ILE:O	1:F:202:VAL:HG12	2.08	0.54
1:H:344:GLY:HA3	1:H:358:CYS:O	2.07	0.54
1:A:232:HIS:ND1	5:A:1101:HOH:O	2.30	0.54
1:A:340:PHE:C	5:A:1107:HOH:O	2.49	0.54
1:G:116:ARG:CZ	1:G:147:MET:HE2	2.37	0.54
1:D:228:VAL:HG23	5:D:1107:HOH:O	2.08	0.54
1:B:327:GLN:HE21	1:B:327:GLN:H	1.56	0.54
1:B:342:ARG:HH21	1:G:291:LYS:HE2	1.72	0.54
1:A:116:ARG:NH2	1:A:151:ASP:OD2	2.36	0.54
1:C:291:LYS:O	1:C:299:LEU:HB2	2.08	0.54
1:F:123:HIS:HE1	1:F:127:GLN:NE2	2.05	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:TYR:HB3	1:F:339:GLU:OE1	2.08	0.54
1:B:243:GLU:O	1:B:244:GLU:C	2.49	0.54
1:B:342:ARG:CG	1:B:342:ARG:NH1	2.70	0.54
1:A:154:HIS:HB2	1:A:157:VAL:HG13	1.89	0.53
1:B:176:LEU:HD23	1:B:313:MET:HE1	1.90	0.53
1:D:249:PHE:O	1:D:257:ARG:NH1	2.40	0.53
1:G:104:LEU:HD11	1:G:109:ILE:CD1	2.37	0.53
1:C:286:MET:CE	1:C:308:GLN:HB2	2.39	0.53
1:E:129:ARG:HG2	1:E:129:ARG:HH11	1.72	0.53
1:A:122:MET:HE2	1:A:198:ALA:CB	2.39	0.53
1:A:324:LYS:HB3	1:A:325:PRO:HD2	1.90	0.53
1:C:116:ARG:O	1:C:120:VAL:HG22	2.09	0.53
1:F:293:THR:O	1:F:296:GLY:N	2.35	0.53
1:A:92:LEU:O	1:A:96:LEU:HG	2.10	0.52
1:H:91:VAL:HG12	1:H:112:LEU:HD13	1.91	0.52
1:B:181:LEU:HD21	1:B:298:LEU:HD12	1.92	0.52
1:B:342:ARG:NH1	1:B:342:ARG:HG2	2.23	0.52
1:F:283:LEU:HD11	1:F:387:LEU:HD22	1.90	0.52
1:E:116:ARG:CZ	1:E:147:MET:HE2	2.40	0.52
1:F:282:ASP:CB	1:F:308:GLN:NE2	2.70	0.52
1:F:340:PHE:CZ	2:F:1001:6PT:C13	2.92	0.52
1:A:340:PHE:CB	5:A:1107:HOH:O	2.52	0.52
1:E:302:ASN:O	1:E:303:TYR:C	2.52	0.52
1:E:343:GLN:O	1:E:347:GLU:HG3	2.09	0.52
1:G:292:VAL:O	1:G:292:VAL:CG2	2.57	0.52
1:E:116:ARG:CZ	1:E:147:MET:CE	2.88	0.52
1:B:321:ASN:HB2	1:B:332:TRP:CD1	2.45	0.51
1:D:323:THR:HB	1:D:395:ILE:HG23	1.91	0.51
1:F:215:THR:O	1:F:216:ASN:C	2.53	0.51
1:G:154:HIS:HB2	1:G:157:VAL:CG1	2.38	0.51
1:G:340:PHE:HZ	2:G:1001:6PT:C13	2.23	0.51
1:D:164:HIS:O	1:D:168:VAL:HG23	2.11	0.51
1:F:254:LYS:C	1:F:256:GLN:N	2.68	0.51
1:H:317:ALA:HA	1:H:320:SER:HB3	1.92	0.51
1:F:326:LEU:HD21	1:F:405:TRP:CE3	2.46	0.51
1:C:321:ASN:N	1:C:322:PRO:CD	2.73	0.51
1:G:292:VAL:O	1:G:293:THR:C	2.52	0.51
1:D:357:MET:HE1	1:D:364:SER:H	1.77	0.50
1:F:349:GLU:O	1:F:350:ARG:C	2.54	0.50
1:A:116:ARG:N	1:A:117:PRO:CD	2.73	0.50
1:C:299:LEU:O	1:C:300:LEU:HD23	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:322:PRO:HG2	1:E:377:VAL:HG21	1.94	0.50
1:F:123:HIS:O	1:F:127:GLN:HG2	2.12	0.50
1:H:326:LEU:HD21	1:H:405:TRP:CD2	2.47	0.50
1:B:184:VAL:HG11	1:B:300:LEU:HD12	1.91	0.50
1:B:321:ASN:CB	1:B:332:TRP:CD1	2.95	0.50
1:F:108:ARG:HH11	1:F:108:ARG:HG3	1.63	0.50
1:F:355:SER:HB3	1:F:356:PRO:CD	2.42	0.50
1:G:135:PHE:CE2	1:G:191:LEU:HD22	2.47	0.50
1:H:303:TYR:O	1:H:304:SER:C	2.55	0.50
1:C:253:THR:HB	1:E:288:GLU:HG3	1.94	0.49
1:H:369:GLN:O	1:H:373:ILE:HG13	2.11	0.49
1:A:200:HIS:NE2	1:A:201:ASP:OD2	2.45	0.49
1:F:302:ASN:H	1:F:302:ASN:HD22	1.58	0.49
1:A:366:GLU:HG2	1:A:409:THR:OG1	2.12	0.49
1:D:301:ASP:N	5:D:1102:HOH:O	2.30	0.49
1:D:357:MET:HE2	1:D:368:SER:OG	2.13	0.49
1:E:123:HIS:CE1	1:E:127:GLN:HE21	2.29	0.49
1:G:302:ASN:O	1:G:303:TYR:C	2.56	0.49
1:C:132:LEU:HD22	1:C:139:VAL:HG23	1.95	0.49
1:C:323:THR:HB	1:C:395:ILE:HG23	1.94	0.49
1:D:282:ASP:HB3	1:D:308:GLN:NE2	2.28	0.49
1:G:302:ASN:O	1:G:306:ARG:HG3	2.12	0.49
1:D:87:GLU:O	1:D:88:GLN:C	2.55	0.49
1:F:293:THR:C	1:F:295:SER:N	2.68	0.49
2:E:1001:6PT:C15	2:E:1001:6PT:C12	2.91	0.49
1:E:366:GLU:HG2	1:E:409:THR:OG1	2.12	0.48
1:G:260:LEU:O	1:G:261:ARG:C	2.56	0.48
1:C:373:ILE:CG2	1:C:399:LEU:HD11	2.43	0.48
1:F:122:MET:SD	1:F:169:VAL:HG11	2.53	0.48
1:G:224:ASN:OD1	1:H:234:LEU:HB3	2.12	0.48
2:G:1001:6PT:C15	2:G:1001:6PT:C12	2.91	0.48
1:D:123:HIS:HE1	1:D:127:GLN:HE21	1.60	0.48
1:D:342:ARG:HH11	1:D:342:ARG:HG3	1.74	0.48
1:B:327:GLN:H	1:B:327:GLN:NE2	2.10	0.48
1:C:337:MET:HG3	1:C:365:VAL:HG22	1.95	0.48
1:A:355:SER:HB3	1:A:356:PRO:CD	2.43	0.48
1:B:323:THR:HG22	1:B:399:LEU:HD13	1.95	0.48
1:F:337:MET:HE3	1:F:365:VAL:HG13	1.96	0.48
1:E:301:ASP:O	1:E:302:ASN:HB3	2.13	0.48
1:F:344:GLY:HA2	1:F:347:GLU:HB2	1.95	0.48
1:A:122:MET:HE2	1:A:198:ALA:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ARG:CG	1:D:342:ARG:NH1	2.53	0.48
1:H:125:ILE:HD13	1:H:173:HIS:CG	2.49	0.48
1:A:352:MET:HE2	1:A:352:MET:HB2	1.71	0.47
1:E:116:ARG:N	1:E:117:PRO:CD	2.77	0.47
1:F:106:VAL:HA	1:F:109:ILE:HD12	1.95	0.47
1:F:344:GLY:CA	5:F:1103:HOH:O	2.62	0.47
1:F:410:ILE:CG2	1:F:411:PRO:HD2	2.44	0.47
2:F:1001:6PT:C12	2:F:1001:6PT:C15	2.92	0.47
1:H:337:MET:HE3	1:H:365:VAL:HA	1.96	0.47
1:F:364:SER:O	1:F:368:SER:OG	2.29	0.47
1:H:100:ASN:OD1	1:H:173:HIS:NE2	2.43	0.47
1:A:315:HIS:CE1	1:A:319:LEU:HD11	2.50	0.47
1:D:316:CYS:HB3	1:D:381:TRP:CZ2	2.50	0.47
2:B:1001:6PT:C12	2:B:1001:6PT:C15	2.93	0.47
1:F:286:MET:HE2	1:F:305:ASP:OD1	2.14	0.47
1:A:178:THR:OG1	1:A:391:ASP:OD2	2.32	0.47
1:D:378:HIS:O	1:D:379:PRO:C	2.54	0.47
1:D:110:ALA:HA	1:D:117:PRO:HD3	1.95	0.47
1:F:234:LEU:HD21	1:F:268:VAL:HB	1.96	0.47
1:F:344:GLY:N	5:F:1103:HOH:O	2.48	0.47
1:G:410:ILE:HG22	1:G:411:PRO:N	2.30	0.47
1:C:178:THR:OG1	1:C:391:ASP:OD2	2.31	0.46
1:D:148:THR:HG22	1:D:240:LEU:HD22	1.97	0.46
1:B:121:ILE:HD12	1:B:166:ALA:HB1	1.97	0.46
1:D:116:ARG:CZ	1:D:147:MET:CE	2.91	0.46
1:D:129:ARG:HB2	1:D:131:LEU:HG	1.98	0.46
1:G:117:PRO:O	1:G:121:ILE:HD12	2.15	0.46
1:A:215:THR:O	1:A:216:ASN:C	2.58	0.46
1:E:182:GLU:O	1:E:183:ALA:HB3	2.16	0.46
1:E:298:LEU:HD13	1:E:300:LEU:CD1	2.43	0.46
1:H:323:THR:HB	1:H:395:ILE:HG23	1.97	0.46
1:G:178:THR:CG2	1:G:181:LEU:HD12	2.45	0.46
1:H:279:LEU:HA	1:H:279:LEU:HD12	1.77	0.46
1:A:348:ARG:HH11	1:A:348:ARG:HB3	1.79	0.46
1:F:157:VAL:HG23	1:F:157:VAL:O	2.16	0.46
1:G:115:ASN:C	1:G:117:PRO:HD2	2.40	0.46
1:H:384:TRP:O	1:H:388:VAL:HG22	2.15	0.46
1:D:407:GLN:CA	1:D:410:ILE:HD12	2.36	0.46
1:E:129:ARG:HG2	1:E:129:ARG:NH1	2.31	0.46
1:G:340:PHE:CZ	2:G:1001:6PT:C13	2.98	0.46
1:F:210:GLN:HE21	1:F:214:ASN:ND2	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:366:GLU:CD	1:H:366:GLU:H	2.24	0.46
1:A:178:THR:OG1	1:A:391:ASP:CB	2.64	0.46
1:A:345:ASP:HA	1:A:348:ARG:HH12	1.81	0.46
1:H:322:PRO:HA	1:H:329:TYR:CD1	2.51	0.46
1:A:316:CYS:O	1:A:320:SER:HB3	2.16	0.45
1:H:347:GLU:OE2	1:H:355:SER:OG	2.31	0.45
1:A:226:SER:O	1:A:227:SER:C	2.59	0.45
1:B:230:GLU:OE2	1:B:272:ASP:HA	2.16	0.45
1:B:331:GLN:HB3	5:B:1122:HOH:O	2.16	0.45
1:C:210:GLN:HE21	1:C:214:ASN:HD21	1.63	0.45
1:H:122:MET:HE2	1:H:198:ALA:CB	2.46	0.45
1:A:367:LYS:HE3	1:A:367:LYS:HB2	1.65	0.45
1:H:298:LEU:HD11	1:H:387:LEU:CD1	2.44	0.45
1:H:376:ILE:C	1:H:379:PRO:HD2	2.41	0.45
1:F:353:GLU:O	1:F:354:ILE:C	2.59	0.45
1:F:358:CYS:CB	5:F:1103:HOH:O	1.90	0.45
1:H:364:SER:O	1:H:368:SER:OG	2.28	0.45
1:A:224:ASN:OD1	1:B:234:LEU:HB3	2.16	0.45
1:E:316:CYS:O	1:E:320:SER:HB3	2.17	0.45
1:F:116:ARG:N	1:F:117:PRO:CD	2.80	0.45
1:A:270:ALA:HB1	1:A:279:LEU:HD21	1.97	0.45
1:A:299:LEU:O	1:A:300:LEU:HD23	2.17	0.45
1:C:301:ASP:O	1:C:302:ASN:CB	2.64	0.45
1:E:121:ILE:HD12	1:E:166:ALA:HB1	1.99	0.45
1:C:367:LYS:HE3	1:C:367:LYS:HB2	1.68	0.45
1:B:342:ARG:NH2	1:G:291:LYS:HE2	2.31	0.45
1:C:301:ASP:O	1:C:302:ASN:HB3	2.17	0.45
1:C:364:SER:HB3	1:C:367:LYS:HB3	1.98	0.45
1:F:323:THR:HG22	1:F:399:LEU:HD13	1.99	0.45
1:G:410:ILE:HB	1:G:411:PRO:HD3	1.98	0.45
1:H:104:LEU:HD11	1:H:109:ILE:CD1	2.47	0.45
1:H:254:LYS:HE3	1:H:254:LYS:HB2	1.64	0.45
1:D:316:CYS:O	1:D:320:SER:HB3	2.17	0.45
1:F:186:THR:N	1:F:189:GLU:OE1	2.42	0.45
1:G:298:LEU:CD1	1:G:300:LEU:HD21	2.45	0.45
1:C:288:GLU:OE2	1:C:288:GLU:HA	2.16	0.45
1:F:108:ARG:NH1	1:F:108:ARG:HG3	2.27	0.45
1:F:250:GLN:HG3	1:F:251:ASN:OD1	2.17	0.45
1:H:156:ASP:OD2	1:H:156:ASP:N	2.51	0.44
1:D:115:ASN:C	1:D:117:PRO:HD2	2.43	0.44
1:D:206:GLY:HA2	1:D:339:GLU:OE2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:247:ASP:O	1:H:250:GLN:HG2	2.17	0.44
1:C:303:TYR:HA	1:C:306:ARG:HD3	1.98	0.44
1:D:223:TYR:CE1	1:D:231:ASN:HB3	2.52	0.44
1:F:240:LEU:O	1:F:241:LEU:C	2.60	0.44
1:B:226:SER:O	1:B:227:SER:C	2.61	0.44
1:C:234:LEU:HD11	1:C:268:VAL:HB	1.99	0.44
1:D:116:ARG:NE	1:D:147:MET:CE	2.80	0.44
1:D:324:LYS:O	1:D:325:PRO:C	2.60	0.44
1:B:329:TYR:CE2	1:B:406:TYR:HE2	2.35	0.44
1:A:191:LEU:HD23	1:A:260:LEU:HD13	1.99	0.44
1:E:381:TRP:O	1:E:385:ALA:N	2.48	0.44
1:B:286:MET:HE3	1:B:286:MET:HB2	1.70	0.44
1:F:117:PRO:O	1:F:121:ILE:HG13	2.17	0.44
1:C:357:MET:HE3	2:C:1001:6PT:C9	2.48	0.44
1:E:229:LEU:HD23	1:E:229:LEU:HA	1.88	0.44
1:E:321:ASN:CB	1:E:332:TRP:CD1	3.01	0.44
1:E:323:THR:HG22	1:E:399:LEU:HD13	2.00	0.44
1:A:355:SER:HB2	1:A:358:CYS:HB2	2.00	0.43
1:D:270:ALA:CB	1:D:311:GLN:HG2	2.47	0.43
1:E:306:ARG:HH11	1:E:306:ARG:CG	2.13	0.43
1:F:357:MET:HA	1:F:357:MET:CE	2.42	0.43
1:F:360:LYS:HG3	1:F:361:HIS:CD2	2.53	0.43
1:B:307:ILE:CG2	1:B:308:GLN:N	2.81	0.43
1:G:88:GLN:OE1	1:G:112:LEU:O	2.36	0.43
1:G:388:VAL:O	1:G:389:HIS:C	2.59	0.43
1:H:104:LEU:HD11	1:H:109:ILE:HD11	2.00	0.43
1:B:181:LEU:CD2	1:B:298:LEU:HD12	2.49	0.43
1:E:116:ARG:NH1	1:E:147:MET:HE2	2.34	0.43
1:H:283:LEU:HG	1:H:383:THR:HG22	1.99	0.43
1:B:302:ASN:OD1	1:B:304:SER:HB3	2.18	0.43
1:B:410:ILE:O	1:B:411:PRO:C	2.61	0.43
1:G:116:ARG:HH21	1:G:147:MET:HE2	1.81	0.43
1:B:272:ASP:OD1	1:B:272:ASP:C	2.62	0.43
1:E:200:HIS:O	1:E:233:HIS:CD2	2.72	0.43
1:F:223:TYR:CE1	1:F:231:ASN:HB3	2.54	0.43
1:A:207:VAL:HG11	1:A:346:ARG:NH1	2.33	0.43
1:B:139:VAL:HG13	1:B:140:ASP:N	2.34	0.43
1:B:154:HIS:HB2	1:B:157:VAL:HG13	2.00	0.43
1:B:345:ASP:O	1:B:346:ARG:C	2.62	0.43
1:D:340:PHE:CZ	2:D:1001:6PT:C13	3.02	0.43
1:F:276:HIS:CD2	1:F:376:ILE:HD12	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASP:HA	1:A:233:HIS:CD2	2.54	0.43
1:D:86:THR:O	1:D:87:GLU:C	2.62	0.43
1:D:88:GLN:HE21	1:D:88:GLN:HB2	1.67	0.43
1:F:322:PRO:HA	1:F:329:TYR:CG	2.54	0.43
1:A:88:GLN:O	1:A:88:GLN:HG2	2.19	0.43
1:A:348:ARG:HG3	1:A:354:ILE:HD11	2.01	0.43
1:B:118:LEU:HB3	1:B:150:GLU:CD	2.43	0.42
1:G:154:HIS:CB	1:G:157:VAL:HG13	2.46	0.42
1:G:344:GLY:HA3	1:G:358:CYS:O	2.19	0.42
1:H:125:ILE:O	1:H:128:GLU:HB3	2.19	0.42
1:A:389:HIS:HA	1:A:390:PRO:HA	1.68	0.42
1:C:121:ILE:O	1:C:125:ILE:HD12	2.19	0.42
1:C:168:VAL:HG21	1:C:200:HIS:CE1	2.54	0.42
1:F:322:PRO:HA	1:F:329:TYR:CD1	2.54	0.42
1:G:267:ILE:HA	1:G:311:GLN:HG2	2.00	0.42
1:B:329:TYR:CE2	1:B:406:TYR:CE2	3.07	0.42
1:D:154:HIS:CB	1:D:157:VAL:HG13	2.48	0.42
1:F:282:ASP:C	1:F:308:GLN:HE22	2.28	0.42
1:G:273:MET:HE3	1:G:273:MET:HB3	1.88	0.42
1:C:253:THR:OG1	1:C:256:GLN:HG3	2.19	0.42
1:F:259:SER:O	1:F:260:LEU:C	2.63	0.42
1:H:302:ASN:H	1:H:302:ASN:ND2	2.17	0.42
1:A:230:GLU:O	1:A:231:ASN:C	2.63	0.42
1:H:122:MET:CE	1:H:198:ALA:HB2	2.49	0.42
1:A:200:HIS:O	1:A:233:HIS:CD2	2.73	0.42
1:B:116:ARG:N	1:B:117:PRO:CD	2.83	0.42
1:E:316:CYS:HB3	1:E:381:TRP:CZ2	2.54	0.42
1:G:272:ASP:HB3	1:G:275:LYS:HD2	2.01	0.42
1:H:326:LEU:HD12	1:H:326:LEU:HA	1.75	0.42
1:C:327:GLN:O	1:C:331:GLN:HG3	2.18	0.42
1:E:146:LEU:HD23	1:E:146:LEU:HA	1.80	0.42
1:E:389:HIS:HA	1:E:390:PRO:HA	1.76	0.42
1:F:357:MET:HE3	1:F:357:MET:CA	2.48	0.42
1:G:165:ALA:O	1:G:169:VAL:HG23	2.20	0.42
1:G:229:LEU:HD23	1:G:229:LEU:HA	1.81	0.42
1:C:127:GLN:OE1	1:C:127:GLN:HA	2.20	0.42
1:G:175:LEU:HD23	1:G:175:LEU:HA	1.91	0.42
1:B:253:THR:HB	5:B:1114:HOH:O	2.20	0.42
1:G:325:PRO:HD2	1:G:328:LEU:HD12	2.02	0.42
1:B:307:ILE:HD12	1:B:307:ILE:HA	1.79	0.41
1:C:348:ARG:O	1:C:349:GLU:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:ARG:O	1:F:117:PRO:C	2.62	0.41
1:F:153:TYR:CE2	1:F:202:VAL:HA	2.55	0.41
1:B:357:MET:HE3	1:B:357:MET:CA	2.27	0.41
1:A:178:THR:OG1	1:A:391:ASP:HB3	2.20	0.41
1:A:378:HIS:HB3	1:A:379:PRO:HD3	2.02	0.41
1:B:176:LEU:HD13	1:B:190:ILE:HG23	2.03	0.41
1:A:201:ASP:HA	1:A:233:HIS:CG	2.56	0.41
1:A:243:GLU:HB2	1:A:246:CYS:SG	2.61	0.41
1:A:346:ARG:HA	1:A:349:GLU:HB2	2.02	0.41
1:E:226:SER:O	1:E:227:SER:C	2.64	0.41
1:G:153:TYR:CE2	1:G:202:VAL:HA	2.55	0.41
1:G:378:HIS:HB3	1:G:379:PRO:HD3	2.02	0.41
1:H:329:TYR:CE2	1:H:406:TYR:HE2	2.38	0.41
1:A:253:THR:OG1	1:A:256:GLN:HB2	2.21	0.41
1:B:302:ASN:O	1:B:306:ARG:HG3	2.21	0.41
1:C:404:GLU:OE1	1:C:404:GLU:HA	2.21	0.41
1:C:410:ILE:HB	1:C:411:PRO:CD	2.50	0.41
1:D:260:LEU:O	1:D:261:ARG:C	2.63	0.41
1:D:321:ASN:CB	1:D:332:TRP:CD1	3.04	0.41
1:F:232:HIS:O	1:F:236:VAL:HG23	2.21	0.41
1:F:327:GLN:HB2	5:F:1115:HOH:O	2.18	0.41
1:B:337:MET:HG3	1:B:365:VAL:HG22	2.03	0.41
1:C:192:ALA:HB2	1:C:263:MET:HE3	2.03	0.41
1:C:337:MET:HE1	2:C:1001:6PT:C8	2.51	0.41
1:D:323:THR:HG22	1:D:399:LEU:HB2	2.02	0.41
1:F:201:ASP:HA	1:F:233:HIS:CD2	2.55	0.41
1:A:201:ASP:HA	1:A:233:HIS:CE1	2.55	0.41
1:A:240:LEU:C	1:A:242:GLN:N	2.78	0.41
1:A:410:ILE:HG22	1:A:411:PRO:N	2.35	0.41
1:C:229:LEU:HB3	1:C:233:HIS:NE2	2.36	0.41
1:C:286:MET:HE1	1:C:308:GLN:CB	2.49	0.41
1:E:352:MET:O	1:E:353:GLU:C	2.63	0.41
1:F:293:THR:O	1:F:294:SER:C	2.62	0.41
1:G:343:GLN:O	1:G:347:GLU:HG3	2.21	0.41
1:H:164:HIS:O	1:H:167:ASP:HB3	2.21	0.41
1:H:396:LEU:HD12	1:H:396:LEU:HA	1.92	0.41
1:E:178:THR:HG22	1:E:181:LEU:HD12	2.03	0.41
1:G:324:LYS:O	1:G:325:PRO:C	2.64	0.41
1:H:122:MET:HE2	1:H:198:ALA:HB2	2.03	0.40
1:H:396:LEU:O	1:H:400:GLU:HG3	2.21	0.40
1:C:170:GLN:O	1:C:173:HIS:HB3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:HIS:O	1:C:379:PRO:C	2.65	0.40
1:F:240:LEU:C	1:F:242:GLN:N	2.79	0.40
1:F:302:ASN:ND2	1:F:302:ASN:N	2.66	0.40
1:F:355:SER:HB3	1:F:356:PRO:HD3	2.04	0.40
1:A:168:VAL:O	1:A:169:VAL:C	2.64	0.40
1:A:388:VAL:O	1:A:389:HIS:C	2.64	0.40
1:D:252:LEU:HB3	1:D:256:GLN:HB2	2.03	0.40
1:D:273:MET:HE3	1:D:273:MET:HB3	1.94	0.40
1:E:115:ASN:C	1:E:117:PRO:HD2	2.46	0.40
1:E:208:SER:O	1:E:209:ASN:C	2.63	0.40
1:F:145:TYR:CE2	1:F:149:LEU:HD22	2.56	0.40
1:B:132:LEU:HD12	1:B:132:LEU:H	1.87	0.40
1:F:249:PHE:O	1:F:257:ARG:NH1	2.54	0.40
1:E:178:THR:O	1:E:179:PRO:C	2.63	0.40
1:F:139:VAL:HG13	1:F:140:ASP:N	2.37	0.40
1:F:261:ARG:O	1:F:265:ILE:HG13	2.21	0.40
1:F:343:GLN:O	1:F:346:ARG:HB2	2.22	0.40
1:F:386:ASP:O	1:F:387:LEU:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	318/326 (98%)	286 (90%)	29 (9%)	3 (1%)	14	28
1	B	324/326 (99%)	306 (94%)	17 (5%)	1 (0%)	36	56
1	C	317/326 (97%)	299 (94%)	18 (6%)	0	100	100
1	D	324/326 (99%)	306 (94%)	18 (6%)	0	100	100
1	E	317/326 (97%)	301 (95%)	16 (5%)	0	100	100
1	F	324/326 (99%)	284 (88%)	35 (11%)	5 (2%)	8	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	318/326 (98%)	293 (92%)	22 (7%)	3 (1%)	14	28
1	H	324/326 (99%)	301 (93%)	20 (6%)	3 (1%)	14	28
All	All	2566/2608 (98%)	2376 (93%)	175 (7%)	15 (1%)	21	39

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	353	GLU
1	F	357	MET
1	G	410	ILE
1	H	304	SER
1	F	349	GLU
1	H	301	ASP
1	A	112	LEU
1	B	290	LYS
1	F	356	PRO
1	H	296	GLY
1	A	355	SER
1	A	410	ILE
1	G	228	VAL
1	F	354	ILE
1	G	116	ARG

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	294/298 (99%)	277 (94%)	17 (6%)	18	37
1	B	297/298 (100%)	282 (95%)	15 (5%)	21	43
1	C	294/298 (99%)	279 (95%)	15 (5%)	21	43
1	D	298/298 (100%)	282 (95%)	16 (5%)	20	40
1	E	294/298 (99%)	283 (96%)	11 (4%)	30	55
1	F	298/298 (100%)	286 (96%)	12 (4%)	28	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	294/298 (99%)	280 (95%)	14 (5%)	23	45
1	H	298/298 (100%)	281 (94%)	17 (6%)	18	38
All	All	2367/2384 (99%)	2250 (95%)	117 (5%)	22	44

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	GLU
1	A	157	VAL
1	A	219	LEU
1	A	221	LEU
1	A	244	GLU
1	A	254	LYS
1	A	255	LYS
1	A	256	GLN
1	A	260	LEU
1	A	279	LEU
1	A	291	LYS
1	A	298	LEU
1	A	327	GLN
1	A	352	MET
1	A	357	MET
1	A	364	SER
1	A	404	GLU
1	B	108	ARG
1	B	133	LYS
1	B	148	THR
1	B	157	VAL
1	B	221	LEU
1	B	245	ASN
1	B	255	LYS
1	B	259	SER
1	B	286	MET
1	B	293	THR
1	B	295	SER
1	B	307	ILE
1	B	327	GLN
1	B	342	ARG
1	B	357	MET
1	C	87	GLU
1	C	88	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	94	LYS
1	C	99	VAL
1	C	139	VAL
1	C	226	SER
1	C	243	GLU
1	C	254	LYS
1	C	259	SER
1	C	287	VAL
1	C	298	LEU
1	C	299	LEU
1	C	304	SER
1	C	354	ILE
1	C	362	ASN
1	D	88	GLN
1	D	104	LEU
1	D	108	ARG
1	D	133	LYS
1	D	134	THR
1	D	157	VAL
1	D	221	LEU
1	D	255	LYS
1	D	287	VAL
1	D	294	SER
1	D	297	VAL
1	D	298	LEU
1	D	321	ASN
1	D	342	ARG
1	D	353	GLU
1	D	364	SER
1	E	89	GLU
1	E	139	VAL
1	E	157	VAL
1	E	221	LEU
1	E	255	LYS
1	E	298	LEU
1	E	299	LEU
1	E	307	ILE
1	E	321	ASN
1	E	355	SER
1	E	382	GLU
1	F	89	GLU
1	F	108	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	177	SER
1	F	221	LEU
1	F	259	SER
1	F	295	SER
1	F	298	LEU
1	F	299	LEU
1	F	302	ASN
1	F	307	ILE
1	F	357	MET
1	F	388	VAL
1	G	87	GLU
1	G	88	GLN
1	G	109	ILE
1	G	157	VAL
1	G	178	THR
1	G	221	LEU
1	G	226	SER
1	G	244	GLU
1	G	292	VAL
1	G	298	LEU
1	G	299	LEU
1	G	327	GLN
1	G	353	GLU
1	G	364	SER
1	H	133	LYS
1	H	147	MET
1	H	163	ILE
1	H	169	VAL
1	H	178	THR
1	H	254	LYS
1	H	259	SER
1	H	274	SER
1	H	288	GLU
1	H	293	THR
1	H	298	LEU
1	H	304	SER
1	H	306	ARG
1	H	336	ILE
1	H	342	ARG
1	H	357	MET
1	H	364	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	123	HIS
1	A	245	ASN
1	A	256	GLN
1	A	321	ASN
1	A	343	GLN
1	B	88	GLN
1	B	123	HIS
1	B	210	GLN
1	B	245	ASN
1	B	250	GLN
1	B	327	GLN
1	C	88	GLN
1	C	210	GLN
1	C	242	GLN
1	C	245	ASN
1	C	250	GLN
1	C	258	GLN
1	C	302	ASN
1	C	312	ASN
1	C	389	HIS
1	D	88	GLN
1	D	123	HIS
1	D	127	GLN
1	D	242	GLN
1	D	245	ASN
1	D	250	GLN
1	D	308	GLN
1	D	361	HIS
1	D	389	HIS
1	E	123	HIS
1	E	210	GLN
1	E	245	ASN
1	E	250	GLN
1	E	308	GLN
1	E	321	ASN
1	E	361	HIS
1	F	88	GLN
1	F	123	HIS
1	F	161	ASN
1	F	210	GLN
1	F	245	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	302	ASN
1	F	308	GLN
1	F	327	GLN
1	F	361	HIS
1	F	362	ASN
1	F	369	GLN
1	F	389	HIS
1	G	88	GLN
1	G	115	ASN
1	G	123	HIS
1	G	242	GLN
1	G	245	ASN
1	G	250	GLN
1	G	258	GLN
1	G	321	ASN
1	G	343	GLN
1	H	88	GLN
1	H	210	GLN
1	H	242	GLN
1	H	245	ASN
1	H	250	GLN
1	H	302	ASN
1	H	308	GLN
1	H	343	GLN
1	H	369	GLN
1	H	407	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	6PT	E	1001	-	30,30,30	1.17	2 (6%)	38,42,42	2.22	13 (34%)
2	6PT	G	1001	-	30,30,30	1.09	2 (6%)	38,42,42	2.25	13 (34%)
2	6PT	A	1001	-	30,30,30	1.09	2 (6%)	38,42,42	2.17	10 (26%)
2	6PT	H	1001	-	30,30,30	1.04	2 (6%)	38,42,42	2.45	13 (34%)
2	6PT	D	1001	-	30,30,30	1.01	1 (3%)	38,42,42	2.28	11 (28%)
2	6PT	F	1001	-	30,30,30	1.06	2 (6%)	38,42,42	2.07	12 (31%)
2	6PT	C	1001	-	30,30,30	0.99	2 (6%)	38,42,42	2.06	9 (23%)
2	6PT	B	1001	-	30,30,30	1.16	3 (10%)	38,42,42	2.25	11 (28%)

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	6PT	E	1001	-	-	1/18/18/18	0/3/3/3
2	6PT	G	1001	-	-	1/18/18/18	0/3/3/3
2	6PT	A	1001	-	-	4/18/18/18	0/3/3/3
2	6PT	H	1001	-	-	3/18/18/18	0/3/3/3
2	6PT	D	1001	-	-	1/18/18/18	0/3/3/3
2	6PT	F	1001	-	-	4/18/18/18	0/3/3/3
2	6PT	C	1001	-	-	4/18/18/18	0/3/3/3
2	6PT	B	1001	-	-	3/18/18/18	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1001	6PT	C1-N1	3.20	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	6PT	C1-N1	3.02	1.36	1.31
2	E	1001	6PT	C1-N1	3.02	1.36	1.31
2	G	1001	6PT	C3-C21	-2.95	1.37	1.42
2	B	1001	6PT	C21-N3	-2.67	1.31	1.39
2	A	1001	6PT	C21-N3	-2.58	1.32	1.39
2	B	1001	6PT	C1-N1	2.57	1.35	1.31
2	D	1001	6PT	C1-N1	2.51	1.35	1.31
2	E	1001	6PT	C2-C3	2.38	1.44	1.38
2	C	1001	6PT	C1-N1	2.25	1.35	1.31
2	B	1001	6PT	C3-C21	-2.17	1.38	1.42
2	F	1001	6PT	O4-C21	2.07	1.27	1.23
2	H	1001	6PT	C2-C12	2.05	1.53	1.46
2	G	1001	6PT	O3-C20	-2.04	1.24	1.30
2	C	1001	6PT	C2-C12	2.02	1.53	1.46
2	F	1001	6PT	C1-N1	2.02	1.34	1.31

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1001	6PT	C21-N3-N1	-7.56	118.45	126.24
2	A	1001	6PT	C4-N3-N1	7.05	122.64	113.46
2	B	1001	6PT	C21-N3-N1	-6.82	119.21	126.24
2	E	1001	6PT	C21-N3-N1	-6.50	119.54	126.24
2	G	1001	6PT	C21-N3-N1	-6.25	119.81	126.24
2	A	1001	6PT	C21-N3-N1	-6.14	119.91	126.24
2	D	1001	6PT	C21-N3-N1	-6.12	119.93	126.24
2	C	1001	6PT	C21-N3-N1	-6.05	120.01	126.24
2	H	1001	6PT	C4-N3-N1	6.02	121.29	113.46
2	B	1001	6PT	C4-N3-N1	5.46	120.57	113.46
2	F	1001	6PT	C21-N3-N1	-5.16	120.93	126.24
2	D	1001	6PT	C4-N3-N1	5.15	120.17	113.46
2	G	1001	6PT	O4-C21-C3	-5.13	116.17	126.64
2	F	1001	6PT	C4-N3-N1	5.13	120.14	113.46
2	G	1001	6PT	C21-C3-N2	-4.62	110.53	118.45
2	H	1001	6PT	O4-C21-C3	-4.46	117.55	126.64
2	E	1001	6PT	O4-C21-C3	-4.45	117.56	126.64
2	H	1001	6PT	C7-C6-C1	-4.30	113.69	120.74
2	B	1001	6PT	O4-C21-C3	-4.27	117.93	126.64
2	D	1001	6PT	O4-C21-C3	-4.23	118.02	126.64
2	E	1001	6PT	C21-C3-N2	-4.15	111.34	118.45
2	D	1001	6PT	O1-C12-C2	-4.04	113.29	120.43
2	C	1001	6PT	C1-C2-C12	-4.02	115.20	124.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1001	6PT	O1-C12-C2	-3.99	113.39	120.43
2	C	1001	6PT	O4-C21-C3	-3.97	118.55	126.64
2	B	1001	6PT	C21-C3-N2	-3.84	111.87	118.45
2	D	1001	6PT	C21-C3-N2	-3.83	111.88	118.45
2	F	1001	6PT	C7-C6-C1	-3.73	114.63	120.74
2	D	1001	6PT	C13-C12-C2	3.59	127.96	120.40
2	G	1001	6PT	C15-C16-C17	-3.58	116.97	120.80
2	H	1001	6PT	C3-C21-N3	3.52	123.07	114.05
2	B	1001	6PT	C3-C21-N3	3.47	122.95	114.05
2	E	1001	6PT	C13-C12-C2	3.46	127.69	120.40
2	C	1001	6PT	C21-C3-N2	-3.45	112.53	118.45
2	E	1001	6PT	C1-N1-N3	3.44	122.60	119.05
2	H	1001	6PT	C13-C12-C2	3.43	127.63	120.40
2	G	1001	6PT	C4-N3-N1	3.42	117.91	113.46
2	H	1001	6PT	C21-C3-N2	-3.42	112.59	118.45
2	F	1001	6PT	C1-C2-C12	-3.41	116.55	124.12
2	D	1001	6PT	C3-C21-N3	3.35	122.64	114.05
2	C	1001	6PT	C13-C12-C2	3.33	127.42	120.40
2	C	1001	6PT	C4-N3-N1	3.26	117.70	113.46
2	A	1001	6PT	C3-C21-N3	3.25	122.38	114.05
2	A	1001	6PT	C7-C6-C1	-3.22	115.47	120.74
2	D	1001	6PT	C1-C2-C12	-3.20	117.03	124.12
2	G	1001	6PT	C1-C2-C12	-3.18	117.07	124.12
2	C	1001	6PT	C3-C21-N3	3.17	122.18	114.05
2	A	1001	6PT	O4-C21-N3	-3.14	115.68	121.17
2	G	1001	6PT	C16-C15-C14	3.13	123.90	120.30
2	A	1001	6PT	C1-C2-C12	-3.12	117.21	124.12
2	G	1001	6PT	C3-C21-N3	3.09	121.98	114.05
2	B	1001	6PT	C1-C2-C12	-3.05	117.36	124.12
2	E	1001	6PT	C2-C1-N1	-2.96	118.99	122.18
2	E	1001	6PT	O1-C12-C2	-2.88	115.34	120.43
2	E	1001	6PT	C1-C2-C12	-2.85	117.79	124.12
2	H	1001	6PT	C11-C6-C1	2.83	125.37	120.74
2	E	1001	6PT	C4-N3-N1	2.82	117.14	113.46
2	F	1001	6PT	C21-C3-N2	-2.79	113.67	118.45
2	G	1001	6PT	C7-C6-C1	-2.77	116.19	120.74
2	F	1001	6PT	O4-C21-C3	-2.72	121.10	126.64
2	B	1001	6PT	O3-C20-C17	2.70	121.77	114.84
2	H	1001	6PT	C1-C2-C12	-2.67	118.20	124.12
2	B	1001	6PT	O1-C12-C2	-2.65	115.74	120.43
2	E	1001	6PT	C6-C1-N1	2.64	118.67	114.12
2	H	1001	6PT	O1-C12-C2	-2.62	115.80	120.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1001	6PT	C13-C12-C2	2.62	125.93	120.40
2	E	1001	6PT	C3-C21-N3	2.61	120.75	114.05
2	H	1001	6PT	C6-C1-N1	2.61	118.61	114.12
2	F	1001	6PT	C3-C21-N3	2.60	120.70	114.05
2	F	1001	6PT	C10-C11-C6	-2.57	117.84	120.36
2	C	1001	6PT	C7-C6-C1	-2.55	116.56	120.74
2	D	1001	6PT	C7-C6-C1	-2.54	116.58	120.74
2	D	1001	6PT	O3-C20-C17	2.49	121.24	114.84
2	D	1001	6PT	O3-C20-O2	-2.45	118.09	123.35
2	A	1001	6PT	C11-C6-C1	2.39	124.65	120.74
2	B	1001	6PT	C13-C12-C2	2.36	125.38	120.40
2	B	1001	6PT	C6-C1-N1	2.35	118.17	114.12
2	G	1001	6PT	C18-C19-C14	-2.33	117.62	120.30
2	A	1001	6PT	C21-C3-N2	-2.32	114.47	118.45
2	C	1001	6PT	O1-C12-C2	-2.31	116.35	120.43
2	A	1001	6PT	O4-C21-C3	-2.31	121.93	126.64
2	A	1001	6PT	O3-C20-C17	2.31	120.76	114.84
2	F	1001	6PT	C11-C6-C1	2.30	124.51	120.74
2	H	1001	6PT	O3-C20-C17	2.22	120.53	114.84
2	G	1001	6PT	O3-C20-C17	2.21	120.52	114.84
2	H	1001	6PT	C6-C1-C2	-2.15	118.07	122.92
2	E	1001	6PT	C14-N2-C3	2.12	133.19	127.89
2	F	1001	6PT	C9-C8-C7	-2.08	117.68	120.24
2	G	1001	6PT	O1-C12-C2	-2.08	116.76	120.43
2	G	1001	6PT	C15-C14-N2	-2.07	113.48	120.41
2	B	1001	6PT	C15-C16-C17	-2.05	118.61	120.80
2	E	1001	6PT	C16-C17-C20	-2.02	116.38	120.37

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1001	6PT	C2-C1-C6-C11
2	F	1001	6PT	C2-C1-C6-C7
2	F	1001	6PT	N1-C1-C6-C11
2	F	1001	6PT	N1-C1-C6-C7
2	A	1001	6PT	C2-C1-C6-C7
2	A	1001	6PT	C2-C1-C6-C11
2	H	1001	6PT	C2-C1-C6-C7
2	C	1001	6PT	C2-C1-C6-C7
2	A	1001	6PT	N1-C1-C6-C11
2	A	1001	6PT	N1-C1-C6-C7

Continued on next page...

Continued from previous page...

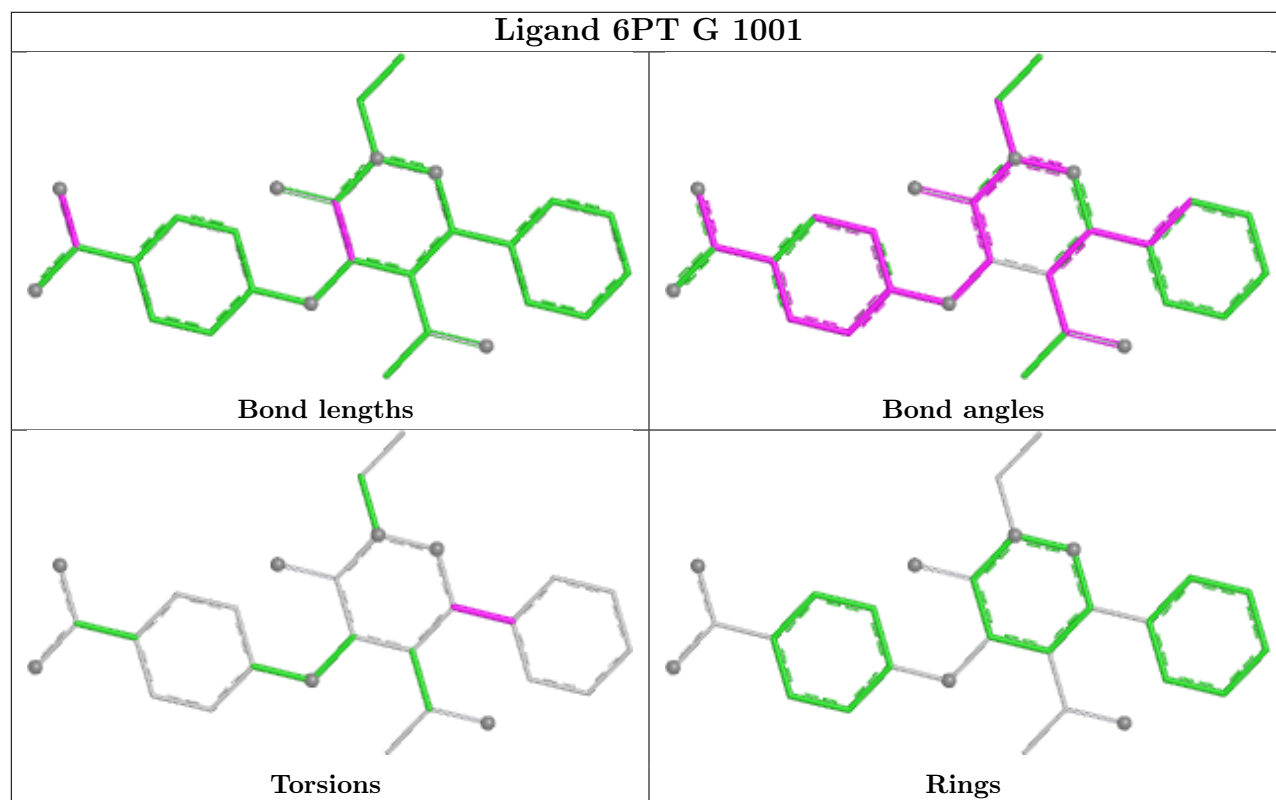
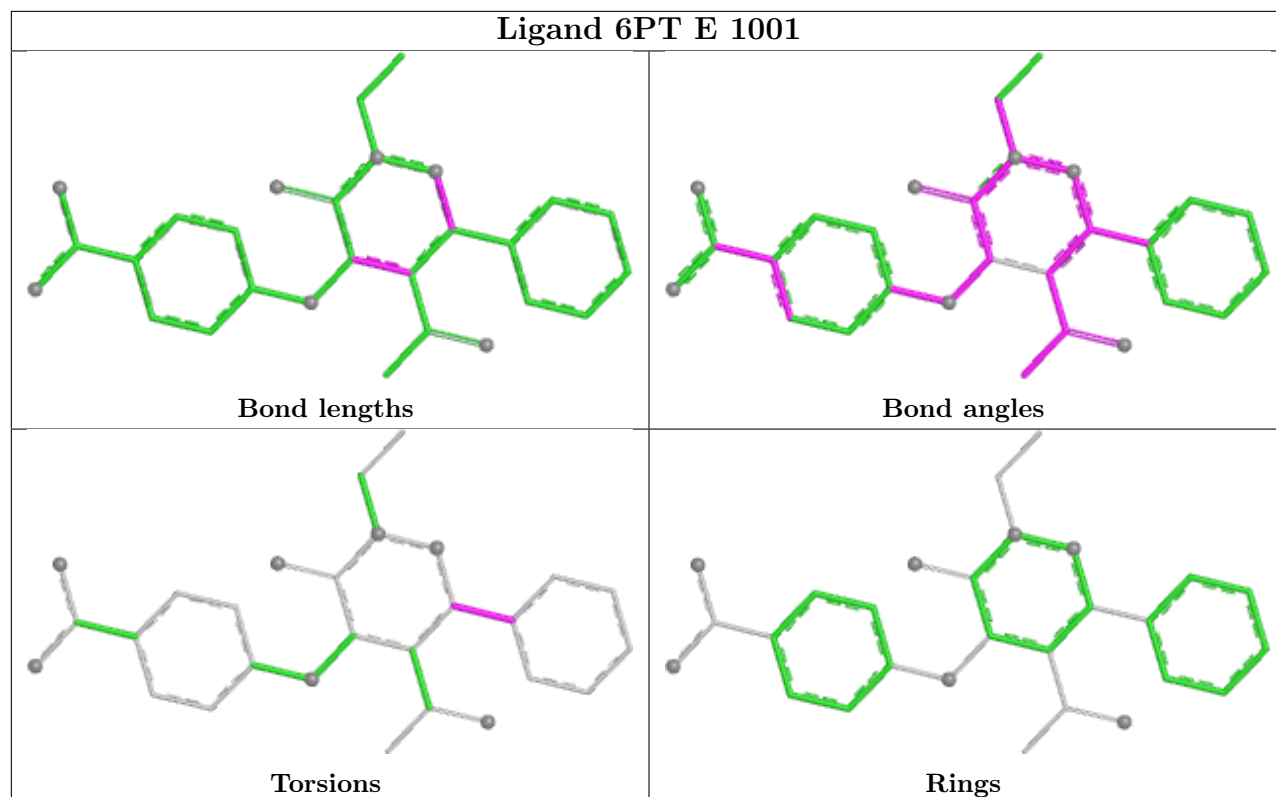
Mol	Chain	Res	Type	Atoms
2	B	1001	6PT	C2-C1-C6-C7
2	C	1001	6PT	C2-C1-C6-C11
2	H	1001	6PT	C2-C1-C6-C11
2	C	1001	6PT	N1-C1-C6-C7
2	C	1001	6PT	N1-C1-C6-C11
2	B	1001	6PT	C2-C1-C6-C11
2	D	1001	6PT	C2-C1-C6-C7
2	E	1001	6PT	C2-C1-C6-C7
2	G	1001	6PT	C2-C1-C6-C7
2	B	1001	6PT	N1-C1-C6-C7
2	H	1001	6PT	N1-C1-C6-C7

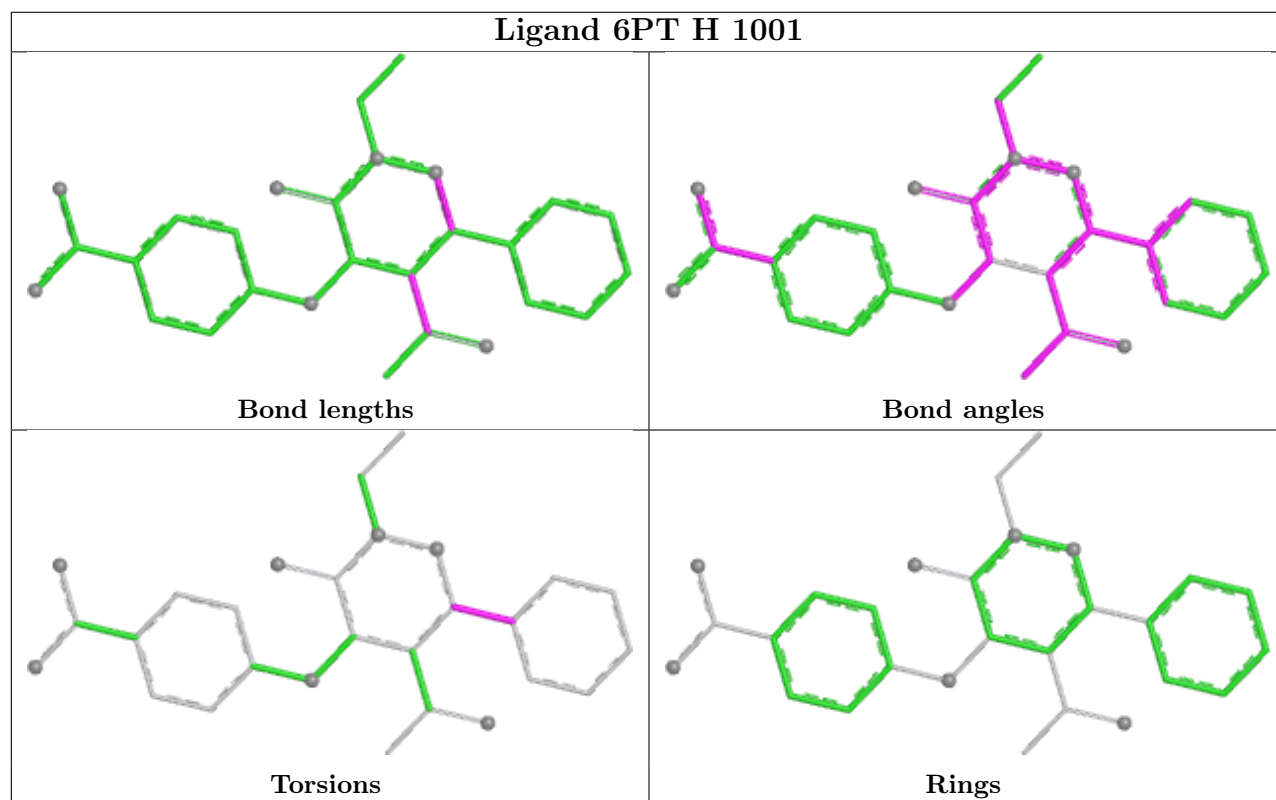
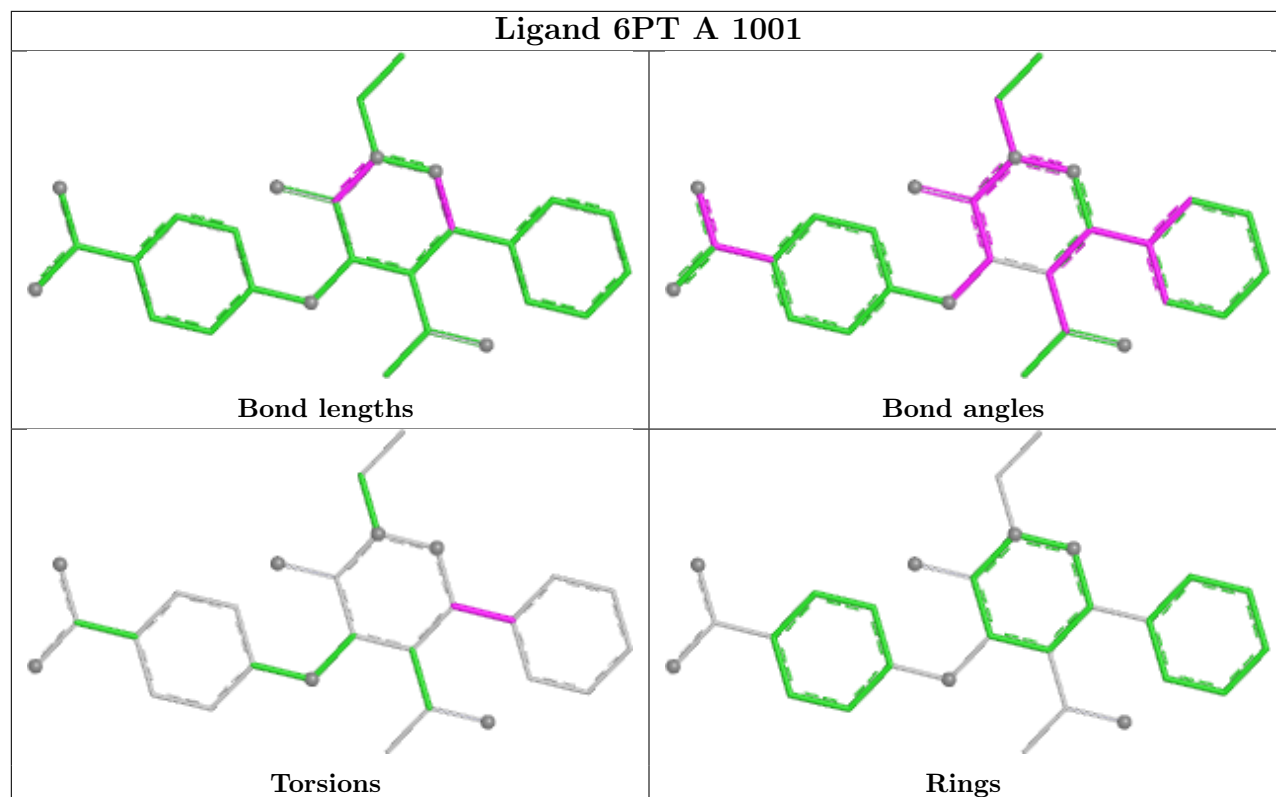
There are no ring outliers.

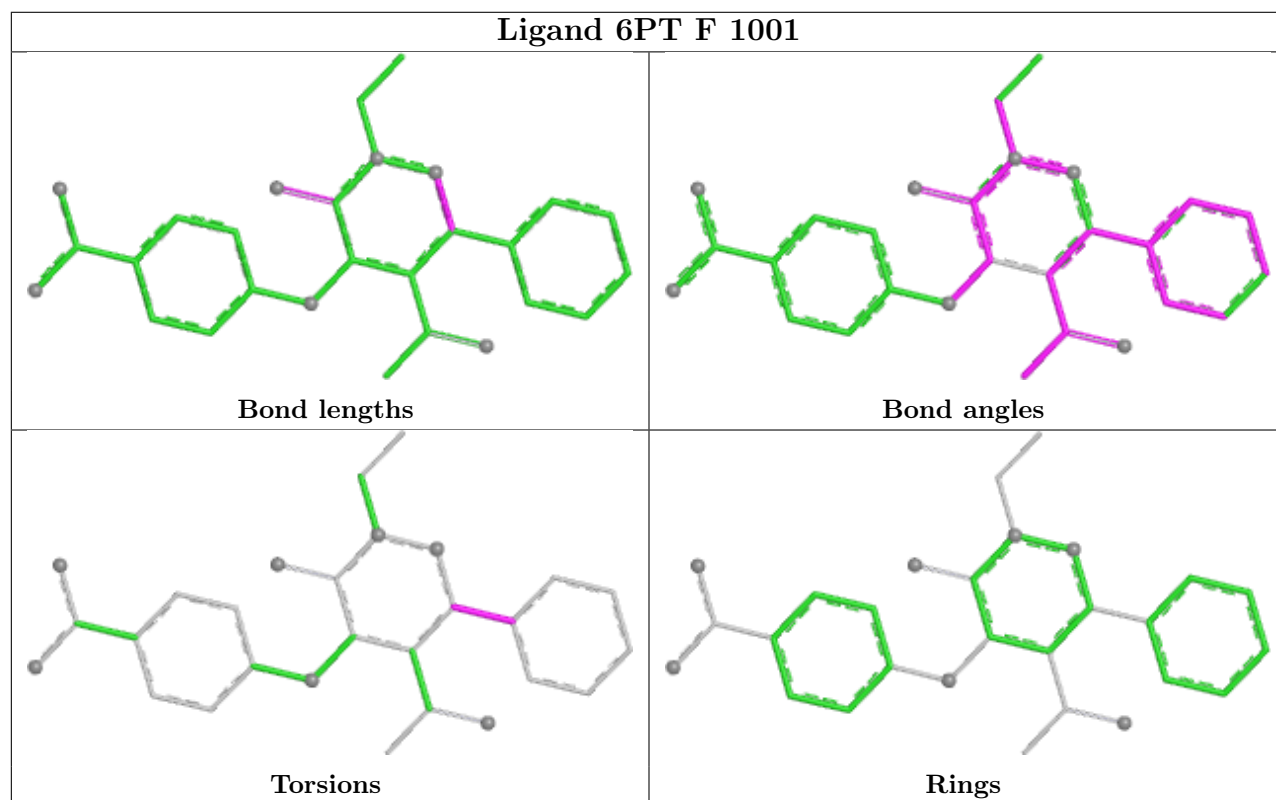
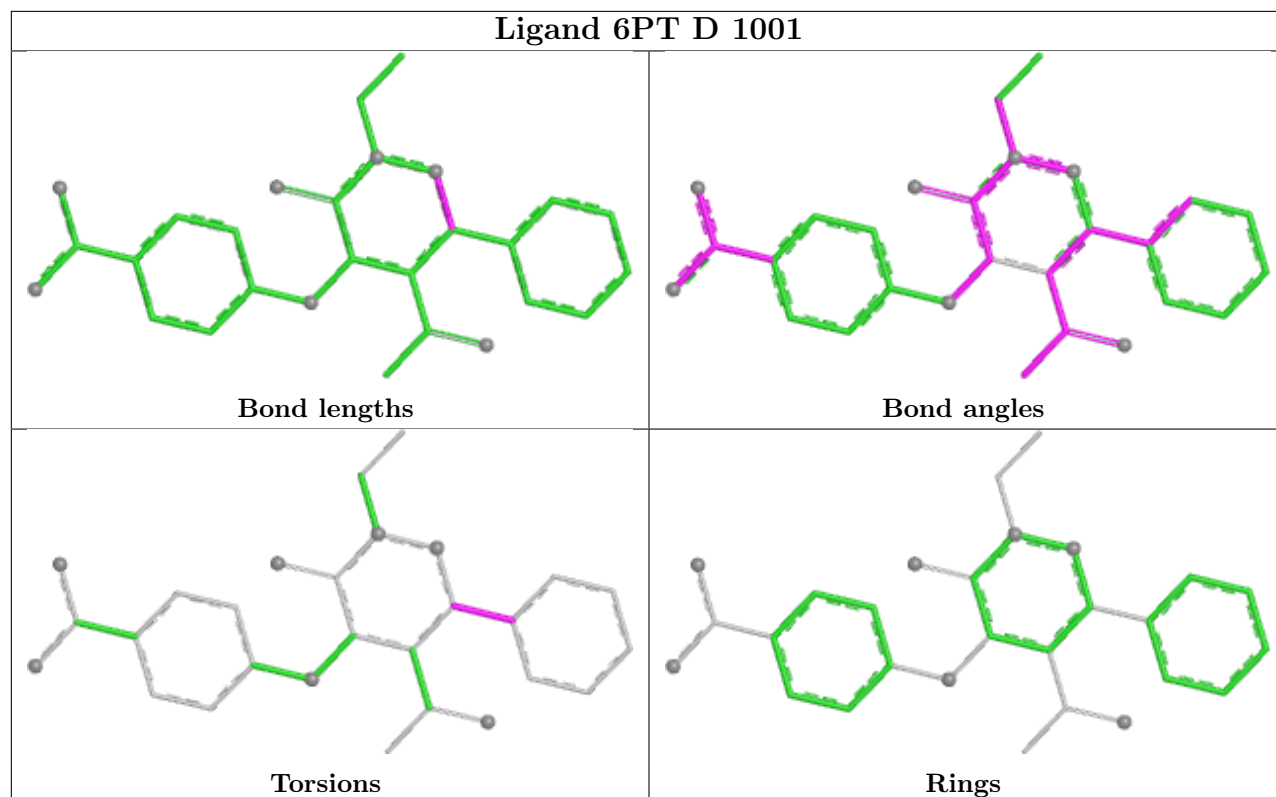
8 monomers are involved in 17 short contacts:

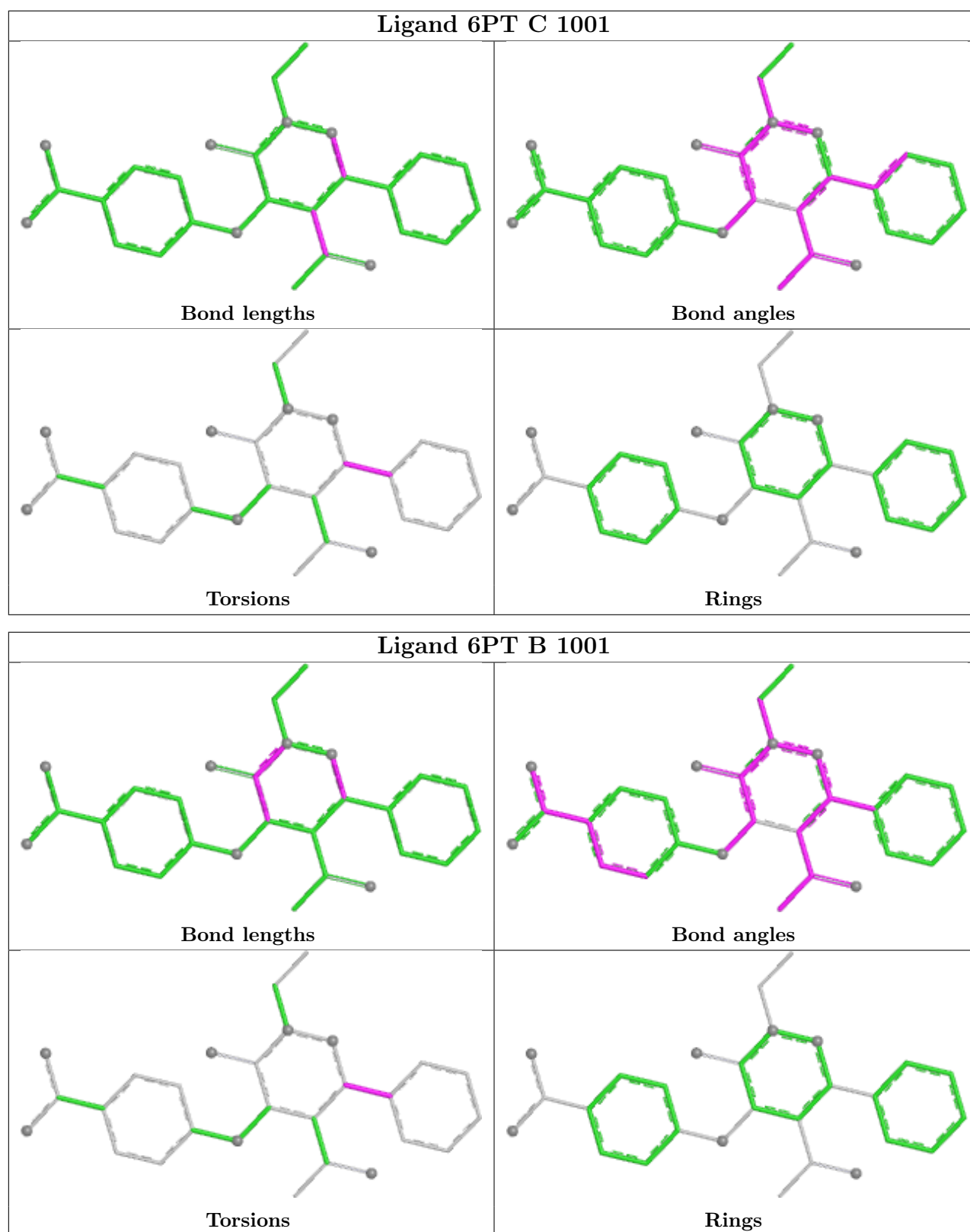
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1001	6PT	1	0
2	G	1001	6PT	3	0
2	A	1001	6PT	1	0
2	H	1001	6PT	1	0
2	D	1001	6PT	2	0
2	F	1001	6PT	3	0
2	C	1001	6PT	3	0
2	B	1001	6PT	3	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	322/326 (98%)	-0.32	2 (0%) 85 83	22, 36, 59, 82	0
1	B	326/326 (100%)	-0.58	1 (0%) 90 88	15, 27, 48, 63	0
1	C	321/326 (98%)	-0.57	0 100 100	17, 26, 44, 55	0
1	D	326/326 (100%)	-0.61	0 100 100	17, 26, 45, 65	0
1	E	321/326 (98%)	-0.65	0 100 100	14, 24, 42, 52	0
1	F	326/326 (100%)	-0.30	4 (1%) 76 73	22, 37, 63, 83	0
1	G	322/326 (98%)	-0.62	2 (0%) 85 83	16, 27, 43, 63	0
1	H	326/326 (100%)	-0.47	3 (0%) 81 78	17, 30, 50, 71	0
All	All	2590/2608 (99%)	-0.51	12 (0%) 87 85	14, 29, 52, 83	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	295	SER	3.3
1	F	411	PRO	2.9
1	G	411	PRO	2.8
1	F	86	THR	2.6
1	B	301	ASP	2.4
1	G	301	ASP	2.4
1	A	411	PRO	2.2
1	H	363	ALA	2.2
1	H	294	SER	2.2
1	F	356	PRO	2.0
1	A	351	GLY	2.0
1	F	353	GLU	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.

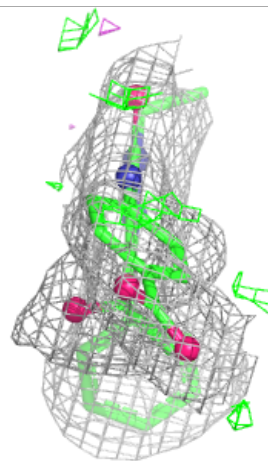
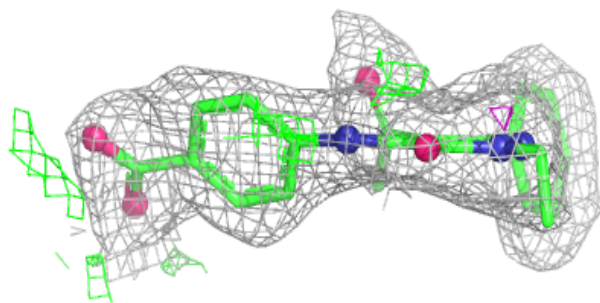
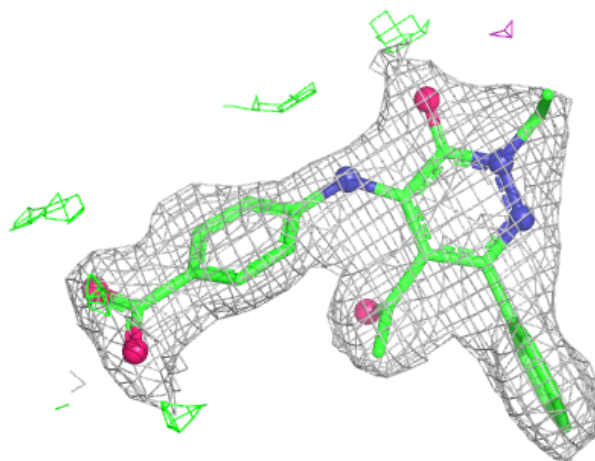
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	E	1003	1/1	0.84	0.34	38,38,38,38	0
4	MG	H	1003	1/1	0.84	0.35	38,38,38,38	0
4	MG	A	1003	1/1	0.87	0.28	42,42,42,42	0
4	MG	F	1003	1/1	0.88	0.28	37,37,37,37	0
4	MG	G	1003	1/1	0.89	0.32	35,35,35,35	0
4	MG	D	1003	1/1	0.89	0.28	34,34,34,34	0
4	MG	B	1003	1/1	0.90	0.33	37,37,37,37	0
2	6PT	F	1001	28/28	0.91	0.09	29,30,31,32	0
2	6PT	A	1001	28/28	0.93	0.09	28,30,31,32	0
2	6PT	C	1001	28/28	0.94	0.08	27,29,30,31	0
2	6PT	G	1001	28/28	0.94	0.09	27,28,30,30	0
2	6PT	E	1001	28/28	0.94	0.09	27,29,30,31	0
2	6PT	B	1001	28/28	0.95	0.09	28,29,29,29	0
2	6PT	D	1001	28/28	0.95	0.08	28,29,30,31	0
4	MG	C	1003	1/1	0.96	0.33	38,38,38,38	0
2	6PT	H	1001	28/28	0.96	0.07	28,29,30,31	0
3	ZN	C	1002	1/1	0.96	0.06	32,32,32,32	0
3	ZN	G	1002	1/1	0.97	0.06	26,26,26,26	0
3	ZN	D	1002	1/1	0.97	0.05	33,33,33,33	0
3	ZN	F	1002	1/1	0.97	0.04	37,37,37,37	0
3	ZN	B	1002	1/1	0.98	0.08	29,29,29,29	0
3	ZN	E	1002	1/1	0.98	0.06	31,31,31,31	0
3	ZN	A	1002	1/1	0.99	0.04	37,37,37,37	0
3	ZN	H	1002	1/1	0.99	0.04	36,36,36,36	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.

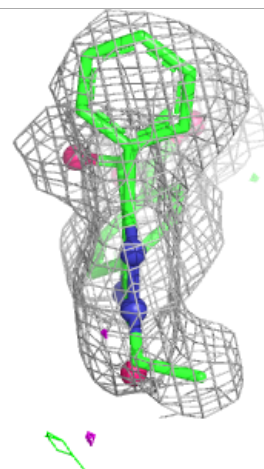
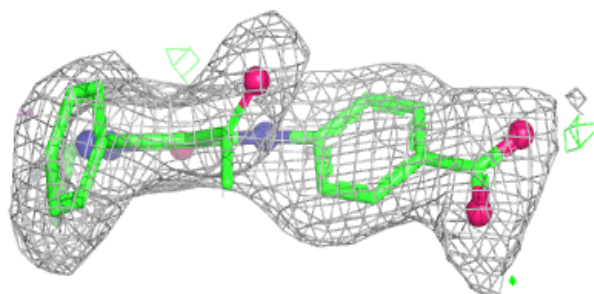
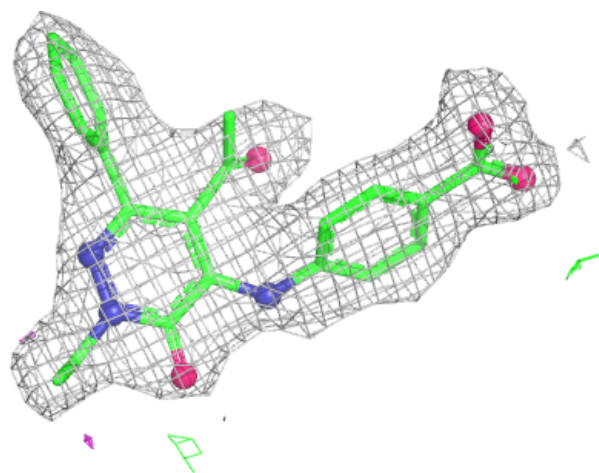
Electron density around 6PT F 1001:

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



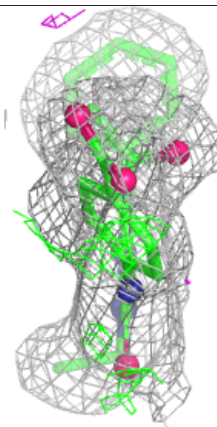
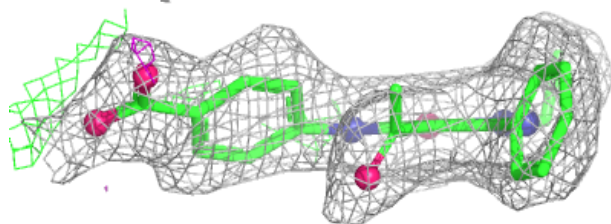
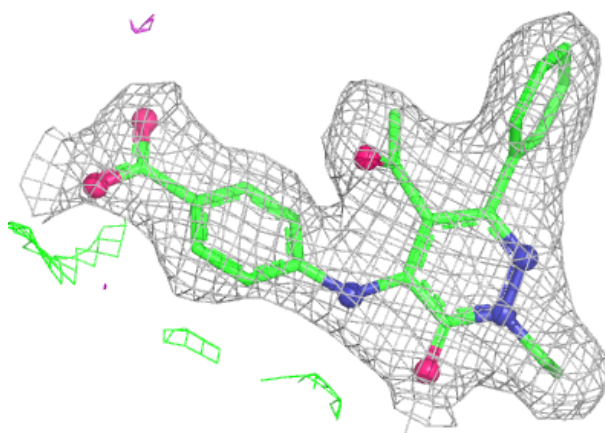
Electron density around 6PT A 1001:

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



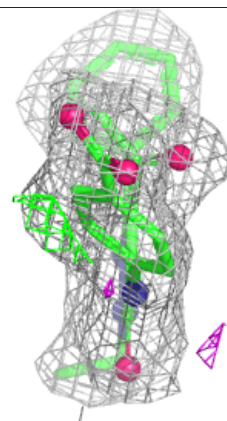
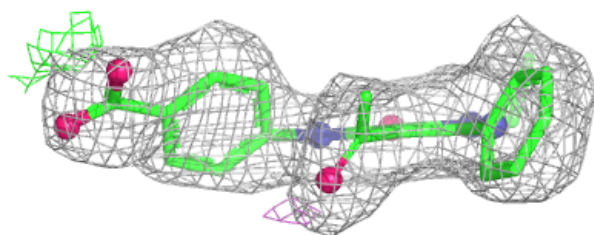
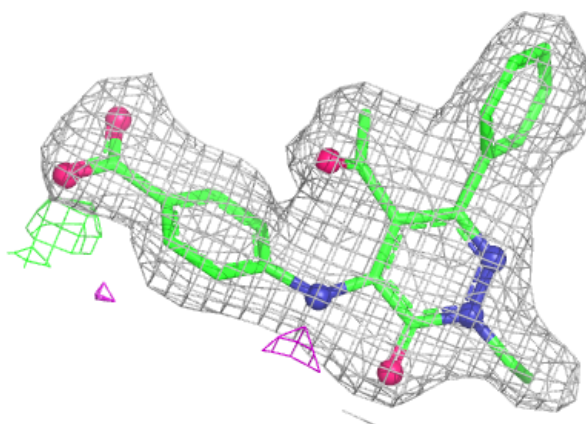
Electron density around 6PT C 1001:

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



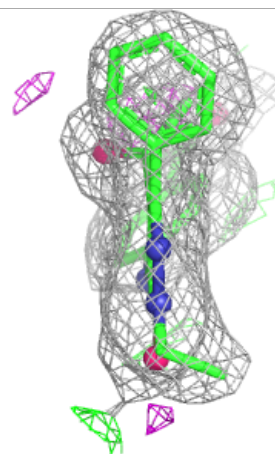
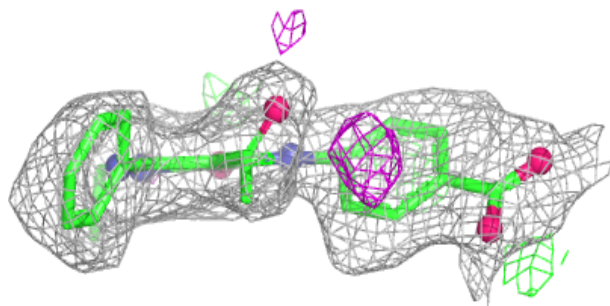
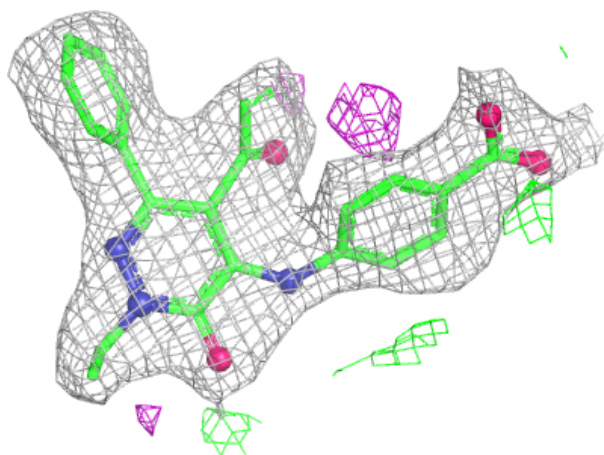
Electron density around 6PT G 1001:

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



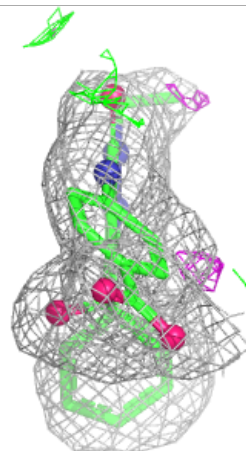
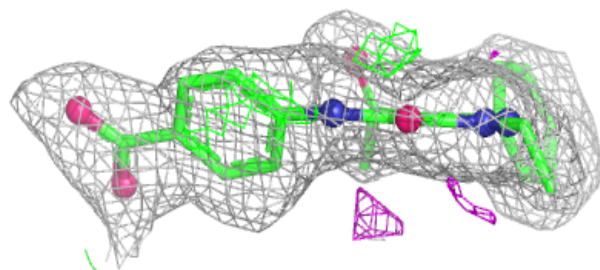
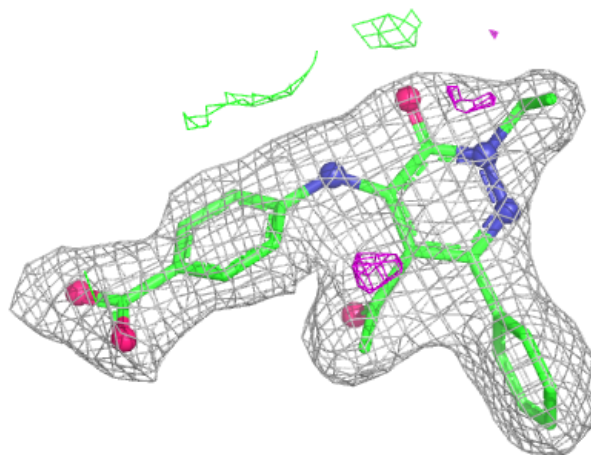
Electron density around 6PT E 1001:

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



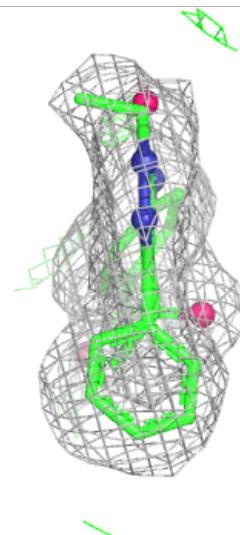
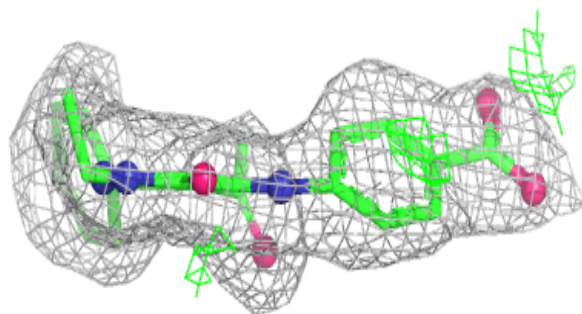
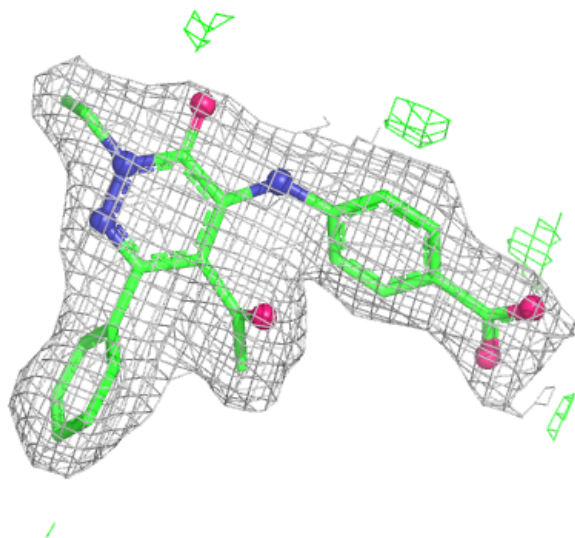
Electron density around 6PT B 1001:

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



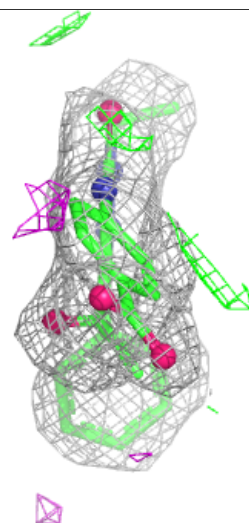
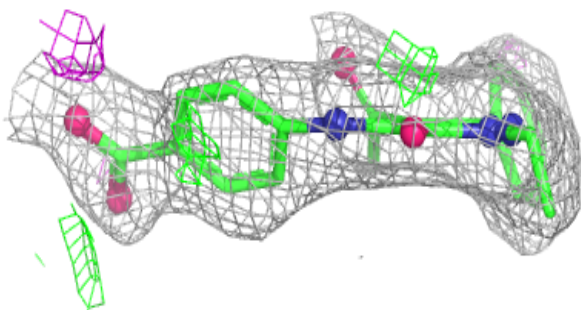
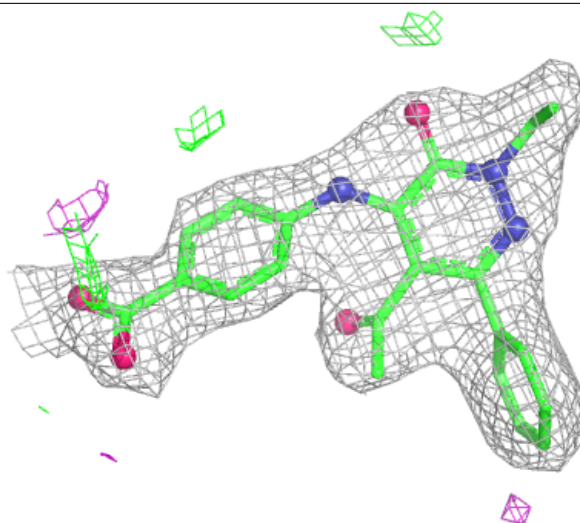
Electron density around 6PT D 1001:

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



Electron density around 6PT H 1001:

$2mF_o-DF_c$ (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.