



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:57 PM UTC

PDB ID : 3UX4 / pdb_00003ux4
Title : Crystal structure of the urea channel from the human gastric pathogen *Helicobacter pylori*
Authors : McNulty, R.; Luecke, H.
Deposited on : 2011-12-03
Resolution : 3.26 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

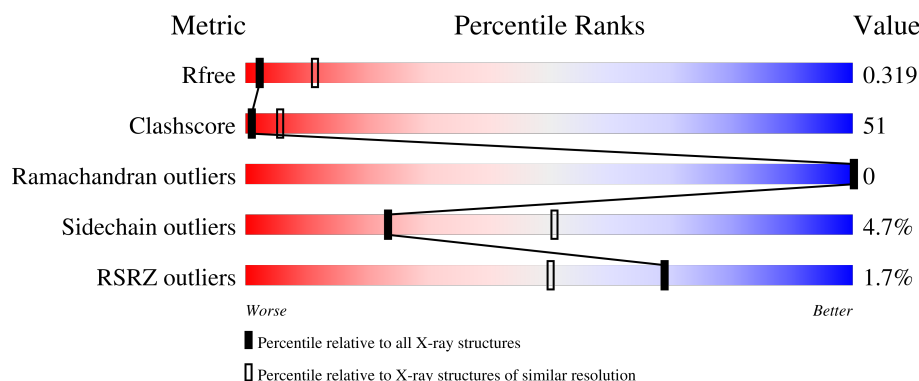
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	201	% 33% 51% 5% 10%
1	B	201	2% 36% 49% • 10%
1	C	201	% 36% 47% 6% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	XP4	B	302	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4482 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.

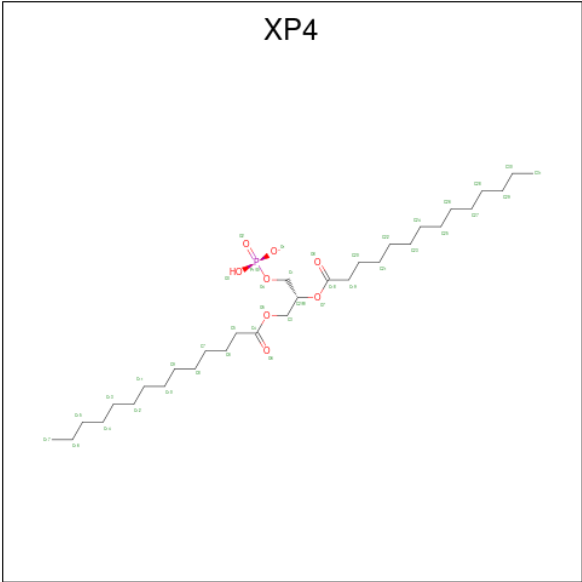
- Molecule 1 is a protein called Acid-activated urea channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1428	972	216	235	5			
1	B	180	Total	C	N	O	S	0	0	0
			1428	972	216	235	5			
1	C	180	Total	C	N	O	S	0	0	0
			1428	972	216	235	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61A	HIS	-	expression tag	UNP P56874
A	61B	HIS	-	expression tag	UNP P56874
A	61C	HIS	-	expression tag	UNP P56874
A	61D	HIS	-	expression tag	UNP P56874
A	61E	HIS	-	expression tag	UNP P56874
A	61F	HIS	-	expression tag	UNP P56874
B	61A	HIS	-	expression tag	UNP P56874
B	61B	HIS	-	expression tag	UNP P56874
B	61C	HIS	-	expression tag	UNP P56874
B	61D	HIS	-	expression tag	UNP P56874
B	61E	HIS	-	expression tag	UNP P56874
B	61F	HIS	-	expression tag	UNP P56874
C	61A	HIS	-	expression tag	UNP P56874
C	61B	HIS	-	expression tag	UNP P56874
C	61C	HIS	-	expression tag	UNP P56874
C	61D	HIS	-	expression tag	UNP P56874
C	61E	HIS	-	expression tag	UNP P56874
C	61F	HIS	-	expression tag	UNP P56874

- Molecule 2 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: XP4) (formula: C₃₁H₆₀O₈P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			17	15	2			
2	A	1	Total	C	O		0	0
			10	8	2			
2	B	1	Total	C	O		0	0
			36	31	5			
2	B	1	Total	C	O	P	0	0
			40	31	8	1		
2	B	1	Total	C	O		0	0
			18	16	2			
2	B	1	Total	C	O		0	0
			17	15	2			
2	B	1	Total	C	O		0	0
			10	8	2			
2	C	1	Total	C	O	P	0	0
			40	31	8	1		
2	C	1	Total	C	O		0	0
			10	8	2			

W142	A143	I144	I145	W146		W149	G150	V151	L152	W153	L154	T155	A156	F157	I158	E159	N160	I161	L162	K163	I164	P165	L166	G167	K168	F169	T170	P171	W172	L173	A174	I175	I176	E177	G178	I179	L180	T181	W183	I184	P185	A186	W187	L188	L189		Q192	H193	W194	V195
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4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	122.90Å 122.90Å 141.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.35 – 3.26 39.35 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.35-3.26) 98.2 (39.35-3.26)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.239 , 0.299 0.244 , 0.319	Depositor DCC
R_{free} test set	872 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	133.8	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 199.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4482	wwPDB-VP
Average B, all atoms (Å ²)	170.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XP4

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	0.79	0/1480	0.96	8/2035 (0.4%)
1	B	0.81	0/1480	0.99	6/2035 (0.3%)
1	C	0.81	0/1480	1.00	8/2035 (0.4%)
All	All	0.80	0/4440	0.98	22/6105 (0.4%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	LEU	N-CA-C	11.65	124.06	111.36
1	B	168	LYS	N-CA-C	-8.06	103.58	113.50
1	A	161	ILE	N-CA-C	6.95	117.91	111.45
1	B	134	LEU	N-CA-C	6.04	117.84	110.41
1	A	137	THR	CB-CA-C	-6.04	109.02	117.23
1	B	137	THR	CB-CA-C	-6.03	109.02	117.23
1	A	163	LYS	N-CA-C	5.76	118.43	111.40
1	B	25	ASP	CA-C-N	5.75	126.14	119.47
1	B	25	ASP	C-N-CA	5.75	126.14	119.47
1	B	163	LYS	N-CA-C	5.64	117.43	111.28
1	C	164	ILE	N-CA-C	5.51	120.78	108.88
1	C	25	ASP	CA-C-N	5.45	125.27	119.28
1	C	25	ASP	C-N-CA	5.45	125.27	119.28
1	A	134	LEU	N-CA-C	5.39	117.04	110.41
1	C	56	THR	N-CA-C	-5.31	102.67	113.29
1	C	134	LEU	N-CA-C	5.31	116.94	110.41
1	A	25	ASP	CA-C-N	5.18	125.48	119.47
1	A	25	ASP	C-N-CA	5.18	125.48	119.47
1	A	167	GLY	N-CA-C	5.13	125.34	113.18
1	C	163	LYS	N-CA-C	5.12	116.86	111.28
1	C	161	ILE	N-CA-C	5.09	115.31	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	ILE	N-CA-C	5.04	119.76	108.88

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	1428	0	1440	178	1
1	B	1428	0	1440	160	0
1	C	1428	0	1440	164	1
2	A	27	0	37	1	0
2	B	121	0	185	29	0
2	C	50	0	70	2	0
All	All	4482	0	4612	465	1

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 51.

All (465) 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:A:53:LEU:HD23	1:A:54:HIS:CE1	1.51	1.45
1:B:53:LEU:HD23	1:B:54:HIS:CE1	1.54	1.42
1:C:53:LEU:HD23	1:C:54:HIS:CE1	1.54	1.42
1:C:56:THR:C	1:C:58:PRO:HD2	1.58	1.28
1:A:53:LEU:CD2	1:A:54:HIS:CE1	2.19	1.24
1:C:19:CYS:O	1:C:23:LYS:HA	1.37	1.23
1:C:53:LEU:CD2	1:C:54:HIS:CE1	2.21	1.22
1:B:53:LEU:CD2	1:B:54:HIS:CE1	2.22	1.20
1:A:11:ILE:HD11	1:B:110:PHE:CD1	1.77	1.19
1:C:57:ALA:N	1:C:58:PRO:HD2	1.53	1.18
1:A:19:CYS:O	1:A:23:LYS:HA	1.41	1.18
1:B:19:CYS:O	1:B:23:LYS:HA	1.39	1.17
1:B:131:HIS:HB2	1:B:133:VAL:HG12	1.20	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:HIS:CB	1:B:133:VAL:HG12	1.77	1.14
1:A:131:HIS:HB2	1:A:133:VAL:HG12	1.23	1.14
1:C:159:GLU:HA	1:C:165:PRO:HD2	1.18	1.13
1:C:131:HIS:CB	1:C:133:VAL:HG12	1.78	1.13
1:C:131:HIS:HB2	1:C:133:VAL:HG12	1.23	1.10
1:A:131:HIS:CB	1:A:133:VAL:HG12	1.81	1.09
1:B:159:GLU:HA	1:B:165:PRO:HD2	1.14	1.09
1:A:57:ALA:N	1:A:58:PRO:HD2	1.63	1.08
1:B:136:ILE:O	1:B:138:GLU:HG2	1.51	1.08
1:A:110:PHE:CD1	1:C:11:ILE:HD11	1.90	1.07
1:A:159:GLU:HA	1:A:165:PRO:HD2	1.11	1.06
1:A:136:ILE:O	1:A:138:GLU:HG2	1.52	1.05
2:B:301:XP4:H47	2:B:302:XP4:H22	1.32	1.05
1:A:137:THR:HG22	1:A:138:GLU:H	1.17	1.05
1:B:137:THR:HG22	1:B:138:GLU:H	1.17	1.05
1:A:11:ILE:HD11	1:B:110:PHE:CE1	1.92	1.05
1:A:110:PHE:CE1	1:C:11:ILE:HD11	1.91	1.04
1:A:187:TRP:CZ2	1:B:117:PRO:HB2	1.91	1.03
1:C:55:PRO:O	1:C:56:THR:HG23	1.59	1.03
1:B:157:PHE:CE1	1:B:161:ILE:HG21	1.94	1.02
1:A:32:MET:HE2	1:B:90:TYR:HE2	1.21	1.01
1:A:117:PRO:HB2	1:C:187:TRP:CZ2	1.96	0.99
1:A:57:ALA:N	1:A:58:PRO:CD	2.25	0.98
1:A:55:PRO:O	1:A:56:THR:HG23	1.64	0.98
1:B:157:PHE:CD1	1:B:161:ILE:HG21	1.98	0.98
1:A:90:TYR:HE2	1:C:32:MET:HE2	1.31	0.95
1:C:57:ALA:N	1:C:58:PRO:CD	2.30	0.94
1:A:24:VAL:HG23	1:B:100:ASP:OD2	1.68	0.94
1:C:55:PRO:C	1:C:56:THR:HG23	1.93	0.94
1:B:53:LEU:HD23	1:B:54:HIS:HE1	1.30	0.93
1:C:169:PHE:O	1:C:172:TRP:N	2.00	0.93
1:A:100:ASP:OD2	1:C:24:VAL:HG23	1.69	0.92
2:B:301:XP4:H9	2:B:304:XP4:H18	1.49	0.91
1:A:53:LEU:HD23	1:A:54:HIS:HE1	1.24	0.91
1:B:137:THR:HG22	1:B:138:GLU:N	1.85	0.90
1:C:116:VAL:HB	1:C:117:PRO:HD3	1.54	0.90
1:B:163:LYS:O	1:B:164:ILE:CG1	2.21	0.89
1:B:157:PHE:O	1:B:161:ILE:HG22	1.73	0.87
1:C:53:LEU:HD23	1:C:54:HIS:HE1	1.29	0.87
1:A:137:THR:HG22	1:A:138:GLU:N	1.85	0.86
1:B:116:VAL:HB	1:B:117:PRO:HD3	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:VAL:HB	1:A:117:PRO:HD3	1.57	0.85
1:A:1:MET:HA	1:B:75:PHE:CZ	2.12	0.85
1:A:159:GLU:HA	1:A:165:PRO:CD	2.04	0.84
1:A:32:MET:HE2	1:B:90:TYR:CE2	2.12	0.84
1:B:163:LYS:O	1:B:164:ILE:HG13	1.77	0.84
1:A:55:PRO:C	1:A:56:THR:HG23	2.02	0.83
1:A:75:PHE:CZ	1:C:1:MET:HA	2.14	0.83
1:B:19:CYS:O	1:B:23:LYS:CA	2.27	0.83
1:B:137:THR:CG2	1:B:138:GLU:H	1.91	0.83
1:C:136:ILE:O	1:C:138:GLU:HG3	1.78	0.81
2:B:301:XP4:H50	2:B:302:XP4:H23	1.63	0.81
1:C:19:CYS:O	1:C:23:LYS:CA	2.26	0.81
1:B:131:HIS:HB2	1:B:133:VAL:CG1	2.08	0.80
1:C:163:LYS:O	1:C:164:ILE:CG1	2.30	0.80
1:B:25:ASP:OD1	1:B:25:ASP:O	1.99	0.79
1:C:157:PHE:CE1	1:C:161:ILE:HG21	2.17	0.79
1:A:25:ASP:OD1	1:A:25:ASP:O	1.99	0.79
1:C:131:HIS:HB3	1:C:133:VAL:HG12	1.65	0.79
2:B:301:XP4:H47	2:B:302:XP4:C12	2.13	0.79
1:C:163:LYS:O	1:C:164:ILE:HG13	1.83	0.79
1:A:157:PHE:CE1	1:A:161:ILE:HG21	2.17	0.78
1:A:19:CYS:O	1:A:23:LYS:CA	2.29	0.78
1:C:55:PRO:O	1:C:56:THR:CG2	2.32	0.78
1:A:56:THR:C	1:A:58:PRO:HD2	2.09	0.77
1:B:159:GLU:HA	1:B:165:PRO:CD	2.07	0.77
1:A:131:HIS:HB2	1:A:133:VAL:CG1	2.11	0.77
1:B:106:TRP:NE1	1:B:161:ILE:HD11	1.99	0.77
1:B:131:HIS:HB3	1:B:133:VAL:HG12	1.67	0.76
1:A:163:LYS:O	1:A:164:ILE:CG1	2.34	0.76
1:C:34:PHE:HB3	2:C:301:XP4:H49	1.68	0.75
1:C:25:ASP:OD1	1:C:25:ASP:O	2.04	0.75
1:C:159:GLU:HA	1:C:165:PRO:CD	2.08	0.75
1:C:56:THR:CA	1:C:58:PRO:HD2	2.15	0.75
1:A:163:LYS:O	1:A:164:ILE:HG13	1.87	0.75
1:B:158:ILE:HD12	1:B:165:PRO:HG3	1.69	0.74
1:C:131:HIS:HB2	1:C:133:VAL:CG1	2.11	0.74
1:C:54:HIS:C	1:C:56:THR:H	1.94	0.74
1:C:170:THR:N	1:C:171:PRO:HD2	2.01	0.74
1:A:11:ILE:CD1	1:B:110:PHE:CD1	2.67	0.73
1:B:55:PRO:C	1:B:56:THR:HG23	2.13	0.73
1:C:158:ILE:HD12	1:C:165:PRO:HG3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ALA:H	1:A:58:PRO:CD	2.01	0.72
1:A:131:HIS:HB3	1:A:133:VAL:HG12	1.71	0.72
1:C:102:ARG:HB2	1:C:103:PRO:HD3	1.72	0.71
1:A:55:PRO:O	1:A:56:THR:CG2	2.38	0.71
1:A:90:TYR:CE2	1:C:32:MET:HE2	2.20	0.71
1:A:187:TRP:HZ2	1:B:117:PRO:HB2	1.54	0.71
1:C:168:LYS:O	1:C:171:PRO:HG2	1.90	0.70
1:A:57:ALA:H	1:A:58:PRO:HD2	1.52	0.70
1:A:102:ARG:HB2	1:A:103:PRO:HD3	1.73	0.70
1:B:163:LYS:O	1:B:164:ILE:HG12	1.91	0.70
1:B:151:VAL:HG12	1:B:173:LEU:HD21	1.71	0.70
1:C:151:VAL:HG12	1:C:173:LEU:HD21	1.74	0.70
1:B:57:ALA:N	1:B:58:PRO:HD2	2.07	0.70
1:A:152:LEU:HG	1:A:173:LEU:HG	1.75	0.69
2:B:302:XP4:H21	2:B:304:XP4:H23	1.75	0.69
1:A:11:ILE:HG12	1:B:110:PHE:CD2	2.28	0.69
1:B:152:LEU:HD11	1:B:174:ALA:HA	1.73	0.68
1:C:1:MET:HE2	1:C:43:CYS:HB3	1.75	0.68
1:B:166:LEU:HD12	1:B:166:LEU:O	1.94	0.68
1:C:128:LEU:HB2	1:C:131:HIS:CE1	2.28	0.68
1:A:152:LEU:HD11	1:A:174:ALA:HA	1.75	0.68
1:B:152:LEU:HG	1:B:173:LEU:HG	1.74	0.68
1:B:102:ARG:HB2	1:B:103:PRO:HD3	1.76	0.67
1:A:151:VAL:HG12	1:A:173:LEU:HD21	1.76	0.67
1:C:55:PRO:C	1:C:56:THR:CG2	2.65	0.67
1:C:152:LEU:HD11	1:C:174:ALA:HA	1.76	0.67
1:C:157:PHE:O	1:C:161:ILE:HG22	1.94	0.66
1:B:128:LEU:HB2	1:B:131:HIS:CE1	2.31	0.66
1:C:53:LEU:HD21	1:C:54:HIS:CE1	2.28	0.66
1:A:158:ILE:O	1:A:163:LYS:HB3	1.96	0.65
1:A:158:ILE:HD12	1:A:165:PRO:HG3	1.76	0.65
1:B:38:GLY:O	1:B:42:VAL:HG23	1.96	0.65
2:B:302:XP4:H5	2:B:302:XP4:O2	1.95	0.65
1:C:94:ASN:HA	1:C:99:LEU:HD12	1.77	0.65
1:C:152:LEU:HG	1:C:173:LEU:HG	1.79	0.65
1:B:53:LEU:HD21	1:B:54:HIS:CE1	2.29	0.65
1:A:108:SER:HB3	1:A:153:TRP:O	1.97	0.65
2:B:302:XP4:O2	2:B:302:XP4:C3	2.45	0.64
1:B:131:HIS:CB	1:B:133:VAL:CG1	2.68	0.64
1:C:172:TRP:HA	1:C:175:ILE:HD12	1.80	0.64
1:A:141:TRP:HE3	1:A:144:ILE:HD11	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ALA:O	1:C:58:PRO:C	2.41	0.64
1:A:110:PHE:CD1	1:C:11:ILE:CD1	2.77	0.63
1:A:1:MET:HE2	1:A:43:CYS:HB3	1.81	0.63
1:A:106:TRP:CD1	1:C:18:ILE:HG21	2.34	0.63
1:B:94:ASN:HA	1:B:99:LEU:HD12	1.78	0.63
1:A:12:VAL:HB	1:A:36:VAL:HG21	1.80	0.63
1:A:110:PHE:CD2	1:C:11:ILE:HG12	2.34	0.63
1:A:117:PRO:HB2	1:C:187:TRP:HZ2	1.55	0.63
1:B:163:LYS:C	1:B:164:ILE:HG12	2.24	0.63
1:A:172:TRP:HA	1:A:175:ILE:HD12	1.80	0.63
1:C:131:HIS:CB	1:C:133:VAL:CG1	2.69	0.63
1:A:173:LEU:O	1:A:177:GLU:HB2	1.99	0.63
1:A:53:LEU:HD21	1:A:54:HIS:CE1	2.27	0.62
1:C:56:THR:C	1:C:58:PRO:CD	2.53	0.62
1:C:161:ILE:HG23	1:C:162:LEU:N	2.13	0.62
2:B:302:XP4:O2	2:B:303:XP4:C2	2.47	0.62
1:A:38:GLY:O	1:A:42:VAL:HG23	1.99	0.62
1:C:38:GLY:O	1:C:42:VAL:HG23	2.00	0.62
1:C:54:HIS:C	1:C:56:THR:N	2.54	0.62
1:B:163:LYS:HB3	1:B:165:PRO:HD3	1.81	0.61
1:A:18:ILE:HG21	1:B:106:TRP:CD1	2.36	0.61
1:C:47:VAL:HG12	1:C:78:PRO:HG3	1.83	0.61
1:B:122:SER:O	1:B:140:ASP:OD2	2.19	0.61
1:B:108:SER:HB3	1:B:153:TRP:O	2.00	0.61
1:A:141:TRP:H	1:A:141:TRP:CD1	2.18	0.61
1:C:128:LEU:CB	1:C:131:HIS:HE1	2.14	0.61
1:A:122:SER:O	1:A:140:ASP:OD2	2.19	0.60
1:B:173:LEU:O	1:B:177:GLU:HB2	2.00	0.60
1:A:11:ILE:HG13	1:B:110:PHE:CE2	2.35	0.60
1:A:158:ILE:HB	1:A:163:LYS:HD3	1.82	0.60
2:B:302:XP4:C12	2:B:304:XP4:H23	2.31	0.60
1:C:46:VAL:O	1:C:50:TYR:HD1	1.85	0.60
1:B:157:PHE:CD1	1:B:161:ILE:CG2	2.80	0.60
1:B:163:LYS:C	1:B:164:ILE:CG1	2.76	0.59
1:B:128:LEU:CB	1:B:131:HIS:HE1	2.15	0.59
1:B:57:ALA:N	1:B:58:PRO:CD	2.66	0.59
1:A:94:ASN:HA	1:A:99:LEU:HD12	1.83	0.59
1:C:141:TRP:HE3	1:C:144:ILE:HD11	1.68	0.59
1:C:159:GLU:CA	1:C:165:PRO:HD2	2.13	0.59
1:B:53:LEU:CD2	1:B:54:HIS:NE2	2.65	0.59
1:C:163:LYS:O	1:C:164:ILE:HG12	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:THR:CG2	1:A:138:GLU:H	1.91	0.59
1:C:108:SER:HB3	1:C:153:TRP:O	2.02	0.59
1:A:46:VAL:O	1:A:50:TYR:HD1	1.87	0.58
1:C:55:PRO:O	1:C:56:THR:CB	2.51	0.58
1:A:11:ILE:CD1	1:B:110:PHE:CE1	2.79	0.58
1:B:12:VAL:HB	1:B:36:VAL:HG21	1.84	0.58
1:C:163:LYS:C	1:C:164:ILE:HG12	2.29	0.58
1:A:163:LYS:C	1:A:164:ILE:HG12	2.29	0.58
1:A:128:LEU:HB2	1:A:131:HIS:CE1	2.38	0.58
1:C:169:PHE:O	1:C:170:THR:C	2.46	0.58
1:A:137:THR:O	1:A:138:GLU:HB2	2.03	0.58
1:C:138:GLU:O	1:C:141:TRP:CD1	2.57	0.58
1:C:53:LEU:O	1:C:55:PRO:HD3	2.03	0.58
1:B:137:THR:O	1:B:138:GLU:HB2	2.03	0.57
2:B:302:XP4:H8	2:B:303:XP4:H8	1.86	0.57
1:B:172:TRP:HA	1:B:175:ILE:HD12	1.84	0.57
1:A:22:THR:HB	1:B:102:ARG:HH21	1.70	0.57
1:C:12:VAL:HB	1:C:36:VAL:HG21	1.85	0.57
1:C:141:TRP:CD1	1:C:141:TRP:H	2.21	0.57
1:A:53:LEU:CG	1:A:54:HIS:CE1	2.88	0.57
1:B:185:PRO:O	1:B:189:LEU:HB2	2.05	0.57
1:A:158:ILE:HG13	1:A:159:GLU:H	1.70	0.57
1:A:185:PRO:O	1:A:189:LEU:HB2	2.04	0.57
1:B:137:THR:CG2	1:B:138:GLU:N	2.55	0.57
1:B:1:MET:HE2	1:B:43:CYS:HB3	1.87	0.57
1:B:170:THR:N	1:B:171:PRO:HD2	2.20	0.57
1:C:20:GLY:O	1:C:23:LYS:HG3	2.05	0.57
1:A:131:HIS:CB	1:A:133:VAL:CG1	2.72	0.56
1:B:102:ARG:CB	1:B:103:PRO:HD3	2.35	0.56
1:B:141:TRP:H	1:B:141:TRP:CD1	2.23	0.56
1:C:128:LEU:HB2	1:C:131:HIS:HE1	1.69	0.56
1:C:102:ARG:CB	1:C:103:PRO:HD3	2.34	0.56
1:C:173:LEU:O	1:C:177:GLU:HB2	2.04	0.56
1:C:53:LEU:CD2	1:C:54:HIS:NE2	2.66	0.56
1:C:168:LYS:O	1:C:171:PRO:CG	2.54	0.56
1:B:141:TRP:HE3	1:B:144:ILE:HD11	1.70	0.56
1:C:158:ILE:HG13	1:C:159:GLU:H	1.71	0.56
1:B:55:PRO:O	1:B:56:THR:HG23	2.04	0.55
1:A:53:LEU:HA	1:C:50:TYR:HE2	1.71	0.55
1:B:157:PHE:CE1	1:B:161:ILE:CG2	2.81	0.55
1:A:141:TRP:O	1:A:144:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:LEU:O	1:C:6:LEU:HB2	2.05	0.55
1:A:123:HIS:HB2	1:A:143:ALA:HB2	1.88	0.55
1:C:149:TRP:HD1	1:C:177:GLU:OE2	1.90	0.55
1:A:47:VAL:HG12	1:A:78:PRO:HG3	1.88	0.55
1:B:46:VAL:O	1:B:50:TYR:HD1	1.90	0.55
1:B:184:ILE:O	1:B:188:LEU:N	2.40	0.55
1:A:11:ILE:HG12	1:B:110:PHE:CG	2.42	0.55
1:A:163:LYS:O	1:A:164:ILE:HG12	2.05	0.55
1:A:149:TRP:HD1	1:A:177:GLU:OE2	1.90	0.55
1:B:110:PHE:CD1	1:B:110:PHE:C	2.84	0.54
1:A:110:PHE:CE1	1:C:11:ILE:CD1	2.80	0.54
1:A:14:ILE:HG13	1:A:178:GLY:HA3	1.88	0.54
1:B:80:THR:HB	1:B:146:TRP:HH2	1.73	0.54
1:A:53:LEU:CD2	1:A:54:HIS:NE2	2.67	0.54
1:A:111:VAL:O	1:A:115:THR:HG23	2.07	0.54
1:B:41:ILE:CG2	2:B:301:XP4:H59	2.38	0.54
1:C:53:LEU:CG	1:C:54:HIS:CE1	2.90	0.54
1:C:141:TRP:O	1:C:144:ILE:HG12	2.08	0.54
1:C:170:THR:N	1:C:171:PRO:CD	2.67	0.54
1:A:11:ILE:CG1	1:B:110:PHE:CD2	2.90	0.54
1:C:163:LYS:C	1:C:164:ILE:CG1	2.79	0.54
1:A:18:ILE:HG21	1:B:106:TRP:NE1	2.23	0.54
1:A:170:THR:N	1:A:171:PRO:HD2	2.22	0.54
1:B:141:TRP:O	1:B:144:ILE:HG12	2.08	0.54
1:A:137:THR:CG2	1:A:138:GLU:N	2.55	0.54
1:A:157:PHE:CD1	1:A:161:ILE:HG21	2.43	0.53
1:B:27:LYS:HZ2	2:B:302:XP4:C1	2.21	0.53
1:C:24:VAL:CG2	1:C:25:ASP:N	2.70	0.53
1:C:137:THR:O	1:C:138:GLU:HB2	2.08	0.53
1:C:123:HIS:HB2	1:C:143:ALA:HB2	1.89	0.53
1:A:159:GLU:CA	1:A:165:PRO:HD2	2.07	0.53
1:B:27:LYS:NZ	2:B:302:XP4:H3	2.24	0.53
1:B:128:LEU:HB2	1:B:131:HIS:HE1	1.70	0.53
1:A:11:ILE:HG21	1:B:107:TYR:HD1	1.74	0.53
1:A:110:PHE:CE2	1:C:11:ILE:HG13	2.43	0.53
1:C:158:ILE:O	1:C:163:LYS:HB3	2.09	0.53
1:A:2:LEU:O	1:A:6:LEU:HB2	2.09	0.52
1:A:53:LEU:HA	1:C:50:TYR:CE2	2.44	0.52
1:A:46:VAL:HG11	1:B:49:THR:HG22	1.91	0.52
1:B:2:LEU:O	1:B:6:LEU:HB2	2.08	0.52
1:C:106:TRP:NE1	1:C:161:ILE:HD11	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:TRP:HD1	1:B:177:GLU:OE2	1.92	0.52
1:B:158:ILE:HG13	1:B:159:GLU:H	1.74	0.52
1:C:80:THR:HB	1:C:146:TRP:HH2	1.75	0.52
1:A:102:ARG:CB	1:A:103:PRO:HD3	2.37	0.52
1:C:111:VAL:O	1:C:115:THR:HG23	2.10	0.52
1:C:1:MET:CE	1:C:43:CYS:HB3	2.39	0.52
1:C:158:ILE:HG13	1:C:159:GLU:N	2.25	0.52
1:A:158:ILE:HG13	1:A:159:GLU:N	2.25	0.52
1:A:163:LYS:C	1:A:164:ILE:CG1	2.80	0.52
1:A:106:TRP:NE1	1:C:18:ILE:HG21	2.24	0.52
1:C:185:PRO:O	1:C:189:LEU:HB2	2.10	0.52
1:A:184:ILE:O	1:A:188:LEU:N	2.40	0.51
1:C:56:THR:N	1:C:58:PRO:HD2	2.26	0.51
1:A:24:VAL:HG22	1:A:25:ASP:N	2.26	0.51
1:A:24:VAL:CG2	1:A:25:ASP:N	2.72	0.51
1:B:24:VAL:CG2	1:B:25:ASP:N	2.73	0.51
1:B:47:VAL:HG12	1:B:78:PRO:HG3	1.91	0.51
1:B:123:HIS:HB2	1:B:143:ALA:HB2	1.93	0.51
1:A:181:THR:O	1:A:185:PRO:HG2	2.10	0.51
1:B:106:TRP:CD1	1:B:161:ILE:CD1	2.94	0.51
1:B:111:VAL:O	1:B:115:THR:HG23	2.11	0.51
1:C:181:THR:O	1:C:185:PRO:HG2	2.10	0.51
1:A:48:ILE:HG21	1:C:1:MET:HE3	1.92	0.51
1:A:50:TYR:HE2	1:B:53:LEU:HA	1.74	0.51
2:B:302:XP4:H17	2:B:304:XP4:H19	1.92	0.51
1:C:55:PRO:C	1:C:57:ALA:H	2.16	0.51
1:C:184:ILE:O	1:C:188:LEU:N	2.40	0.51
1:A:24:VAL:HG13	1:A:29:THR:HG22	1.91	0.51
1:A:128:LEU:CB	1:A:131:HIS:HE1	2.24	0.51
1:A:157:PHE:CE1	1:A:161:ILE:CG2	2.91	0.51
1:B:14:ILE:HG13	1:B:178:GLY:HA3	1.92	0.51
1:B:154:LEU:O	1:B:157:PHE:HB3	2.11	0.51
1:A:25:ASP:OD1	1:A:25:ASP:C	2.54	0.51
1:B:24:VAL:HG22	1:B:25:ASP:N	2.26	0.51
1:A:55:PRO:O	1:A:56:THR:CB	2.58	0.51
1:B:106:TRP:CE2	1:B:161:ILE:HG12	2.46	0.51
1:B:54:HIS:C	1:B:56:THR:H	2.18	0.50
1:B:106:TRP:CD1	1:B:161:ILE:HD11	2.45	0.50
1:C:14:ILE:HG13	1:C:178:GLY:HA3	1.92	0.50
1:C:138:GLU:O	1:C:141:TRP:HD1	1.93	0.50
1:A:11:ILE:HD13	1:B:107:TYR:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LEU:HG	1:B:54:HIS:CD2	2.46	0.50
1:C:87:THR:HG21	1:C:153:TRP:NE1	2.26	0.50
1:A:134:LEU:N	1:A:134:LEU:HD12	2.27	0.50
2:B:302:XP4:H21	2:B:304:XP4:C13	2.40	0.50
1:C:53:LEU:HG	1:C:54:HIS:CD2	2.46	0.50
1:C:110:PHE:CD1	1:C:110:PHE:C	2.90	0.50
1:A:1:MET:CE	1:A:43:CYS:HB3	2.42	0.49
1:A:110:PHE:CD1	1:A:110:PHE:C	2.90	0.49
1:B:53:LEU:CG	1:B:54:HIS:CE1	2.92	0.49
1:B:55:PRO:C	1:B:56:THR:CG2	2.83	0.49
1:C:154:LEU:O	1:C:157:PHE:HB3	2.12	0.49
1:A:75:PHE:O	1:A:78:PRO:HD2	2.11	0.49
1:C:27:LYS:HD2	2:C:301:XP4:O8	2.12	0.49
1:A:157:PHE:O	1:A:161:ILE:HG22	2.12	0.49
1:A:9:VAL:HA	1:A:12:VAL:HG12	1.93	0.49
1:A:50:TYR:CE2	1:B:53:LEU:HA	2.47	0.49
2:A:201:XP4:H18	2:B:301:XP4:H13	1.94	0.49
1:B:25:ASP:OD1	1:B:25:ASP:C	2.55	0.49
1:B:129:ASP:O	1:B:130:ASP:OD1	2.31	0.49
1:C:176:ILE:HG13	1:C:177:GLU:N	2.27	0.49
1:A:176:ILE:HG13	1:A:177:GLU:N	2.28	0.49
1:B:43:CYS:O	1:B:46:VAL:HG22	2.12	0.49
1:B:176:ILE:HG13	1:B:177:GLU:N	2.28	0.49
1:B:50:TYR:O	1:B:53:LEU:HB3	2.13	0.49
1:A:11:ILE:CG1	1:B:110:PHE:CE2	2.96	0.48
1:B:27:LYS:HZ2	2:B:302:XP4:H2	1.78	0.48
1:B:181:THR:O	1:B:185:PRO:HG2	2.12	0.48
1:A:48:ILE:CG2	1:C:1:MET:HE3	2.43	0.48
1:A:163:LYS:HG2	1:A:165:PRO:HD3	1.95	0.48
1:B:53:LEU:O	1:B:55:PRO:HD3	2.13	0.48
1:C:161:ILE:CG2	1:C:162:LEU:N	2.77	0.48
1:B:27:LYS:NZ	2:B:302:XP4:C1	2.77	0.48
1:B:168:LYS:O	1:B:171:PRO:HG2	2.13	0.48
1:A:102:ARG:HH21	1:C:22:THR:HB	1.77	0.48
1:B:158:ILE:HG13	1:B:159:GLU:N	2.28	0.48
2:B:302:XP4:O2	2:B:302:XP4:H6	2.13	0.48
1:C:12:VAL:HG11	1:C:36:VAL:HG11	1.96	0.48
1:A:56:THR:CA	1:A:58:PRO:HD2	2.43	0.47
1:A:110:PHE:CG	1:C:11:ILE:HG12	2.49	0.47
1:A:167:GLY:O	1:A:171:PRO:HD2	2.14	0.47
2:B:302:XP4:H8	2:B:303:XP4:C5	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TRP:O	1:A:176:ILE:HG12	2.15	0.47
1:A:50:TYR:O	1:A:53:LEU:HB3	2.15	0.47
1:B:12:VAL:HG11	1:B:36:VAL:HG11	1.96	0.47
1:A:128:LEU:HB2	1:A:131:HIS:HE1	1.80	0.47
1:A:192:GLN:O	1:A:193:HIS:HB2	2.15	0.47
1:A:190:PHE:CE1	1:B:76:TYR:HA	2.50	0.46
2:B:301:XP4:C27	2:B:302:XP4:H23	2.41	0.46
1:A:9:VAL:HG13	1:A:88:TYR:OH	2.15	0.46
1:C:24:VAL:HG22	1:C:25:ASP:N	2.29	0.46
1:C:34:PHE:CD2	1:C:92:ALA:HB1	2.51	0.46
1:A:103:PRO:CG	1:C:24:VAL:HG11	2.46	0.46
1:B:75:PHE:O	1:B:78:PRO:HD2	2.16	0.46
1:C:50:TYR:O	1:C:53:LEU:HB3	2.15	0.46
1:C:169:PHE:O	1:C:171:PRO:N	2.48	0.46
1:A:49:THR:HG22	1:C:46:VAL:HG11	1.98	0.46
1:B:9:VAL:HA	1:B:12:VAL:HG12	1.98	0.46
1:B:87:THR:HG21	1:B:153:TRP:NE1	2.31	0.46
1:A:179:ILE:O	1:A:183:TRP:HB3	2.16	0.46
1:B:134:LEU:N	1:B:134:LEU:HD12	2.30	0.46
1:B:161:ILE:HG23	1:B:162:LEU:N	2.30	0.46
1:C:142:TRP:HA	1:C:145:ILE:HD12	1.98	0.46
1:A:53:LEU:HG	1:A:54:HIS:CD2	2.52	0.45
1:B:1:MET:CE	1:B:43:CYS:HB3	2.46	0.45
1:B:192:GLN:O	1:B:193:HIS:HB2	2.15	0.45
1:C:54:HIS:O	1:C:56:THR:N	2.49	0.45
1:B:178:GLY:O	1:B:183:TRP:HB2	2.16	0.45
1:B:9:VAL:HG13	1:B:88:TYR:OH	2.16	0.45
1:B:24:VAL:O	1:B:25:ASP:C	2.59	0.45
1:B:80:THR:HB	1:B:146:TRP:CH2	2.52	0.45
2:B:301:XP4:H7	2:B:301:XP4:H40	1.97	0.45
1:A:154:LEU:O	1:A:157:PHE:HB3	2.15	0.45
1:A:20:GLY:O	1:A:23:LYS:HG3	2.16	0.45
1:A:24:VAL:O	1:A:25:ASP:C	2.60	0.45
1:B:142:TRP:HA	1:B:145:ILE:HD12	1.99	0.45
1:C:192:GLN:O	1:C:193:HIS:HB2	2.16	0.45
1:A:55:PRO:C	1:A:56:THR:CG2	2.74	0.45
1:A:110:PHE:CE2	1:C:11:ILE:CG1	3.00	0.45
2:B:302:XP4:C3	2:B:302:XP4:P1	3.05	0.45
1:A:80:THR:HB	1:A:146:TRP:HH2	1.82	0.44
2:B:301:XP4:H40	2:B:301:XP4:C5	2.47	0.44
1:C:129:ASP:O	1:C:130:ASP:OD1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ASN:ND2	1:C:183:TRP:CZ2	2.84	0.44
1:B:179:ILE:O	1:B:183:TRP:HB3	2.18	0.44
2:B:302:XP4:H6	2:B:302:XP4:P1	2.57	0.44
1:A:34:PHE:CD2	1:A:92:ALA:HB1	2.52	0.44
1:A:43:CYS:O	1:A:46:VAL:HG22	2.17	0.44
2:B:301:XP4:C25	2:B:302:XP4:H22	2.24	0.44
1:A:110:PHE:CD2	1:C:11:ILE:CG1	2.99	0.44
1:C:55:PRO:O	1:C:56:THR:OG1	2.30	0.44
1:A:1:MET:HE3	1:B:48:ILE:CG2	2.47	0.44
1:A:12:VAL:HG11	1:A:36:VAL:HG11	2.00	0.44
1:C:157:PHE:CD1	1:C:161:ILE:HG21	2.52	0.44
1:C:106:TRP:CZ3	1:C:157:PHE:HE1	2.36	0.44
1:C:180:LEU:HD23	1:C:180:LEU:C	2.43	0.44
1:C:134:LEU:HD12	1:C:134:LEU:N	2.32	0.44
1:A:141:TRP:CE3	1:A:144:ILE:HD11	2.47	0.44
1:B:183:TRP:CD1	1:B:183:TRP:C	2.95	0.44
1:C:1:MET:HE2	1:C:43:CYS:CB	2.44	0.44
1:C:45:VAL:O	1:C:49:THR:HG23	2.16	0.44
1:A:25:ASP:HA	1:A:26:PRO:HD3	1.69	0.44
1:B:106:TRP:NE1	1:B:161:ILE:CD1	2.76	0.43
1:B:158:ILE:O	1:B:163:LYS:HB3	2.17	0.43
1:C:43:CYS:O	1:C:46:VAL:HG22	2.17	0.43
1:B:148:ALA:O	1:B:151:VAL:HB	2.18	0.43
2:B:301:XP4:H35	2:B:301:XP4:O5	2.18	0.43
1:C:179:ILE:O	1:C:183:TRP:HB3	2.18	0.43
1:A:156:ALA:O	1:A:160:ASN:HB2	2.17	0.43
1:B:20:GLY:O	1:B:23:LYS:HG3	2.19	0.43
1:C:140:ASP:H	1:C:195:VAL:HG11	1.84	0.43
1:C:183:TRP:CD1	1:C:183:TRP:C	2.95	0.43
1:B:106:TRP:CZ3	1:B:157:PHE:HE1	2.36	0.43
1:A:11:ILE:HG13	1:B:110:PHE:CZ	2.52	0.43
1:C:47:VAL:CG1	1:C:78:PRO:HG3	2.49	0.43
1:C:141:TRP:CE3	1:C:144:ILE:HD11	2.52	0.43
1:C:145:ILE:HG12	1:C:181:THR:HG23	2.01	0.43
1:A:30:ALA:O	1:A:31:VAL:C	2.60	0.43
1:A:145:ILE:HG12	1:A:181:THR:HG23	2.00	0.43
1:C:25:ASP:OD1	1:C:25:ASP:C	2.56	0.43
1:B:55:PRO:O	1:B:56:THR:CB	2.66	0.43
1:B:55:PRO:O	1:B:56:THR:OG1	2.30	0.43
1:A:129:ASP:O	1:A:130:ASP:OD1	2.37	0.43
1:A:142:TRP:HA	1:A:145:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LYS:CB	1:B:165:PRO:HD3	2.47	0.42
1:C:9:VAL:HA	1:C:12:VAL:HG12	2.00	0.42
1:A:100:ASP:HB2	1:C:24:VAL:HG21	2.01	0.42
1:C:167:GLY:O	1:C:171:PRO:HD2	2.19	0.42
1:A:183:TRP:C	1:A:183:TRP:CD1	2.97	0.42
1:B:151:VAL:O	1:B:155:THR:HG23	2.19	0.42
1:B:151:VAL:HG12	1:B:152:LEU:N	2.33	0.42
1:A:103:PRO:HG3	1:C:24:VAL:HG11	2.02	0.42
1:C:20:GLY:O	1:C:23:LYS:CG	2.67	0.42
1:C:178:GLY:O	1:C:183:TRP:HB2	2.20	0.42
1:A:154:LEU:HD12	1:A:157:PHE:HB3	2.02	0.42
1:B:27:LYS:HZ2	2:B:302:XP4:H3	1.85	0.42
1:C:24:VAL:O	1:C:25:ASP:C	2.63	0.42
1:C:136:ILE:C	1:C:137:THR:OG1	2.63	0.42
1:A:53:LEU:O	1:A:55:PRO:HD3	2.20	0.42
1:A:55:PRO:O	1:A:56:THR:OG1	2.36	0.42
1:B:141:TRP:CE3	1:B:144:ILE:HD11	2.52	0.42
1:A:141:TRP:H	1:A:141:TRP:HD1	1.65	0.41
1:C:53:LEU:HG	1:C:54:HIS:NE2	2.35	0.41
1:C:154:LEU:HD12	1:C:157:PHE:HB3	2.02	0.41
1:A:11:ILE:CG1	1:B:110:PHE:CG	3.03	0.41
1:B:126:ASP:O	1:B:128:LEU:HG	2.20	0.41
1:C:156:ALA:O	1:C:160:ASN:HB2	2.20	0.41
1:A:1:MET:HE3	1:B:48:ILE:HG21	2.01	0.41
1:A:24:VAL:CG2	1:B:100:ASP:OD2	2.55	0.41
1:A:148:ALA:O	1:A:151:VAL:HB	2.20	0.41
1:C:55:PRO:C	1:C:57:ALA:N	2.77	0.41
1:A:24:VAL:HG11	1:B:103:PRO:CG	2.50	0.41
1:A:151:VAL:HG12	1:A:152:LEU:N	2.34	0.41
1:C:126:ASP:O	1:C:128:LEU:HG	2.20	0.41
1:A:110:PHE:CZ	1:C:11:ILE:HG13	2.55	0.41
1:B:54:HIS:C	1:B:56:THR:N	2.79	0.41
1:A:47:VAL:CG1	1:A:78:PRO:HG3	2.51	0.41
1:B:172:TRP:O	1:B:176:ILE:HG12	2.20	0.41
1:C:158:ILE:HB	1:C:163:LYS:HD3	2.03	0.41
1:C:172:TRP:O	1:C:176:ILE:HG12	2.21	0.41
1:B:34:PHE:CD2	1:B:92:ALA:HB1	2.56	0.41
1:A:35:PHE:CE1	1:B:89:LEU:HG	2.56	0.40
1:B:145:ILE:HG12	1:B:181:THR:HG23	2.03	0.40
1:C:161:ILE:HG23	1:C:162:LEU:H	1.82	0.40
1:C:184:ILE:N	1:C:185:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ILE:HG21	2:B:301:XP4:H59	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ASP:OD2	1:C:25:ASP:OD2[7_555]	2.06	0.14

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	176/201 (88%)	153 (87%)	23 (13%)	0	100	100
1	B	176/201 (88%)	153 (87%)	23 (13%)	0	100	100
1	C	176/201 (88%)	154 (88%)	22 (12%)	0	100	100
All	All	528/603 (88%)	460 (87%)	68 (13%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	150/169 (89%)	143 (95%)	7 (5%)	23	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	150/169 (89%)	144 (96%)	6 (4%)	28	54
1	C	150/169 (89%)	142 (95%)	8 (5%)	20	48
All	All	450/507 (89%)	429 (95%)	21 (5%)	23	51

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	46	VAL
1	A	109	LEU
1	A	121	LEU
1	A	127	MET
1	A	142	TRP
1	A	151	VAL
1	B	45	VAL
1	B	46	VAL
1	B	109	LEU
1	B	142	TRP
1	B	151	VAL
1	B	166	LEU
1	C	4	LEU
1	C	24	VAL
1	C	45	VAL
1	C	46	VAL
1	C	109	LEU
1	C	121	LEU
1	C	142	TRP
1	C	151	VAL

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	54	HIS
1	A	95	HIS
1	A	193	HIS
1	B	54	HIS
1	B	95	HIS
1	B	193	HIS
1	C	54	HIS
1	C	95	HIS

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Mol	Chain	Res	Type
1	C	193	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	XP4	B	305	-	9,9,39	1.99	1 (11%)	9,9,44	1.19	1 (11%)
2	XP4	B	302	-	39,39,39	1.39	2 (5%)	42,44,44	1.94	10 (23%)
2	XP4	A	201	-	16,16,39	1.42	1 (6%)	16,16,44	1.30	1 (6%)
2	XP4	B	301	-	35,35,39	1.25	2 (5%)	37,37,44	1.97	6 (16%)
2	XP4	C	301	-	39,39,39	1.44	3 (7%)	42,44,44	2.23	9 (21%)
2	XP4	B	303	-	17,17,39	1.56	1 (5%)	17,17,44	1.56	3 (17%)
2	XP4	A	202	-	9,9,39	1.81	1 (11%)	9,9,44	1.62	1 (11%)
2	XP4	C	302	-	9,9,39	1.71	1 (11%)	9,9,44	1.25	1 (11%)
2	XP4	B	304	-	16,16,39	1.39	1 (6%)	16,16,44	1.40	2 (12%)

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	XP4	B	305	-	-	3/8/8/41	-
2	XP4	B	302	-	-	19/41/41/41	-
2	XP4	A	201	-	-	3/15/15/41	-
2	XP4	B	301	-	-	13/37/37/41	-
2	XP4	C	301	-	-	22/41/41/41	-
2	XP4	B	303	-	-	3/16/16/41	-
2	XP4	A	202	-	-	4/8/8/41	-
2	XP4	C	302	-	-	4/8/8/41	-
2	XP4	B	304	-	-	0/15/15/41	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	XP4	O7-C18	6.07	1.51	1.34
2	B	303	XP4	O5-C4	5.96	1.50	1.33
2	B	302	XP4	O7-C18	5.68	1.50	1.34
2	B	305	XP4	O5-C4	5.61	1.50	1.33
2	B	302	XP4	O5-C4	5.35	1.48	1.33
2	A	202	XP4	O5-C4	5.22	1.49	1.33
2	B	304	XP4	O5-C4	5.20	1.49	1.33
2	A	201	XP4	O5-C4	5.17	1.49	1.33
2	B	301	XP4	O7-C18	5.02	1.48	1.34
2	C	302	XP4	O5-C4	4.81	1.47	1.33
2	C	301	XP4	O5-C4	4.42	1.46	1.33
2	B	301	XP4	O5-C4	4.30	1.45	1.33
2	C	301	XP4	P1-O4	2.47	1.68	1.60

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	XP4	O5-C4-C5	7.96	136.09	111.83
2	B	301	XP4	O5-C4-C5	6.92	132.94	111.83
2	B	302	XP4	O5-C4-C5	6.67	132.17	111.83
2	C	301	XP4	C3-C2-C1	-6.33	97.03	111.78
2	B	302	XP4	O7-C18-C19	5.97	124.40	111.48
2	B	301	XP4	O7-C18-C19	5.94	124.34	111.48
2	B	303	XP4	C3-O5-C4	4.67	129.93	116.67
2	A	201	XP4	C3-O5-C4	4.60	130.80	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	XP4	O6-C4-C5	-4.55	105.98	123.78
2	C	301	XP4	O7-C18-C19	4.50	121.21	111.48
2	B	304	XP4	C3-O5-C4	4.11	129.24	116.07
2	A	202	XP4	C3-O5-C4	4.06	129.06	116.07
2	B	302	XP4	O6-C4-C5	-3.95	108.34	123.78
2	B	301	XP4	O5-C4-O6	-3.89	113.89	123.63
2	C	301	XP4	O4-P1-O2	3.54	116.00	106.44
2	C	302	XP4	C3-O5-C4	3.37	126.87	116.07
2	B	301	XP4	O4-C1-C2	3.16	119.91	111.77
2	B	302	XP4	O3-P1-O4	-2.78	99.43	106.67
2	B	305	XP4	C3-O5-C4	2.77	124.95	116.07
2	C	301	XP4	O7-C2-C1	2.74	118.19	108.34
2	B	301	XP4	O6-C4-C5	-2.74	113.08	123.78
2	B	302	XP4	O3-P1-O1	2.71	117.95	107.80
2	B	301	XP4	O7-C18-O8	-2.67	117.46	123.70
2	B	303	XP4	O5-C3-C2	2.59	117.69	108.40
2	C	301	XP4	O1-P1-O4	-2.56	99.98	106.67
2	B	302	XP4	C2-O7-C18	-2.48	111.86	117.80
2	C	301	XP4	O5-C3-C2	2.36	115.20	108.40
2	B	302	XP4	O7-C18-O8	-2.34	118.24	123.70
2	C	301	XP4	O5-C4-O6	-2.33	117.81	123.63
2	B	302	XP4	C3-O5-C4	2.29	125.49	117.12
2	B	303	XP4	O5-C4-C5	2.21	118.58	111.83
2	B	304	XP4	C7-C6-C5	-2.11	105.36	113.13
2	B	302	XP4	O5-C3-C2	2.09	114.42	108.40
2	B	302	XP4	C7-C6-C5	2.02	120.53	113.13

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	XP4	C19-C18-O7-C2
2	B	302	XP4	C2-C1-O4-P1
2	B	302	XP4	C19-C18-O7-C2
2	C	301	XP4	C1-O4-P1-O1
2	C	301	XP4	C1-O4-P1-O2
2	C	301	XP4	C1-O4-P1-O3
2	C	301	XP4	C19-C18-O7-C2
2	B	301	XP4	O8-C18-O7-C2
2	B	302	XP4	O8-C18-O7-C2
2	C	301	XP4	O8-C18-O7-C2
2	C	301	XP4	C5-C4-O5-C3

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Mol	Chain	Res	Type	Atoms
2	C	301	XP4	O6-C4-O5-C3
2	C	302	XP4	C5-C4-O5-C3
2	A	202	XP4	C4-C5-C6-C7
2	B	305	XP4	C4-C5-C6-C7
2	A	202	XP4	C5-C4-O5-C3
2	B	305	XP4	C5-C4-O5-C3
2	B	301	XP4	C11-C12-C13-C14
2	B	302	XP4	C4-C5-C6-C7
2	C	302	XP4	C4-C5-C6-C7
2	C	302	XP4	O6-C4-O5-C3
2	B	301	XP4	C4-C5-C6-C7
2	C	301	XP4	C11-C12-C13-C14
2	B	302	XP4	C11-C12-C13-C14
2	B	301	XP4	C12-C13-C14-C15
2	C	301	XP4	C25-C26-C27-C28
2	B	302	XP4	O6-C4-O5-C3
2	B	301	XP4	C19-C20-C21-C22
2	C	301	XP4	C12-C13-C14-C15
2	A	202	XP4	O6-C4-O5-C3
2	B	301	XP4	C25-C26-C27-C28
2	C	301	XP4	C19-C20-C21-C22
2	C	301	XP4	C5-C6-C7-C8
2	B	302	XP4	C1-O4-P1-O2
2	A	201	XP4	C11-C12-C13-C14
2	B	302	XP4	C25-C26-C27-C28
2	B	302	XP4	C12-C13-C14-C15
2	B	305	XP4	O6-C4-O5-C3
2	B	302	XP4	C5-C4-O5-C3
2	B	301	XP4	C13-C14-C15-C16
2	B	302	XP4	O4-C1-C2-C3
2	C	301	XP4	O4-C1-C2-C3
2	C	301	XP4	C28-C29-C30-C31
2	B	301	XP4	C28-C29-C30-C31
2	B	302	XP4	O4-C1-C2-O7
2	B	302	XP4	C14-C15-C16-C17
2	B	301	XP4	C14-C15-C16-C17
2	C	301	XP4	O4-C1-C2-O7
2	C	301	XP4	C7-C8-C9-C10
2	B	302	XP4	C13-C14-C15-C16
2	B	302	XP4	C28-C29-C30-C31
2	C	301	XP4	C2-C1-O4-P1
2	C	301	XP4	C23-C24-C25-C26

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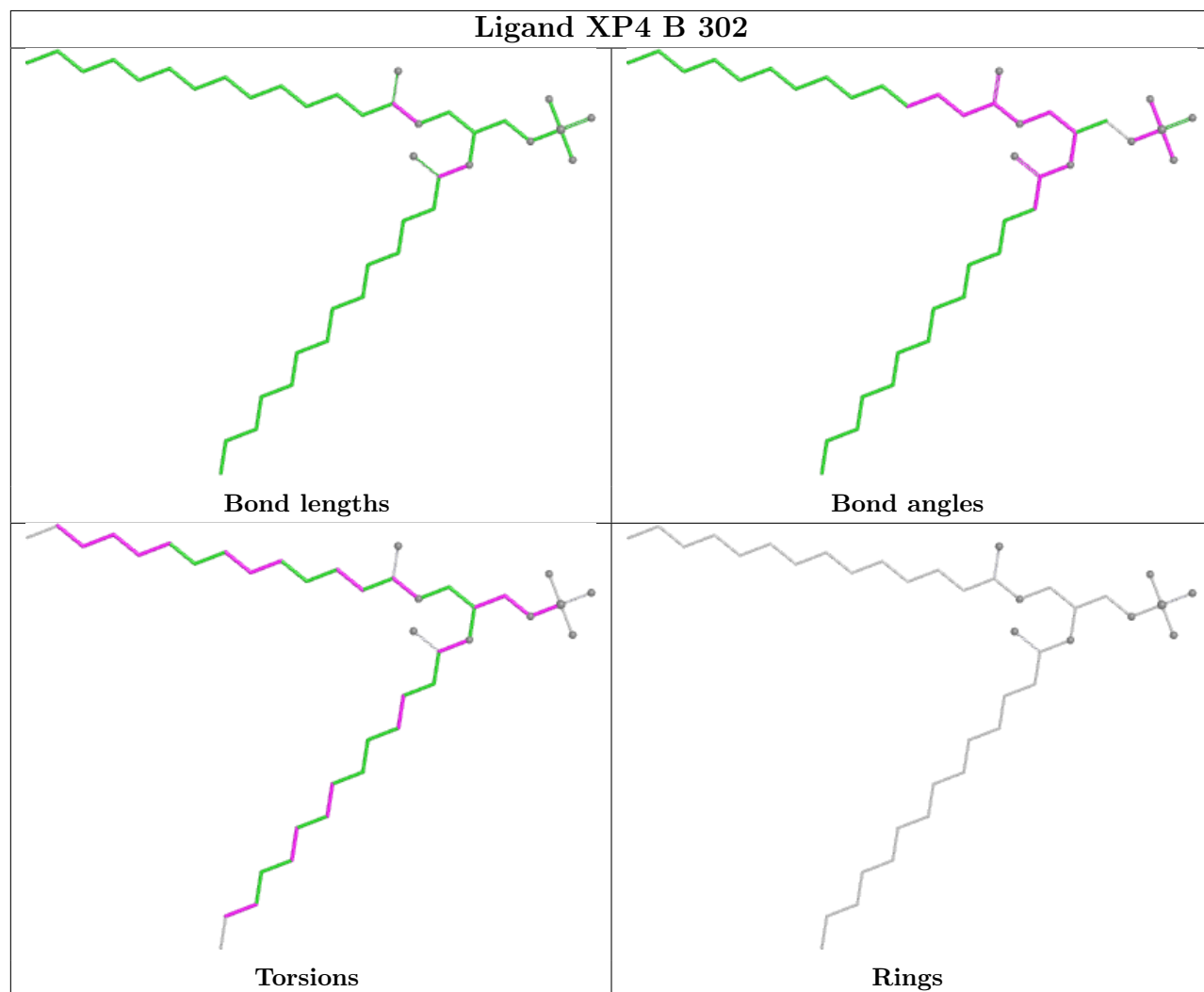
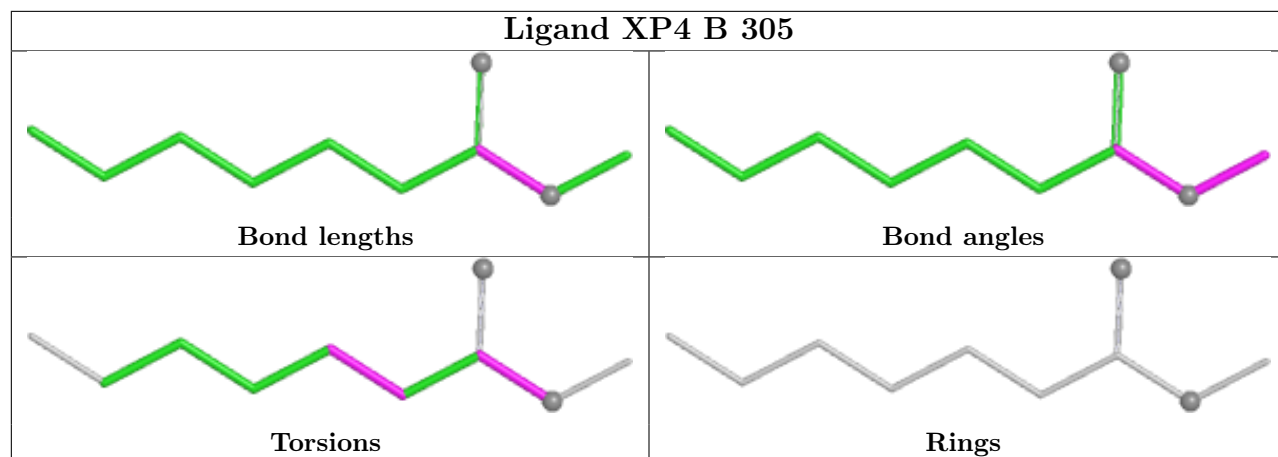
Mol	Chain	Res	Type	Atoms
2	B	302	XP4	C19-C20-C21-C22
2	B	302	XP4	C23-C24-C25-C26
2	A	202	XP4	C5-C6-C7-C8
2	B	301	XP4	C11-C10-C9-C8
2	C	301	XP4	C14-C15-C16-C17
2	B	301	XP4	C23-C24-C25-C26
2	B	303	XP4	C11-C12-C13-C14
2	B	302	XP4	C11-C10-C9-C8
2	C	301	XP4	C21-C22-C23-C24
2	B	301	XP4	C7-C8-C9-C10
2	B	302	XP4	C7-C8-C9-C10
2	B	303	XP4	C2-C3-O5-C4
2	C	301	XP4	C13-C14-C15-C16
2	C	301	XP4	O7-C2-C3-O5
2	C	302	XP4	C5-C6-C7-C8
2	A	201	XP4	O5-C4-C5-C6
2	A	201	XP4	O6-C4-C5-C6
2	B	303	XP4	C12-C13-C14-C15

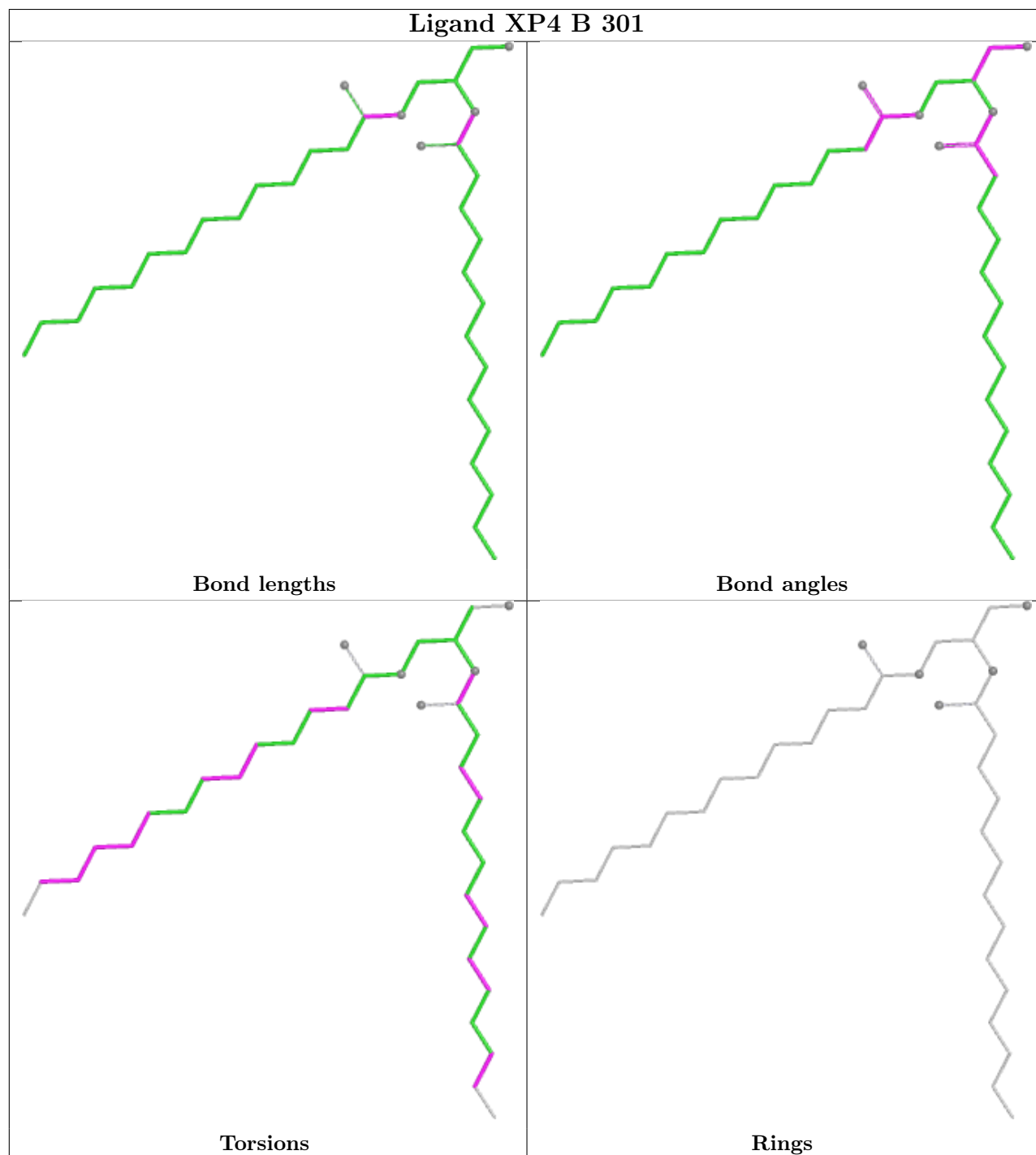
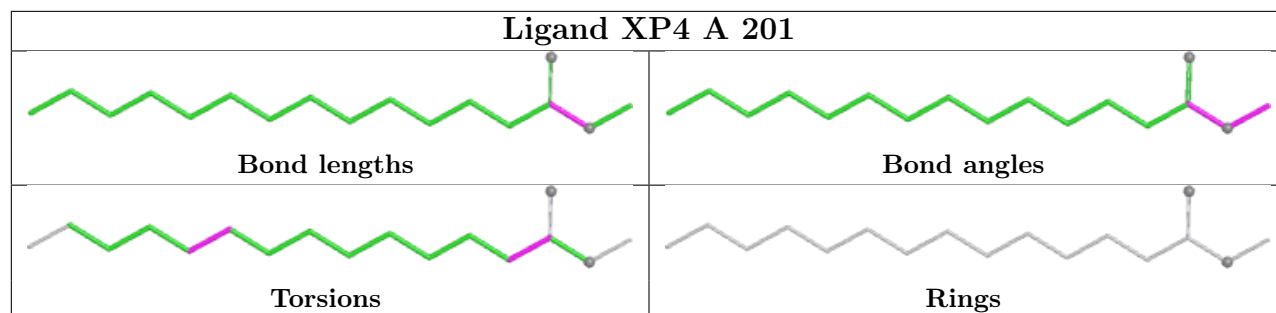
There are no ring outliers.

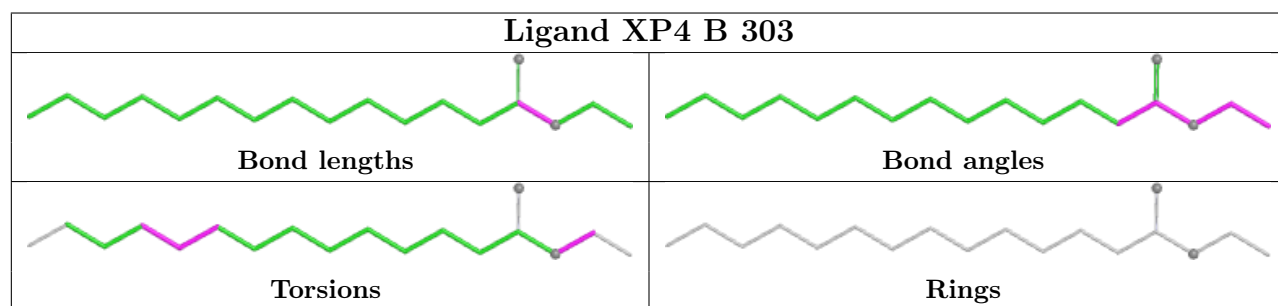
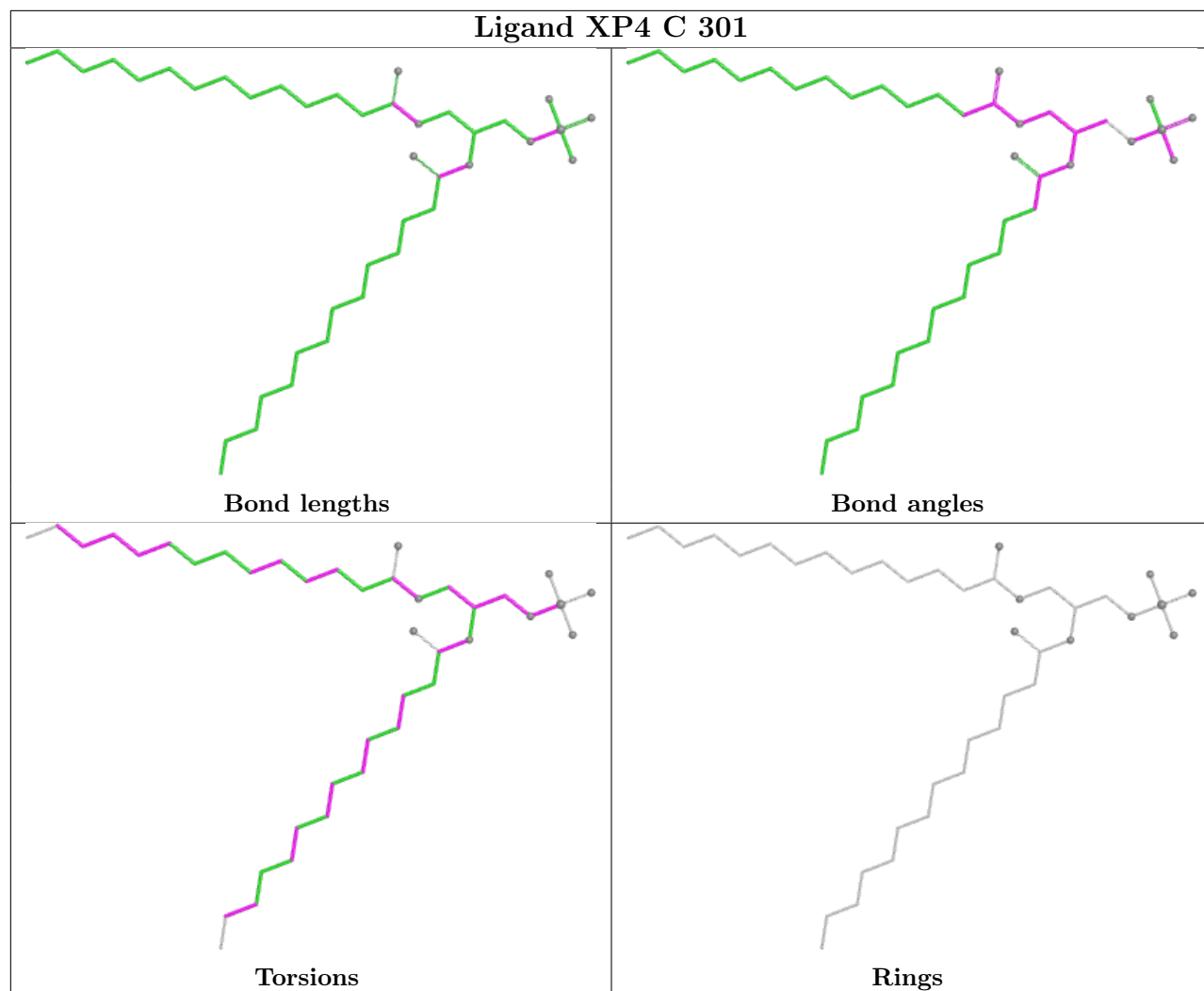
6 monomers are involved in 31 short contacts:

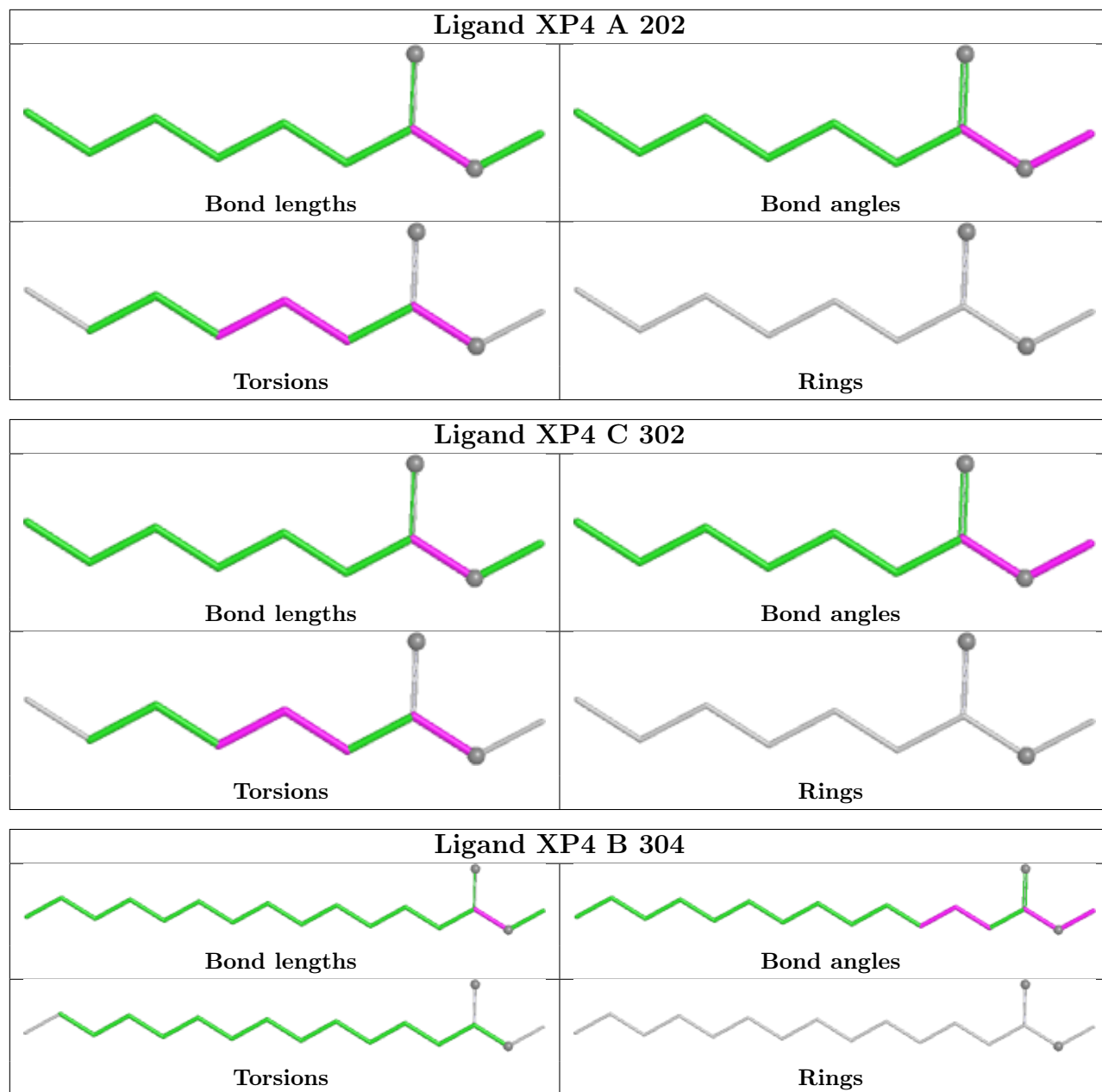
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	302	XP4	22	0
2	A	201	XP4	1	0
2	B	301	XP4	12	0
2	C	301	XP4	2	0
2	B	303	XP4	3	0
2	B	304	XP4	5	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	180/201 (89%)	-0.18	3 (1%) 69 50	81, 155, 259, 304	0
1	B	180/201 (89%)	-0.07	4 (2%) 62 43	75, 178, 277, 312	0
1	C	180/201 (89%)	-0.15	2 (1%) 78 60	73, 170, 257, 286	0
All	All	540/603 (89%)	-0.13	9 (1%) 69 50	73, 163, 261, 312	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	100	ASP	4.8
1	B	25	ASP	4.4
1	A	127	MET	3.0
1	B	195	VAL	2.9
1	A	50	TYR	2.8
1	C	125	SER	2.8
1	B	129	ASP	2.4
1	B	50	TYR	2.3
1	A	121	LEU	2.1

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 ⓘ

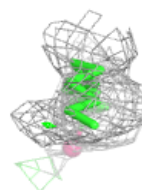
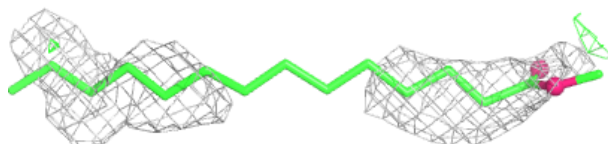
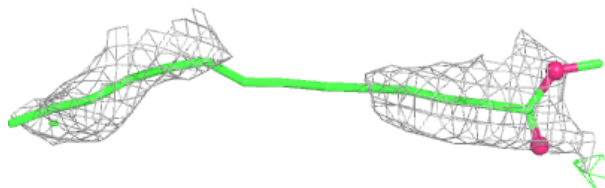
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	XP4	A	201	17/40	0.77	0.15	110,191,275,281	0
2	XP4	B	304	17/40	0.80	0.15	83,148,243,243	0
2	XP4	B	303	18/40	0.85	0.15	112,144,186,252	0
2	XP4	B	301	36/40	0.88	0.15	79,134,186,192	0
2	XP4	A	202	10/40	0.91	0.08	105,174,230,267	0
2	XP4	C	301	40/40	0.92	0.12	63,127,258,273	0
2	XP4	C	302	10/40	0.92	0.12	150,163,217,238	0
2	XP4	B	302	40/40	0.94	0.12	72,136,217,291	0
2	XP4	B	305	10/40	0.95	0.11	96,176,231,244	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.

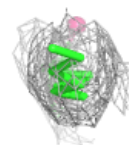
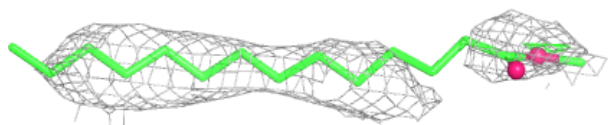
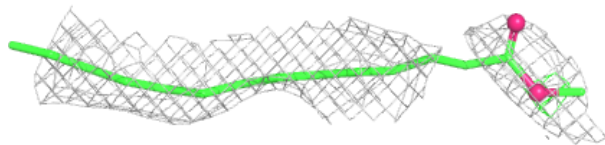
Electron density around XP4 A 201:

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

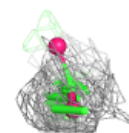
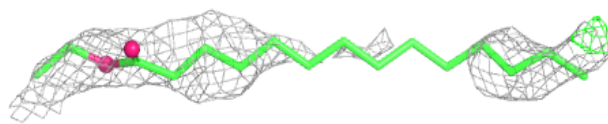
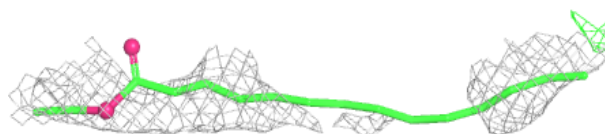


Electron density around XP4 B 304:

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

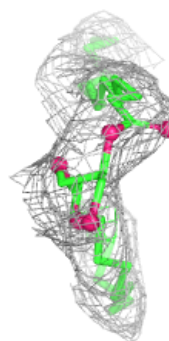
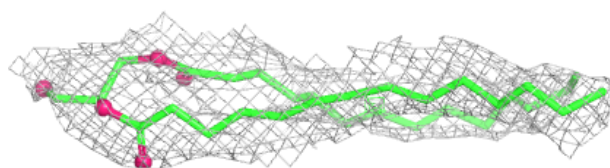
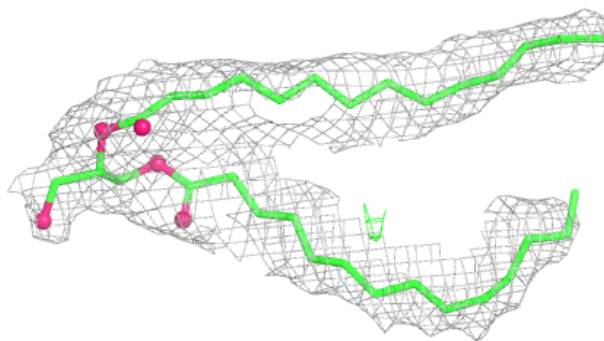
**Electron density around XP4 B 303:**

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

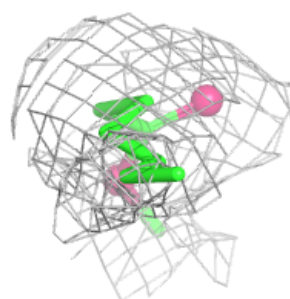
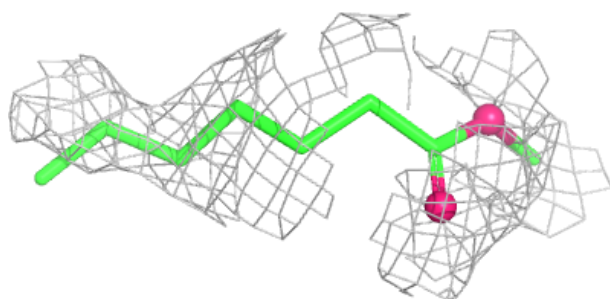
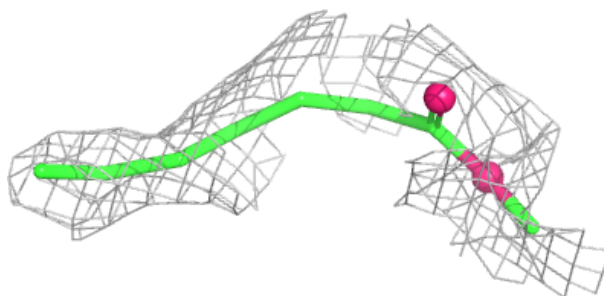


Electron density around XP4 B 301:

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

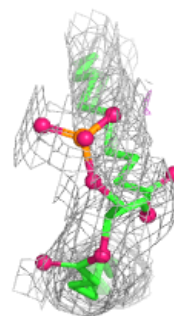
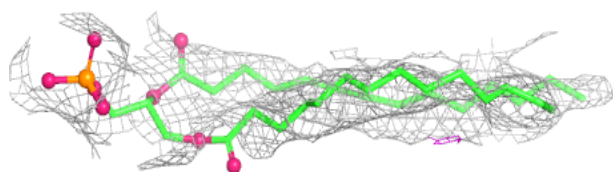
**Electron density around XP4 A 202:**

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

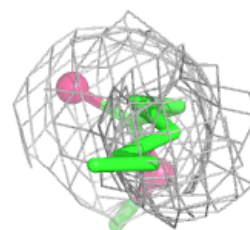
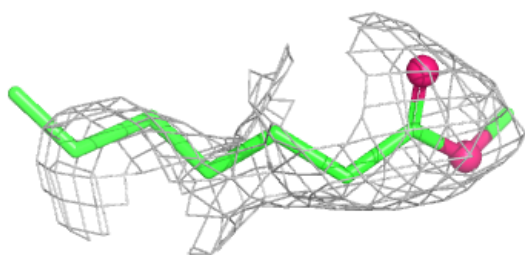
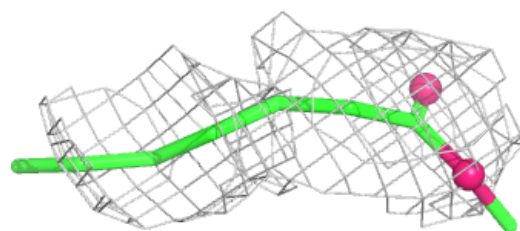


Electron density around XP4 C 301:

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

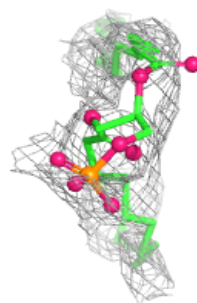
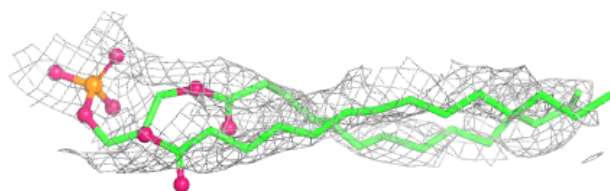
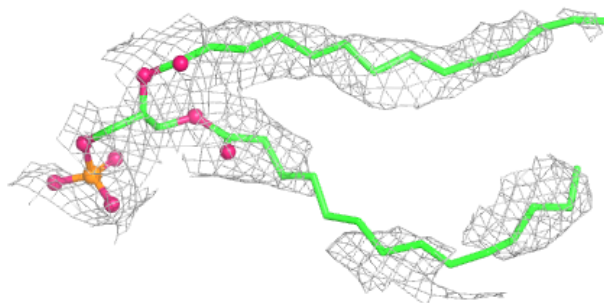
**Electron density around XP4 C 302:**

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

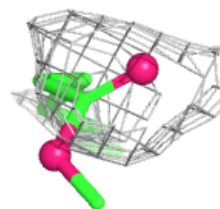
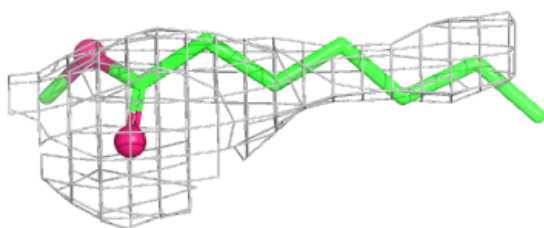
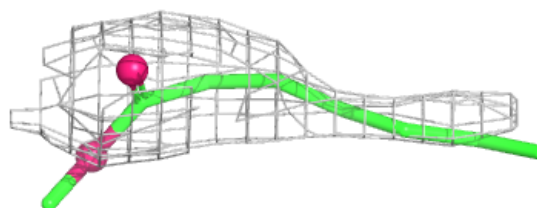


Electron density around XP4 B 302:

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

**Electron density around XP4 B 305:**

$2mF_o-DF_c$ (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.