



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 01:38 AM EST

PDB ID : 3UX4
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

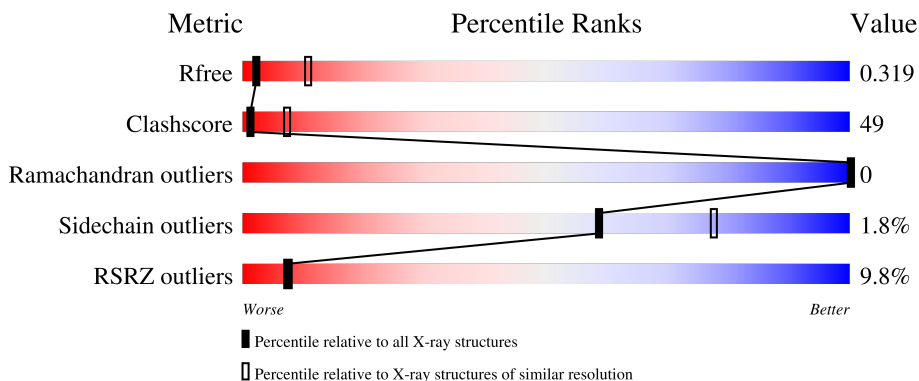
1 Overall quality at a glance

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}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (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	 8% 36% 51% 10%
1	B	201	 10% 38% 49% 10%
1	C	201	 8% 38% 50% 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	A	201	-	-	-	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.

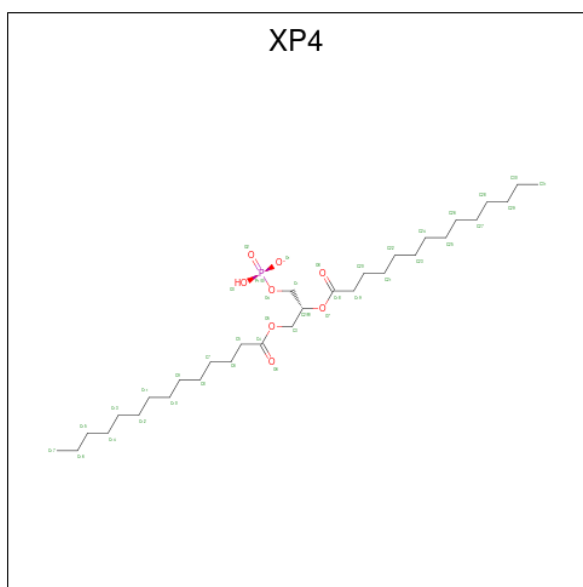
- Molecule 1 is a protein called Acid-activated urea channel.

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

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 (three-letter code: XP4) (formula: C₃₁H₆₀O₈P).

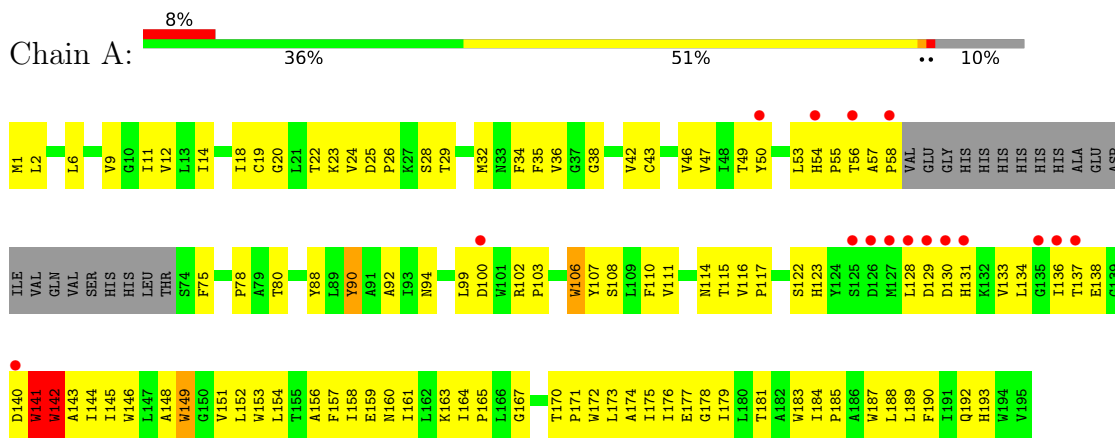


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 17 15 2	0	0
2	A	1	Total C O 10 8 2	0	0
2	B	1	Total C O 36 31 5	0	0
2	B	1	Total C O P 40 31 8 1	0	0
2	B	1	Total C O 18 16 2	0	0
2	B	1	Total C O 17 15 2	0	0
2	B	1	Total C O 10 8 2	0	0
2	C	1	Total C O P 40 31 8 1	0	0
2	C	1	Total C O 10 8 2	0	0

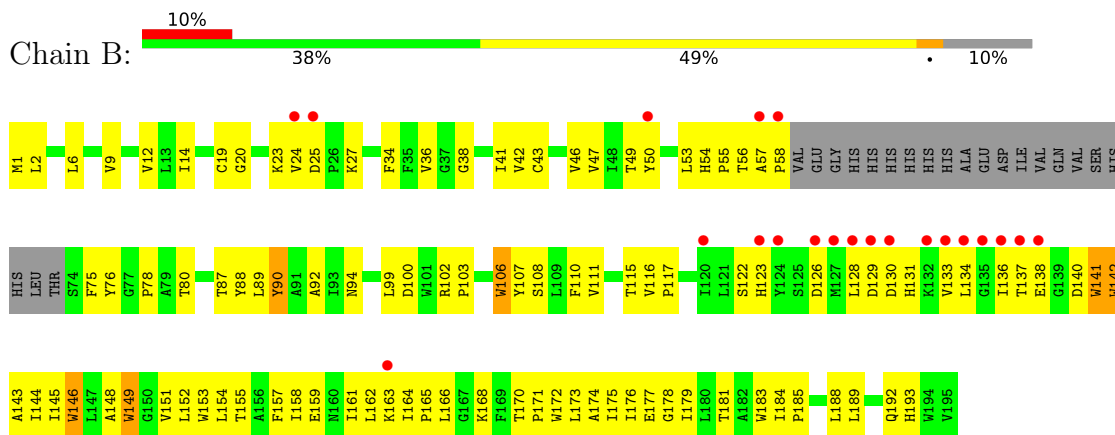
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

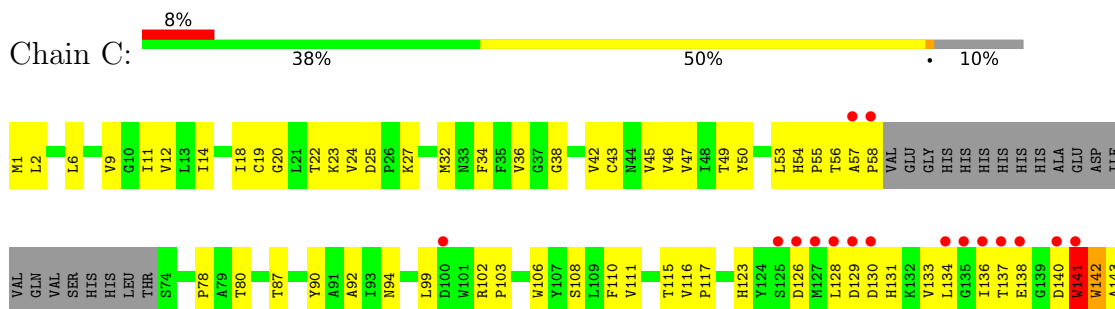
- Molecule 1: Acid-activated urea channel



- Molecule 1: Acid-activated urea channel



- Molecule 1: Acid-activated urea channel



I144	I145	W146	W149	G150	W151	L152	W153	L154	T155	A156	F157	I158	E159	N160	I161	L162	K163	L164	P165	L166	G167	K168	F169	T170	P171	W172	L173	A174	I175	I176	E177	G178	I179	L180	T181	A182	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 42 21 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) 98.0 (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)	Xtrriage
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 (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	133.8	Xtrriage
Anisotropy	0.404	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 152.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.71	4/1480 (0.3%)	0.65	0/2035
1	B	0.72	4/1480 (0.3%)	0.64	0/2035
1	C	0.70	3/1480 (0.2%)	0.63	0/2035
All	All	0.71	11/4440 (0.2%)	0.64	0/6105

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	TRP	CD2-CE2	5.50	1.48	1.41
1	C	141	TRP	CD2-CE2	5.46	1.48	1.41
1	A	141	TRP	CD2-CE2	5.35	1.47	1.41
1	B	141	TRP	CD2-CE2	5.30	1.47	1.41
1	C	146	TRP	CD2-CE2	5.21	1.47	1.41
1	A	106	TRP	CD2-CE2	5.20	1.47	1.41
1	C	149	TRP	CD2-CE2	5.16	1.47	1.41
1	B	146	TRP	CD2-CE2	5.16	1.47	1.41
1	B	106	TRP	CD2-CE2	5.14	1.47	1.41
1	B	149	TRP	CD2-CE2	5.07	1.47	1.41
1	A	142	TRP	CD2-CE2	5.02	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1428	0	1440	173	1
1	B	1428	0	1440	154	0
1	C	1428	0	1440	155	1
2	A	27	0	37	1	0
2	B	121	0	185	27	0
2	C	50	0	70	2	0
All	All	4482	0	4612	447	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 49.

All (447) 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: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:56:THR:C	1:C:58:PRO:HD2	1.58	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:1:MET:HE2	1:C:43:CYS:HB3	1.44	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: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: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:1:MET:HE2	1:A:43:CYS:HB3	1.50	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:C:55:PRO:C	1:C:56:THR:HG23	1.93	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
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:B:163:LYS:O	1:B:164:ILE:HG13	1.77	0.84
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:55:PRO:C	1:A:56:THR:HG23	2.02	0.78
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: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:C:1:MET:HE2	1:C:43:CYS:CB	2.16	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: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:C:158:ILE:HD12	1:C:165:PRO:HG3	1.71	0.73
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:A:56:THR:C	1:A:58:PRO:HD2	2.09	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: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:C:54:HIS:C	1:C:56:THR:H	1.94	0.69
1:A:152:LEU:HG	1:A:173:LEU:HG	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:XP4:H21	2:B:304:XP4:H23	1.75	0.69
1:B:55:PRO:C	1:B:56:THR:HG23	2.13	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: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: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
1:A:110:PHE:CD1	1:C:11:ILE:CD1	2.77	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: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:C:55:PRO:C	1:C:56:THR:CG2	2.65	0.63
1:A:53:LEU:HD21	1:A:54:HIS:CE1	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HE2	1:A:43:CYS:CB	2.25	0.61
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: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:90:TYR:HE2	1:C:32:MET:HE2	1.67	0.60
1:C:54:HIS:C	1:C:56:THR:N	2.54	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:A:32:MET:CE	1:B:90:TYR:HE2	2.15	0.60
1:B:157:PHE:CD1	1:B:161:ILE:CG2	2.80	0.60
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:32:MET:HE2	1:B:90:TYR:HE2	1.66	0.59
1:A:94:ASN:HA	1:A:99:LEU:HD12	1.83	0.59
1:C:56:THR:C	1:C:58:PRO:CD	2.53	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:57:ALA:O	1:C:58:PRO:C	2.41	0.59
1:C:163:LYS:O	1:C:164:ILE:HG12	2.01	0.59
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:137:THR:O	1:B:138:GLU:HB2	2.03	0.58
1:B:12:VAL:HB	1:B:36:VAL:HG21	1.84	0.58
1:A:128:LEU:HB2	1:A:131:HIS:CE1	2.38	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
2:B:302:XP4:H8	2:B:303:XP4:H8	1.86	0.57
1:B:55:PRO:O	1:B:56:THR:HG23	2.04	0.57
1:B:172:TRP:HA	1:B:175:ILE:HD12	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:163:LYS:C	1:B:164:ILE:HG12	2.24	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: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: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
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:B:163:LYS:C	1:B:164:ILE:CG1	2.76	0.55
1:A:149:TRP:HD1	1:A:177:GLU:OE2	1.90	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:CG1	1:B:110:PHE:CD2	2.90	0.54
1:A:90:TYR:HE2	1:C:32:MET:CE	2.20	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:C:163:LYS:C	1:C:164:ILE:HG12	2.29	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:169:PHE:O	1:C:170:THR:C	2.46	0.53
1:A:163:LYS:C	1:A:164:ILE:HG12	2.29	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
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:158:ILE:HG13	1:C:159:GLU:N	2.25	0.52
1:A:24:VAL:CG2	1:A:25:ASP:N	2.72	0.52
1:A:158:ILE:HG13	1:A:159:GLU:N	2.25	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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
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:B:110:PHE:CD1	1:B:110:PHE:C	2.84	0.50
1:C:53:LEU:HG	1:C:54:HIS:CD2	2.46	0.50
1:B:53:LEU:CG	1:B:54:HIS:CE1	2.92	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:C:163:LYS:C	1:C:164:ILE:CG1	2.79	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: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:181:THR:O	1:B:185:PRO:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:55:PRO:C	1:C:57:ALA:H	2.16	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:25:ASP:OD1	1:A:25:ASP:C	2.54	0.46
1:A:103:PRO:CG	1:C:24:VAL:HG11	2.46	0.46
1:A:163:LYS:C	1:A:164:ILE:CG1	2.80	0.46
1:B:75:PHE:O	1:B:78:PRO:HD2	2.16	0.46
1:B:54:HIS:C	1:B:56:THR:H	2.18	0.46
1:B:161:ILE:HG23	1:B:162:LEU:N	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:110:PHE:CD1	1:C:110:PHE:C	2.90	0.45
1:A:110:PHE:CD1	1:A:110:PHE:C	2.90	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:B:55:PRO:C	1:B:56:THR:CG2	2.83	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
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:B:25:ASP:OD1	1:B:25:ASP:C	2.55	0.44
1:C:55:PRO:O	1:C:56:THR:OG1	2.30	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HE2	1:B:43:CYS:HB3	1.99	0.43
1:C:140:ASP:H	1:C:195:VAL:HG11	1.84	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:145:ILE:HG12	1:A:181:THR:HG23	2.00	0.43
1:A:25:ASP:OD1	1:A:28:SER:OG	2.31	0.43
1:B:27:LYS:HZ1	2:B:302:XP4:H3	1.82	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
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: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:A:53:LEU:O	1:A:55:PRO:HD3	2.20	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:24:VAL:CG2	1:B:100:ASP:OD2	2.55	0.41
1:A:32:MET:HE3	1:B:107:TYR:CD1	2.56	0.41
1:A:148:ALA:O	1:A:151:VAL:HB	2.20	0.41
1:A:24:VAL:HG11	1:B:103:PRO:CG	2.50	0.41
1:A:55:PRO:C	1:A:56:THR:CG2	2.74	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:A:47:VAL:CG1	1:A:78:PRO:HG3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:107:TYR:CD1	1:C:32:MET:HE3	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:B:24:VAL:O	1:B:25:ASP:C	2.59	0.40
1:C:184:ILE:N	1:C:185:PRO:CD	2.84	0.40
1:A:24:VAL:O	1:A:25:ASP:C	2.60	0.40
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%)	147 (98%)	3 (2%)	55	76
1	B	150/169 (89%)	148 (99%)	2 (1%)	69	82
1	C	150/169 (89%)	147 (98%)	3 (2%)	55	76
All	All	450/507 (89%)	442 (98%)	8 (2%)	59	77

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	TYR
1	A	141	TRP
1	A	142	TRP
1	B	90	TYR
1	B	142	TRP
1	C	90	TYR
1	C	141	TRP
1	C	142	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	95	HIS
1	A	193	HIS
1	B	95	HIS
1	B	193	HIS
1	C	54	HIS
1	C	95	HIS
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 monosaccharides 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	1.93	1 (11%)	9,9,44	1.15	1 (11%)
2	XP4	A	201	-	16,16,39	1.38	1 (6%)	16,16,44	1.27	1 (6%)
2	XP4	B	302	-	39,39,39	1.38	2 (5%)	43,44,44	1.95	11 (25%)
2	XP4	B	303	-	17,17,39	1.54	1 (5%)	17,17,44	1.53	3 (17%)
2	XP4	A	202	-	9,9,39	1.77	1 (11%)	9,9,44	1.57	1 (11%)
2	XP4	C	301	-	39,39,39	1.43	3 (7%)	43,44,44	2.51	10 (23%)
2	XP4	C	302	-	9,9,39	1.67	1 (11%)	9,9,44	1.21	1 (11%)
2	XP4	B	301	-	35,35,39	1.24	2 (5%)	37,37,44	1.94	6 (16%)
2	XP4	B	304	-	16,16,39	1.35	1 (6%)	16,16,44	1.38	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	A	201	-	-	3/15/15/41	-
2	XP4	B	302	-	-	19/41/41/41	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XP4	B	303	-	-	3/16/16/41	-
2	XP4	A	202	-	-	4/8/8/41	-
2	XP4	C	301	-	-	22/41/41/41	-
2	XP4	C	302	-	-	4/8/8/41	-
2	XP4	B	301	-	-	13/37/37/41	-
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	6.08	1.51	1.34
2	B	303	XP4	O5-C4	5.94	1.50	1.33
2	B	302	XP4	O7-C18	5.69	1.50	1.34
2	B	305	XP4	O5-C4	5.46	1.50	1.33
2	B	302	XP4	O5-C4	5.34	1.48	1.33
2	A	202	XP4	O5-C4	5.08	1.49	1.33
2	B	304	XP4	O5-C4	5.06	1.49	1.33
2	A	201	XP4	O5-C4	5.04	1.49	1.33
2	B	301	XP4	O7-C18	5.02	1.48	1.34
2	C	302	XP4	O5-C4	4.69	1.47	1.33
2	C	301	XP4	O5-C4	4.41	1.46	1.33
2	B	301	XP4	O5-C4	4.29	1.45	1.33
2	C	301	XP4	P1-O4	2.46	1.68	1.60

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	XP4	P1-O4-C1	8.32	141.22	118.30
2	C	301	XP4	O5-C4-C5	7.71	136.09	111.91
2	B	301	XP4	O5-C4-C5	6.70	132.94	111.91
2	B	302	XP4	O5-C4-C5	6.46	132.17	111.91
2	C	301	XP4	C3-C2-C1	-6.24	97.03	111.79
2	B	302	XP4	O7-C18-C19	5.98	124.40	111.50
2	B	301	XP4	O7-C18-C19	5.96	124.34	111.50
2	C	301	XP4	O6-C4-C5	-4.55	105.98	123.73
2	B	303	XP4	C3-O5-C4	4.54	129.93	116.73
2	C	301	XP4	O7-C18-C19	4.51	121.21	111.50
2	A	201	XP4	C3-O5-C4	4.46	130.80	116.11
2	B	304	XP4	C3-O5-C4	3.99	129.24	116.11
2	B	302	XP4	O6-C4-C5	-3.95	108.34	123.73
2	A	202	XP4	C3-O5-C4	3.93	129.06	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	XP4	O5-C4-O6	-3.85	113.89	123.59
2	C	301	XP4	O4-P1-O2	3.40	116.00	106.47
2	C	302	XP4	C3-O5-C4	3.27	126.87	116.11
2	B	301	XP4	O4-C1-C2	3.06	119.91	111.78
2	B	302	XP4	P1-O4-C1	2.96	126.45	118.30
2	B	302	XP4	O3-P1-O4	-2.75	99.43	106.73
2	B	301	XP4	O6-C4-C5	-2.73	113.08	123.73
2	C	301	XP4	O7-C2-C1	2.70	118.19	108.40
2	B	302	XP4	O3-P1-O1	2.70	117.95	107.64
2	B	305	XP4	C3-O5-C4	2.68	124.95	116.11
2	B	301	XP4	O7-C18-O8	-2.58	117.46	123.70
2	C	301	XP4	O1-P1-O4	-2.54	99.98	106.73
2	B	303	XP4	O5-C3-C2	2.52	117.69	108.42
2	B	302	XP4	C2-O7-C18	-2.41	111.86	117.79
2	C	301	XP4	O5-C3-C2	2.32	115.20	108.43
2	C	301	XP4	O5-C4-O6	-2.29	117.81	123.59
2	B	302	XP4	O7-C18-O8	-2.26	118.24	123.70
2	B	302	XP4	C3-O5-C4	2.26	125.49	117.12
2	B	304	XP4	C7-C6-C5	-2.18	105.36	113.19
2	B	303	XP4	O5-C4-C5	2.13	118.58	111.91
2	B	302	XP4	O5-C3-C2	2.06	114.42	108.43
2	B	302	XP4	C7-C6-C5	2.04	120.53	113.19

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
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

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

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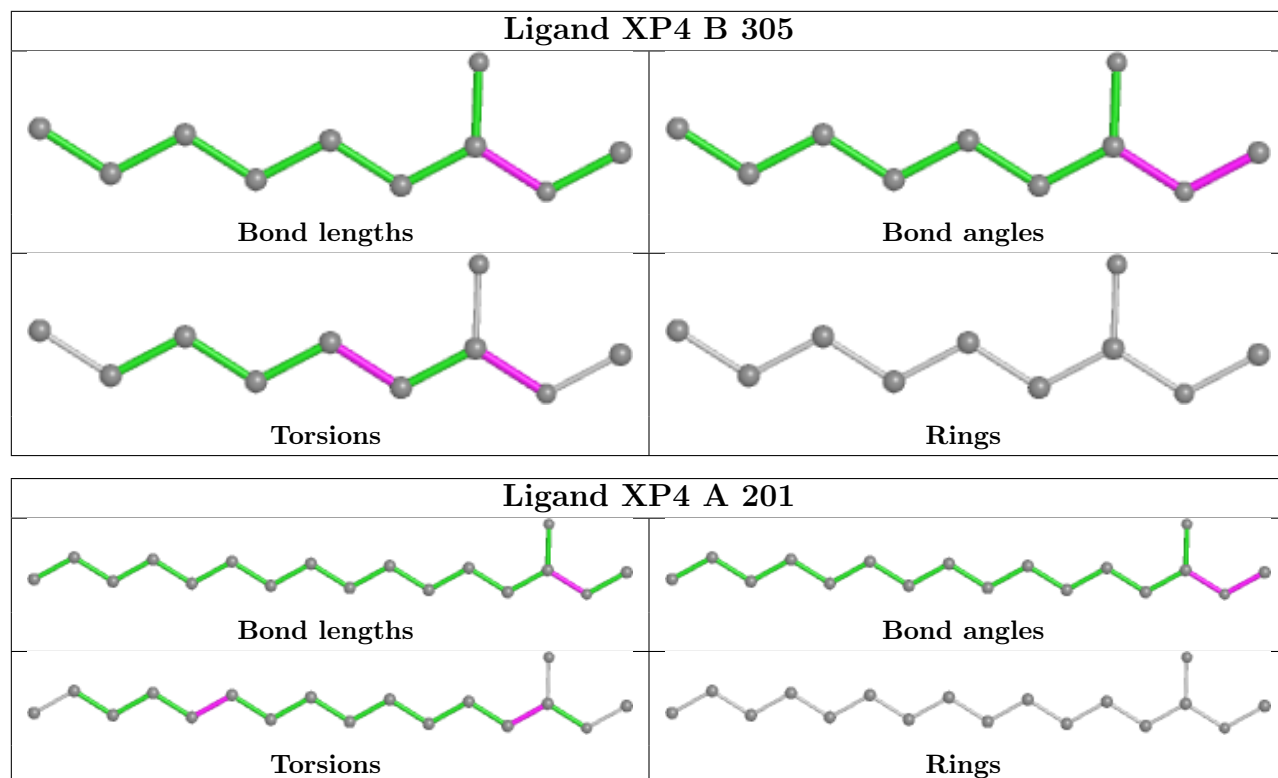
Mol	Chain	Res	Type	Atoms
2	C	301	XP4	C14-C15-C16-C17
2	B	301	XP4	C23-C24-C25-C26
2	B	303	XP4	C11-C12-C13-C14
2	B	302	XP4	C11-C10-C9-C8
2	C	301	XP4	C21-C22-C23-C24
2	B	301	XP4	C7-C8-C9-C10
2	B	302	XP4	C7-C8-C9-C10
2	C	301	XP4	C13-C14-C15-C16
2	B	303	XP4	C2-C3-O5-C4
2	C	301	XP4	O7-C2-C3-O5
2	C	302	XP4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

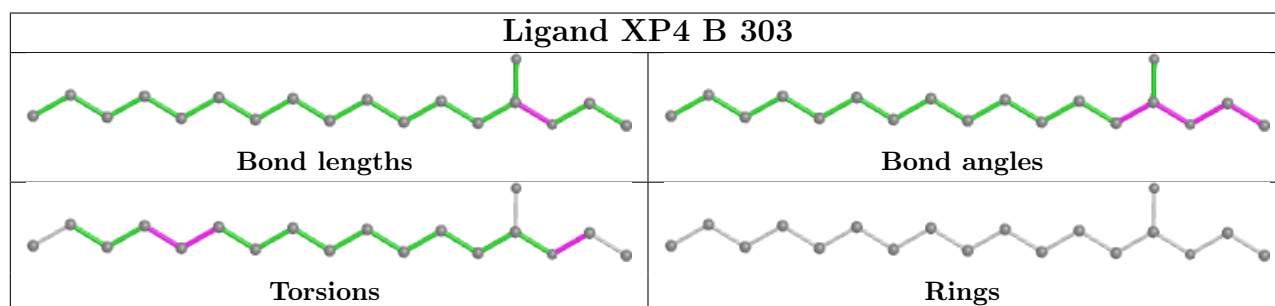
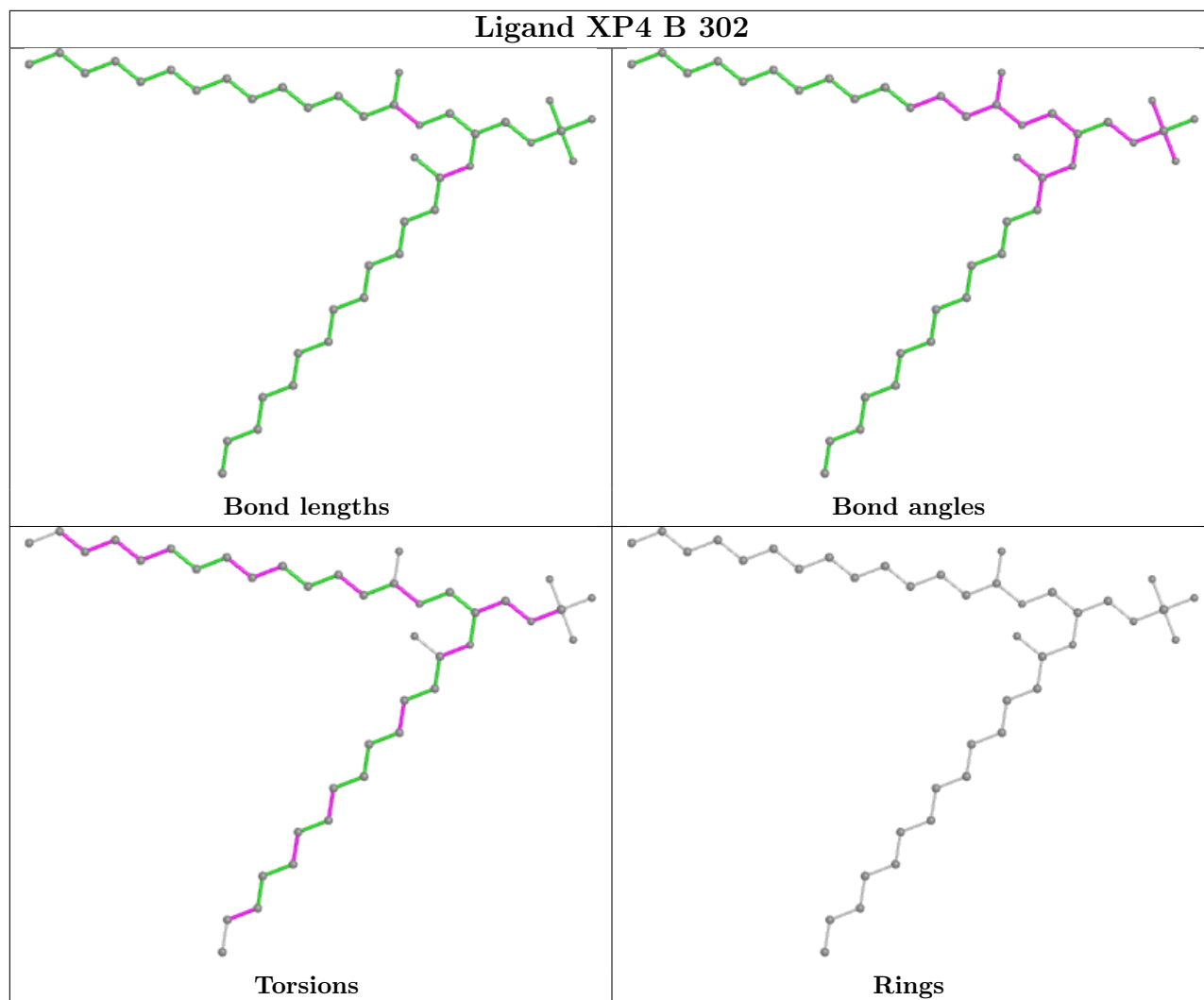
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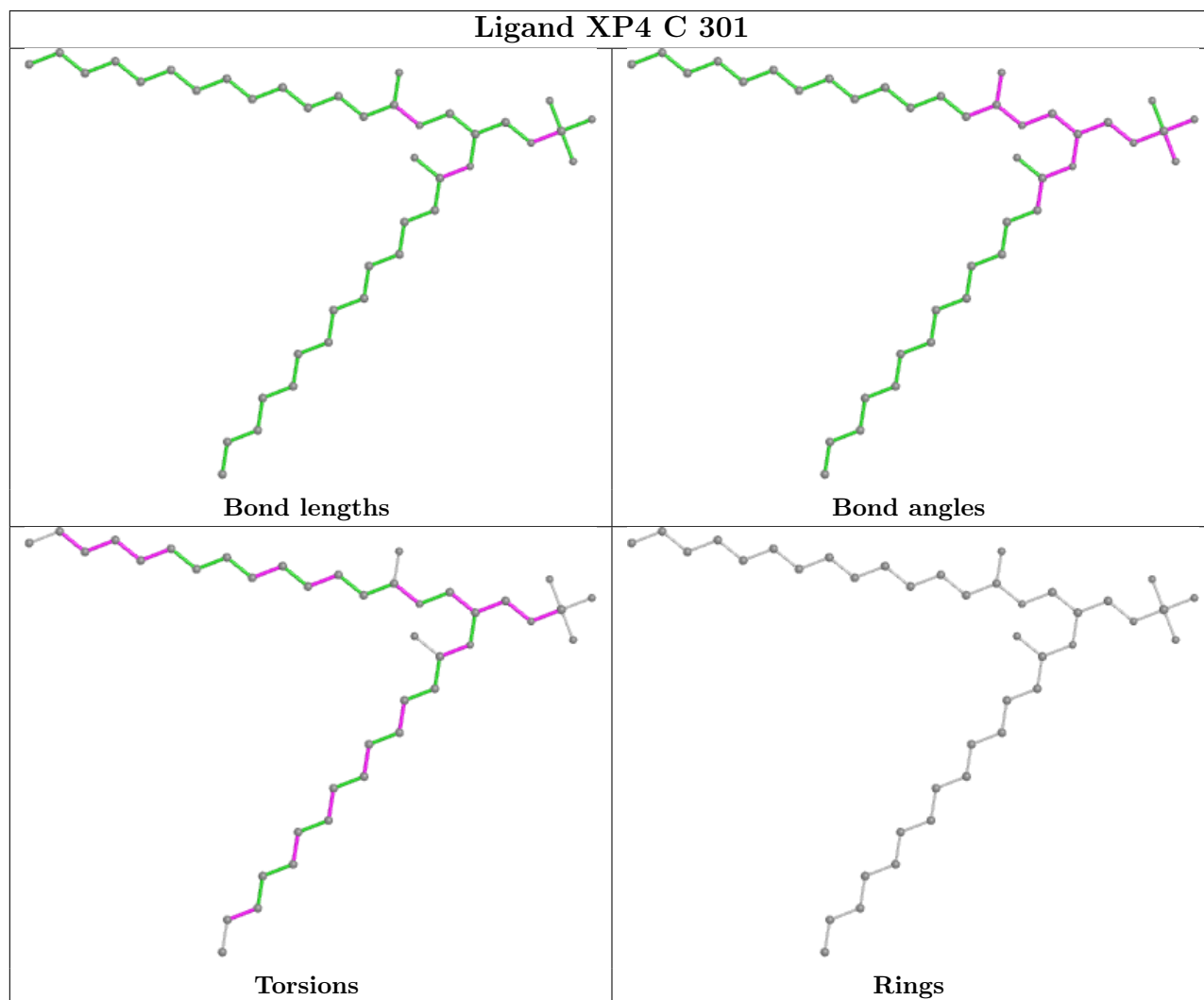
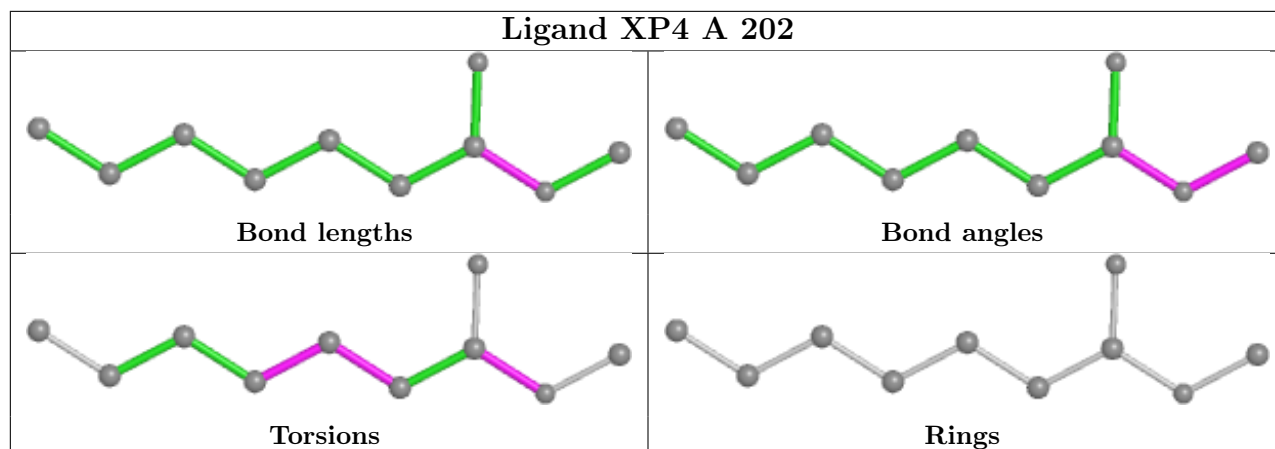
6 monomers are involved in 29 short contacts:

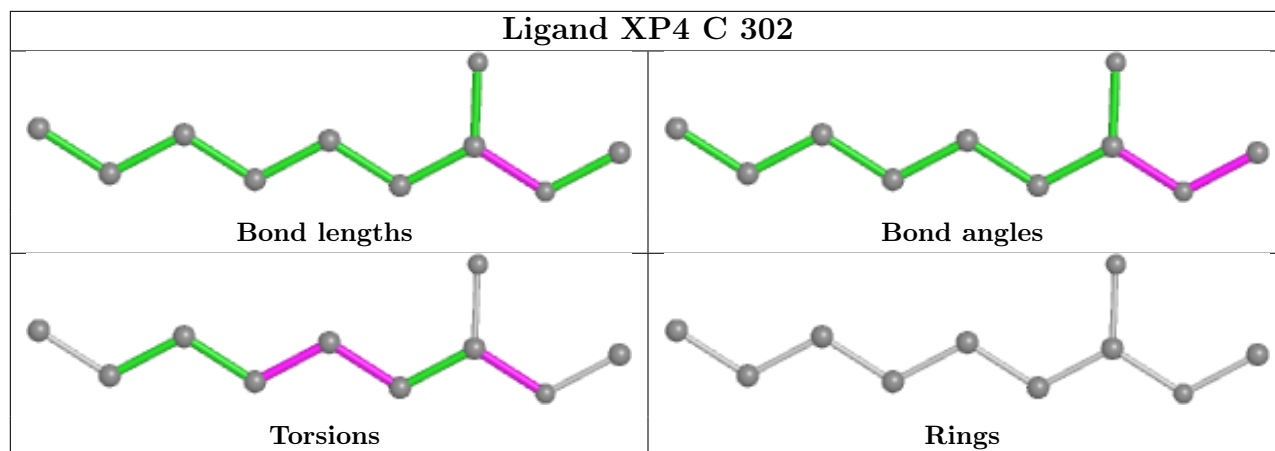
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	XP4	1	0
2	B	302	XP4	20	0
2	B	303	XP4	3	0
2	C	301	XP4	2	0
2	B	301	XP4	12	0
2	B	304	XP4	5	0

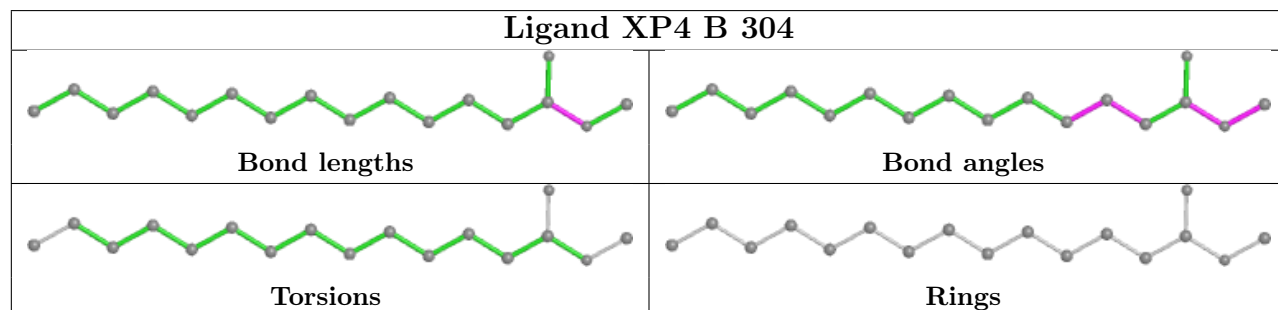
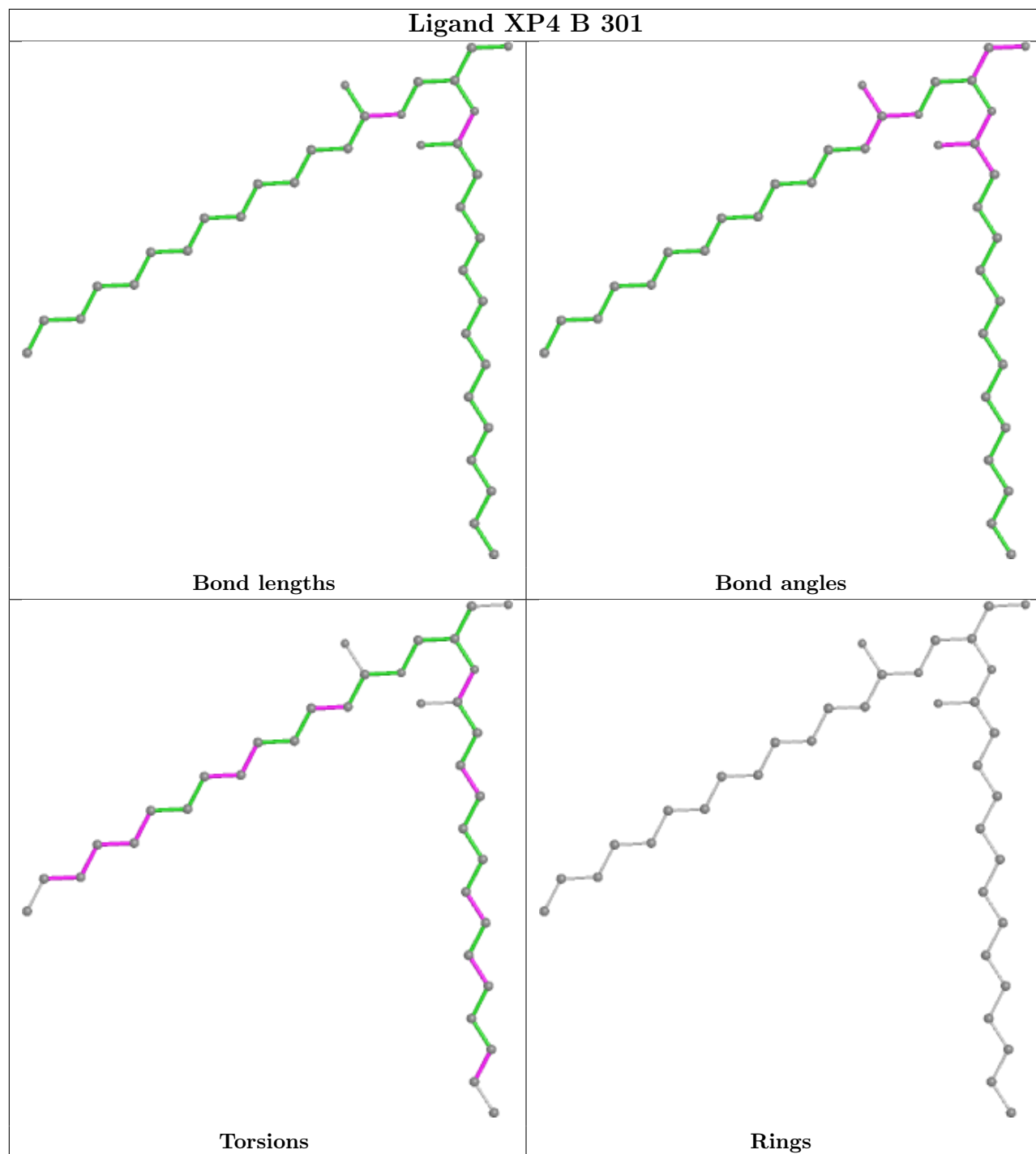
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

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	180/201 (89%)	0.31	16 (8%) 9 10	81, 155, 259, 304	0
1	B	180/201 (89%)	0.43	21 (11%) 4 4	75, 178, 277, 312	0
1	C	180/201 (89%)	0.22	16 (8%) 9 10	73, 170, 257, 286	0
All	All	540/603 (89%)	0.32	53 (9%) 7 7	73, 163, 261, 312	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	ASP	11.4
1	B	129	ASP	8.6
1	A	127	MET	7.0
1	B	137	THR	6.9
1	A	58	PRO	6.9
1	B	135	GLY	6.5
1	B	57	ALA	6.1
1	A	137	THR	6.1
1	B	58	PRO	5.5
1	B	130	ASP	5.0
1	B	134	LEU	4.9
1	A	131	HIS	4.3
1	B	126	ASP	4.3
1	B	127	MET	4.1
1	C	136	ILE	4.1
1	C	135	GLY	4.0
1	A	130	ASP	4.0
1	C	58	PRO	4.0
1	A	129	ASP	4.0
1	A	54	HIS	3.7
1	A	128	LEU	3.7
1	C	127	MET	3.5
1	A	135	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	129	ASP	3.5
1	B	136	ILE	3.5
1	C	126	ASP	3.4
1	B	128	LEU	3.3
1	C	137	THR	3.2
1	C	100	ASP	3.2
1	C	125	SER	3.2
1	C	130	ASP	3.2
1	C	134	LEU	3.1
1	B	25	ASP	2.9
1	B	138	GLU	2.9
1	C	57	ALA	2.9
1	B	124	TYR	2.8
1	B	163	LYS	2.6
1	A	136	ILE	2.6
1	B	132	LYS	2.5
1	A	125	SER	2.5
1	B	123	HIS	2.5
1	A	140	ASP	2.5
1	C	138	GLU	2.5
1	C	128	LEU	2.3
1	A	56	THR	2.3
1	A	50	TYR	2.2
1	B	120	ILE	2.1
1	A	100	ASP	2.1
1	B	133	VAL	2.1
1	B	50	TYR	2.1
1	C	140	ASP	2.0
1	C	141	TRP	2.0
1	B	24	VAL	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 [\(i\)](#)

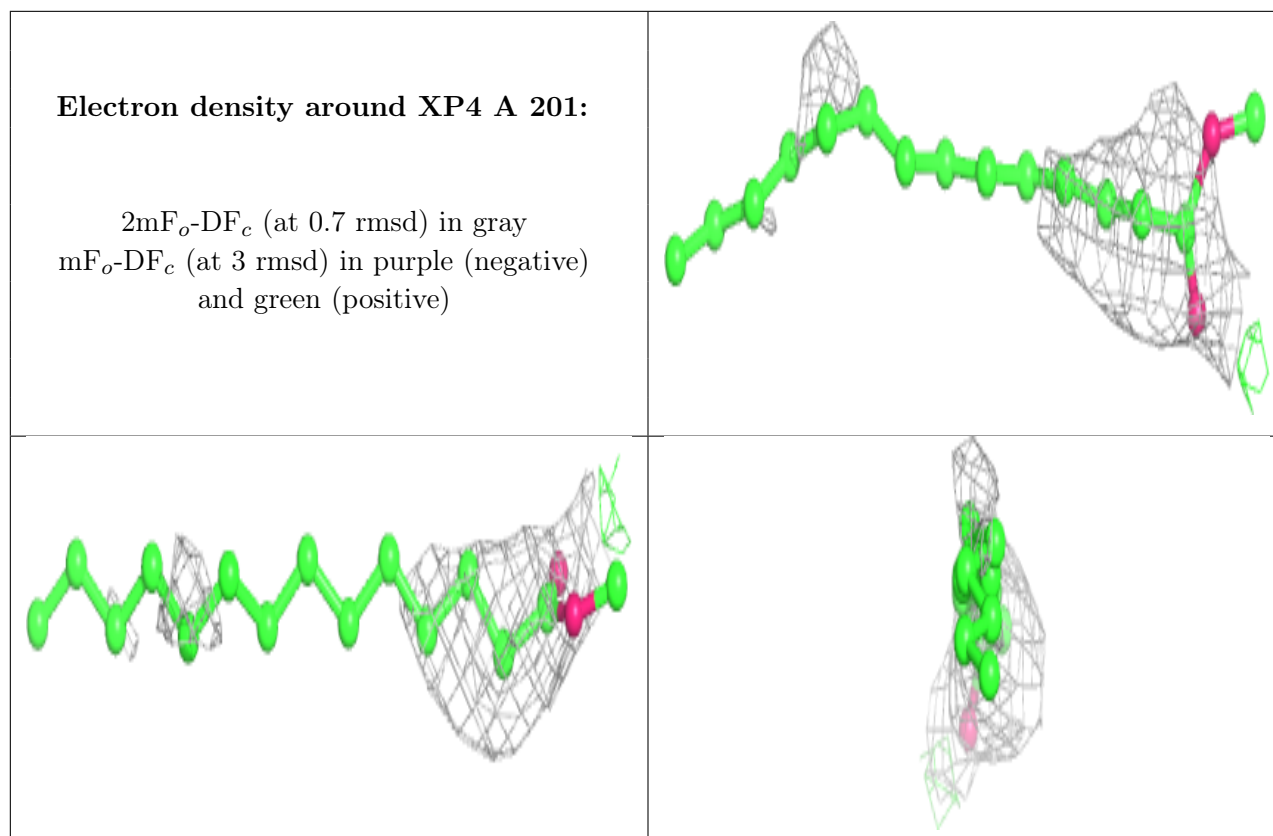
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

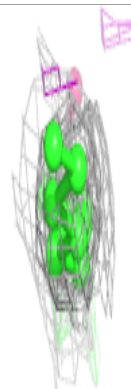
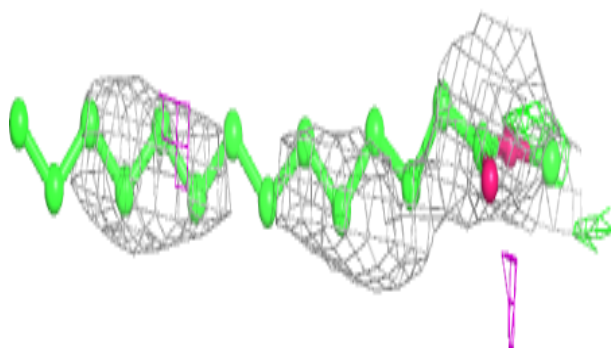
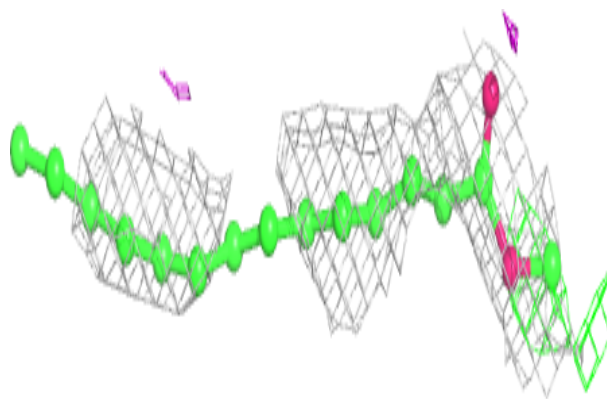
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	XP4	A	201	17/40	0.69	0.45	110,191,275,281	0
2	XP4	B	304	17/40	0.72	0.40	83,148,243,243	0
2	XP4	B	303	18/40	0.74	0.39	112,144,186,252	0
2	XP4	B	301	36/40	0.76	0.39	79,134,186,192	0
2	XP4	B	305	10/40	0.84	0.39	96,176,231,244	0
2	XP4	B	302	40/40	0.85	0.29	72,136,217,291	0
2	XP4	C	301	40/40	0.85	0.33	63,127,258,273	0
2	XP4	C	302	10/40	0.85	0.38	150,163,217,238	0
2	XP4	A	202	10/40	0.89	0.51	105,174,230,267	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.

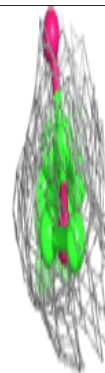
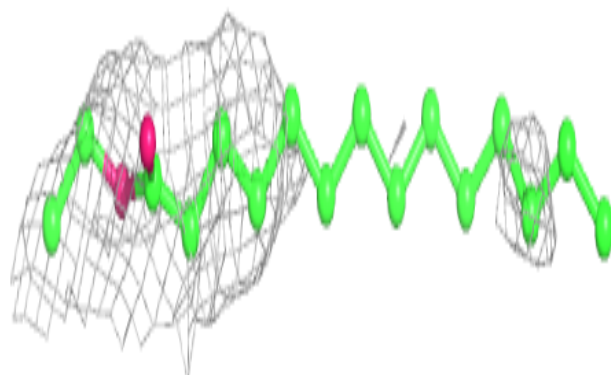
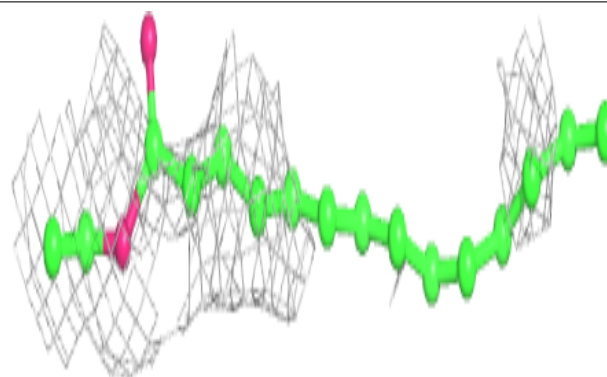


Electron density around XP4 B 304:

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

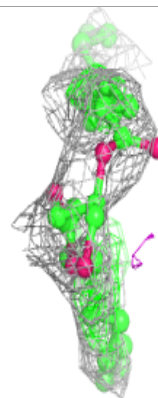
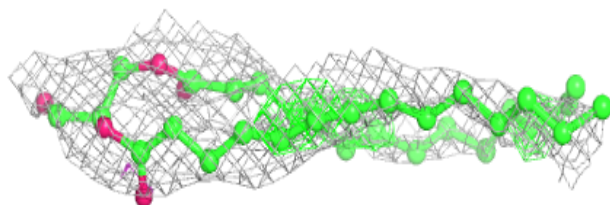
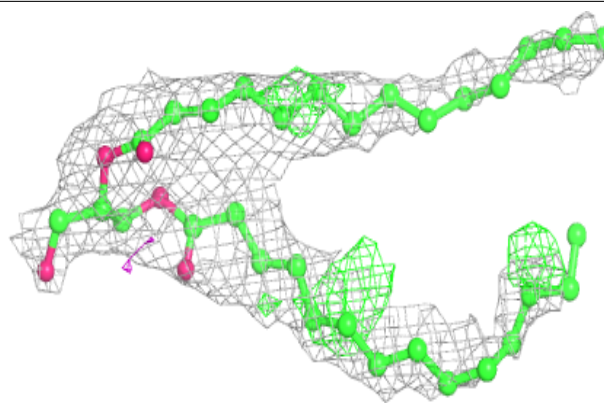
**Electron density around XP4 B 303:**

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

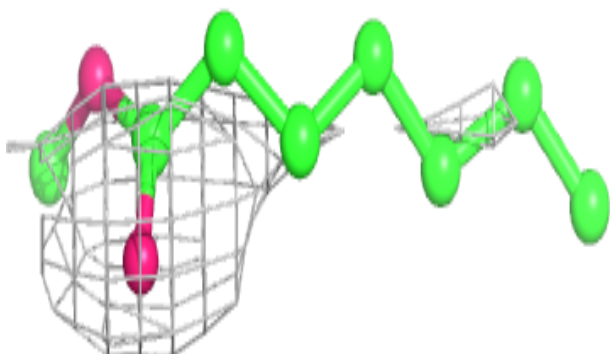
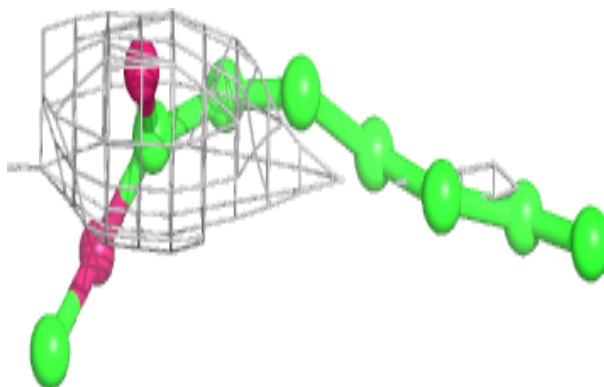


Electron density around XP4 B 301:

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

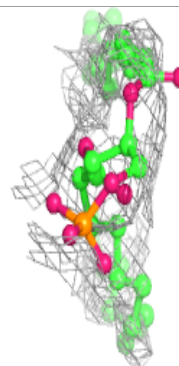
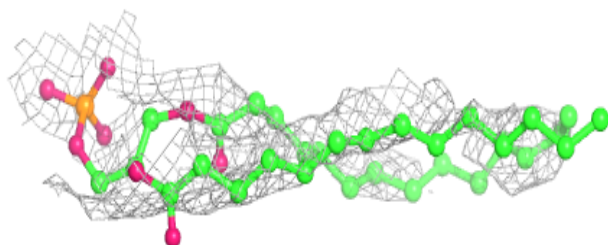
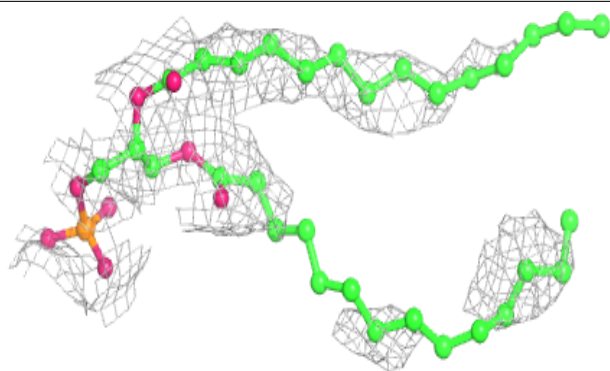
**Electron density around XP4 B 305:**

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

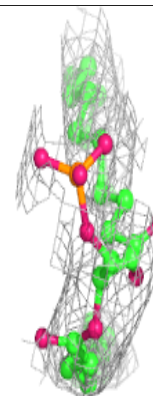
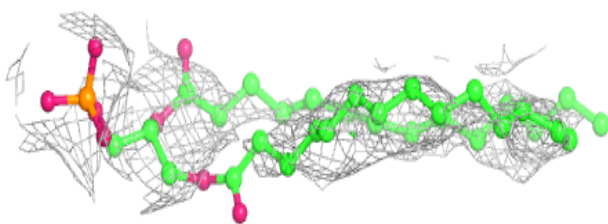
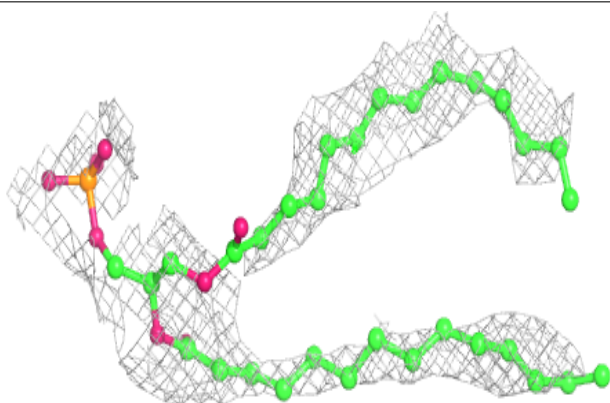


Electron density around XP4 B 302:

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

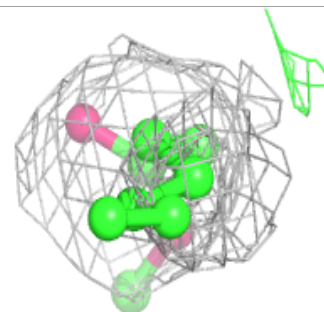
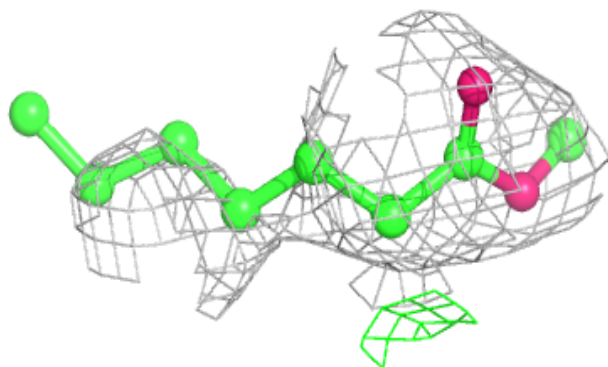
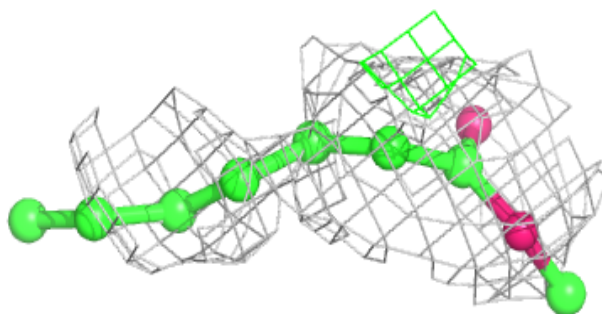
**Electron density around XP4 C 301:**

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

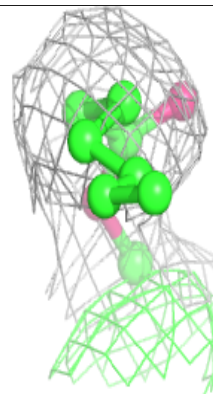
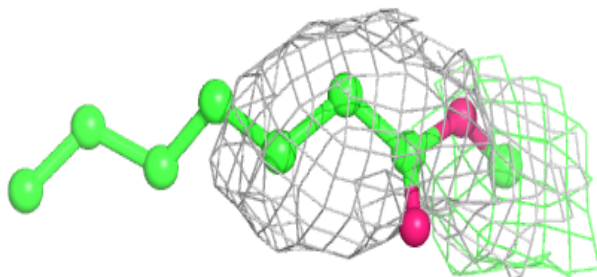
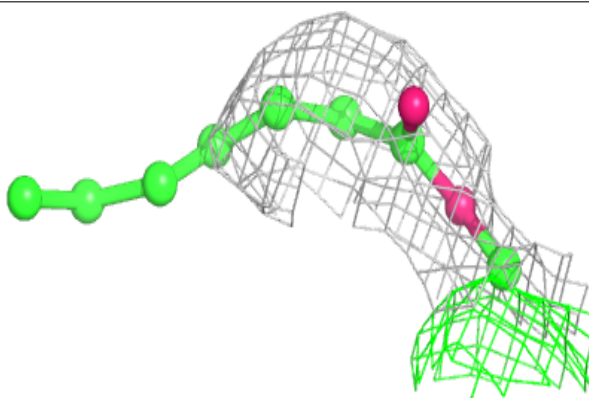


Electron density around XP4 C 302:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.