



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:14 PM UTC

PDB ID : 3LNM / pdb_00003lnm
Title : F233W mutant of the Kv2.1 paddle-Kv1.2 chimera channel
Authors : Tao, X.; Lee, A.; Limapichat, W.; Dougherty, D.A.; MacKinnon, R.
Deposited on : 2010-02-02
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

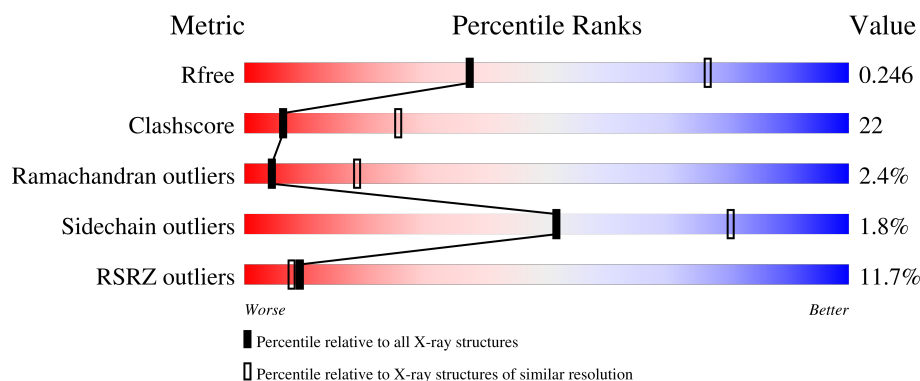
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	333	3% 74% 22% ..
1	C	333	2% 69% 27% ..
2	B	514	11% 43% 30% 24%
2	D	514	17% 29% 30% 38%

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
4	PGW	B	603	-	-	-	X
4	PGW	B	604	-	-	-	X
4	PGW	B	612	-	-	-	X
4	PGW	D	601	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11308 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 Voltage-gated potassium channel subunit beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2556	1627	443	470	16			
1	C	326	Total	C	N	O	S	0	0	0
			2556	1627	443	470	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	initiating methionine	UNP P62483
C	35	MET	-	initiating methionine	UNP P62483

- Molecule 2 is a protein called F233W mutant of the Kv2.1 paddle-Kv1.2 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	389	Total	C	N	O	S	0	0	0
			3116	2038	510	554	14			
2	D	318	Total	C	N	O	S	0	0	0
			2584	1702	419	451	12			

There are 50 discrepancies between the modelled and reference sequences:

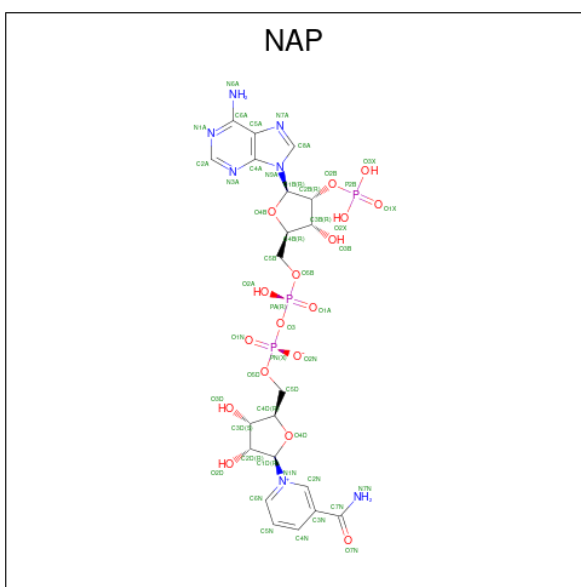
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	expression tag	UNP P63142
B	-17	ALA	-	expression tag	UNP P63142
B	-16	HIS	-	expression tag	UNP P63142
B	-15	HIS	-	expression tag	UNP P63142
B	-14	HIS	-	expression tag	UNP P63142
B	-13	HIS	-	expression tag	UNP P63142
B	-12	HIS	-	expression tag	UNP P63142
B	-11	HIS	-	expression tag	UNP P63142
B	-10	HIS	-	expression tag	UNP P63142
B	-9	HIS	-	expression tag	UNP P63142

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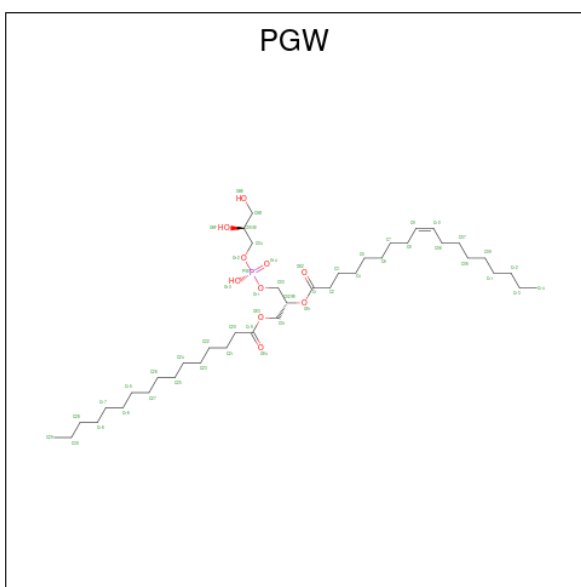
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP P63142
B	-7	HIS	-	expression tag	UNP P63142
B	-6	GLY	-	expression tag	UNP P63142
B	-5	LEU	-	expression tag	UNP P63142
B	-4	VAL	-	expression tag	UNP P63142
B	-3	PRO	-	expression tag	UNP P63142
B	-2	ARG	-	expression tag	UNP P63142
B	-1	GLY	-	expression tag	UNP P63142
B	0	SER	-	expression tag	UNP P63142
B	31	SER	CYS	engineered mutation	UNP P63142
B	32	SER	CYS	engineered mutation	UNP P63142
B	207	GLN	ASN	engineered mutation	UNP P63142
B	233	TRP	PHE	engineered mutation	UNP P63142
B	431	SER	CYS	engineered mutation	UNP P63142
B	478	SER	CYS	engineered mutation	UNP P63142
D	-18	MET	-	expression tag	UNP P63142
D	-17	ALA	-	expression tag	UNP P63142
D	-16	HIS	-	expression tag	UNP P63142
D	-15	HIS	-	expression tag	UNP P63142
D	-14	HIS	-	expression tag	UNP P63142
D	-13	HIS	-	expression tag	UNP P63142
D	-12	HIS	-	expression tag	UNP P63142
D	-11	HIS	-	expression tag	UNP P63142
D	-10	HIS	-	expression tag	UNP P63142
D	-9	HIS	-	expression tag	UNP P63142
D	-8	HIS	-	expression tag	UNP P63142
D	-7	HIS	-	expression tag	UNP P63142
D	-6	GLY	-	expression tag	UNP P63142
D	-5	LEU	-	expression tag	UNP P63142
D	-4	VAL	-	expression tag	UNP P63142
D	-3	PRO	-	expression tag	UNP P63142
D	-2	ARG	-	expression tag	UNP P63142
D	-1	GLY	-	expression tag	UNP P63142
D	0	SER	-	expression tag	UNP P63142
D	31	SER	CYS	engineered mutation	UNP P63142
D	32	SER	CYS	engineered mutation	UNP P63142
D	207	GLN	ASN	engineered mutation	UNP P63142
D	233	TRP	PHE	engineered mutation	UNP P63142
D	431	SER	CYS	engineered mutation	UNP P63142
D	478	SER	CYS	engineered mutation	UNP P63142

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			19	15	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C 5 5	0	0
4	B	1	Total C 5 5	0	0
4	B	1	Total C 5 5	0	0
4	B	1	Total C 8 8	0	0
4	B	1	Total C 7 7	0	0
4	B	1	Total C 7 7	0	0
4	B	1	Total C O P 20 11 8 1	0	0
4	B	1	Total C 6 6	0	0
4	B	1	Total C O P 28 17 10 1	0	0
4	B	1	Total C 9 9	0	0
4	B	1	Total C 6 6	0	0
4	D	1	Total C O 22 17 5	0	0

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	5	Total K 5 5	0	0
5	D	5	Total K 5 5	0	0

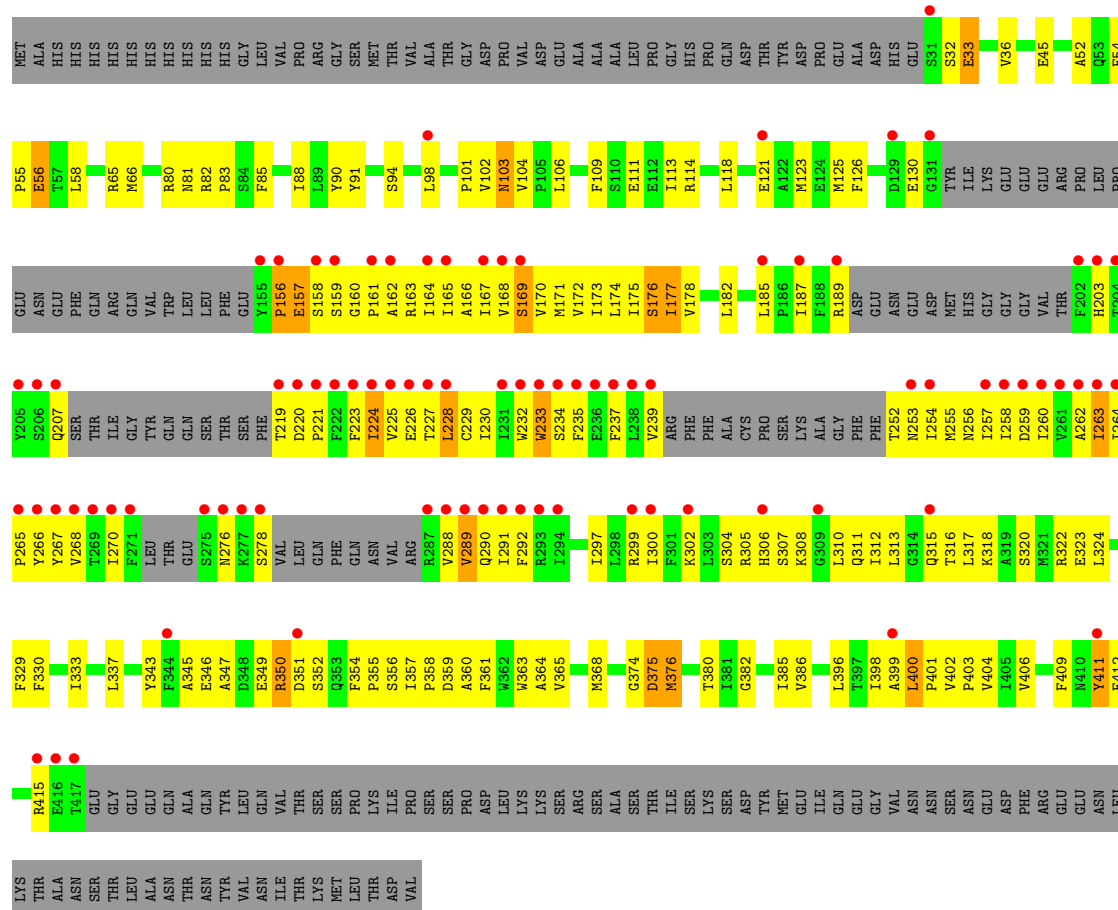
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	92	Total O 92 92	0	0
6	B	46	Total O 46 46	0	0
6	C	91	Total O 91 91	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	14	Total	O	0	0
			14	14		



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	144.27Å 144.27Å 284.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.64 – 2.90 49.64 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.64-2.90) 99.5 (49.64-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.211 , 0.247 0.212 , 0.246	Depositor DCC
R_{free} test set	3245 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 69.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11308	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: PGW, NAP, K

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	0.51	0/2608	0.93	5/3524 (0.1%)
1	C	0.46	0/2608	0.92	7/3524 (0.2%)
2	B	0.40	0/3199	0.92	10/4334 (0.2%)
2	D	0.38	0/2646	0.91	9/3581 (0.3%)
All	All	0.44	0/11061	0.92	31/14963 (0.2%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	PHE	CA-C-N	8.01	128.44	119.32
2	B	54	PHE	C-N-CA	8.01	128.44	119.32
2	B	85	PHE	N-CA-C	7.93	119.93	111.28
2	D	385	ILE	N-CA-C	-7.40	103.47	110.42
1	A	228	GLN	N-CA-C	7.36	118.99	110.97
1	C	315	GLU	N-CA-C	-6.91	105.12	113.97
2	B	252	THR	N-CA-C	-6.55	105.30	113.55
1	C	316	GLY	N-CA-C	-6.38	106.75	114.66
1	C	157	ALA	N-CA-C	-6.36	97.33	108.20
2	D	85	PHE	N-CA-C	6.11	118.74	111.71
1	C	228	GLN	N-CA-C	6.09	119.91	112.23
1	A	224	LYS	N-CA-C	6.07	117.56	111.07
2	D	176	SER	N-CA-C	-5.91	104.96	111.82
2	B	43	ARG	N-CA-C	5.89	118.34	108.73
1	A	157	ALA	N-CA-C	-5.68	97.99	107.99
2	D	350	ARG	N-CA-C	-5.65	106.60	112.93
2	B	234	SER	N-CA-C	-5.64	105.28	111.82
2	B	80	ARG	N-CA-C	5.54	116.67	108.86
2	D	228	LEU	N-CA-C	-5.47	106.31	112.87
1	A	67	GLU	N-CA-C	-5.43	105.26	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	138	ARG	CA-C-N	5.43	125.42	120.21
2	B	138	ARG	C-N-CA	5.43	125.42	120.21
1	C	191	SER	N-CA-C	-5.41	103.25	110.55
1	C	67	GLU	N-CA-C	-5.28	105.60	111.36
2	D	177	ILE	N-CA-C	-5.27	105.71	110.82
2	D	169	SER	N-CA-C	-5.26	107.23	113.97
2	B	144	GLU	N-CA-C	-5.18	106.98	113.15
1	A	229	LEU	N-CA-C	5.18	120.51	113.16
1	C	327	ALA	N-CA-C	5.13	117.61	111.71
2	D	54	PHE	CA-C-N	5.10	126.22	119.84
2	D	54	PHE	C-N-CA	5.10	126.22	119.84

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	2556	0	2582	60	0
1	C	2556	0	2582	67	0
2	B	3116	0	3052	149	0
2	D	2584	0	2598	204	0
3	A	48	0	25	2	0
3	C	48	0	25	3	0
4	B	125	0	141	8	0
4	D	22	0	25	7	0
5	B	5	0	0	0	0
5	D	5	0	0	0	0
6	A	92	0	0	2	0
6	B	46	0	0	2	0
6	C	91	0	0	3	0
6	D	14	0	0	2	0
All	All	11308	0	11030	485	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (485) 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)
2:B:213:GLN:HE22	2:B:219:THR:HB	1.29	0.95
2:B:400:LEU:HB2	2:B:401:PRO:HD3	1.49	0.93
2:D:400:LEU:HB2	2:D:401:PRO:HD3	1.48	0.93
2:D:103:ASN:HD22	2:D:103:ASN:H	1.11	0.92
1:C:295:ILE:HD12	1:C:295:ILE:H	1.37	0.89
2:D:264:ILE:HB	2:D:265:PRO:HD3	1.54	0.89
1:C:333:ASN:HD21	3:C:1001:NAP:H61A	1.22	0.86
2:B:103:ASN:H	2:B:103:ASN:HD22	1.21	0.85
2:B:236:GLU:HB3	2:B:240:ARG:HH12	1.39	0.84
2:D:260:ILE:HG22	2:D:264:ILE:HD11	1.60	0.84
2:D:182:LEU:HA	2:D:185:LEU:HD13	1.59	0.83
2:B:236:GLU:HB3	2:B:240:ARG:NH1	1.94	0.82
2:B:213:GLN:HB3	2:B:220:ASP:HB2	1.60	0.82
2:D:103:ASN:H	2:D:103:ASN:ND2	1.78	0.80
2:B:152:LEU:HB2	2:B:165:ILE:HD12	1.64	0.77
1:C:75:LEU:HD23	1:C:331:MET:HE3	1.66	0.77
2:D:267:TYR:HA	2:D:270:ILE:HD12	1.64	0.77
1:C:338:GLN:O	1:C:341:PRO:HD2	1.85	0.76
1:C:217:TYR:HB2	1:C:225:VAL:HG21	1.68	0.76
2:D:225:VAL:HG13	2:D:228:LEU:HD23	1.68	0.76
2:D:355:PRO:HB2	2:D:359:ASP:OD2	1.86	0.75
2:B:82:ARG:HB2	2:B:83:PRO:HD3	1.67	0.74
2:B:98:LEU:HD21	2:B:113:ILE:HD13	1.70	0.74
2:D:259:ASP:HB2	2:D:302:LYS:NZ	2.02	0.74
2:D:265:PRO:HA	2:D:292:PHE:HD2	1.53	0.73
2:B:186:PRO:HG3	2:B:189:ARG:NH2	2.03	0.72
2:D:257:ILE:HD13	2:D:260:ILE:HD12	1.71	0.72
2:B:350:ARG:HB3	2:B:350:ARG:NH1	2.05	0.72
2:B:323:GLU:CD	2:B:323:GLU:H	1.98	0.72
2:D:260:ILE:O	2:D:264:ILE:HG13	1.90	0.72
2:B:244:CYS:HB3	2:B:247:LYS:HD3	1.71	0.72
2:D:264:ILE:O	2:D:268:VAL:HG23	1.90	0.71
2:B:73:ARG:HD3	6:B:2061:HOH:O	1.89	0.71
2:B:244:CYS:H	2:B:247:LYS:HZ3	1.36	0.70
2:B:168:VAL:O	2:B:172:VAL:HG23	1.90	0.70
2:D:363:TRP:HB2	2:D:376:MET:HE2	1.73	0.70
2:D:98:LEU:HD21	2:D:113:ILE:HD13	1.72	0.70
2:B:213:GLN:NE2	2:B:219:THR:HB	2.06	0.69
1:C:326:ASN:ND2	1:C:329:GLN:HG3	2.07	0.69
1:C:73:MET:HE3	1:C:84:PHE:CD2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ASN:HD21	3:A:1001:NAP:H61A	1.39	0.69
2:B:152:LEU:HB3	2:B:162:ALA:HB2	1.73	0.69
2:D:166:ALA:HB1	2:D:306:HIS:CD2	2.28	0.69
2:D:288:VAL:HG12	2:D:289:VAL:H	1.55	0.69
2:D:288:VAL:O	2:D:289:VAL:HG22	1.93	0.69
2:B:260:ILE:HG22	2:B:264:ILE:HD11	1.75	0.68
2:B:361:PHE:HB2	4:B:601:PGW:H2	1.75	0.68
1:A:118:LYS:HG3	1:A:156:PHE:HB2	1.74	0.68
1:C:295:ILE:HD12	1:C:295:ILE:N	2.08	0.68
2:B:282:PHE:C	2:B:284:ASN:H	2.02	0.67
2:D:82:ARG:HB2	2:D:83:PRO:HD3	1.77	0.67
2:D:237:PHE:HE1	2:D:260:ILE:HG12	1.60	0.66
2:D:411:TYR:CZ	2:D:415:ARG:HD3	2.30	0.66
2:D:227:THR:HA	2:D:230:ILE:HB	1.76	0.66
2:D:230:ILE:HG21	2:D:266:TYR:CE2	2.30	0.66
2:B:315:GLN:HE21	4:B:610:PGW:H01	1.61	0.66
2:D:254:ILE:HG23	2:D:255:MET:H	1.60	0.65
2:B:109:PHE:CE2	2:B:113:ILE:HD11	2.31	0.65
2:D:322:ARG:HH11	2:D:322:ARG:HG3	1.62	0.65
2:D:173:ILE:HD13	2:D:302:LYS:HB3	1.80	0.64
2:D:227:THR:HA	2:D:230:ILE:CG1	2.28	0.64
2:D:109:PHE:CE2	2:D:113:ILE:HD11	2.33	0.64
2:D:343:TYR:CE1	2:D:356:SER:HA	2.33	0.64
2:D:288:VAL:HG12	2:D:289:VAL:N	2.14	0.63
2:B:164:ILE:O	2:B:168:VAL:HG23	1.99	0.63
2:B:120:GLU:O	2:B:124:GLU:HG3	1.98	0.63
2:B:350:ARG:HB3	2:B:350:ARG:HH11	1.64	0.63
2:B:396:LEU:O	2:B:400:LEU:HG	1.99	0.63
2:D:349:GLU:HB2	2:D:352:SER:HB2	1.79	0.63
1:A:326:ASN:ND2	1:A:329:GLN:H	1.97	0.62
2:D:106:LEU:HD11	2:D:130:GLU:HG2	1.80	0.62
2:B:280:LEU:HD12	2:B:280:LEU:H	1.64	0.62
2:D:221:PRO:C	2:D:223:PHE:H	2.06	0.62
2:D:288:VAL:C	2:D:290:GLN:H	2.06	0.62
2:D:81:ASN:HA	6:D:2057:HOH:O	1.99	0.62
1:A:326:ASN:HD22	1:A:328:GLU:N	1.97	0.62
1:C:295:ILE:H	1:C:295:ILE:CD1	2.10	0.61
2:B:240:ARG:HH11	2:B:240:ARG:HG3	1.65	0.61
2:D:56:GLU:CD	2:D:56:GLU:H	2.08	0.61
2:D:121:GLU:O	2:D:125:MET:HG2	2.01	0.61
2:B:210:ILE:HD11	2:B:273:THR:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:TYR:CE2	2:D:94:SER:HB3	2.36	0.60
1:C:167:GLU:HG3	1:C:205:PHE:CE1	2.37	0.60
1:A:40:ARG:HD2	1:A:318:SER:O	2.01	0.60
2:D:357:ILE:HB	2:D:358:PRO:HD3	1.83	0.60
2:B:331:LEU:O	2:B:335:VAL:HG23	2.01	0.60
2:D:32:SER:O	2:D:33:GLU:C	2.44	0.60
2:D:402:VAL:HB	2:D:403:PRO:HD3	1.84	0.60
2:B:213:GLN:HB3	2:B:220:ASP:CB	2.32	0.59
1:C:141:LYS:HD2	6:C:2091:HOH:O	2.00	0.59
1:A:73:MET:HE3	1:A:84:PHE:CD2	2.37	0.59
2:B:276:ASN:HB3	2:B:281:GLN:HB3	1.85	0.59
2:D:173:ILE:C	2:D:175:ILE:H	2.08	0.59
1:A:326:ASN:HD21	1:A:328:GLU:HB2	1.67	0.59
2:D:235:PHE:O	2:D:239:VAL:HG23	2.03	0.59
2:D:58:LEU:C	2:D:58:LEU:HD23	2.26	0.59
2:B:262:ALA:CB	2:B:302:LYS:HD2	2.32	0.59
2:D:364:ALA:O	2:D:368:MET:HG3	2.02	0.59
1:C:292:LEU:HA	1:C:295:ILE:HD13	1.85	0.59
2:D:185:LEU:O	2:D:189:ARG:HG2	2.03	0.59
2:D:52:ALA:O	2:D:55:PRO:HD3	2.03	0.58
2:D:375:ASP:O	2:D:376:MET:HB2	2.01	0.58
2:D:162:ALA:HA	2:D:165:ILE:CD1	2.32	0.58
2:D:172:VAL:HG12	2:D:172:VAL:O	2.02	0.58
2:D:227:THR:HA	2:D:230:ILE:CB	2.33	0.58
1:C:236:ILE:HG13	1:C:238:VAL:HG23	1.85	0.58
2:D:254:ILE:HG23	2:D:255:MET:N	2.18	0.58
2:B:361:PHE:CB	4:B:601:PGW:H2	2.33	0.58
4:B:608:PGW:O11	4:B:608:PGW:O02	2.22	0.58
2:D:227:THR:C	2:D:229:CYS:H	2.11	0.58
2:D:255:MET:HG3	2:D:305:ARG:NH2	2.18	0.57
1:A:326:ASN:HD21	1:A:329:GLN:H	1.52	0.57
2:B:264:ILE:O	2:B:268:VAL:HG23	2.03	0.57
1:A:258:GLY:O	1:A:260:PRO:HD3	2.05	0.57
2:D:259:ASP:HB2	2:D:302:LYS:HZ3	1.66	0.57
2:D:396:LEU:O	2:D:400:LEU:HG	2.05	0.57
2:B:244:CYS:H	2:B:247:LYS:NZ	2.03	0.57
2:D:113:ILE:HG23	2:D:118:LEU:HD12	1.87	0.57
2:D:227:THR:C	2:D:229:CYS:N	2.62	0.57
2:D:253:ASN:HB3	2:D:256:ASN:ND2	2.19	0.57
4:B:601:PGW:H01	4:B:601:PGW:O02	2.03	0.57
2:D:160:GLY:O	2:D:164:ILE:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:267:TYR:HA	2:D:270:ILE:CD1	2.34	0.57
2:D:365:VAL:HG21	4:D:601:PGW:H6A	1.87	0.57
2:D:109:PHE:O	2:D:113:ILE:HG13	2.05	0.56
2:B:382:GLY:O	2:B:386:VAL:HG23	2.06	0.56
4:D:601:PGW:H01	4:D:601:PGW:O02	2.04	0.56
2:B:294:ILE:O	2:B:297:ILE:HG22	2.06	0.56
2:D:171:MET:C	2:D:173:ILE:H	2.13	0.56
2:B:414:HIS:C	2:B:416:GLU:H	2.14	0.56
1:A:159:ARG:HA	1:A:188:SER:O	2.06	0.56
2:D:374:GLY:C	2:D:376:MET:H	2.13	0.56
1:C:73:MET:HE3	1:C:84:PHE:CE2	2.41	0.56
1:C:326:ASN:HD21	1:C:329:GLN:HG3	1.70	0.56
1:C:104:LYS:HZ2	1:C:148:GLN:HE22	1.54	0.55
2:B:53:GLN:C	2:B:55:PRO:HD3	2.31	0.55
2:B:281:GLN:O	2:B:284:ASN:HB3	2.07	0.55
2:D:350:ARG:HD2	2:D:350:ARG:O	2.07	0.55
2:D:165:ILE:O	2:D:168:VAL:HG12	2.07	0.54
2:B:309:GLY:HA2	2:B:312:ILE:HD12	1.87	0.54
2:D:402:VAL:O	2:D:406:VAL:HG23	2.06	0.54
2:B:103:ASN:H	2:B:103:ASN:ND2	1.97	0.54
2:D:103:ASN:HD22	2:D:103:ASN:N	1.93	0.54
2:D:156:PRO:O	2:D:158:SER:N	2.35	0.54
1:C:340:LEU:HB3	1:C:341:PRO:HD3	1.88	0.54
2:D:227:THR:OG1	2:D:230:ILE:HD12	2.07	0.54
2:B:282:PHE:C	2:B:284:ASN:N	2.66	0.54
1:A:302:THR:OG1	1:A:305:GLN:HG3	2.08	0.54
2:D:171:MET:SD	2:D:171:MET:N	2.80	0.54
1:A:338:GLN:N	1:A:338:GLN:CD	2.65	0.54
2:D:266:TYR:O	2:D:270:ILE:HG13	2.08	0.54
1:A:326:ASN:ND2	1:A:328:GLU:HB2	2.23	0.53
1:A:147:LEU:HB3	1:A:149:LEU:HD12	1.89	0.53
1:C:247:ALA:O	1:C:248:CYS:HB2	2.08	0.53
1:C:347:ILE:O	1:C:351:ILE:HG13	2.09	0.53
2:B:255:MET:HB3	2:B:305:ARG:NH2	2.23	0.53
2:D:237:PHE:CE1	2:D:260:ILE:HG12	2.43	0.53
2:D:350:ARG:HG3	2:D:350:ARG:HH11	1.73	0.53
2:D:114:ARG:HG3	2:D:114:ARG:HH11	1.74	0.53
2:D:203:HIS:O	2:D:207:GLN:HB3	2.08	0.53
2:B:103:ASN:HD22	2:B:103:ASN:N	2.00	0.53
2:D:346:GLU:OE2	2:D:380:THR:HG23	2.09	0.53
2:B:241:PHE:O	2:B:247:LYS:NZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:PHE:CD1	2:B:376:MET:HE2	2.43	0.53
1:C:187:THR:O	1:C:213:GLU:HA	2.09	0.53
2:D:308:LYS:O	2:D:312:ILE:HG13	2.09	0.53
1:A:251:VAL:O	1:A:251:VAL:HG12	2.08	0.52
2:B:163:ARG:O	2:B:167:ILE:HG12	2.09	0.52
2:D:178:VAL:O	2:D:182:LEU:HG	2.08	0.52
2:D:189:ARG:HG3	2:D:189:ARG:HH11	1.74	0.52
1:A:326:ASN:HD22	1:A:328:GLU:H	1.57	0.52
1:C:152:VAL:O	1:C:182:ALA:HA	2.08	0.52
1:C:214:GLN:HA	1:C:241:MET:O	2.09	0.52
1:C:350:GLU:O	1:C:354:ILE:HG13	2.10	0.52
2:D:337:LEU:HD23	2:D:337:LEU:C	2.34	0.52
1:A:71:HIS:CD2	1:A:327:ALA:HB2	2.45	0.52
1:C:218:HIS:CE1	1:C:220:PHE:HB2	2.45	0.52
2:D:313:LEU:O	2:D:317:LEU:HG	2.09	0.52
2:B:277:LYS:HE3	6:B:2123:HOH:O	2.10	0.52
2:B:262:ALA:HB1	2:B:302:LYS:HD2	1.90	0.52
2:D:349:GLU:HB3	2:D:352:SER:H	1.75	0.52
1:A:303:LEU:HB3	1:A:304:PRO:HD3	1.92	0.52
2:B:311:GLN:O	2:B:315:GLN:HG3	2.10	0.52
2:D:259:ASP:HA	2:D:262:ALA:HB3	1.92	0.52
2:D:361:PHE:HD2	4:D:601:PGW:H20A	1.75	0.52
2:D:363:TRP:CB	2:D:376:MET:HE2	2.39	0.52
2:B:415:ARG:HH11	2:B:415:ARG:HG2	1.76	0.51
1:C:120:PHE:O	1:C:129:ARG:HA	2.10	0.51
2:B:244:CYS:N	2:B:247:LYS:HZ3	2.07	0.51
1:C:120:PHE:CE2	1:C:159:ARG:HD3	2.46	0.51
1:C:104:LYS:NZ	1:C:148:GLN:HE22	2.07	0.51
2:D:156:PRO:C	2:D:158:SER:H	2.17	0.51
2:D:351:ASP:O	2:D:352:SER:C	2.53	0.51
1:C:68:MET:HA	1:C:68:MET:HE2	1.92	0.51
1:A:120:PHE:O	1:A:129:ARG:HA	2.10	0.51
1:C:114:VAL:HA	1:C:153:ASP:OD2	2.10	0.51
2:B:324:LEU:HD13	2:B:405:ILE:HD13	1.93	0.51
2:D:316:THR:HG21	2:D:409:PHE:HB2	1.92	0.51
2:D:354:PHE:CD1	2:D:376:MET:HE3	2.46	0.51
2:B:414:HIS:O	2:B:416:GLU:N	2.37	0.51
2:B:280:LEU:HD12	2:B:280:LEU:N	2.26	0.50
2:D:88:ILE:O	2:D:91:TYR:HB3	2.11	0.50
2:D:343:TYR:C	2:D:345:ALA:H	2.20	0.50
2:B:246:SER:C	2:B:248:ALA:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:TRP:O	1:C:313:ARG:HG2	2.11	0.50
1:A:326:ASN:ND2	1:A:328:GLU:N	2.59	0.50
2:D:258:ILE:CG2	2:D:302:LYS:HA	2.41	0.50
2:D:400:LEU:O	2:D:403:PRO:HD2	2.11	0.50
2:D:221:PRO:HA	2:D:224:ILE:HB	1.93	0.50
2:D:329:PHE:O	2:D:333:ILE:HG12	2.12	0.50
2:D:162:ALA:HA	2:D:165:ILE:HD12	1.93	0.50
2:D:259:ASP:O	2:D:263:ILE:HG12	2.12	0.50
2:D:400:LEU:HB2	2:D:401:PRO:CD	2.32	0.50
2:B:360:ALA:O	2:B:361:PHE:C	2.55	0.50
2:D:169:SER:O	2:D:173:ILE:HG13	2.12	0.50
2:B:357:ILE:HB	2:B:358:PRO:HD3	1.94	0.50
2:D:177:ILE:HD11	2:D:300:ILE:HG13	1.94	0.50
2:D:304:SER:HA	2:D:310:LEU:HD23	1.92	0.50
2:B:102:VAL:HG23	2:B:103:ASN:N	2.27	0.50
1:A:326:ASN:HD22	1:A:326:ASN:C	2.20	0.49
2:B:29:HIS:HB2	2:B:52:ALA:HB3	1.93	0.49
2:B:362:TRP:O	2:B:366:VAL:HG23	2.12	0.49
2:B:318:LYS:HD2	4:B:610:PGW:H22	1.94	0.49
2:D:260:ILE:HG22	2:D:264:ILE:CD1	2.37	0.49
1:A:313:ARG:HH11	1:A:313:ARG:HG2	1.76	0.49
2:B:243:ALA:N	2:B:247:LYS:HZ1	2.10	0.49
2:D:253:ASN:O	2:D:257:ILE:HG12	2.12	0.49
2:B:169:SER:O	2:B:173:ILE:HG13	2.12	0.49
1:C:302:THR:OG1	1:C:304:PRO:HD2	2.13	0.49
2:D:123:MET:O	2:D:126:PHE:HB3	2.11	0.49
2:B:343:TYR:CE1	2:B:356:SER:HA	2.48	0.49
2:B:261:VAL:HA	2:B:264:ILE:HD12	1.95	0.49
1:C:333:ASN:ND2	3:C:1001:NAP:H61A	2.02	0.49
2:D:308:LYS:HA	2:D:311:GLN:CG	2.43	0.49
1:A:52:LEU:HD13	1:A:322:LEU:HD11	1.93	0.49
2:D:361:PHE:CD2	4:D:601:PGW:H20A	2.48	0.49
2:B:240:ARG:NH1	2:B:240:ARG:HG3	2.27	0.49
2:D:288:VAL:C	2:D:290:GLN:N	2.70	0.49
2:B:141:PRO:O	2:B:143:ASN:N	2.46	0.49
2:B:53:GLN:O	2:B:55:PRO:HD3	2.13	0.49
2:B:296:ARG:HE	2:B:299:ARG:NH2	2.11	0.49
1:C:268:LYS:NZ	1:C:268:LYS:HB3	2.28	0.49
1:A:118:LYS:CG	1:A:156:PHE:HB2	2.43	0.48
2:B:221:PRO:O	2:B:225:VAL:HG23	2.12	0.48
1:C:331:MET:HE1	1:C:334:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:THR:HG22	1:A:60:PHE:CD1	2.48	0.48
2:B:146:GLN:C	2:B:148:GLN:H	2.21	0.48
1:C:120:PHE:CD1	1:C:159:ARG:HG3	2.48	0.48
2:B:70:ASP:C	2:B:70:ASP:OD1	2.55	0.48
2:B:141:PRO:O	2:B:142:GLU:C	2.57	0.48
2:B:227:THR:O	2:B:231:ILE:HG12	2.12	0.48
2:B:243:ALA:H	2:B:247:LYS:NZ	2.11	0.48
1:C:295:ILE:HD11	1:C:354:ILE:HD11	1.94	0.48
2:D:403:PRO:O	2:D:406:VAL:HB	2.12	0.48
1:A:67:GLU:CD	1:A:67:GLU:H	2.22	0.48
1:A:120:PHE:CD1	1:A:159:ARG:HG3	2.48	0.48
2:B:322:ARG:HG3	2:B:322:ARG:HH11	1.79	0.48
2:B:355:PRO:HG2	2:B:359:ASP:OD2	2.13	0.48
2:D:173:ILE:C	2:D:175:ILE:N	2.72	0.48
2:D:187:ILE:HG22	2:D:187:ILE:O	2.13	0.48
2:D:227:THR:HA	2:D:230:ILE:HG13	1.95	0.48
1:A:323:GLY:HA3	3:A:1001:NAP:H51A	1.95	0.48
2:B:230:ILE:HG12	2:B:266:TYR:CG	2.49	0.48
2:B:308:LYS:O	2:B:312:ILE:HG13	2.14	0.48
1:C:40:ARG:HD2	1:C:51:CYS:HB3	1.95	0.48
1:C:52:LEU:HD13	1:C:322:LEU:HD11	1.96	0.48
2:D:346:GLU:O	2:D:347:ALA:C	2.57	0.48
1:A:57:TRP:CD2	1:A:58:VAL:HG23	2.48	0.48
2:D:233:TRP:HA	2:D:233:TRP:CE3	2.48	0.47
1:A:310:TRP:O	1:A:313:ARG:HG2	2.14	0.47
1:C:323:GLY:HA3	3:C:1001:NAP:H51A	1.96	0.47
1:C:333:ASN:N	1:C:333:ASN:HD22	2.11	0.47
2:D:350:ARG:HG3	2:D:350:ARG:NH1	2.28	0.47
2:B:29:HIS:HB2	2:B:52:ALA:CB	2.44	0.47
1:C:42:LEU:HD11	1:C:212:CYS:SG	2.54	0.47
2:B:58:LEU:HD23	2:B:58:LEU:C	2.39	0.47
2:B:282:PHE:HA	2:B:285:VAL:HG12	1.96	0.47
1:C:40:ARG:HD3	1:C:318:SER:O	2.14	0.47
2:D:288:VAL:O	2:D:290:GLN:N	2.47	0.47
2:B:217:SER:O	2:B:218:PHE:C	2.58	0.47
1:C:291:GLU:O	1:C:294:ALA:HB3	2.14	0.47
2:D:175:ILE:HA	2:D:178:VAL:CG2	2.45	0.47
2:D:264:ILE:HB	2:D:265:PRO:CD	2.37	0.47
1:A:187:THR:O	1:A:213:GLU:HA	2.14	0.47
4:B:606:PGW:H3	4:B:609:PGW:H17	1.96	0.47
1:C:85:ASP:OD1	1:C:118:LYS:NZ	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:TRP:O	1:C:276:LYS:HG2	2.15	0.47
2:D:80:ARG:HG2	6:D:2061:HOH:O	2.15	0.47
2:D:322:ARG:HG3	2:D:322:ARG:NH1	2.28	0.47
2:B:189:ARG:HG3	2:B:189:ARG:HH11	1.80	0.47
1:C:292:LEU:HD21	1:C:351:ILE:HG23	1.96	0.47
2:B:399:ALA:O	2:B:403:PRO:HD3	2.14	0.47
1:C:357:ASN:O	1:C:358:LYS:C	2.58	0.47
1:C:217:TYR:HB3	1:C:242:THR:HB	1.96	0.47
2:D:171:MET:C	2:D:173:ILE:N	2.72	0.47
2:D:171:MET:HB3	2:D:175:ILE:HD12	1.95	0.47
1:A:326:ASN:ND2	1:A:326:ASN:C	2.72	0.46
2:B:346:GLU:O	2:B:349:GLU:HB2	2.15	0.46
2:D:361:PHE:CB	4:D:601:PGW:H2	2.45	0.46
2:D:182:LEU:O	2:D:185:LEU:HB2	2.16	0.46
2:D:266:TYR:HD2	2:D:267:TYR:CE1	2.34	0.46
2:B:246:SER:C	2:B:248:ALA:N	2.73	0.46
2:B:264:ILE:HB	2:B:265:PRO:HD3	1.96	0.46
2:D:98:LEU:HD23	2:D:126:PHE:HB2	1.98	0.46
1:C:303:LEU:HB3	1:C:304:PRO:HD3	1.97	0.46
2:D:157:GLU:HA	2:D:163:ARG:CG	2.46	0.46
2:B:214:GLN:NE2	2:B:270:ILE:HG12	2.30	0.46
2:B:226:GLU:O	2:B:230:ILE:HD13	2.16	0.46
2:B:408:ASN:O	2:B:412:PHE:HD2	1.99	0.46
2:D:111:GLU:O	2:D:114:ARG:HB3	2.16	0.46
2:B:153:PHE:CE2	2:B:239:VAL:HG11	2.51	0.46
1:C:91:ALA:O	1:C:94:LYS:HB2	2.16	0.46
2:D:207:GLN:C	2:D:207:GLN:CD	2.84	0.46
2:D:291:ILE:HG22	2:D:291:ILE:O	2.15	0.46
2:B:149:VAL:O	2:B:152:LEU:HD12	2.16	0.46
1:C:146:ARG:HD3	6:C:2049:HOH:O	2.15	0.46
2:D:101:PRO:HB2	2:D:104:VAL:HG23	1.98	0.46
2:B:186:PRO:O	2:B:190:ASP:HB2	2.16	0.45
2:D:266:TYR:CZ	2:D:270:ILE:HD11	2.51	0.45
1:A:183:MET:HB3	1:A:184:TYR:CD1	2.52	0.45
2:B:109:PHE:O	2:B:113:ILE:HG13	2.15	0.45
2:B:414:HIS:C	2:B:416:GLU:N	2.74	0.45
2:D:258:ILE:O	2:D:302:LYS:HD3	2.17	0.45
2:D:308:LYS:HA	2:D:311:GLN:HG2	1.98	0.45
2:B:82:ARG:HB2	2:B:83:PRO:CD	2.44	0.45
2:D:360:ALA:O	2:D:361:PHE:C	2.59	0.45
1:C:98:VAL:O	1:C:102:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:MET:HG3	1:C:185:TRP:CE3	2.51	0.45
2:D:176:SER:OG	2:D:299:ARG:NH1	2.49	0.45
1:C:252:SER:OG	1:C:254:LYS:HG2	2.16	0.45
2:B:170:VAL:HG12	2:B:171:MET:HE2	1.98	0.45
2:B:202:PHE:HB2	2:B:279:VAL:CG2	2.47	0.45
2:B:369:THR:OG1	2:B:371:VAL:HG23	2.17	0.45
2:D:230:ILE:HG21	2:D:266:TYR:CD2	2.51	0.45
1:A:85:ASP:OD1	1:A:118:LYS:NZ	2.49	0.45
2:D:354:PHE:HD1	2:D:376:MET:HE3	1.80	0.45
2:B:235:PHE:O	2:B:239:VAL:HG23	2.17	0.45
2:B:226:GLU:OE1	2:B:296:ARG:NH2	2.49	0.45
2:D:229:CYS:HA	2:D:232:TRP:CB	2.47	0.45
2:D:324:LEU:H	2:D:324:LEU:HD22	1.83	0.44
2:B:307:SER:O	2:B:311:GLN:HG3	2.17	0.44
2:B:323:GLU:CD	2:B:323:GLU:N	2.72	0.44
2:B:400:LEU:CB	2:B:401:PRO:HD3	2.33	0.44
4:B:608:PGW:O12	4:B:608:PGW:H02	2.17	0.44
2:D:106:LEU:CD1	2:D:130:GLU:HG2	2.45	0.44
1:A:68:MET:HE3	1:A:326:ASN:HA	1.99	0.44
1:A:344:SER:O	1:A:348:VAL:HG23	2.18	0.44
1:C:251:VAL:HG12	1:C:251:VAL:O	2.17	0.44
1:A:71:HIS:HD2	1:A:327:ALA:HB2	1.81	0.44
1:A:217:TYR:HB3	1:A:242:THR:HB	1.99	0.44
1:A:314:ASN:HB2	6:A:2035:HOH:O	2.18	0.44
2:D:167:ILE:HA	2:D:170:VAL:HG23	1.99	0.44
2:D:256:ASN:C	2:D:258:ILE:N	2.75	0.44
2:B:255:MET:HE2	2:B:305:ARG:HB2	2.00	0.44
2:B:400:LEU:HB2	2:B:401:PRO:CD	2.34	0.44
1:C:75:LEU:CD2	1:C:331:MET:HE3	2.42	0.44
2:D:304:SER:CA	2:D:310:LEU:HD23	2.48	0.44
2:D:172:VAL:HG12	2:D:233:TRP:CZ2	2.53	0.44
2:D:330:PHE:O	2:D:333:ILE:HB	2.17	0.44
1:A:260:PRO:HA	1:A:261:PRO:HD3	1.90	0.43
2:B:243:ALA:N	2:B:247:LYS:NZ	2.65	0.43
2:D:109:PHE:HE2	2:D:113:ILE:HD11	1.79	0.43
2:D:220:ASP:O	2:D:224:ILE:HG13	2.17	0.43
2:D:302:LYS:HA	2:D:302:LYS:HD2	1.82	0.43
1:A:301:CYS:HB2	1:A:305:GLN:OE1	2.18	0.43
2:B:253:ASN:OD1	2:B:255:MET:HB2	2.18	0.43
1:C:352:ASP:CG	1:C:358:LYS:HD2	2.42	0.43
2:D:297:ILE:C	2:D:299:ARG:N	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:LEU:O	2:B:65:ARG:NH1	2.49	0.43
2:D:102:VAL:HG23	2:D:103:ASN:N	2.33	0.43
2:D:176:SER:OG	2:D:299:ARG:HD3	2.18	0.43
2:D:233:TRP:HA	2:D:233:TRP:HE3	1.84	0.43
2:D:264:ILE:CB	2:D:265:PRO:HD3	2.35	0.43
1:C:331:MET:CE	1:C:334:ILE:HD12	2.48	0.43
2:D:219:THR:O	2:D:220:ASP:HB2	2.17	0.43
2:D:225:VAL:HG13	2:D:228:LEU:CD2	2.45	0.43
1:A:347:ILE:O	1:A:351:ILE:HG13	2.19	0.43
2:B:285:VAL:O	2:B:285:VAL:HG22	2.18	0.43
2:D:233:TRP:C	2:D:235:PHE:H	2.26	0.43
2:B:298:LEU:C	2:B:300:ILE:N	2.77	0.43
2:B:316:THR:HG21	2:B:409:PHE:HB2	2.00	0.43
2:D:165:ILE:O	2:D:165:ILE:HG22	2.18	0.43
2:D:400:LEU:CB	2:D:401:PRO:HD3	2.32	0.43
1:A:106:LYS:HG3	1:A:108:TRP:CH2	2.54	0.43
1:A:159:ARG:HB2	1:A:160:PRO:HD2	2.00	0.43
1:A:134:LYS:O	1:A:138:GLU:HG3	2.19	0.43
2:B:127:ARG:HH11	2:B:127:ARG:HG2	1.84	0.43
2:B:254:ILE:O	2:B:258:ILE:HG13	2.19	0.43
2:D:114:ARG:HG3	2:D:114:ARG:NH1	2.34	0.43
2:D:221:PRO:HA	2:D:224:ILE:HD12	1.99	0.43
2:D:318:LYS:C	2:D:320:SER:H	2.27	0.43
2:D:175:ILE:HA	2:D:178:VAL:HG23	2.01	0.42
1:A:63:GLN:NE2	1:A:267:LEU:HD11	2.35	0.42
2:B:150:TRP:HE1	2:B:155:TYR:HE2	1.66	0.42
2:D:221:PRO:C	2:D:223:PHE:N	2.74	0.42
1:A:114:VAL:HA	1:A:153:ASP:OD2	2.19	0.42
1:A:119:ILE:O	1:A:120:PHE:HB2	2.19	0.42
2:B:343:TYR:HE1	2:B:356:SER:HA	1.83	0.42
2:B:404:VAL:O	2:B:407:SER:HB3	2.19	0.42
2:D:164:ILE:HG22	2:D:164:ILE:O	2.18	0.42
2:D:382:GLY:O	2:D:386:VAL:HG23	2.20	0.42
2:B:127:ARG:HG2	2:B:127:ARG:NH1	2.35	0.42
2:B:349:GLU:HB2	2:B:352:SER:HB2	2.01	0.42
1:A:51:CYS:SG	1:A:337:ILE:HD11	2.59	0.42
2:B:209:THR:O	2:B:293:ARG:HD2	2.19	0.42
2:B:255:MET:CE	2:B:305:ARG:HB2	2.50	0.42
2:B:304:SER:CA	2:B:310:LEU:HD23	2.50	0.42
2:B:402:VAL:HB	2:B:403:PRO:HD3	2.00	0.42
2:D:168:VAL:HG22	2:D:168:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:361:PHE:HB2	4:D:601:PGW:H2	2.02	0.42
2:D:374:GLY:C	2:D:376:MET:N	2.78	0.42
1:C:268:LYS:C	1:C:268:LYS:HD2	2.44	0.42
2:D:171:MET:O	2:D:175:ILE:HB	2.18	0.42
1:A:65:THR:HB	1:A:67:GLU:OE1	2.19	0.42
1:A:284:ARG:HB2	1:A:284:ARG:NH1	2.33	0.42
2:B:155:TYR:C	2:B:157:GLU:H	2.27	0.42
2:B:218:PHE:HB3	2:B:224:ILE:HG12	2.00	0.42
1:C:124:LYS:HG3	6:C:2082:HOH:O	2.19	0.42
1:C:216:GLU:HB2	1:C:243:TRP:CZ2	2.55	0.42
2:D:323:GLU:OE1	2:D:404:VAL:HG11	2.20	0.42
2:B:153:PHE:O	2:B:154:GLU:HB2	2.20	0.42
2:D:56:GLU:CD	2:D:56:GLU:N	2.76	0.42
2:D:164:ILE:C	2:D:166:ALA:H	2.27	0.42
2:D:160:GLY:C	2:D:163:ARG:HB3	2.45	0.42
2:D:307:SER:O	2:D:311:GLN:HG2	2.20	0.42
1:A:173:MET:HG3	1:A:185:TRP:CE3	2.55	0.42
1:A:218:HIS:CE1	1:A:221:GLN:HB2	2.55	0.42
2:B:230:ILE:HG21	2:B:266:TYR:CD2	2.55	0.42
2:B:277:LYS:HG3	2:B:277:LYS:O	2.20	0.42
2:D:225:VAL:HG12	2:D:225:VAL:O	2.20	0.42
2:B:284:ASN:OD1	2:B:284:ASN:C	2.62	0.41
2:D:233:TRP:C	2:D:235:PHE:N	2.77	0.41
2:B:72:LEU:HD23	2:B:72:LEU:HA	1.89	0.41
2:D:252:THR:HG22	2:D:253:ASN:N	2.35	0.41
2:D:276:ASN:C	2:D:278:SER:N	2.78	0.41
1:A:327:ALA:HB1	1:A:331:MET:HE2	2.03	0.41
1:A:337:ILE:HD13	1:A:337:ILE:HA	1.87	0.41
1:C:255:TYR:OH	1:C:263:SER:HB2	2.20	0.41
2:D:343:TYR:C	2:D:345:ALA:N	2.78	0.41
1:C:235:LYS:HB2	2:D:66:MET:HE1	2.02	0.41
2:D:65:ARG:O	2:D:66:MET:C	2.63	0.41
2:B:80:ARG:NH1	2:B:112:GLU:OE2	2.53	0.41
2:B:298:LEU:C	2:B:300:ILE:H	2.28	0.41
2:D:36:VAL:HG22	2:D:45:GLU:HG2	2.01	0.41
2:D:160:GLY:CA	2:D:163:ARG:HB3	2.50	0.41
2:D:166:ALA:HB1	2:D:306:HIS:HD2	1.84	0.41
2:B:244:CYS:N	2:B:247:LYS:NZ	2.68	0.41
2:B:399:ALA:O	2:B:403:PRO:CD	2.69	0.41
2:B:402:VAL:O	2:B:403:PRO:C	2.62	0.41
1:C:164:THR:HA	1:C:165:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:258:ILE:HG22	2:D:302:LYS:HA	2.02	0.41
2:D:258:ILE:HG21	2:D:302:LYS:HA	2.01	0.41
2:B:304:SER:HA	2:B:310:LEU:HD23	2.01	0.41
4:D:601:PGW:O02	4:D:601:PGW:H03A	2.20	0.41
2:B:257:ILE:O	2:B:261:VAL:HG23	2.21	0.41
2:B:282:PHE:O	2:B:284:ASN:N	2.54	0.41
1:C:225:VAL:O	1:C:230:PRO:HD3	2.21	0.41
2:D:160:GLY:O	2:D:163:ARG:HB3	2.20	0.41
2:D:226:GLU:HG3	2:D:230:ILE:HD11	2.03	0.41
2:D:234:SER:HA	2:D:237:PHE:HB3	2.01	0.41
2:D:258:ILE:O	2:D:258:ILE:HG22	2.19	0.41
2:D:262:ALA:O	2:D:263:ILE:HG23	2.20	0.41
2:D:288:VAL:CG1	2:D:289:VAL:H	2.28	0.41
2:D:398:ILE:O	2:D:402:VAL:HG23	2.21	0.41
2:D:229:CYS:HA	2:D:232:TRP:HB2	2.03	0.41
1:A:214:GLN:HA	1:A:241:MET:O	2.21	0.40
1:A:302:THR:OG1	1:A:304:PRO:HD2	2.21	0.40
2:B:357:ILE:N	2:B:358:PRO:CD	2.84	0.40
1:C:313:ARG:HG2	1:C:313:ARG:HH11	1.86	0.40
2:D:173:ILE:HG12	2:D:233:TRP:HZ2	1.86	0.40
2:D:225:VAL:O	2:D:228:LEU:HB3	2.21	0.40
2:B:210:ILE:HD11	2:B:273:THR:CG2	2.51	0.40
2:B:353:GLN:O	2:B:376:MET:HE3	2.22	0.40
1:A:211:ILE:HG23	6:A:2003:HOH:O	2.20	0.40
1:A:313:ARG:HG2	1:A:313:ARG:NH1	2.37	0.40
2:B:264:ILE:N	2:B:265:PRO:CD	2.85	0.40
2:D:255:MET:HG3	2:D:305:ARG:CZ	2.52	0.40
1:A:73:MET:HE3	1:A:84:PHE:CE2	2.55	0.40
2:B:399:ALA:O	2:B:400:LEU:C	2.64	0.40
1:C:292:LEU:C	1:C:294:ALA:N	2.80	0.40
2:D:161:PRO:C	2:D:163:ARG:H	2.27	0.40
2:D:224:ILE:HG22	2:D:225:VAL:N	2.36	0.40
2:D:288:VAL:CG1	2:D:289:VAL:N	2.83	0.40
2:B:143:ASN:C	2:B:145:PHE:H	2.29	0.40
2:D:315:GLN:C	2:D:317:LEU:N	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/333 (97%)	305 (94%)	18 (6%)	1 (0%)	36	65
1	C	324/333 (97%)	307 (95%)	14 (4%)	3 (1%)	14	41
2	B	387/514 (75%)	321 (83%)	52 (13%)	14 (4%)	2	11
2	D	304/514 (59%)	238 (78%)	52 (17%)	14 (5%)	2	7
All	All	1339/1694 (79%)	1171 (88%)	136 (10%)	32 (2%)	4	18

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	133	ILE
2	B	141	PRO
2	B	142	GLU
2	B	154	GLU
2	D	157	GLU
2	D	289	VAL
1	A	120	PHE
2	B	158	SER
1	C	120	PHE
1	C	223	GLU
2	D	156	PRO
2	D	376	MET
2	B	243	ALA
2	B	283	GLN
2	B	399	ALA
2	D	159	SER
2	D	399	ALA
2	D	400	LEU
2	D	412	PHE
2	B	218	PHE
2	D	33	GLU
2	D	174	LEU

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Mol	Chain	Res	Type
2	D	263	ILE
2	D	375	ASP
2	D	411	TYR
2	B	128	GLU
2	B	400	LEU
2	B	415	ARG
2	B	416	GLU
1	C	342	LYS
2	B	279	VAL
2	D	224	ILE

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	273/280 (98%)	269 (98%)	4 (2%)	57	84
1	C	273/280 (98%)	264 (97%)	9 (3%)	33	67
2	B	335/459 (73%)	330 (98%)	5 (2%)	57	84
2	D	284/459 (62%)	281 (99%)	3 (1%)	65	88
All	All	1165/1478 (79%)	1144 (98%)	21 (2%)	51	80

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

Mol	Chain	Res	Type
1	A	73	MET
1	A	75	LEU
1	A	183	MET
1	A	326	ASN
2	B	103	ASN
2	B	152	LEU
2	B	283	GLN
2	B	284	ASN
2	B	323	GLU
1	C	37	GLN
1	C	40	ARG

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Mol	Chain	Res	Type
1	C	73	MET
1	C	75	LEU
1	C	223	GLU
1	C	231	GLU
1	C	268	LYS
1	C	283	ARG
1	C	295	ILE
2	D	56	GLU
2	D	103	ASN
2	D	233	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	71	HIS
1	A	148	GLN
1	A	204	GLN
1	A	206	ASN
1	A	271	GLN
1	A	285	GLN
1	A	286	GLN
1	A	326	ASN
1	A	333	ASN
2	B	103	ASN
2	B	196	HIS
2	B	213	GLN
2	B	214	GLN
2	B	276	ASN
2	B	315	GLN
2	B	410	ASN
2	B	414	HIS
1	C	37	GLN
1	C	71	HIS
1	C	148	GLN
1	C	163	ASN
1	C	175	HIS
1	C	204	GLN
1	C	314	ASN
1	C	333	ASN
2	D	47	GLN
2	D	53	GLN

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Mol	Chain	Res	Type
2	D	103	ASN
2	D	315	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 10 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAP	A	1001	-	50,52,52	1.27	6 (12%)	71,80,80	1.00	2 (2%)
4	PGW	B	605	-	7,7,50	0.36	0	6,6,56	0.52	0
4	PGW	D	601	-	21,21,50	0.61	0	23,23,56	1.20	2 (8%)
4	PGW	B	608	-	19,19,50	0.84	0	22,24,56	1.28	3 (13%)
4	PGW	B	610	-	27,27,50	0.72	0	28,32,56	1.16	2 (7%)
4	PGW	B	606	-	6,6,50	0.36	0	5,5,56	0.49	0
4	PGW	B	609	-	5,5,50	0.36	0	4,4,56	0.43	0
4	PGW	B	601	-	18,18,50	0.60	0	19,19,56	1.25	3 (15%)
4	PGW	B	612	-	5,5,50	0.37	0	4,4,56	0.41	0
4	PGW	B	604	-	4,4,50	0.38	0	3,3,56	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	C	1001	-	50,52,52	1.31	5 (10%)	71,80,80	0.99	2 (2%)
4	PGW	B	603	-	4,4,50	0.37	0	3,3,56	0.41	0
4	PGW	B	611	-	8,8,50	0.36	0	7,7,56	0.51	0
4	PGW	B	607	-	6,6,50	0.37	0	5,5,56	0.48	0
4	PGW	B	602	-	4,4,50	0.38	0	3,3,56	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	A	1001	-	-	3/35/67/67	0/5/5/5
4	PGW	B	605	-	-	0/5/5/55	-
4	PGW	D	601	-	-	1/23/23/55	-
4	PGW	B	608	-	-	5/21/21/55	-
4	PGW	B	610	-	-	5/31/31/55	-
4	PGW	B	606	-	-	0/4/4/55	-
4	PGW	B	609	-	-	0/3/3/55	-
4	PGW	B	601	-	-	1/18/18/55	-
4	PGW	B	612	-	-	0/3/3/55	-
4	PGW	B	604	-	-	0/2/2/55	-
3	NAP	C	1001	-	-	2/35/67/67	0/5/5/5
4	PGW	B	603	-	-	0/2/2/55	-
4	PGW	B	611	-	-	0/6/6/55	-
4	PGW	B	607	-	-	0/4/4/55	-
4	PGW	B	602	-	-	0/2/2/55	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1001	NAP	C6N-N1N	3.84	1.44	1.35
3	C	1001	NAP	C4N-C3N	3.68	1.45	1.39
3	A	1001	NAP	C6N-N1N	3.61	1.43	1.35
3	A	1001	NAP	C4N-C3N	3.18	1.44	1.39
3	C	1001	NAP	C4A-N3A	2.94	1.39	1.34
3	A	1001	NAP	C4A-N3A	2.68	1.39	1.34
3	A	1001	NAP	C5A-N7A	-2.63	1.34	1.39
3	A	1001	NAP	PN-O3	-2.61	1.56	1.59
3	C	1001	NAP	PA-O3	2.56	1.62	1.59
3	C	1001	NAP	C5A-N7A	-2.17	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	NAP	C2N-N1N	2.06	1.37	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	610	PGW	O01-C1-O02	-4.62	119.78	125.70
4	D	601	PGW	O01-C1-C2	3.30	118.62	111.48
4	B	608	PGW	O01-C1-C2	2.98	117.93	111.48
3	C	1001	NAP	C6N-N1N-C2N	-2.96	119.36	121.88
4	B	608	PGW	O03-C19-C20	2.74	119.46	111.15
3	A	1001	NAP	C2A-N1A-C6A	2.52	122.87	118.73
4	B	601	PGW	O03-C19-C20	2.52	119.50	111.83
3	A	1001	NAP	C6N-N1N-C2N	-2.51	119.74	121.88
4	B	608	PGW	O11-P-O14	2.39	112.89	106.44
4	B	601	PGW	C01-O03-C19	-2.36	109.52	116.90
4	D	601	PGW	O03-C19-C20	2.35	118.99	111.83
3	C	1001	NAP	C2A-N1A-C6A	2.34	122.57	118.73
4	B	601	PGW	O01-C1-C2	2.33	118.95	111.83
4	B	610	PGW	O03-C19-C20	2.24	118.66	111.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

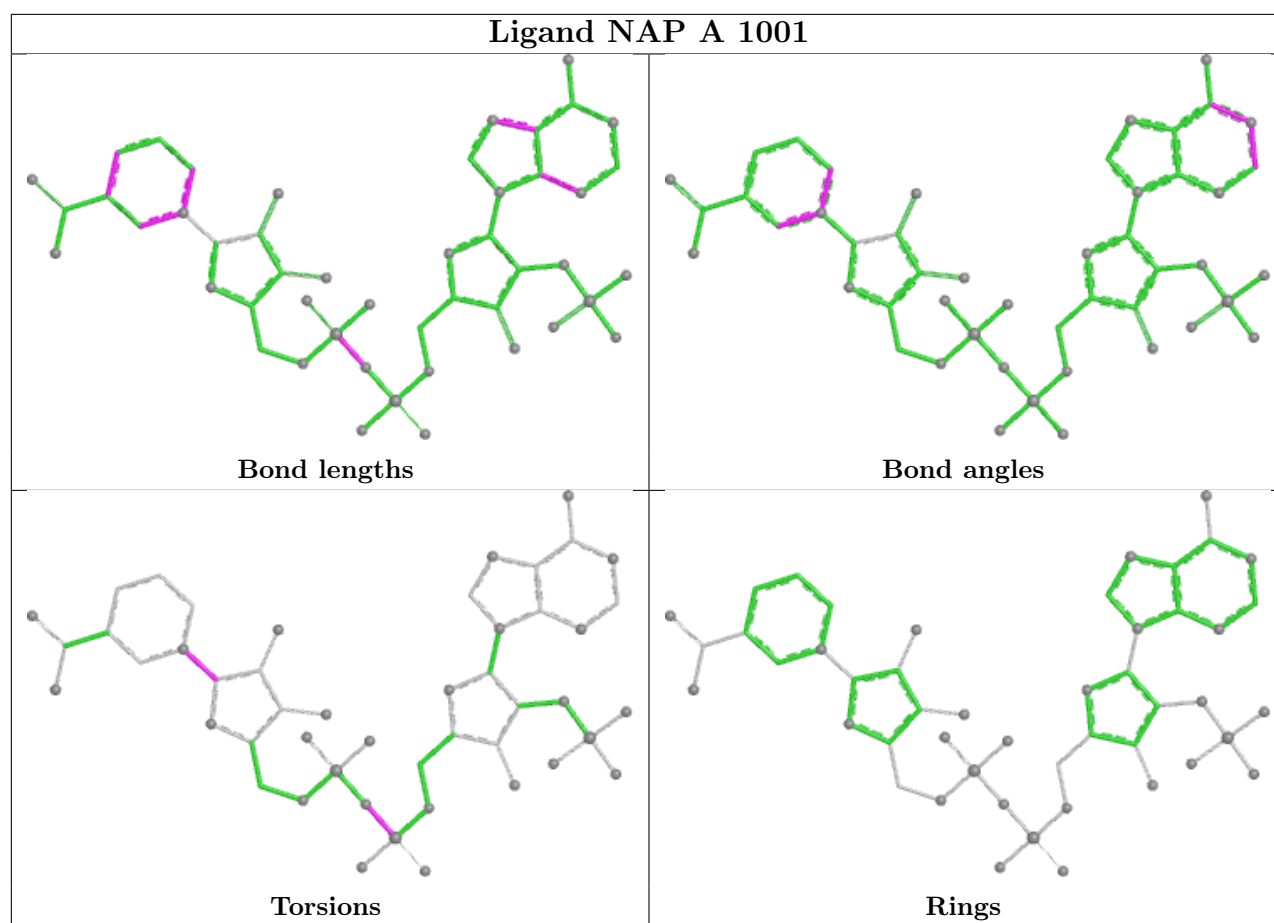
Mol	Chain	Res	Type	Atoms
3	A	1001	NAP	PN-O3-PA-O5B
4	B	601	PGW	C01-C02-O01-C1
4	B	608	PGW	C02-C03-O11-P
4	B	610	PGW	O02-C1-O01-C02
4	D	601	PGW	C01-C02-O01-C1
4	B	608	PGW	C01-C02-O01-C1
4	B	608	PGW	C03-C02-O01-C1
3	A	1001	NAP	O4D-C1D-N1N-C2N
3	A	1001	NAP	O4D-C1D-N1N-C6N
3	C	1001	NAP	O4D-C1D-N1N-C2N
3	C	1001	NAP	O4D-C1D-N1N-C6N
4	B	610	PGW	C01-C02-O01-C1
4	B	610	PGW	C03-C02-O01-C1
4	B	610	PGW	O03-C19-C20-C21
4	B	608	PGW	O01-C1-C2-C3
4	B	608	PGW	O02-C1-C2-C3
4	B	610	PGW	O04-C19-C20-C21

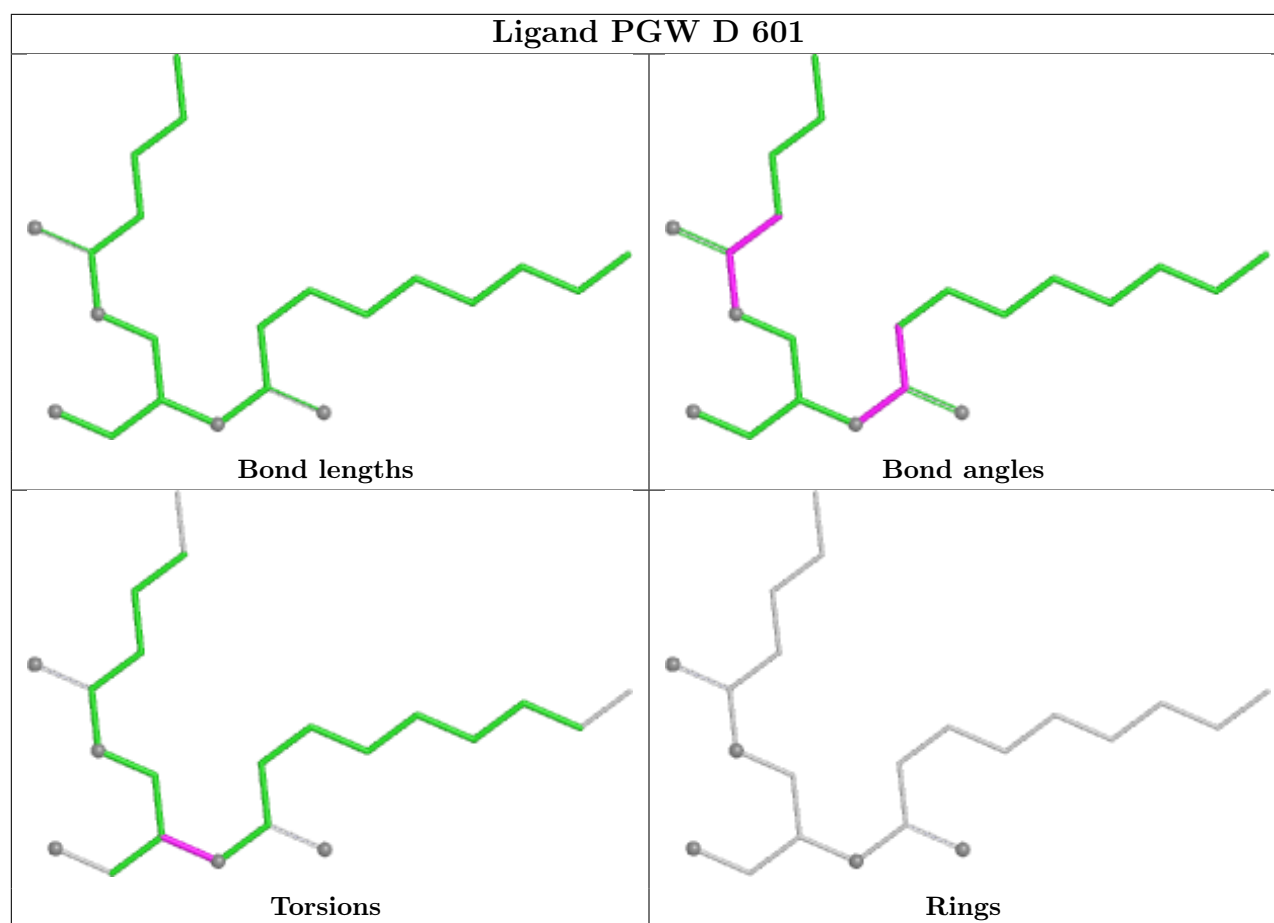
There are no ring outliers.

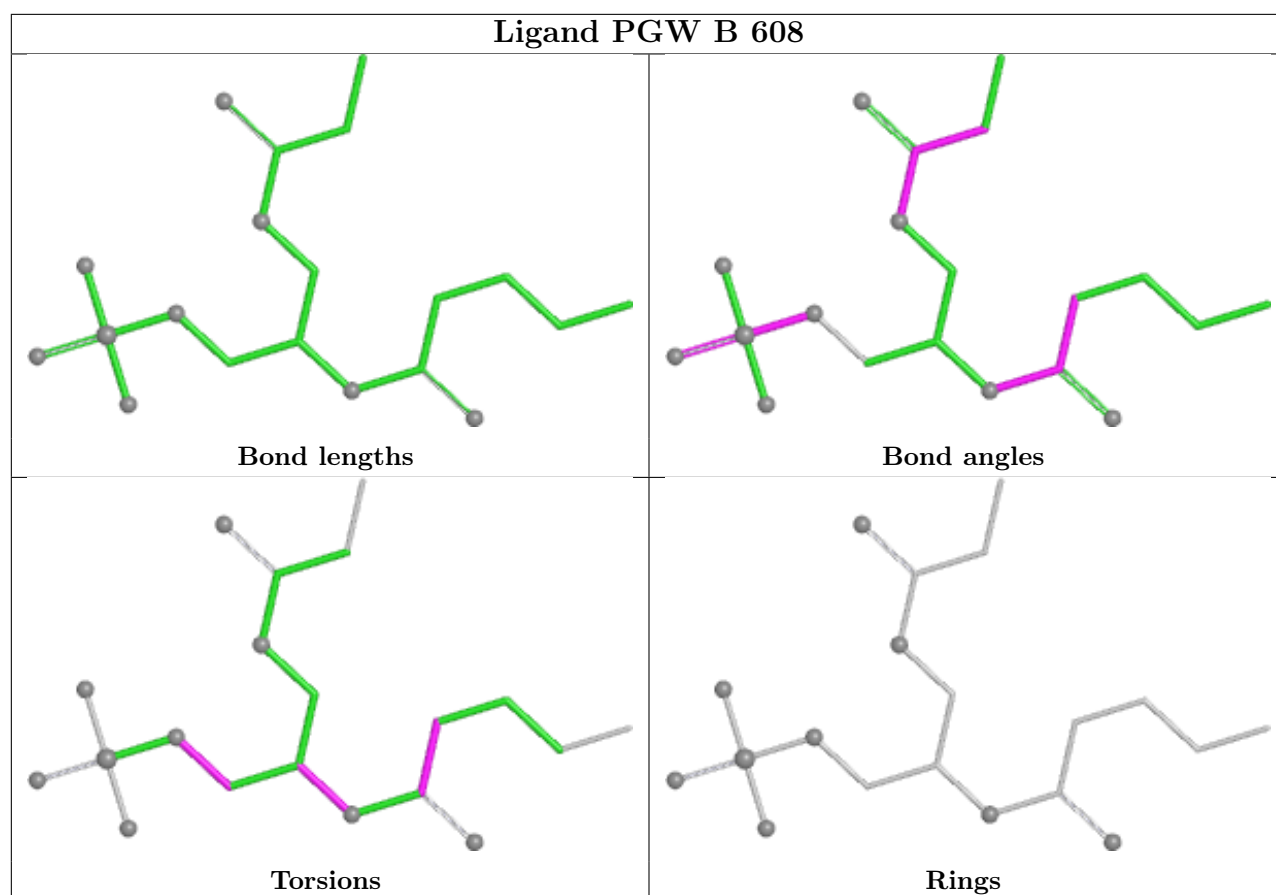
8 monomers are involved in 20 short contacts:

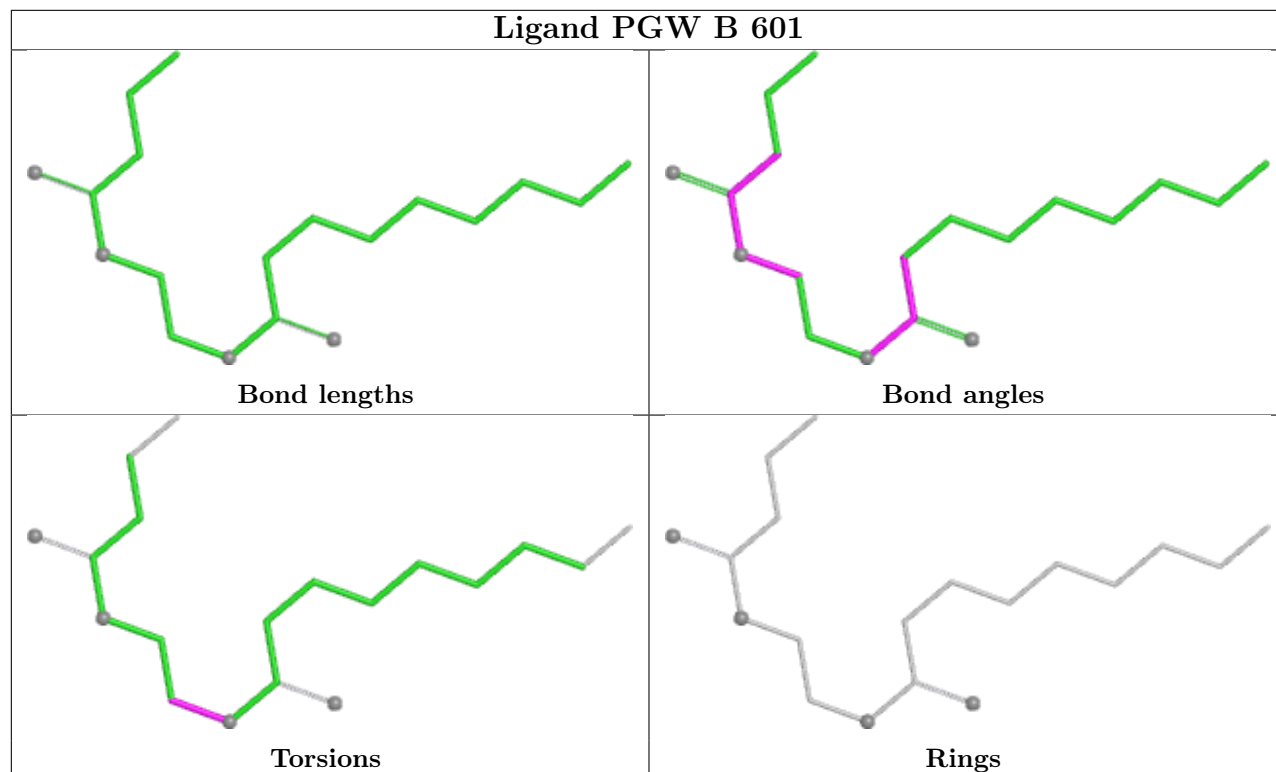
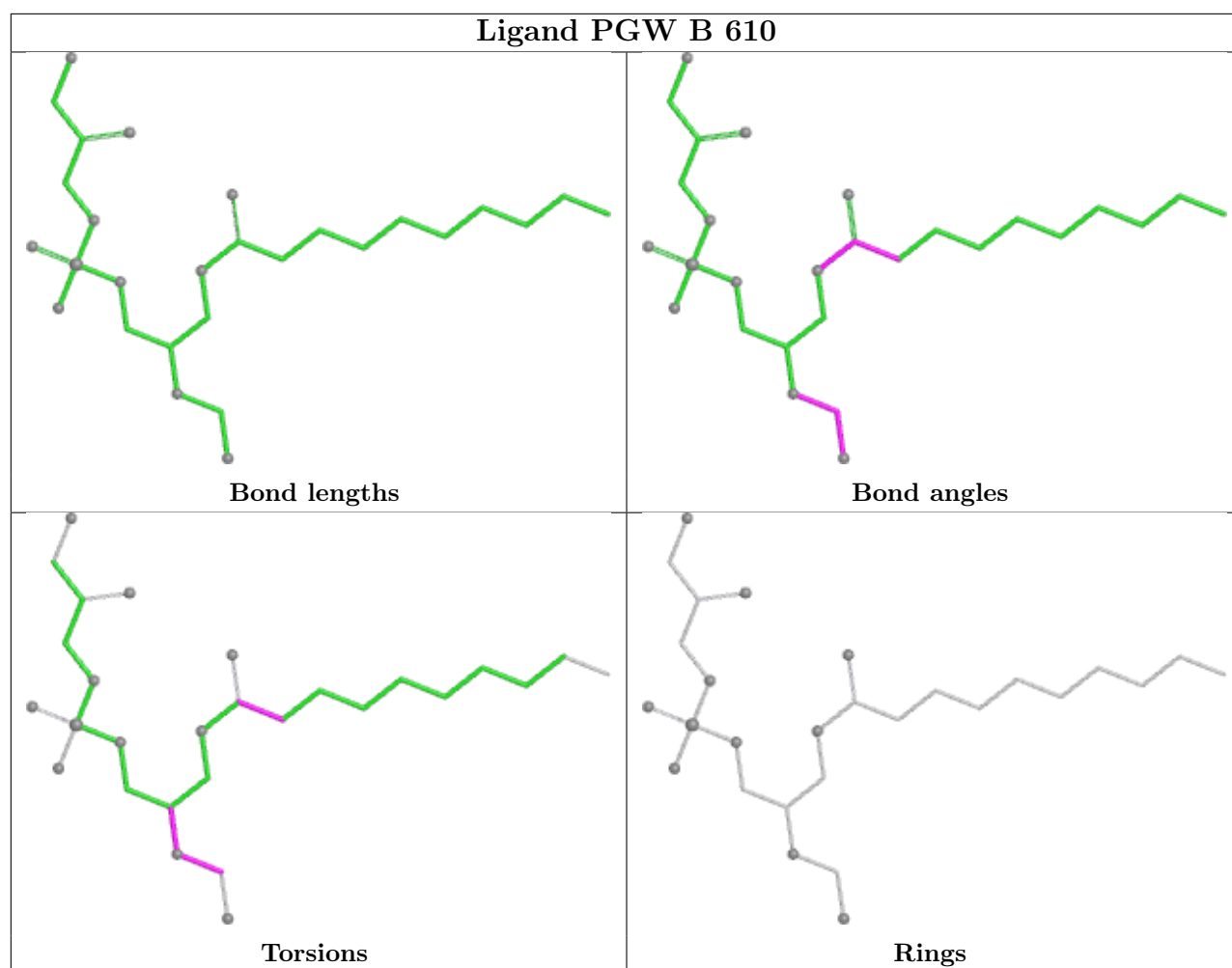
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	NAP	2	0
4	D	601	PGW	7	0
4	B	608	PGW	2	0
4	B	610	PGW	2	0
4	B	606	PGW	1	0
4	B	609	PGW	1	0
4	B	601	PGW	3	0
3	C	1001	NAP	3	0

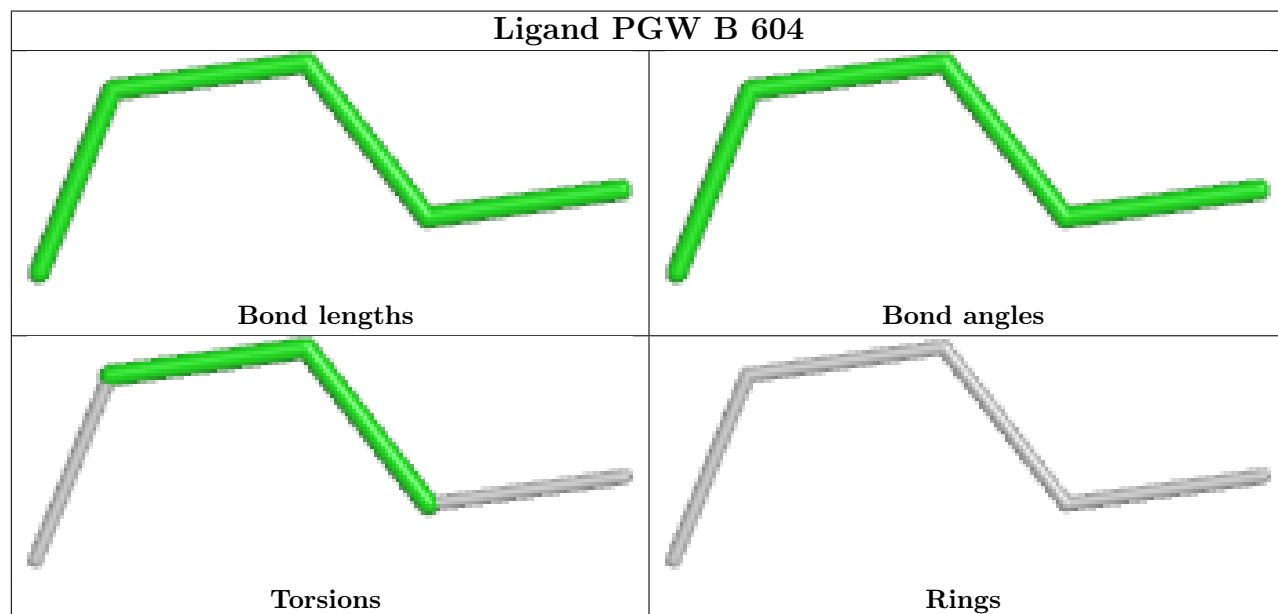
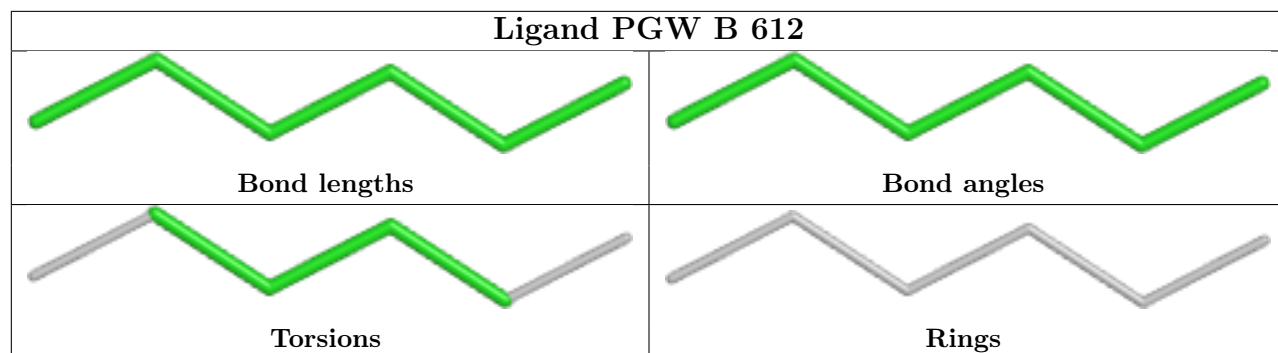
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

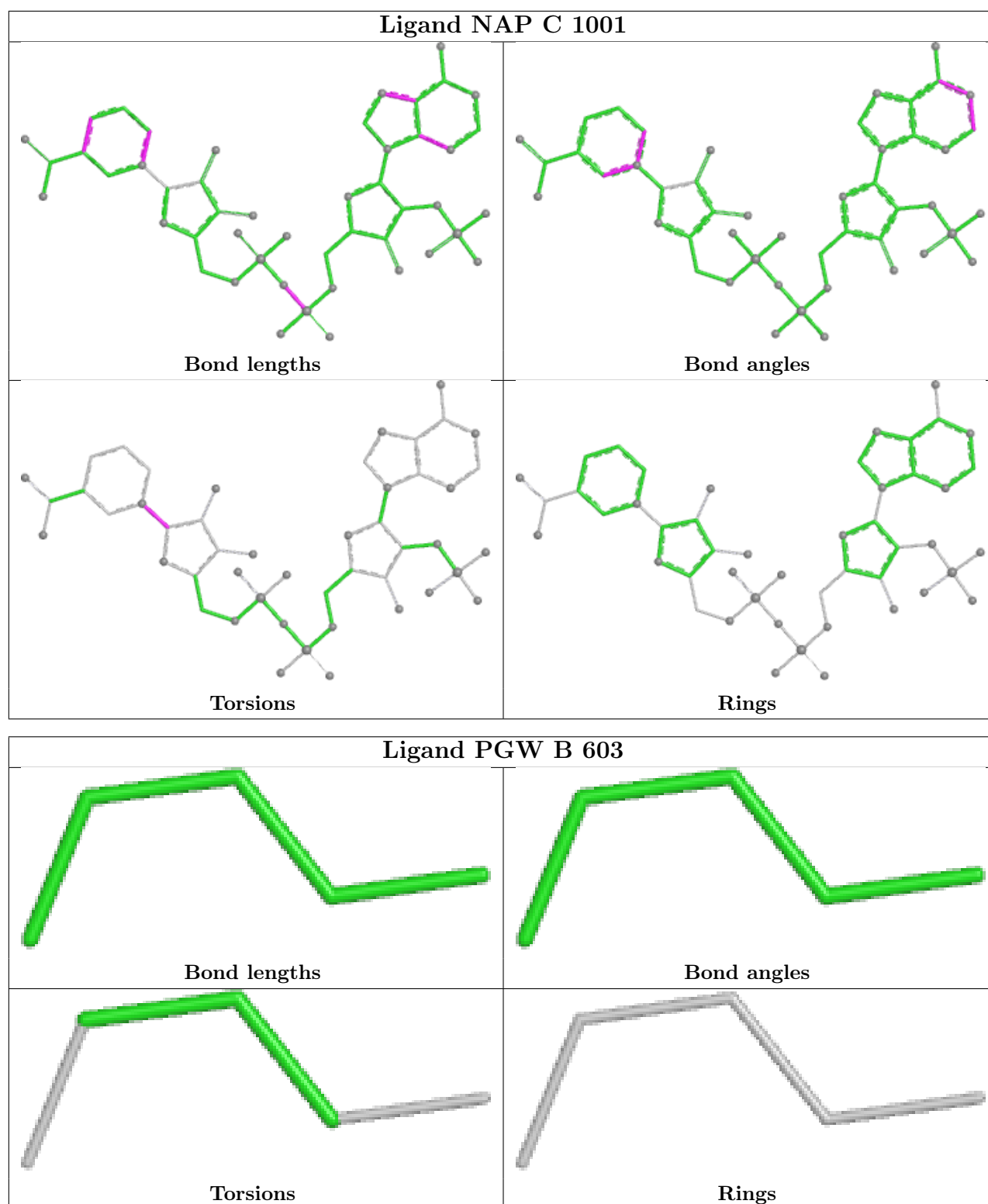












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	326/333 (97%)	-0.21	10 (3%) 51 42	22, 42, 68, 94	0
1	C	326/333 (97%)	-0.20	6 (1%) 67 59	24, 46, 77, 102	0
2	B	389/514 (75%)	0.85	57 (14%) 6 4	33, 79, 137, 146	0
2	D	318/514 (61%)	1.34	86 (27%) 1 1	39, 97, 171, 187	0
All	All	1359/1694 (80%)	0.46	159 (11%) 9 8	22, 61, 149, 187	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	269	THR	7.0
2	B	197	GLY	6.2
2	D	162	ALA	6.1
2	B	200	VAL	6.0
2	D	288	VAL	5.9
2	D	291	ILE	5.8
2	D	168	VAL	5.4
2	D	415	ARG	5.0
2	D	165	ILE	4.9
2	B	153	PHE	4.9
2	B	196	HIS	4.9
2	D	278	SER	4.8
2	D	239	VAL	4.7
2	B	274	GLU	4.6
2	D	262	ALA	4.6
2	D	294	ILE	4.6
2	D	222	PHE	4.6
2	D	164	ILE	4.5
2	D	131	GLY	4.5
2	B	195	MET	4.5
2	D	271	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
2	D	225	VAL	4.4
2	D	167	ILE	4.3
2	B	192	ASN	4.2
2	D	204	THR	4.1
2	B	375	ASP	4.1
2	D	289	VAL	4.1
2	B	202	PHE	4.1
2	B	280	LEU	4.0
2	B	145	PHE	4.0
2	D	219	THR	4.0
2	B	193	GLU	4.0
2	B	194	ASP	3.9
1	A	36	LEU	3.9
1	A	360	TYR	3.9
2	D	155	TYR	3.9
2	D	270	ILE	3.9
2	B	152	LEU	3.9
2	D	237	PHE	3.8
2	B	155	TYR	3.8
2	D	205	TYR	3.8
2	D	351	ASP	3.8
2	B	199	GLY	3.8
2	D	261	VAL	3.7
2	B	203	HIS	3.7
2	B	205	TYR	3.7
2	D	268	VAL	3.7
2	D	206	SER	3.7
2	D	266	TYR	3.7
2	B	417	THR	3.6
2	D	277	LYS	3.6
2	B	188	PHE	3.6
2	B	190	ASP	3.6
2	D	287	ARG	3.5
2	D	223	PHE	3.5
2	D	156	PRO	3.4
2	D	290	GLN	3.4
2	D	416	GLU	3.4
2	D	275	SER	3.3
2	D	129	ASP	3.2
1	C	36	LEU	3.2
2	D	207	GLN	3.2
2	D	233	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	359	ASP	3.2
2	B	204	THR	3.1
2	D	231	ILE	3.1
2	B	214	GLN	3.1
2	D	187	ILE	3.1
2	B	151	LEU	3.1
2	D	202	PHE	3.1
2	B	242	PHE	3.0
2	D	417	THR	3.0
2	B	154	GLU	3.0
2	B	156	PRO	2.9
2	D	254	ILE	2.9
2	B	219	THR	2.9
2	D	221	PRO	2.9
2	D	235	PHE	2.9
1	C	360	TYR	2.8
2	B	191	GLU	2.8
2	D	228	LEU	2.8
2	D	264	ILE	2.8
1	C	231	GLU	2.8
2	D	267	TYR	2.8
2	D	257	ILE	2.8
2	D	253	ASN	2.8
2	D	399	ALA	2.8
2	B	201	THR	2.7
2	B	374	GLY	2.7
2	D	31	SER	2.7
2	D	158	SER	2.6
2	B	140	LEU	2.6
2	D	236	GLU	2.6
2	D	276	ASN	2.6
1	C	361	SER	2.6
1	C	268	LYS	2.6
1	A	361	SER	2.5
2	D	189	ARG	2.5
2	B	231	ILE	2.5
2	D	121	GLU	2.5
2	B	187	ILE	2.5
2	B	213	GLN	2.5
2	D	302	LYS	2.5
2	D	185	LEU	2.5
2	B	215	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	349	HIS	2.5
2	D	260	ILE	2.4
2	D	203	HIS	2.4
1	A	121	TRP	2.4
2	D	411	TYR	2.4
2	B	181	CYS	2.4
2	B	146	GLN	2.4
2	B	129	ASP	2.4
2	D	220	ASP	2.4
2	D	344	PHE	2.4
1	A	223	GLU	2.4
1	A	231	GLU	2.4
2	B	137	GLU	2.4
2	D	258	ILE	2.4
2	B	143	ASN	2.3
2	B	283	GLN	2.3
2	D	234	SER	2.3
2	B	279	VAL	2.3
2	D	299	ARG	2.3
2	D	238	LEU	2.3
2	B	150	TRP	2.3
2	D	159	SER	2.3
2	B	275	SER	2.3
1	A	228	GLN	2.2
2	D	232	TRP	2.2
2	B	125	MET	2.2
2	B	286	ARG	2.2
2	D	161	PRO	2.2
2	B	234	SER	2.2
2	B	147	ARG	2.2
1	A	66	ASP	2.2
2	B	30	GLU	2.2
2	D	306	HIS	2.1
2	D	265	PRO	2.1
2	D	98	LEU	2.1
2	D	292	PHE	2.1
2	D	263	ILE	2.1
2	D	227	THR	2.1
1	C	280	GLU	2.1
2	B	206	SER	2.1
2	D	226	GLU	2.1
2	D	300	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	315	GLN	2.1
2	B	149	VAL	2.1
1	A	43	GLY	2.1
2	D	309	GLY	2.1
2	B	251	PHE	2.1
2	B	183	GLU	2.1
2	D	259	ASP	2.0
2	B	304	SER	2.0
2	D	169	SER	2.0
2	D	293	ARG	2.0
2	D	224	ILE	2.0
2	B	128	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PGW	B	602	5/51	0.44	0.38	80,81,82,82	0
4	PGW	B	612	6/51	0.44	0.48	94,96,96,97	0
4	PGW	B	603	5/51	0.70	0.47	85,87,88,88	0
4	PGW	B	601	19/51	0.71	0.37	72,84,97,97	0
4	PGW	B	610	28/51	0.73	0.26	122,148,154,155	0
4	PGW	D	601	22/51	0.75	0.41	95,113,118,118	0
4	PGW	B	604	5/51	0.77	0.42	87,87,88,88	0
4	PGW	B	608	20/51	0.78	0.27	141,146,153,153	0
4	PGW	B	611	9/51	0.81	0.35	83,84,85,85	0
4	PGW	B	607	7/51	0.82	0.33	94,96,98,98	0
4	PGW	B	609	6/51	0.83	0.44	73,73,73,74	0

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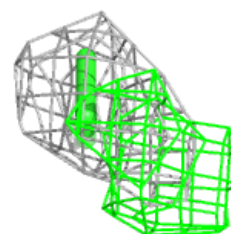
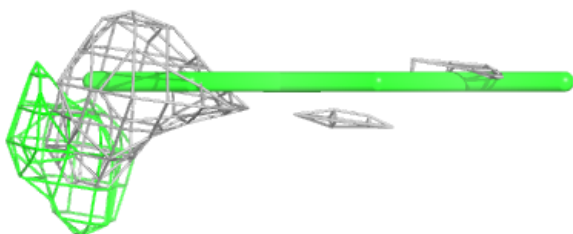
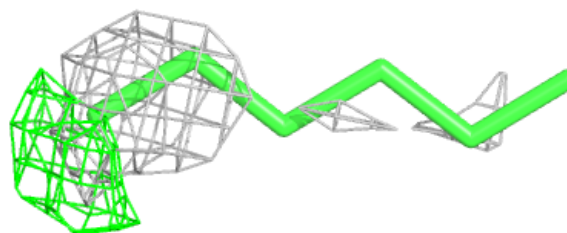
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PGW	B	606	7/51	0.84	0.34	90,91,93,93	0
5	K	B	505	1/1	0.84	0.21	64,64,64,64	1
5	K	D	502	1/1	0.85	0.19	34,34,34,34	1
4	PGW	B	605	8/51	0.91	0.24	74,74,75,75	0
5	K	D	501	1/1	0.91	0.27	37,37,37,37	1
5	K	B	501	1/1	0.91	0.27	32,32,32,32	1
5	K	B	503	1/1	0.93	0.13	28,28,28,28	1
5	K	B	504	1/1	0.95	0.18	26,26,26,26	1
5	K	B	502	1/1	0.95	0.17	21,21,21,21	1
5	K	D	504	1/1	0.95	0.24	26,26,26,26	1
5	K	D	505	1/1	0.96	0.41	53,53,53,53	1
5	K	D	503	1/1	0.97	0.11	41,41,41,41	1
3	NAP	A	1001	48/48	0.97	0.08	35,43,47,48	0
3	NAP	C	1001	48/48	0.97	0.08	38,45,53,54	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.

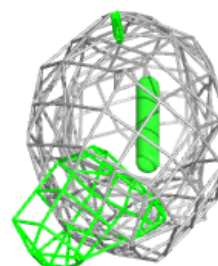
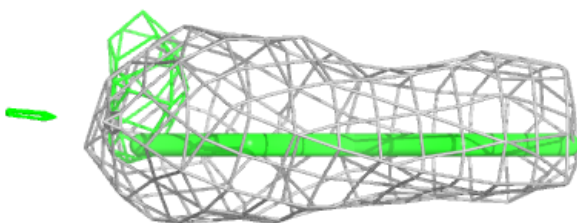
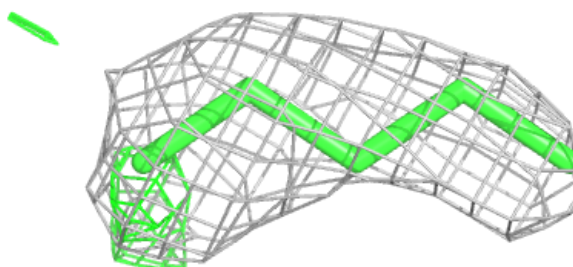
Electron density around PGW B 612:

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

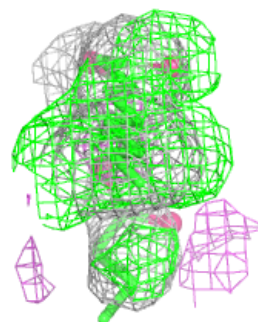
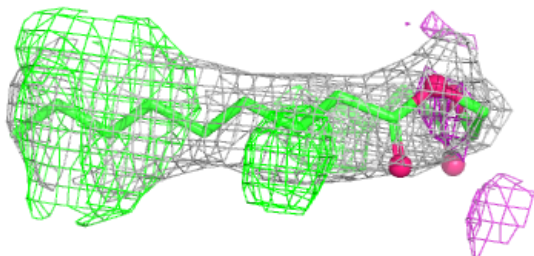
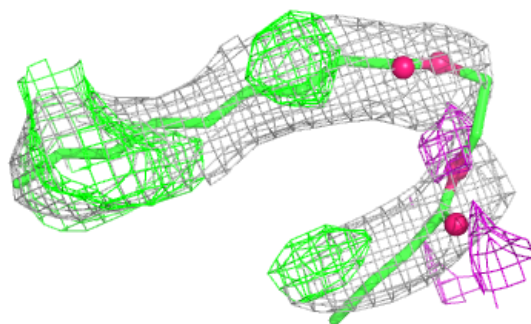


Electron density around PGW B 603:

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

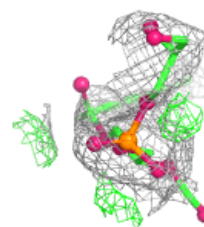
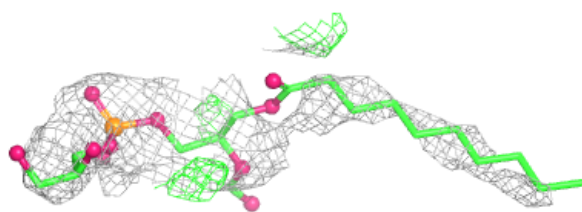
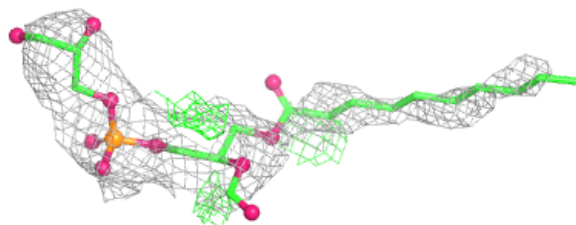
**Electron density around PGW B 601:**

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

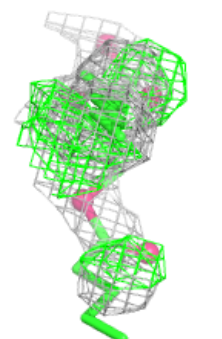
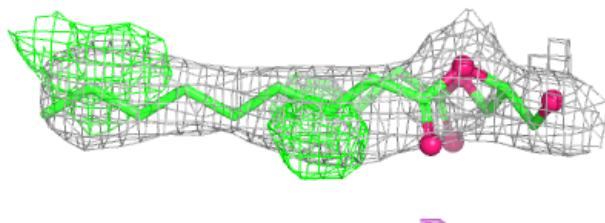
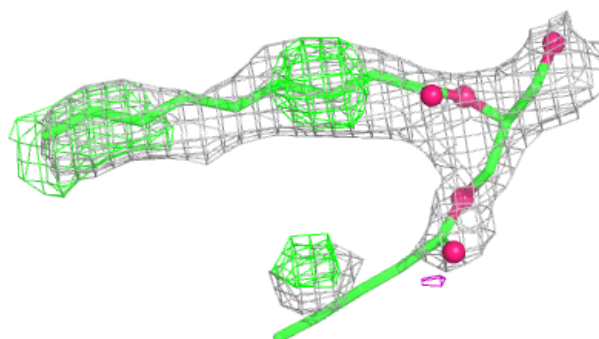


Electron density around PGW B 610:

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

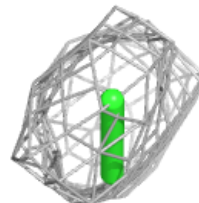
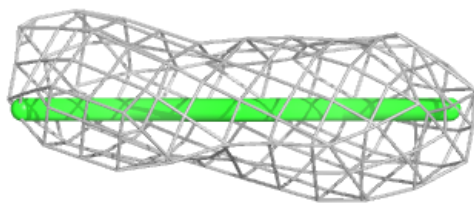
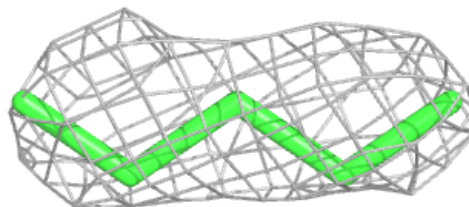
**Electron density around PGW D 601:**

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



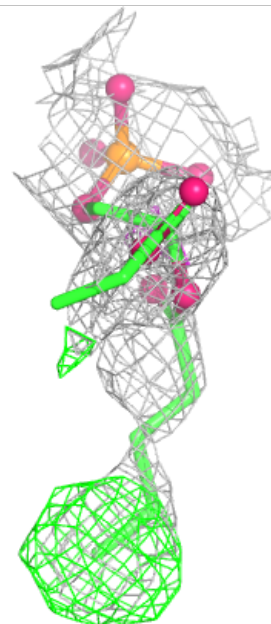
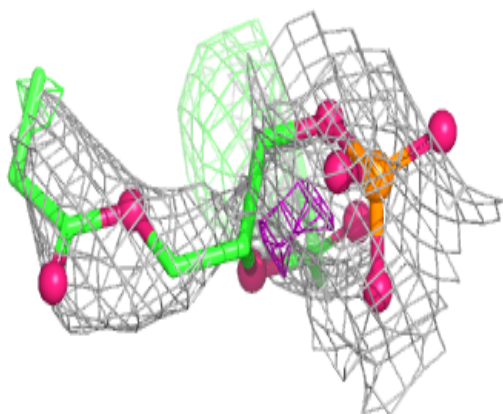
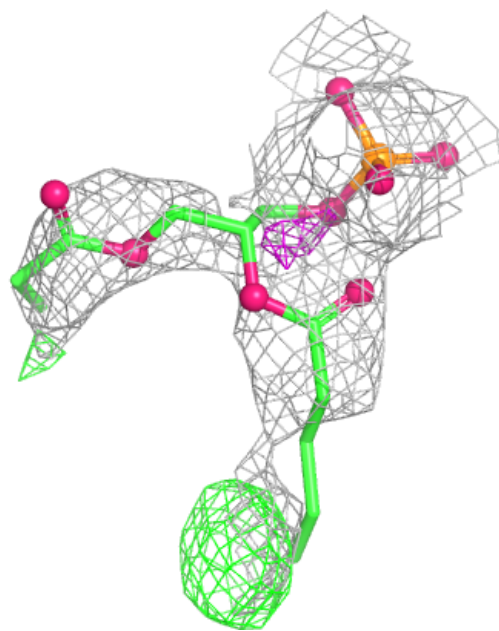
Electron density around PGW B 604:

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



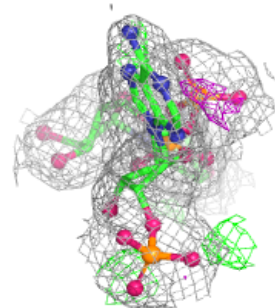
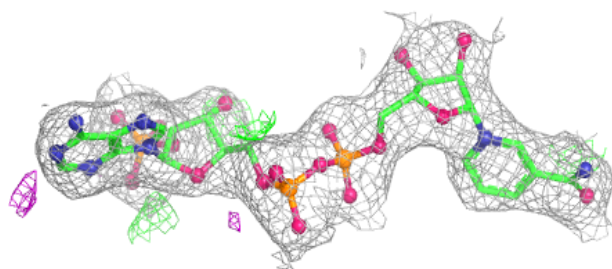
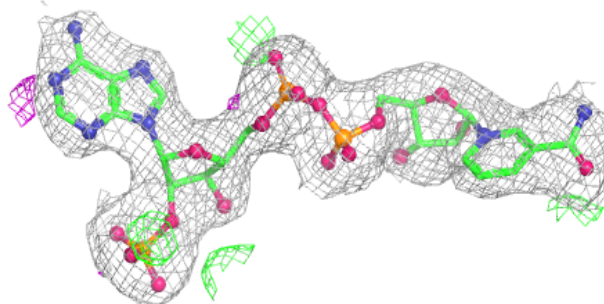
Electron density around PGW B 608:

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

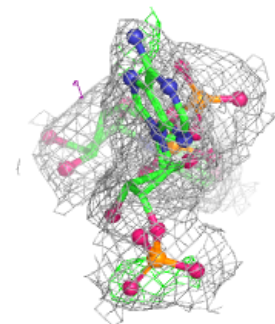
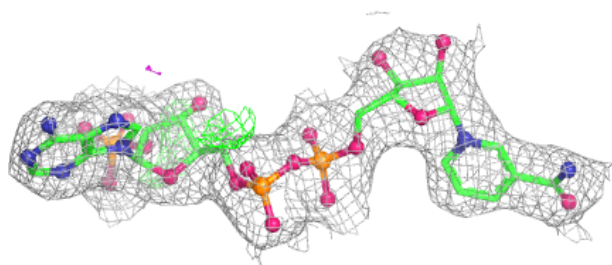
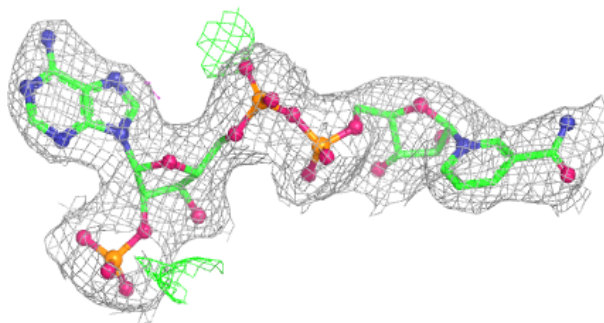


Electron density around NAP A 1001:

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

**Electron density around NAP C 1001:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.