



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:17 PM UTC

PDB ID : 7XYO / pdb_00007xyo
Title : Crystal Structure of a M61 aminopeptidase family member from Myxococcus fulvus
Authors : Chen, X.; Wang, X.; Huo, L.; Wu, D.
Deposited on : 2022-06-02
Resolution : 2.70 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

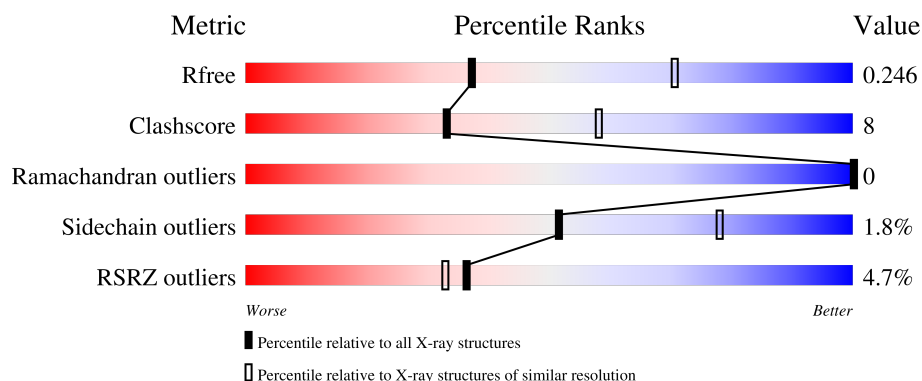
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	557	4% 77% 15% 6%
1	B	557	5% 77% 16% 6%

2 Entry composition [i](#)

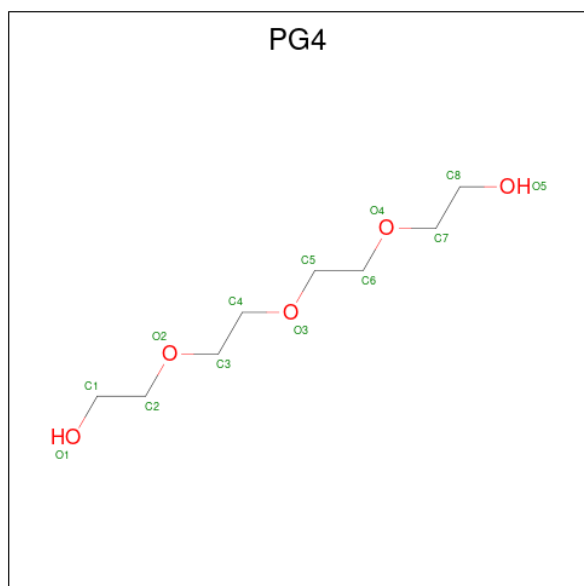
There are 5 unique types of molecules in this entry. The entry contains 8444 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aminopeptidase M61.

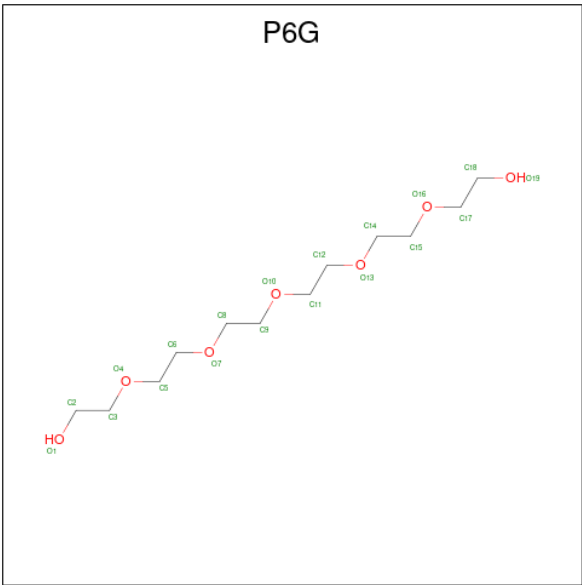
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			4137	2633	755	740	9			
1	B	522	Total	C	N	O	S	0	0	0
			4121	2623	753	736	9			

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			19	12 7		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

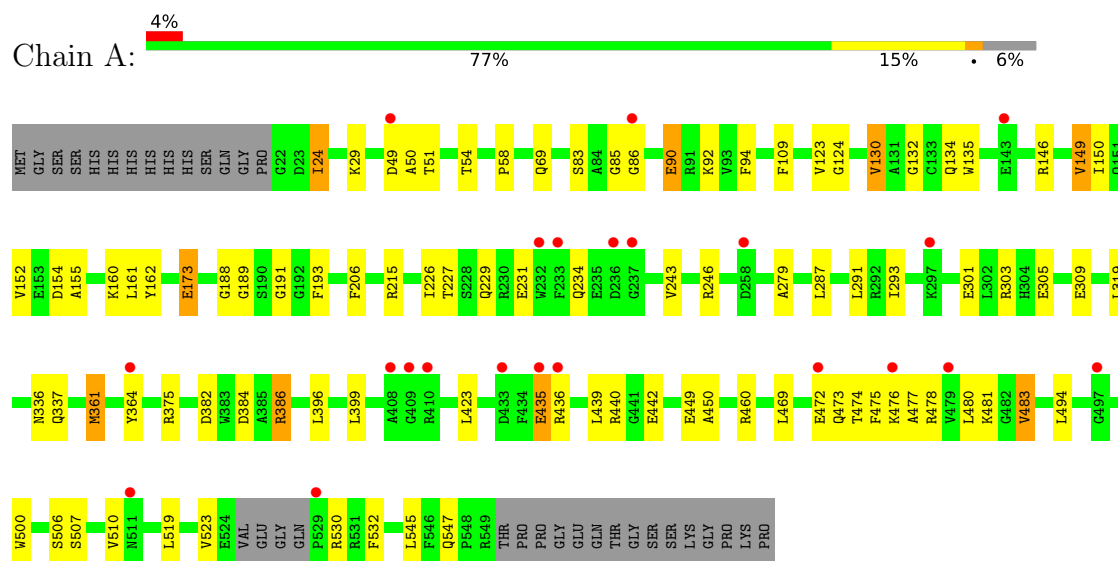
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		
5	B	67	Total	O	0	0
			67	67		

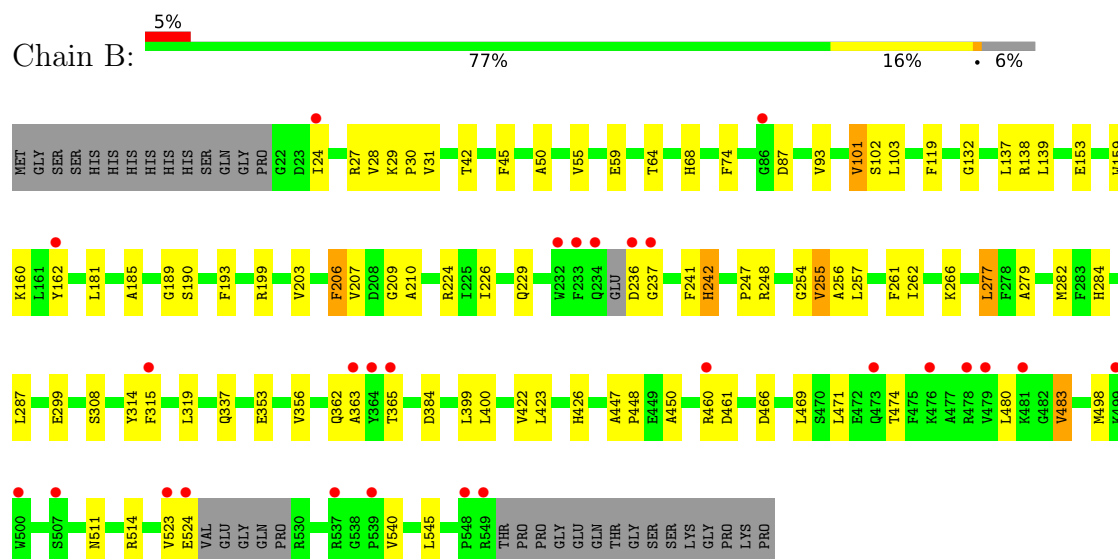
3 Residue-property plots [i](#)

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: Aminopeptidase M61



• Molecule 1: Aminopeptidase M61



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.68Å 113.28Å 132.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.11 – 2.70 41.11 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.3 (41.11-2.70) 87.8 (41.11-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.217 , 0.250 0.225 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (5.36%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8444	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0178e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, P6G, PG4

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	1.28	27/4247 (0.6%)	0.88	11/5751 (0.2%)
1	B	1.25	40/4229 (0.9%)	0.88	17/5725 (0.3%)
All	All	1.26	67/8476 (0.8%)	0.88	28/11476 (0.2%)

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	GLY	C-O	-10.44	1.17	1.24
1	B	466	ASP	C-O	-7.38	1.19	1.25
1	B	64	THR	CA-C	-6.80	1.45	1.53
1	A	215	ARG	C-O	-6.59	1.16	1.24
1	A	24	ILE	C-O	-6.52	1.17	1.24
1	A	303	ARG	CA-C	-6.52	1.43	1.52
1	B	210	ALA	C-O	-6.50	1.16	1.24
1	B	262	ILE	C-O	-6.47	1.16	1.24
1	B	248	ARG	C-O	-6.43	1.15	1.23
1	B	206	PHE	C-O	-6.43	1.16	1.24
1	A	243	VAL	C-O	-6.42	1.17	1.24
1	B	256	ALA	CA-C	-6.40	1.45	1.52
1	B	30	PRO	C-O	-6.34	1.17	1.23
1	A	287	LEU	C-O	-6.28	1.19	1.25
1	B	28	VAL	C-O	-6.27	1.17	1.24
1	A	94	PHE	C-N	6.24	1.41	1.33
1	A	130	VAL	C-O	-6.23	1.17	1.24
1	A	226	ILE	C-O	-6.07	1.17	1.24
1	B	261	PHE	C-O	-6.01	1.17	1.24
1	B	337	GLN	C-O	-5.96	1.17	1.24
1	B	279	ALA	C-O	-5.94	1.16	1.24
1	A	206	PHE	C-O	-5.94	1.17	1.24
1	B	356	VAL	C-N	-5.93	1.25	1.34
1	A	279	ALA	C-O	-5.93	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	VAL	C-O	-5.89	1.16	1.23
1	B	29	LYS	C-O	-5.86	1.17	1.24
1	A	150	ILE	C-O	-5.83	1.17	1.24
1	B	193	PHE	N-CA	-5.74	1.38	1.46
1	B	42	THR	C-O	-5.74	1.16	1.24
1	B	160	LYS	C-O	-5.70	1.16	1.24
1	B	287	LEU	C-N	5.68	1.45	1.34
1	A	160	LYS	N-CA	-5.67	1.39	1.46
1	B	207	VAL	C-O	-5.67	1.18	1.24
1	B	247	PRO	C-O	-5.67	1.18	1.23
1	B	181	LEU	N-CA	-5.63	1.38	1.46
1	B	189	GLY	C-O	-5.56	1.18	1.23
1	A	337	GLN	C-O	-5.55	1.17	1.24
1	A	29	LYS	C-O	-5.54	1.18	1.24
1	A	173	GLU	C-O	-5.47	1.17	1.23
1	B	450	ALA	CA-C	-5.44	1.45	1.52
1	A	173	GLU	CA-CB	-5.39	1.45	1.53
1	B	101	VAL	C-O	-5.35	1.18	1.24
1	A	375	ARG	N-CA	-5.35	1.40	1.46
1	B	287	LEU	N-CA	-5.34	1.39	1.46
1	B	209	GLY	C-O	-5.33	1.17	1.23
1	A	149	VAL	C-O	-5.32	1.18	1.24
1	A	109	PHE	C-O	-5.32	1.17	1.24
1	B	31	VAL	C-O	-5.32	1.18	1.23
1	B	224	ARG	C-O	-5.30	1.17	1.24
1	A	94	PHE	C-O	-5.29	1.17	1.24
1	B	153	GLU	C-O	-5.25	1.17	1.23
1	B	255	VAL	C-O	-5.22	1.18	1.24
1	A	336	ASN	C-O	-5.16	1.18	1.24
1	B	132	GLY	C-O	-5.16	1.17	1.23
1	B	242	HIS	C-O	-5.16	1.17	1.24
1	B	277	LEU	C-O	-5.14	1.17	1.24
1	A	124	GLY	C-O	-5.11	1.17	1.24
1	B	68	HIS	C-O	-5.10	1.17	1.24
1	B	203	VAL	C-O	-5.09	1.19	1.24
1	B	257	LEU	N-CA	-5.09	1.39	1.45
1	A	69	GLN	CD-OE1	5.09	1.33	1.23
1	B	474	THR	CA-C	-5.08	1.46	1.52
1	B	27	ARG	C-O	-5.08	1.18	1.24
1	B	308	SER	C-O	-5.04	1.17	1.24
1	A	132	GLY	C-O	-5.03	1.17	1.23
1	B	226	ILE	C-O	-5.02	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	PHE	C-O	-5.02	1.17	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	ALA	N-CA-C	7.73	121.81	112.38
1	B	237	GLY	CA-C-N	7.18	127.16	119.76
1	B	237	GLY	C-N-CA	7.18	127.16	119.76
1	A	303	ARG	N-CA-C	6.55	120.13	111.75
1	B	511	ASN	N-CA-C	6.45	120.00	111.75
1	B	450	ALA	N-CA-C	6.26	120.17	112.54
1	B	254	GLY	O-C-N	-6.16	118.59	123.27
1	B	363	ALA	N-CA-C	-6.12	101.07	109.71
1	B	362	GLN	N-CA-C	5.89	120.04	112.86
1	A	90	GLU	N-CA-C	5.76	119.35	110.42
1	A	483	VAL	CB-CA-C	-5.58	104.55	111.08
1	B	448	PRO	N-CA-C	5.39	120.66	114.03
1	A	134	GLN	N-CA-C	5.38	119.69	113.18
1	B	287	LEU	CA-C-O	-5.34	114.67	119.59
1	B	474	THR	CB-CA-C	-5.32	102.49	110.90
1	A	58	PRO	N-CA-C	5.32	119.44	111.14
1	A	189	GLY	N-CA-C	5.30	118.31	110.42
1	A	155	ALA	CA-C-N	-5.29	114.51	119.85
1	A	155	ALA	C-N-CA	-5.29	114.51	119.85
1	B	365	THR	N-CA-C	5.28	116.74	110.19
1	A	150	ILE	N-CA-C	5.15	115.27	107.75
1	B	356	VAL	CB-CA-C	-5.14	103.93	112.26
1	B	299	GLU	CB-CA-C	5.10	116.06	108.87
1	B	185	ALA	N-CA-C	5.09	117.12	109.23
1	B	447	ALA	CA-C-N	-5.09	114.58	119.87
1	B	447	ALA	C-N-CA	-5.09	114.58	119.87
1	B	50	ALA	N-CA-C	5.08	119.05	113.21
1	A	109	PHE	N-CA-CB	-5.01	102.19	109.95

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	4137	0	4060	71	0
1	B	4121	0	4045	57	0
2	A	13	0	18	0	0
2	B	13	0	18	2	0
3	A	19	0	26	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	72	0	0	0	0
5	B	67	0	0	0	0
All	All	8444	0	8167	129	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 8.

All (129) 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:B:460:ARG:HD3	1:B:545:LEU:CD1	1.63	1.25
1:B:460:ARG:CD	1:B:545:LEU:HD12	1.70	1.21
1:A:399:LEU:HD21	1:A:423:LEU:CD2	1.72	1.18
1:A:477:ALA:HB2	1:A:481:LYS:NZ	1.57	1.17
1:A:477:ALA:CB	1:A:481:LYS:HE3	1.76	1.12
1:A:477:ALA:HB3	1:A:481:LYS:HE3	1.30	1.09
1:A:49:ASP:OD2	1:A:51:THR:HG23	1.53	1.08
1:B:74:PHE:CZ	1:B:103:LEU:HD23	1.97	1.00
1:A:231:GLU:O	1:A:234:GLN:HG3	1.61	0.99
1:A:460:ARG:HD3	1:A:545:LEU:HD22	1.46	0.98
1:A:477:ALA:CB	1:A:481:LYS:CE	2.44	0.96
1:A:477:ALA:HB2	1:A:481:LYS:CE	2.00	0.91
1:B:460:ARG:HD3	1:B:545:LEU:HD12	0.91	0.90
1:A:477:ALA:HB2	1:A:481:LYS:HZ1	1.35	0.89
3:A:702:P6G:H182	3:A:702:P6G:H21	1.53	0.88
1:A:152:VAL:HG11	1:A:161:LEU:CD1	2.03	0.86
1:A:399:LEU:HD21	1:A:423:LEU:HD22	1.59	0.84
1:A:478:ARG:NH1	1:A:500:TRP:HZ3	1.75	0.84
1:A:399:LEU:HD21	1:A:423:LEU:HD21	1.59	0.83
1:B:162:TYR:HB3	1:B:206:PHE:CZ	2.17	0.80
1:A:477:ALA:CB	1:A:481:LYS:NZ	2.44	0.79
1:A:86:GLY:HA3	1:A:90:GLU:OE2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LEU:HD23	1:A:188:GLY:HA3	1.64	0.79
1:B:137:LEU:HB3	1:B:139:LEU:HD11	1.66	0.77
1:A:152:VAL:HG11	1:A:161:LEU:HD13	1.65	0.77
1:A:460:ARG:HD2	1:A:547:GLN:HE22	1.48	0.76
1:A:24:ILE:HD11	1:A:146:ARG:HD3	1.68	0.76
1:B:74:PHE:CZ	1:B:103:LEU:CD2	2.68	0.75
1:A:227:THR:O	1:A:231:GLU:HG3	1.88	0.72
1:B:523:VAL:HG12	1:B:524:GLU:N	2.03	0.72
1:A:477:ALA:HB3	1:A:481:LYS:CE	2.14	0.71
1:B:138:ARG:C	1:B:139:LEU:HD12	2.15	0.71
1:A:477:ALA:HB2	1:A:481:LYS:HZ2	1.55	0.71
1:A:472:GLU:H	1:A:472:GLU:CD	2.01	0.69
1:B:74:PHE:CE1	1:B:103:LEU:HD23	2.27	0.69
1:A:507:SER:OG	1:A:510:VAL:HG22	1.94	0.67
1:B:55:VAL:HG12	1:B:139:LEU:HG	1.76	0.67
1:A:152:VAL:HG11	1:A:161:LEU:HD11	1.75	0.67
1:A:545:LEU:HD12	1:A:545:LEU:N	2.10	0.66
1:A:86:GLY:CA	1:A:90:GLU:OE2	2.43	0.65
1:A:530:ARG:NH1	1:A:532:PHE:CE1	2.66	0.64
1:B:399:LEU:HD21	1:B:423:LEU:HD22	1.79	0.63
1:A:86:GLY:N	1:A:90:GLU:OE2	2.31	0.63
1:A:436:ARG:O	1:A:442:GLU:HB2	1.99	0.62
1:A:478:ARG:NH1	1:A:500:TRP:CZ3	2.65	0.61
1:B:137:LEU:HB3	1:B:139:LEU:CD1	2.31	0.60
1:A:475:PHE:CE1	1:A:500:TRP:CZ2	2.90	0.60
1:B:24:ILE:HD13	1:B:45:PHE:CB	2.32	0.59
1:B:461:ASP:HB3	1:B:540:VAL:CG1	2.32	0.58
1:A:472:GLU:OE1	1:A:472:GLU:N	2.28	0.58
1:A:507:SER:OG	1:A:510:VAL:CG2	2.52	0.57
1:A:85:GLY:HA3	1:A:90:GLU:HG3	1.85	0.57
1:A:24:ILE:CD1	1:A:146:ARG:HD3	2.34	0.57
1:B:315:PHE:CE2	1:B:400:LEU:HD22	2.39	0.57
1:B:498:MET:SD	1:B:523:VAL:HG11	2.44	0.57
1:B:119:PHE:CE1	1:B:255:VAL:HG13	2.41	0.56
1:B:523:VAL:HG12	1:B:524:GLU:H	1.70	0.56
1:A:384:ASP:OD1	1:A:396:LEU:N	2.33	0.56
1:A:472:GLU:O	1:A:476:LYS:HG3	2.06	0.55
1:B:139:LEU:HD12	1:B:139:LEU:N	2.22	0.55
1:A:399:LEU:CD2	1:A:423:LEU:CD2	2.66	0.55
1:B:523:VAL:CG1	1:B:524:GLU:N	2.69	0.54
1:B:514:ARG:HH11	1:B:514:ARG:HG3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:LEU:C	1:B:469:LEU:HD12	2.32	0.54
1:A:399:LEU:HD21	1:A:423:LEU:HD23	1.83	0.54
1:A:473:GLN:O	1:A:481:LYS:HD2	2.08	0.54
1:B:87:ASP:OD1	1:B:87:ASP:N	2.31	0.53
1:B:199:ARG:HE	1:B:236:ASP:N	2.06	0.53
1:B:24:ILE:HD13	1:B:45:PHE:HB3	1.89	0.52
1:A:545:LEU:N	1:A:545:LEU:CD1	2.73	0.52
1:B:461:ASP:HB3	1:B:540:VAL:HG11	1.90	0.52
1:A:530:ARG:NH1	1:A:532:PHE:CZ	2.78	0.52
1:A:49:ASP:CG	1:A:50:ALA:N	2.68	0.51
1:B:399:LEU:HD13	1:B:426:HIS:CD2	2.45	0.51
1:B:399:LEU:HD11	1:B:422:VAL:HG12	1.92	0.51
1:B:315:PHE:CZ	1:B:400:LEU:HD22	2.45	0.51
1:B:266:LYS:HZ1	2:B:601:PG4:H22	1.76	0.50
1:B:266:LYS:NZ	2:B:601:PG4:H22	2.27	0.50
1:B:480:LEU:HD12	1:B:498:MET:HB3	1.94	0.50
1:A:301:GLU:O	1:A:301:GLU:HG3	2.11	0.50
1:A:382:ASP:O	1:A:386:ARG:HG3	2.12	0.50
1:A:435:GLU:O	1:A:440:ARG:NE	2.45	0.50
1:A:436:ARG:HG2	1:A:440:ARG:NH1	2.27	0.49
1:B:353:GLU:OE1	1:B:353:GLU:N	2.42	0.49
1:A:399:LEU:HD11	1:A:423:LEU:HD23	1.94	0.49
1:B:460:ARG:CD	1:B:545:LEU:CD1	2.53	0.49
1:B:74:PHE:CE1	1:B:103:LEU:CD2	2.95	0.49
1:B:159:TRP:CD1	1:B:190:SER:HB3	2.48	0.49
1:B:314:TYR:OH	1:B:384:ASP:OD2	2.29	0.49
1:A:162:TYR:HE2	1:A:246:ARG:NH2	2.11	0.49
1:A:305:GLU:O	1:A:309:GLU:HB2	2.12	0.49
1:A:83:SER:OG	1:A:92:LYS:HB3	2.13	0.48
1:A:49:ASP:CG	1:A:50:ALA:H	2.21	0.48
1:A:149:VAL:HG22	1:A:173:GLU:HG3	1.95	0.48
1:A:460:ARG:HD2	1:A:547:GLN:NE2	2.24	0.48
1:B:229:GLN:HG3	1:B:319:LEU:HD11	1.96	0.48
1:B:241:PHE:CE2	1:B:282:MET:HE3	2.49	0.47
1:B:162:TYR:HB2	1:B:242:HIS:CG	2.49	0.47
1:A:231:GLU:O	1:A:234:GLN:CG	2.50	0.47
1:A:436:ARG:O	1:A:442:GLU:CB	2.63	0.47
1:B:102:SER:C	1:B:103:LEU:HD12	2.40	0.46
1:B:523:VAL:CG1	1:B:524:GLU:H	2.27	0.46
1:B:469:LEU:HD11	1:B:471:LEU:HD23	1.97	0.46
1:B:139:LEU:CD1	1:B:139:LEU:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:PHE:HE2	1:B:282:MET:HE3	1.81	0.45
1:A:475:PHE:CD1	1:A:500:TRP:CZ2	3.05	0.44
1:B:514:ARG:HG3	1:B:514:ARG:NH1	2.33	0.44
1:A:480:LEU:HD11	1:A:494:LEU:HD22	1.99	0.44
1:A:384:ASP:OD1	1:A:396:LEU:HB2	2.19	0.43
1:A:361:MET:HE2	1:A:361:MET:HB2	1.86	0.43
1:B:162:TYR:O	1:B:162:TYR:CG	2.71	0.43
1:B:74:PHE:HZ	1:B:103:LEU:CD2	2.28	0.42
1:B:137:LEU:CB	1:B:139:LEU:HD11	2.43	0.42
1:B:162:TYR:HB3	1:B:206:PHE:CE1	2.53	0.42
1:A:435:GLU:HA	1:A:439:LEU:HB2	2.02	0.42
1:B:423:LEU:N	1:B:423:LEU:HD23	2.34	0.42
1:A:291:LEU:C	1:A:291:LEU:HD12	2.45	0.42
1:B:483:VAL:O	1:B:483:VAL:HG12	2.20	0.42
1:A:86:GLY:H	1:A:90:GLU:CD	2.28	0.42
1:B:399:LEU:HD13	1:B:426:HIS:CE1	2.55	0.42
1:A:506:SER:HA	1:A:519:LEU:CD1	2.49	0.41
1:B:24:ILE:HD13	1:B:45:PHE:HB2	2.01	0.41
1:B:461:ASP:HB3	1:B:540:VAL:HG13	2.00	0.41
1:B:101:VAL:HG12	1:B:103:LEU:HD13	2.03	0.41
1:A:229:GLN:HG3	1:A:319:LEU:HD11	2.03	0.41
1:A:293:ILE:HD13	1:A:293:ILE:HG21	1.83	0.41
1:A:130:VAL:HG21	1:A:135:TRP:CD1	2.56	0.40
1:A:494:LEU:CD2	1:A:523:VAL:HG11	2.51	0.40
1:A:475:PHE:CE1	1:A:500:TRP:CE2	3.10	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	520/557 (93%)	502 (96%)	18 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	516/557 (93%)	496 (96%)	20 (4%)	0	100	100
All	All	1036/1114 (93%)	998 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	419/446 (94%)	409 (98%)	10 (2%)	43	72
1	B	417/446 (94%)	412 (99%)	5 (1%)	63	84
All	All	836/892 (94%)	821 (98%)	15 (2%)	51	78

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	THR
1	A	154	ASP
1	A	361	MET
1	A	364	TYR
1	A	386	ARG
1	A	435	GLU
1	A	449	GLU
1	A	469	LEU
1	A	474	THR
1	A	483	VAL
1	B	59	GLU
1	B	93	VAL
1	B	277	LEU
1	B	284	HIS
1	B	483	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	217	GLN
1	A	547	GLN
1	B	284	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	P6G	A	702	-	18,18,18	0.75	0	17,17,17	0.90	1 (5%)
2	PG4	A	701	-	12,12,12	0.68	0	11,11,11	0.74	0
2	PG4	B	601	-	12,12,12	0.54	0	11,11,11	0.21	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	P6G	A	702	-	-	9/16/16/16	-
2	PG4	A	701	-	-	1/10/10/10	-
2	PG4	B	601	-	-	6/10/10/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	P6G	C11-O10-C9	2.50	124.21	113.26

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	P6G	O4-C5-C6-O7
3	A	702	P6G	C9-C8-O7-C6
2	B	601	PG4	O2-C3-C4-O3
3	A	702	P6G	O7-C8-C9-O10
2	A	701	PG4	O4-C7-C8-O5
2	B	601	PG4	O3-C5-C6-O4
3	A	702	P6G	C2-C3-O4-C5
3	A	702	P6G	C15-C14-O13-C12
3	A	702	P6G	C8-C9-O10-C11
2	B	601	PG4	C1-C2-O2-C3
3	A	702	P6G	O10-C11-C12-O13
2	B	601	PG4	O1-C1-C2-O2
3	A	702	P6G	C18-C17-O16-C15
2	B	601	PG4	C4-C3-O2-C2
3	A	702	P6G	C5-C6-O7-C8
2	B	601	PG4	O4-C7-C8-O5

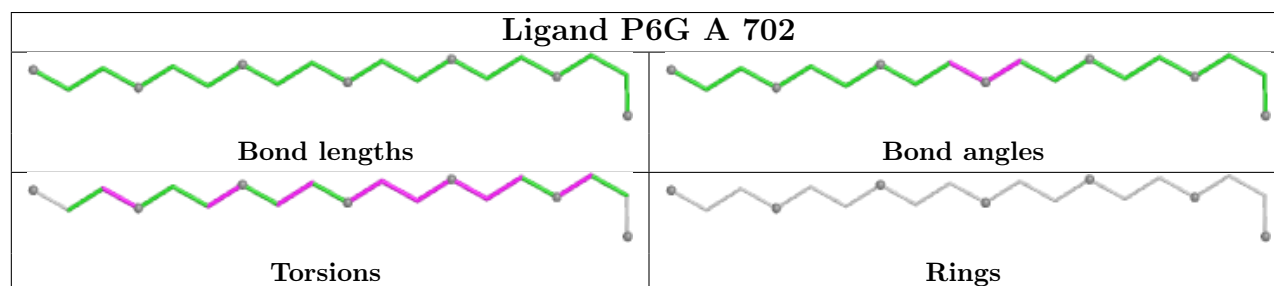
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	P6G	1	0
2	B	601	PG4	2	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	524/557 (94%)	0.21	22 (4%) 40 37	21, 40, 78, 163	0
1	B	522/557 (93%)	0.29	27 (5%) 33 29	21, 42, 85, 121	0
All	All	1046/1114 (93%)	0.25	49 (4%) 36 33	21, 41, 81, 163	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	GLY	8.4
1	B	232	TRP	5.3
1	B	363	ALA	4.6
1	B	236	ASP	3.8
1	B	524	GLU	3.8
1	B	364	TYR	3.5
1	B	233	PHE	3.5
1	B	162	TYR	3.4
1	B	537	ARG	3.3
1	B	234	GLN	3.3
1	B	460	ARG	3.2
1	A	364	TYR	3.0
1	A	232	TRP	2.9
1	B	479	VAL	2.9
1	A	297	LYS	2.9
1	A	476	LYS	2.9
1	A	49	ASP	2.7
1	B	539	PRO	2.7
1	A	143	GLU	2.7
1	A	410	ARG	2.7
1	B	237	GLY	2.6
1	A	433	ASP	2.6
1	A	511	ASN	2.6
1	A	86	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	497	GLY	2.4
1	A	529	PRO	2.4
1	A	233	PHE	2.4
1	B	478	ARG	2.4
1	A	435	GLU	2.4
1	B	481	LYS	2.3
1	B	500	TRP	2.3
1	B	86	GLY	2.3
1	B	507	SER	2.3
1	A	472	GLU	2.3
1	B	523	VAL	2.2
1	A	258	ASP	2.2
1	B	549	ARG	2.2
1	A	408	ALA	2.1
1	B	476	LYS	2.1
1	A	479	VAL	2.1
1	B	24	ILE	2.1
1	B	473	GLN	2.1
1	B	548	PRO	2.1
1	A	236	ASP	2.1
1	B	315	PHE	2.1
1	A	436	ARG	2.1
1	B	365	THR	2.0
1	B	499	LYS	2.0
1	A	237	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

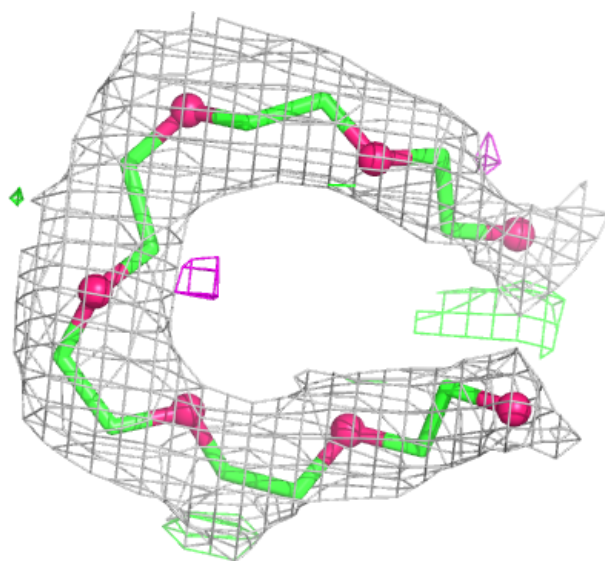
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	P6G	A	702	19/19	0.86	0.17	45,47,50,50	0
2	PG4	B	601	13/13	0.93	0.12	22,25,26,27	0
2	PG4	A	701	13/13	0.94	0.08	20,25,28,28	0
4	ZN	B	602	1/1	0.96	0.05	52,52,52,52	0
4	ZN	A	703	1/1	0.99	0.02	48,48,48,48	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.

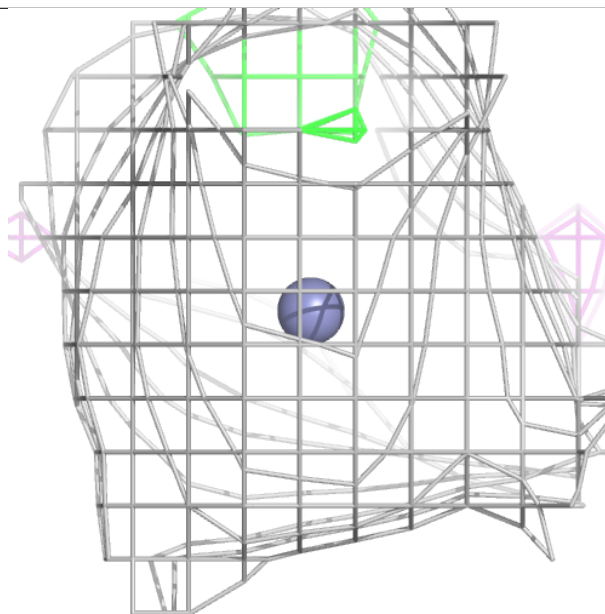
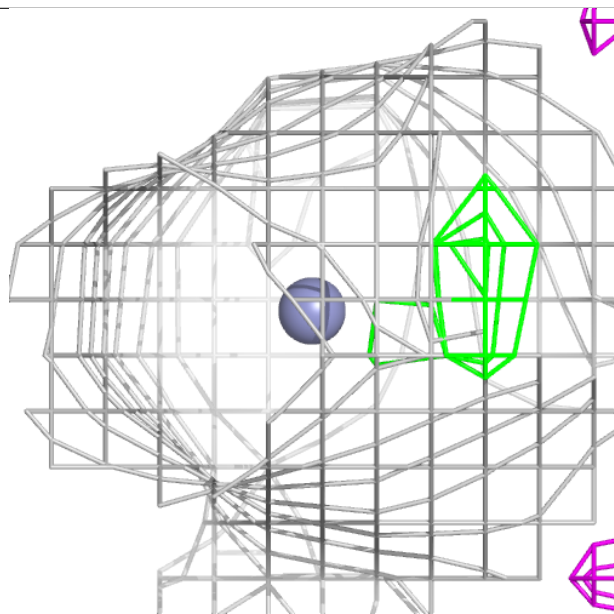
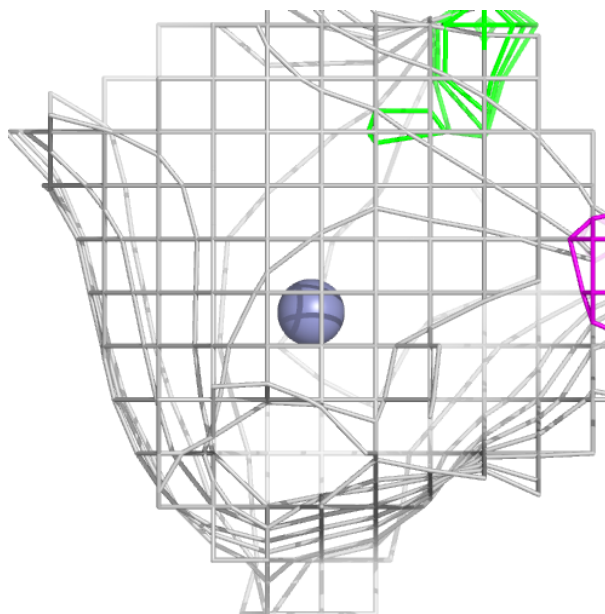
Electron density around P6G A 702:

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



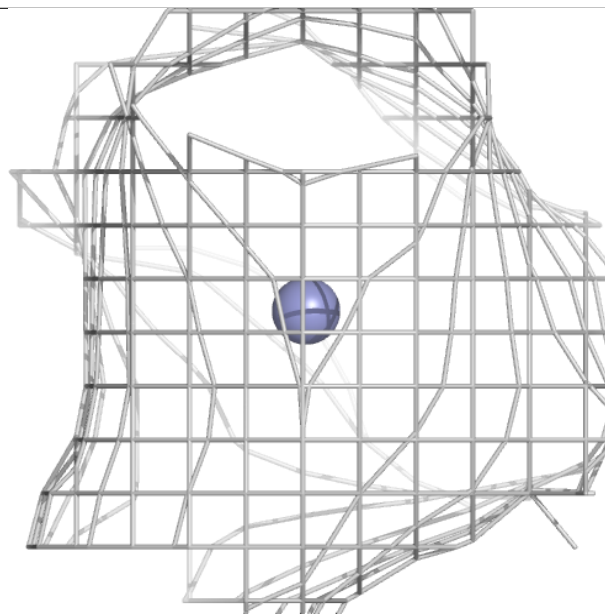
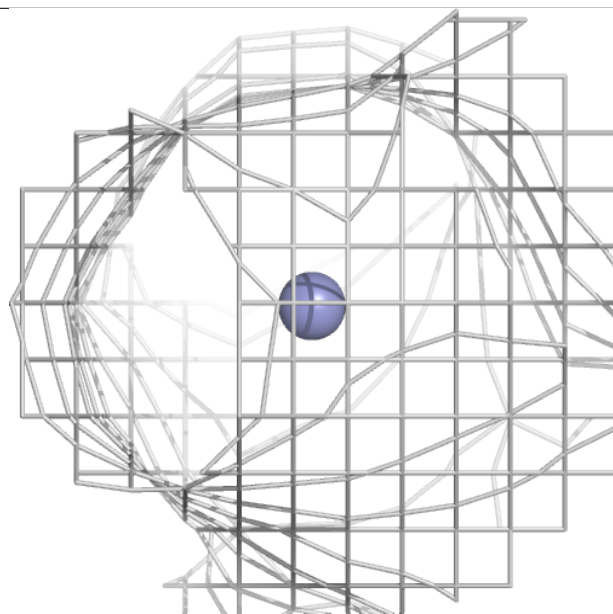
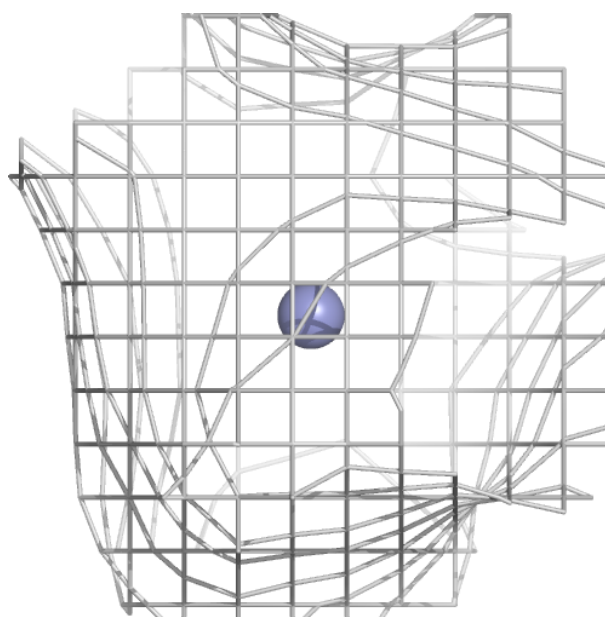
Electron density around ZN B 602:

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



Electron density around ZN A 703:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.