



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 01:53 AM UTC

PDB ID : 4PHZ / pdb_00004phz
Title : Crystal structure of particulate methane monooxygenase from *Methylocystis* sp. ATCC 49242 (Rockwell)
Authors : Sirajuddin, S.; Rosenzweig, A.C.
Deposited on : 2014-05-07
Resolution : 2.59 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

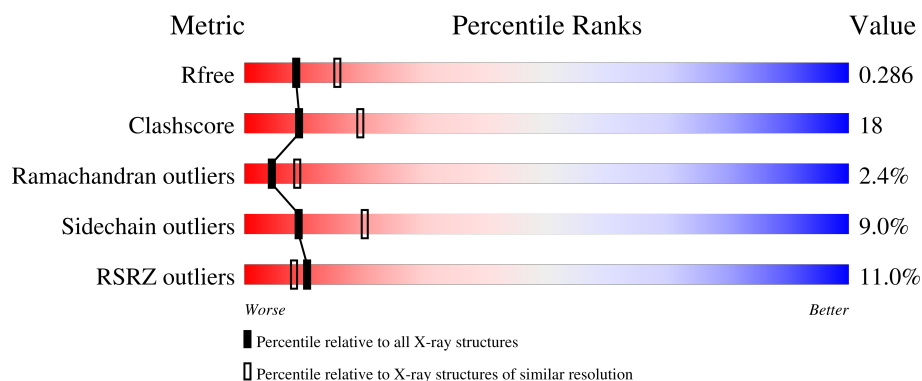
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	24	
1	H	24	
1	N	24	
2	C	256	
2	G	256	

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Mol	Chain	Length	Quality of chain
2	K	256	
3	A	420	
3	E	420	
3	I	420	
4	B	252	
4	F	252	
4	J	252	

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
6	PGT	K	302	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20853 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 unknown peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	D	19	Total	C	N	O	0	0	0
			95	57	19	19			
1	H	20	Total	C	N	O	0	0	0
			100	60	20	20			
1	N	24	Total	C	N	O	0	0	0
			120	72	24	24			

- Molecule 2 is a protein called Particulate methane monooxygenase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	213	Total	C	N	O	S	0	0	0
			1738	1166	275	289	8			
2	C	214	Total	C	N	O	S	0	0	0
			1742	1168	276	290	8			
2	G	212	Total	C	N	O	S	0	0	0
			1731	1161	274	288	8			

- Molecule 3 is a protein called Particulate methane monooxygenase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	388	Total	C	N	O	S	0	0	0
			3026	1946	521	555	4			
3	E	388	Total	C	N	O	S	0	0	0
			3026	1946	521	555	4			
3	I	388	Total	C	N	O	S	0	0	0
			3026	1946	521	555	4			

- Molecule 4 is a protein called Particulate methane monooxygenase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	244	Total	C	N	O	S	0	0	0
			1974	1336	311	316	11			

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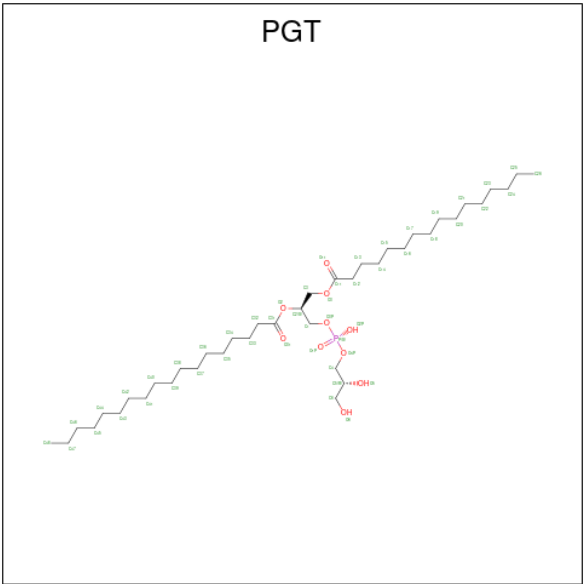
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	244	Total	C	N	O	S	0	0	0
			1974	1336	311	316	11			
4	J	244	Total	C	N	O	S	0	0	0
			1974	1336	311	316	11			

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	K	1	Total	Cu	0	0
			1	1		
5	A	1	Total	Cu	0	0
			1	1		
5	E	1	Total	Cu	0	0
			1	1		
5	I	1	Total	Cu	0	0
			1	1		
5	C	1	Total	Cu	0	0
			1	1		
5	G	1	Total	Cu	0	0
			1	1		

- Molecule 6 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	K	1	Total	C	O	P	0	0
			51	40	10	1		
6	C	1	Total	C	O	P	0	0
			51	40	10	1		
6	G	1	Total	C	O	P	0	0
			51	40	10	1		
6	G	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 7 is water.

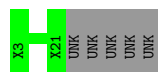
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	K	7	Total	O	0	0
			7	7		
7	A	13	Total	O	0	0
			13	13		
7	B	11	Total	O	0	0
			11	11		
7	E	25	Total	O	0	0
			25	25		
7	I	12	Total	O	0	0
			12	12		
7	F	18	Total	O	0	0
			18	18		
7	J	16	Total	O	0	0
			16	16		
7	C	4	Total	O	0	0
			4	4		
7	G	11	Total	O	0	0
			11	11		

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.

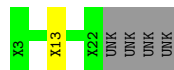
- Molecule 1: unknown peptide

Chain D: 



- Molecule 1: unknown peptide

Chain H: 



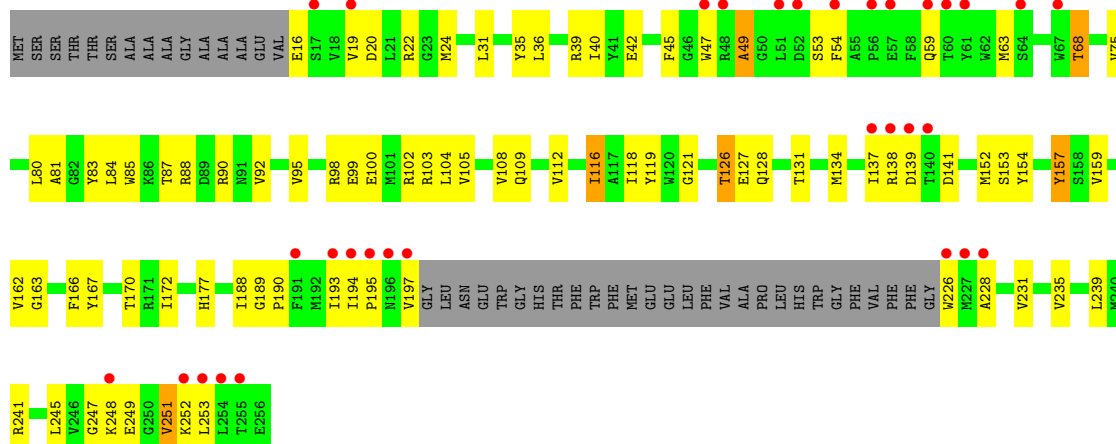
- Molecule 1: unknown peptide

Chain N: 

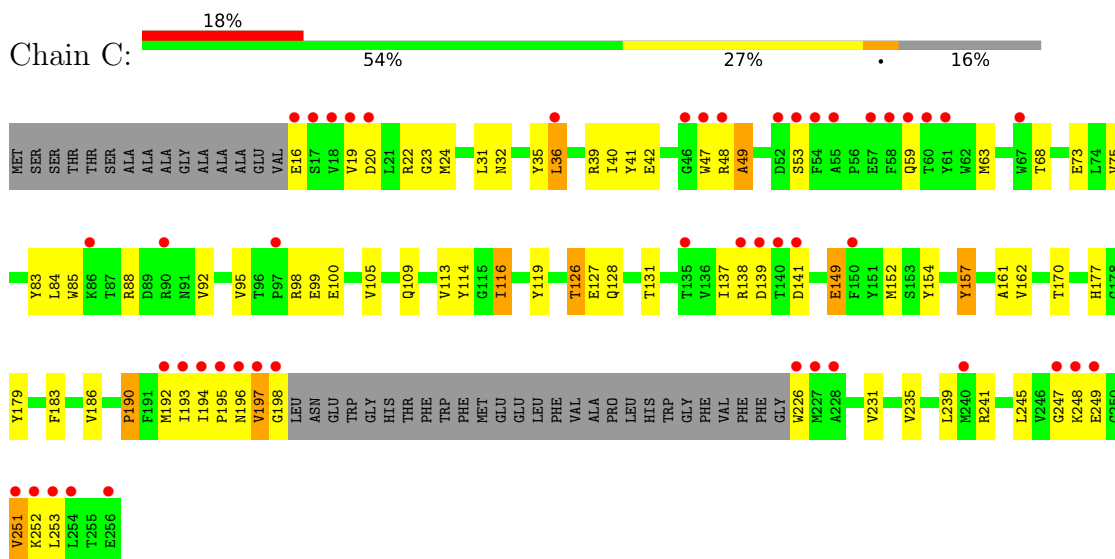


- Molecule 2: Particulate methane monooxygenase subunit C

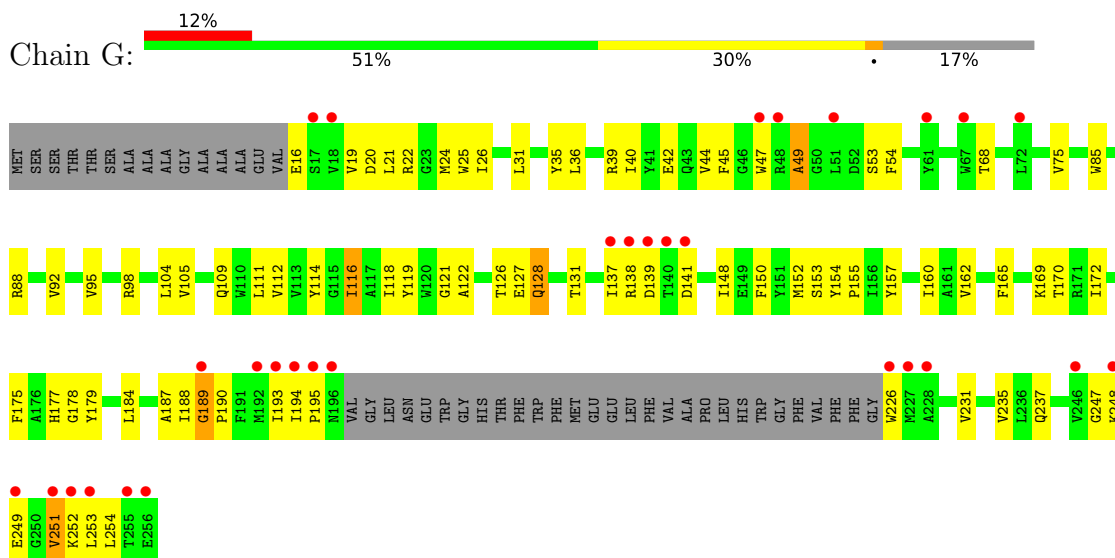
Chain K: 



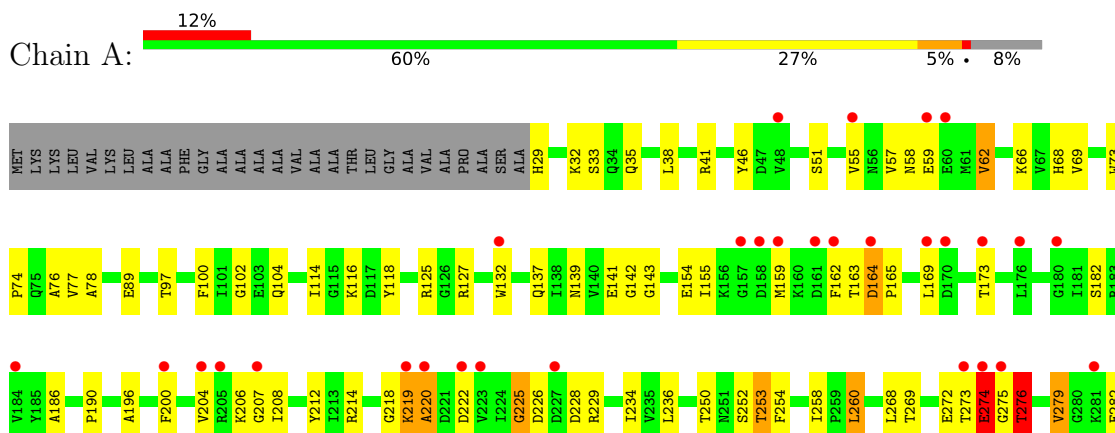
- Molecule 2: Particulate methane monooxygenase subunit C

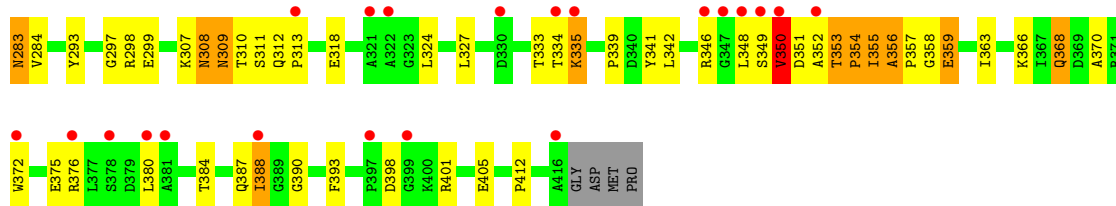


- Molecule 2: Particulate methane monooxygenase subunit C

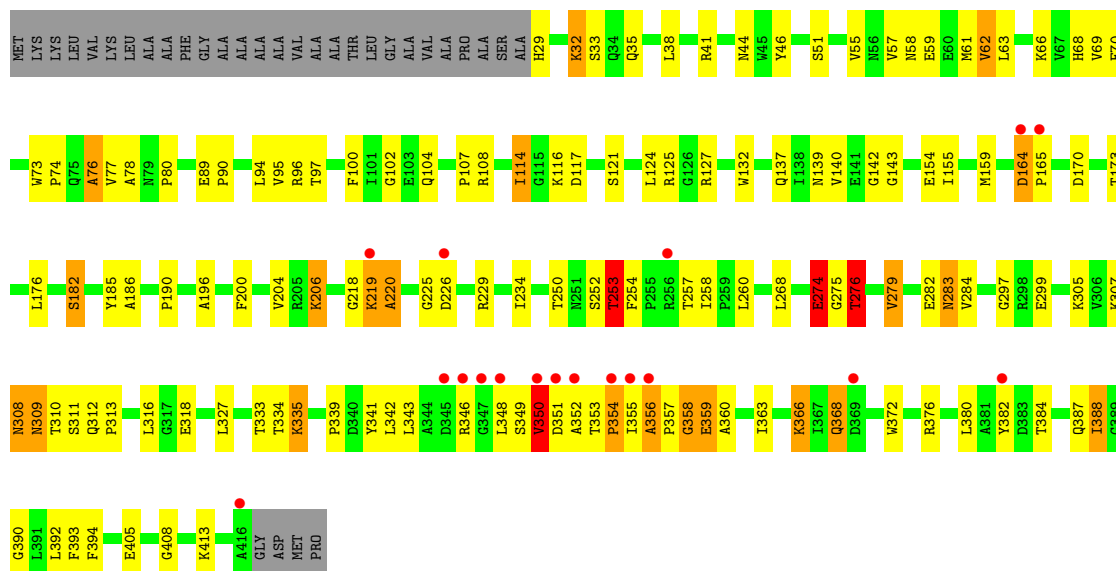


- Molecule 3: Particulate methane monooxygenase subunit B

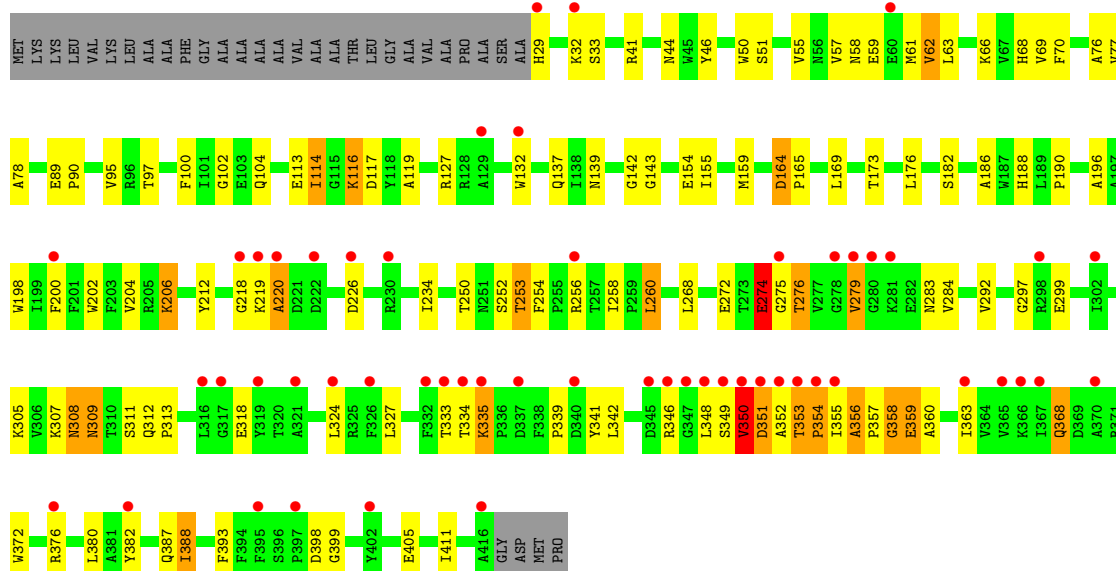




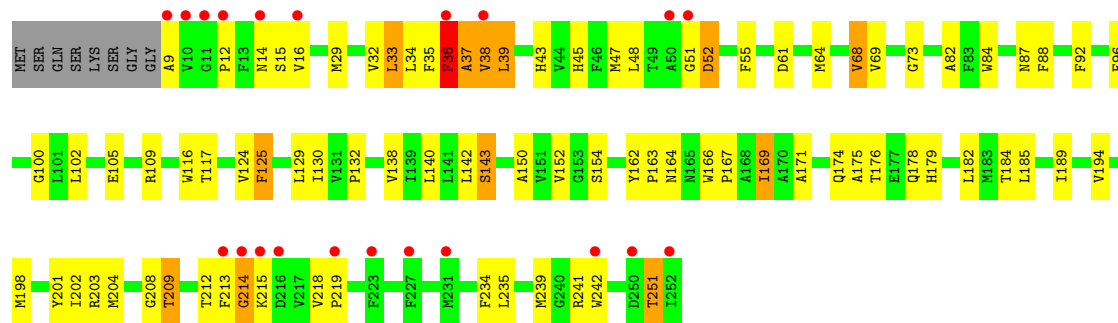
• Molecule 3: Particulate methane monooxygenase subunit B



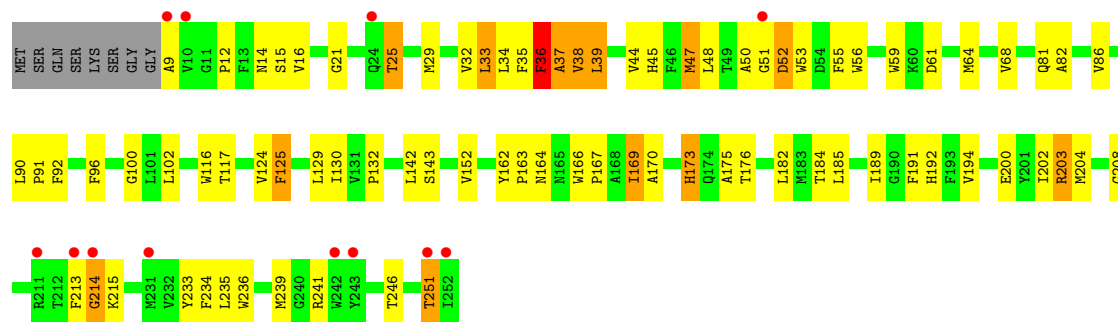
• Molecule 3: Particulate methane monooxygenase subunit B



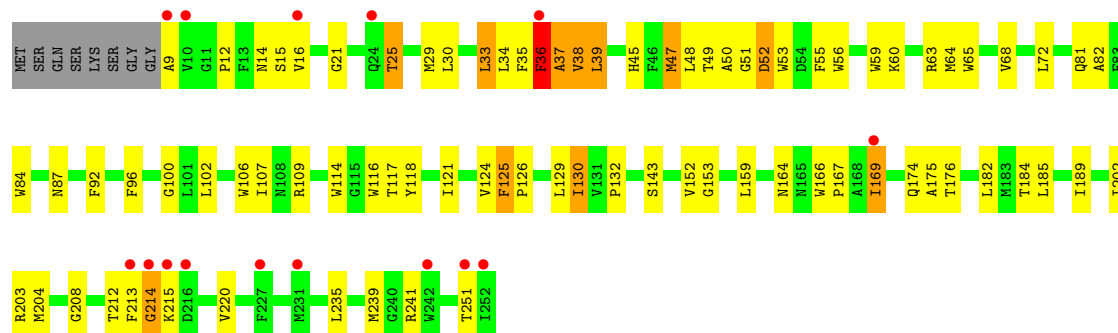
• Molecule 4: Particulate methane monooxygenase subunit A



• Molecule 4: Particulate methane monooxygenase subunit A



• Molecule 4: Particulate methane monooxygenase subunit A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.46Å 184.53Å 189.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.59 50.00 – 2.59	Depositor EDS
% Data completeness (in resolution range)	72.3 (50.00-2.59) 72.7 (50.00-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.237 , 0.289 0.235 , 0.286	Depositor DCC
R_{free} test set	4678 reflections (3.63%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20853	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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: PGT, CU

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	$\# Z > 5$
2	C	0.86	0/1796	0.99	0/2449
2	G	0.90	0/1785	1.02	2/2434 (0.1%)
2	K	0.92	0/1792	1.01	0/2444
3	A	0.84	1/3103 (0.0%)	1.10	12/4227 (0.3%)
3	E	0.97	1/3103 (0.0%)	1.16	10/4227 (0.2%)
3	I	0.86	2/3103 (0.1%)	1.14	11/4227 (0.3%)
4	B	0.94	2/2052 (0.1%)	1.11	5/2814 (0.2%)
4	F	1.09	2/2052 (0.1%)	1.16	12/2814 (0.4%)
4	J	1.10	2/2052 (0.1%)	1.21	12/2814 (0.4%)
All	All	0.94	10/20838 (0.0%)	1.11	64/28450 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1
3	E	0	2
3	I	0	2
4	B	0	1
4	F	0	2
4	J	0	2
All	All	0	10

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	45	HIS	CG-CD2	6.19	1.42	1.35
4	F	45	HIS	CG-CD2	6.08	1.42	1.35
3	A	254	PHE	N-CA	5.96	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	188	HIS	CG-CD2	5.69	1.42	1.35
3	I	254	PHE	N-CA	5.67	1.50	1.46
3	E	254	PHE	N-CA	5.46	1.50	1.46
4	B	45	HIS	CG-CD2	5.33	1.41	1.35
4	B	84	TRP	CA-C	-5.29	1.46	1.52
4	J	45	HIS	CE1-NE2	5.27	1.37	1.32
4	F	173	HIS	CG-CD2	5.02	1.41	1.35

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	87	ASN	N-CA-C	8.44	121.61	111.82
3	A	208	ILE	N-CA-C	-7.53	103.89	110.74
4	F	36	PHE	N-CA-C	7.48	119.91	107.20
4	J	214	GLY	N-CA-C	-7.46	103.06	111.63
3	I	226	ASP	N-CA-C	-7.36	99.13	110.10
4	J	36	PHE	N-CA-C	7.36	119.71	107.20
4	F	143	SER	N-CA-C	-7.30	100.75	110.24
3	E	226	ASP	N-CA-C	-7.05	100.01	110.23
3	A	226	ASP	N-CA-C	-7.04	100.31	110.24
3	I	206	LYS	CA-C-N	-6.96	115.38	122.27
3	I	206	LYS	C-N-CA	-6.96	115.38	122.27
3	I	297	GLY	N-CA-C	6.92	119.90	110.69
4	F	125	PHE	CA-C-N	6.83	126.77	120.21
4	F	125	PHE	C-N-CA	6.83	126.77	120.21
3	I	254	PHE	CB-CA-C	-6.62	105.24	111.00
4	B	125	PHE	CA-C-N	6.57	126.52	120.21
4	B	125	PHE	C-N-CA	6.57	126.52	120.21
4	J	143	SER	N-CA-C	-6.47	101.95	110.43
4	F	214	GLY	N-CA-C	-6.46	104.20	111.63
4	F	194	VAL	N-CA-C	6.40	117.57	108.93
3	A	253	THR	N-CA-C	-6.34	97.30	110.80
4	J	53	TRP	N-CA-C	-6.33	105.38	113.23
3	E	390	GLY	N-CA-C	6.30	119.32	110.38
4	B	36	PHE	N-CA-C	6.28	117.88	107.20
4	J	220	VAL	N-CA-CB	6.12	118.41	110.57
3	E	254	PHE	CB-CA-C	-6.12	105.68	111.00
3	A	297	GLY	N-CA-C	6.01	118.68	110.69
3	E	413	LYS	N-CA-C	-5.98	98.66	108.41
4	B	214	GLY	N-CA-C	-5.96	104.70	111.85
3	E	206	LYS	CA-C-N	-5.83	113.92	121.96
3	E	206	LYS	C-N-CA	-5.83	113.92	121.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	192	HIS	N-CA-C	5.81	117.28	111.07
4	B	251	THR	N-CA-C	5.75	117.53	108.96
4	J	30	LEU	N-CA-C	-5.70	103.89	111.24
3	E	253	THR	N-CA-C	-5.63	98.81	110.80
3	A	254	PHE	CB-CA-C	-5.62	106.11	111.00
3	I	275	GLY	CA-C-N	5.61	131.80	121.70
3	I	275	GLY	C-N-CA	5.61	131.80	121.70
4	J	153	GLY	N-CA-C	-5.53	105.80	112.49
3	E	308	ASN	CA-C-N	5.51	131.62	121.70
3	E	308	ASN	C-N-CA	5.51	131.62	121.70
3	A	390	GLY	N-CA-C	5.50	118.05	110.56
3	I	119	ALA	N-CA-C	-5.49	100.94	109.72
3	A	353	THR	CA-C-N	5.42	126.62	119.84
3	A	353	THR	C-N-CA	5.42	126.62	119.84
3	A	225	GLY	N-CA-C	-5.36	102.93	111.18
3	E	297	GLY	N-CA-C	5.32	117.76	110.69
3	A	228	ASP	N-CA-C	-5.20	105.69	111.36
4	J	125	PHE	CA-C-N	5.19	125.17	120.03
4	J	125	PHE	C-N-CA	5.19	125.17	120.03
4	F	53	TRP	N-CA-C	-5.18	106.81	113.23
2	G	254	LEU	N-CA-C	5.17	116.77	111.03
3	A	308	ASN	CA-C-N	5.12	130.92	121.70
3	A	308	ASN	C-N-CA	5.12	130.92	121.70
3	I	351	ASP	N-CA-C	-5.12	106.28	112.88
4	F	36	PHE	CA-C-N	5.10	130.88	121.70
4	F	36	PHE	C-N-CA	5.10	130.88	121.70
3	I	308	ASN	CA-C-N	5.08	130.84	121.70
3	I	308	ASN	C-N-CA	5.08	130.84	121.70
2	G	128	GLN	N-CA-C	-5.06	105.68	111.14
4	F	203	ARG	N-CA-C	5.04	119.69	111.37
4	J	214	GLY	CA-C-N	5.03	130.76	121.70
4	J	214	GLY	C-N-CA	5.03	130.76	121.70
4	F	56	TRP	N-CA-C	5.01	116.58	108.41

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	333	THR	Peptide
4	B	36	PHE	Peptide
3	E	274	GLU	Peptide
3	E	333	THR	Peptide

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Mol	Chain	Res	Type	Group
4	F	36	PHE	Peptide
4	F	50	ALA	Peptide
3	I	274	GLU	Peptide
3	I	333	THR	Peptide
4	J	36	PHE	Peptide
4	J	50	ALA	Peptide

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	D	95	0	22	0	0
1	H	100	0	23	2	0
1	N	120	0	28	5	0
2	C	1742	0	1749	70	0
2	G	1731	0	1737	72	0
2	K	1738	0	1746	163	0
3	A	3026	0	3015	104	0
3	E	3026	0	3015	111	0
3	I	3026	0	3015	90	0
4	B	1974	0	1932	67	0
4	F	1974	0	1932	69	0
4	J	1974	0	1932	76	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
5	K	1	0	0	0	0
6	C	51	0	78	4	0
6	G	102	0	156	7	0
6	K	51	0	78	94	0
7	A	13	0	0	4	0
7	B	11	0	0	1	0
7	C	4	0	0	2	0
7	E	25	0	0	9	0
7	F	18	0	0	1	0
7	G	11	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	12	0	0	0	0
7	J	16	0	0	2	0
7	K	7	0	0	4	0
All	All	20853	0	20458	757	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 18.

All (757) 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:K:84:LEU:HD13	6:K:302:PGT:C36	1.15	1.53
2:K:84:LEU:CD2	6:K:302:PGT:H341	1.42	1.47
2:K:84:LEU:CD1	6:K:302:PGT:H362	0.99	1.46
2:K:81:ALA:HA	6:K:302:PGT:C40	1.57	1.32
2:K:84:LEU:HD13	6:K:302:PGT:C35	1.58	1.31
2:K:166:PHE:CB	6:K:302:PGT:H372	1.65	1.25
2:K:81:ALA:CA	6:K:302:PGT:H402	1.67	1.24
2:K:81:ALA:HB1	6:K:302:PGT:C41	1.68	1.23
3:E:334:THR:HA	3:E:335:LYS:HB2	1.27	1.17
3:I:334:THR:HA	3:I:335:LYS:HB2	1.26	1.16
2:K:84:LEU:HD22	6:K:302:PGT:C34	1.72	1.16
2:K:166:PHE:HB2	6:K:302:PGT:H372	1.25	1.15
3:E:356:ALA:HB1	3:E:357:PRO:C	1.74	1.12
3:A:78:ALA:CB	3:A:142:GLY:HA3	1.78	1.12
2:K:167:TYR:HB2	6:K:302:PGT:H352	1.24	1.12
3:E:78:ALA:CB	3:E:142:GLY:HA3	1.80	1.11
2:G:188:ILE:HD11	6:G:303:PGT:H361	1.17	1.10
3:A:356:ALA:HB1	3:A:357:PRO:C	1.76	1.10
2:K:81:ALA:HB1	6:K:302:PGT:H412	1.10	1.09
3:A:274:GLU:H	3:A:275:GLY:HA2	1.12	1.09
3:I:219:LYS:HA	3:I:220:ALA:HB3	1.34	1.09
3:A:334:THR:HA	3:A:335:LYS:HB2	1.33	1.08
3:I:78:ALA:CB	3:I:142:GLY:HA3	1.82	1.08
2:K:84:LEU:HD21	6:K:302:PGT:H321	1.31	1.07
4:B:51:GLY:HA3	4:B:52:ASP:HB2	1.36	1.07
2:K:84:LEU:CD1	6:K:302:PGT:C36	1.84	1.07
2:K:81:ALA:HA	6:K:302:PGT:C39	1.85	1.06
3:I:356:ALA:HB1	3:I:357:PRO:C	1.81	1.05
3:A:219:LYS:HA	3:A:220:ALA:HB3	1.38	1.04
3:A:78:ALA:HB3	3:A:142:GLY:HA3	1.39	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:84:LEU:CB	6:K:302:PGT:H371	1.88	1.03
4:J:51:GLY:HA3	4:J:52:ASP:HB2	1.39	1.03
3:E:78:ALA:HB3	3:E:142:GLY:HA3	1.39	1.02
2:K:81:ALA:HA	6:K:302:PGT:H402	1.05	1.02
2:C:23:GLY:HA3	6:C:302:PGT:O11	1.60	1.02
2:K:84:LEU:HD12	6:K:302:PGT:H362	1.04	1.01
3:E:275:GLY:HA2	3:E:276:THR:HB	1.42	1.01
2:K:81:ALA:CB	6:K:302:PGT:H402	1.91	1.00
3:E:219:LYS:HA	3:E:220:ALA:HB3	1.39	1.00
4:F:51:GLY:HA3	4:F:52:ASP:CB	1.91	1.00
2:K:167:TYR:CA	6:K:302:PGT:H351	1.91	0.99
2:K:167:TYR:HA	6:K:302:PGT:H351	1.44	0.98
4:B:116:TRP:O	2:C:47:TRP:CH2	2.16	0.98
2:C:251:VAL:HG12	2:C:252:LYS:N	1.78	0.98
2:K:81:ALA:CB	6:K:302:PGT:H412	1.94	0.97
4:B:51:GLY:HA3	4:B:52:ASP:CB	1.91	0.97
2:K:167:TYR:CD1	6:K:302:PGT:H331	2.00	0.97
4:J:51:GLY:HA3	4:J:52:ASP:CB	1.94	0.96
2:C:251:VAL:HG12	2:C:252:LYS:H	1.31	0.96
4:J:51:GLY:CA	4:J:52:ASP:HB2	1.95	0.96
2:K:47:TRP:CH2	4:J:116:TRP:O	2.18	0.95
2:K:166:PHE:CB	6:K:302:PGT:C37	2.43	0.95
2:K:81:ALA:CA	6:K:302:PGT:C40	2.33	0.95
2:K:84:LEU:CD2	6:K:302:PGT:C34	2.38	0.94
3:I:334:THR:HA	3:I:335:LYS:CB	1.96	0.94
4:F:51:GLY:CA	4:F:52:ASP:HB2	1.98	0.94
3:A:334:THR:HA	3:A:335:LYS:CB	1.98	0.93
2:G:138:ARG:HH12	2:G:141:ASP:HA	1.33	0.93
3:E:274:GLU:H	3:E:275:GLY:HA2	1.33	0.92
3:I:78:ALA:HB3	3:I:142:GLY:HA3	1.48	0.92
3:E:334:THR:HA	3:E:335:LYS:CB	2.00	0.92
2:K:166:PHE:HB2	6:K:302:PGT:C37	1.99	0.92
2:K:167:TYR:CB	6:K:302:PGT:H352	1.99	0.92
2:K:81:ALA:CB	6:K:302:PGT:C41	2.46	0.92
4:B:242:TRP:HB3	7:B:305:HOH:O	1.70	0.91
4:B:51:GLY:CA	4:B:52:ASP:HB2	2.02	0.90
2:K:81:ALA:O	6:K:302:PGT:H391	1.71	0.89
2:K:166:PHE:HB3	6:K:302:PGT:H372	1.52	0.89
2:K:84:LEU:HB3	6:K:302:PGT:H371	1.55	0.89
3:I:78:ALA:HB2	3:I:142:GLY:HA3	1.51	0.89
2:K:166:PHE:CZ	6:K:302:PGT:H411	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:78:ALA:HB2	3:A:142:GLY:HA3	1.54	0.88
2:K:84:LEU:HD22	6:K:302:PGT:H341	0.89	0.87
2:K:81:ALA:C	6:K:302:PGT:H421	2.00	0.87
2:K:251:VAL:HG12	2:K:252:LYS:N	1.88	0.87
2:K:84:LEU:HD13	6:K:302:PGT:C34	2.05	0.86
1:N:3:UNK:C	1:N:5:UNK:H	1.85	0.86
2:K:166:PHE:CG	6:K:302:PGT:H392	2.10	0.86
3:E:283:ASN:O	3:E:309:ASN:HB3	1.73	0.86
2:C:24:MET:HB2	2:C:109:GLN:HG2	1.55	0.86
2:K:166:PHE:HB3	6:K:302:PGT:C37	2.06	0.86
2:K:167:TYR:CA	6:K:302:PGT:C35	2.53	0.86
2:K:167:TYR:HD1	6:K:302:PGT:C34	1.89	0.85
2:K:138:ARG:HH12	2:K:141:ASP:HA	1.40	0.85
4:F:51:GLY:HA3	4:F:52:ASP:HB2	1.53	0.85
3:E:78:ALA:HB2	3:E:142:GLY:HA3	1.57	0.85
3:E:356:ALA:HB1	3:E:357:PRO:CA	2.07	0.84
2:K:84:LEU:CG	6:K:302:PGT:H341	2.09	0.83
2:C:138:ARG:HH12	2:C:141:ASP:HA	1.44	0.82
3:A:318:GLU:HG3	3:A:327:LEU:HD23	1.60	0.82
4:F:129:LEU:O	4:F:132:PRO:HD2	1.78	0.82
2:K:81:ALA:CB	6:K:302:PGT:C40	2.55	0.82
2:G:251:VAL:HG12	2:G:252:LYS:N	1.95	0.82
3:E:55:VAL:HG22	3:E:59:GLU:HB3	1.62	0.81
2:G:138:ARG:NH1	2:G:141:ASP:HA	1.95	0.81
4:F:116:TRP:O	2:G:47:TRP:CH2	2.33	0.81
2:K:47:TRP:CZ3	4:J:116:TRP:O	2.33	0.81
3:A:308:ASN:HA	3:A:309:ASN:HB2	1.61	0.81
3:E:312:GLN:HG3	7:E:615:HOH:O	1.80	0.81
2:K:47:TRP:HZ3	4:J:116:TRP:CD1	1.99	0.80
2:K:167:TYR:HD1	6:K:302:PGT:H331	1.44	0.80
6:K:302:PGT:C16	6:K:302:PGT:H122	2.10	0.80
2:K:167:TYR:HD1	6:K:302:PGT:C33	1.92	0.80
2:K:84:LEU:HB2	6:K:302:PGT:H371	1.60	0.80
3:A:275:GLY:HA2	3:A:276:THR:HB	1.63	0.80
2:K:167:TYR:HD1	6:K:302:PGT:H342	1.47	0.80
4:B:116:TRP:CD1	2:C:47:TRP:HZ3	1.99	0.79
2:C:138:ARG:NH1	2:C:141:ASP:HA	1.95	0.79
2:K:138:ARG:NH1	2:K:141:ASP:HA	1.97	0.79
2:K:167:TYR:N	6:K:302:PGT:H351	1.97	0.79
6:K:302:PGT:H122	6:K:302:PGT:H162	1.64	0.79
3:A:274:GLU:H	3:A:275:GLY:CA	1.90	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:51:SER:HB3	3:E:62:VAL:H	1.47	0.78
3:I:356:ALA:HB1	3:I:357:PRO:CA	2.13	0.78
2:G:194:ILE:HG23	2:G:195:PRO:HD3	1.62	0.78
4:J:63:ARG:HD3	7:J:304:HOH:O	1.82	0.78
3:I:219:LYS:HA	3:I:220:ALA:CB	2.09	0.78
3:A:308:ASN:CA	3:A:309:ASN:HB2	2.14	0.78
3:A:356:ALA:HB1	3:A:357:PRO:CA	2.13	0.78
3:A:283:ASN:O	3:A:309:ASN:HB3	1.83	0.78
4:F:235:LEU:HG	4:F:239:MET:HE2	1.65	0.78
3:A:219:LYS:HA	3:A:220:ALA:CB	2.14	0.77
2:K:109:GLN:HB3	6:K:302:PGT:H132	1.66	0.77
3:E:334:THR:CA	3:E:335:LYS:HB2	2.13	0.77
4:J:33:LEU:O	4:J:37:ALA:HB2	1.84	0.77
2:K:167:TYR:HA	6:K:302:PGT:C35	2.11	0.77
3:I:334:THR:CA	3:I:335:LYS:HB2	2.13	0.77
2:G:188:ILE:HD11	6:G:303:PGT:C36	2.08	0.77
3:I:308:ASN:HA	3:I:309:ASN:HB2	1.67	0.77
2:K:92:VAL:O	2:K:95:VAL:HG12	1.85	0.76
3:A:274:GLU:N	3:A:275:GLY:HA2	1.95	0.76
3:E:219:LYS:HA	3:E:220:ALA:CB	2.14	0.76
2:K:167:TYR:HB2	6:K:302:PGT:C35	2.13	0.76
4:F:116:TRP:CD1	2:G:47:TRP:HZ3	2.04	0.76
3:E:62:VAL:HB	7:E:612:HOH:O	1.86	0.76
2:G:35:TYR:HE1	2:G:152:MET:HE3	1.51	0.75
3:E:346:ARG:HD2	3:E:368:GLN:HG2	1.69	0.75
3:E:350:VAL:HB	3:E:352:ALA:H	1.52	0.75
3:E:356:ALA:CB	3:E:357:PRO:CA	2.64	0.75
4:F:51:GLY:CA	4:F:52:ASP:CB	2.60	0.74
2:K:84:LEU:CD1	6:K:302:PGT:C34	2.65	0.74
2:C:226:TRP:HA	2:C:226:TRP:CE3	2.22	0.74
3:E:308:ASN:HA	3:E:309:ASN:HB2	1.69	0.74
2:C:92:VAL:O	2:C:95:VAL:HG12	1.88	0.74
3:I:283:ASN:O	3:I:309:ASN:HB3	1.87	0.73
2:G:226:TRP:CE3	2:G:226:TRP:HA	2.22	0.73
3:A:346:ARG:HD2	3:A:368:GLN:HG2	1.71	0.73
3:A:275:GLY:CA	3:A:276:THR:HB	2.19	0.72
2:C:251:VAL:CG1	2:C:252:LYS:N	2.51	0.72
4:F:33:LEU:O	4:F:37:ALA:HB2	1.89	0.72
3:A:350:VAL:HB	3:A:352:ALA:H	1.54	0.71
2:K:24:MET:HB2	2:K:109:GLN:HG2	1.72	0.71
3:I:346:ARG:HD2	3:I:368:GLN:HG2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:36:PHE:HD1	4:B:36:PHE:O	1.73	0.71
4:J:235:LEU:HG	4:J:239:MET:HE2	1.72	0.71
2:C:194:ILE:HG23	2:C:195:PRO:HD3	1.73	0.71
2:G:45:PHE:O	2:G:49:ALA:HB3	1.91	0.71
4:B:116:TRP:O	2:C:47:TRP:CZ3	2.42	0.71
4:B:235:LEU:HG	4:B:239:MET:HE2	1.72	0.71
3:I:350:VAL:HB	3:I:352:ALA:H	1.56	0.71
2:K:251:VAL:HG12	2:K:252:LYS:H	1.53	0.71
2:K:84:LEU:CB	6:K:302:PGT:C37	2.67	0.71
4:J:166:TRP:HB3	4:J:167:PRO:HD3	1.71	0.70
2:K:166:PHE:CD2	6:K:302:PGT:H392	2.25	0.70
2:K:226:TRP:HA	2:K:226:TRP:CE3	2.25	0.70
3:I:55:VAL:HG22	3:I:59:GLU:HB3	1.72	0.70
3:E:348:LEU:HB2	7:E:601:HOH:O	1.90	0.70
3:A:334:THR:CA	3:A:335:LYS:HB2	2.18	0.70
3:E:274:GLU:N	3:E:275:GLY:HA2	2.07	0.70
4:F:51:GLY:HA3	4:F:52:ASP:HB3	1.73	0.70
3:I:51:SER:HB3	3:I:62:VAL:H	1.57	0.69
3:I:308:ASN:CA	3:I:309:ASN:HB2	2.22	0.69
2:K:35:TYR:HE1	2:K:152:MET:HE3	1.57	0.69
2:K:166:PHE:CB	6:K:302:PGT:H392	2.21	0.69
2:C:35:TYR:HE1	2:C:152:MET:HE3	1.57	0.69
2:C:113:VAL:HG21	6:C:302:PGT:H162	1.75	0.69
4:B:36:PHE:O	4:B:36:PHE:CD1	2.45	0.69
2:K:167:TYR:CB	6:K:302:PGT:C35	2.69	0.69
3:E:78:ALA:HB3	3:E:142:GLY:CA	2.20	0.69
2:K:84:LEU:HD21	6:K:302:PGT:C32	2.17	0.69
3:A:352:ALA:O	3:A:354:PRO:HD3	1.92	0.69
2:G:154:TYR:HD1	2:G:157:TYR:HE2	1.39	0.69
3:A:250:THR:HG21	4:B:167:PRO:HA	1.74	0.69
2:K:84:LEU:CD1	6:K:302:PGT:C37	2.70	0.69
2:K:47:TRP:CH2	4:J:117:THR:HA	2.27	0.69
3:I:250:THR:HG21	4:J:167:PRO:HA	1.73	0.68
2:K:194:ILE:HG23	2:K:195:PRO:HD3	1.74	0.68
3:A:51:SER:HB3	3:A:62:VAL:H	1.58	0.68
3:E:275:GLY:CA	3:E:276:THR:HB	2.18	0.68
3:A:55:VAL:HG22	3:A:59:GLU:HB3	1.76	0.68
3:E:308:ASN:CA	3:E:309:ASN:HB2	2.23	0.68
3:E:182:SER:HA	7:E:610:HOH:O	1.93	0.68
4:B:82:ALA:HB1	4:B:241:ARG:HD2	1.76	0.67
2:K:84:LEU:CD1	6:K:302:PGT:H341	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:185:LEU:O	4:F:189:ILE:HG13	1.95	0.67
3:A:356:ALA:CB	3:A:357:PRO:CA	2.72	0.67
3:I:78:ALA:HB3	3:I:142:GLY:CA	2.24	0.67
2:C:31:LEU:HD23	2:C:116:ILE:HG22	1.77	0.67
2:K:84:LEU:HB2	6:K:302:PGT:C37	2.25	0.66
3:A:163:THR:HB	7:A:608:HOH:O	1.93	0.66
3:E:318:GLU:HG3	3:E:327:LEU:HD23	1.77	0.66
2:K:167:TYR:CD1	6:K:302:PGT:H342	2.28	0.66
2:K:81:ALA:HB1	6:K:302:PGT:C42	2.26	0.66
3:A:78:ALA:HB3	3:A:142:GLY:CA	2.19	0.66
4:B:33:LEU:O	4:B:37:ALA:HB2	1.95	0.66
2:K:166:PHE:HB2	6:K:302:PGT:C38	2.26	0.66
2:C:226:TRP:HA	2:C:226:TRP:HE3	1.61	0.65
3:A:41:ARG:NE	3:A:387:GLN:HG2	2.11	0.65
2:K:81:ALA:HA	6:K:302:PGT:H391	1.75	0.65
2:K:90:ARG:HG2	7:K:407:HOH:O	1.96	0.65
4:J:34:LEU:O	4:J:38:VAL:HG13	1.97	0.65
3:E:250:THR:HG21	4:F:167:PRO:HA	1.79	0.65
3:I:318:GLU:HB3	3:I:393:PHE:HB2	1.78	0.65
2:G:31:LEU:HD23	2:G:116:ILE:HG22	1.79	0.65
2:G:226:TRP:HA	2:G:226:TRP:HE3	1.61	0.65
3:I:308:ASN:ND2	3:I:356:ALA:HB3	2.11	0.65
3:I:356:ALA:CB	3:I:357:PRO:CA	2.74	0.65
3:I:218:GLY:O	3:I:219:LYS:HE2	1.98	0.64
2:G:24:MET:HB2	2:G:109:GLN:HG2	1.79	0.64
2:K:31:LEU:HD23	2:K:116:ILE:HG22	1.80	0.64
2:K:80:LEU:O	6:K:302:PGT:H382	1.97	0.64
3:I:334:THR:CA	3:I:335:LYS:CB	2.73	0.64
3:A:269:THR:HG23	7:A:602:HOH:O	1.97	0.64
4:B:166:TRP:HB3	4:B:167:PRO:HD3	1.79	0.64
3:I:164:ASP:OD2	3:I:176:LEU:HB2	1.97	0.64
4:F:166:TRP:HB3	4:F:167:PRO:HD3	1.77	0.64
2:K:112:VAL:HA	4:J:33:LEU:HB2	1.79	0.64
4:B:117:THR:HA	2:C:47:TRP:CH2	2.33	0.64
2:K:47:TRP:CZ3	4:J:116:TRP:CD1	2.86	0.63
3:E:334:THR:CA	3:E:335:LYS:CB	2.76	0.63
3:A:308:ASN:ND2	3:A:356:ALA:HB3	2.14	0.63
4:B:35:PHE:HA	4:B:96:PHE:CZ	2.34	0.63
2:G:251:VAL:HG12	2:G:252:LYS:H	1.60	0.63
4:F:36:PHE:O	4:F:36:PHE:CD1	2.52	0.63
3:A:356:ALA:CB	3:A:359:GLU:H	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:228:ALA:HB2	7:K:403:HOH:O	1.99	0.62
4:J:9:ALA:HA	4:J:14:ASN:O	2.00	0.62
2:C:251:VAL:CG1	2:C:252:LYS:H	2.03	0.62
4:F:116:TRP:O	2:G:47:TRP:CZ3	2.52	0.62
3:A:356:ALA:HB1	3:A:359:GLU:H	1.64	0.62
2:G:154:TYR:CD1	2:G:157:TYR:HE2	2.16	0.62
2:K:84:LEU:HD21	6:K:302:PGT:H341	1.67	0.62
2:K:226:TRP:HA	2:K:226:TRP:HE3	1.65	0.61
4:F:117:THR:HA	2:G:47:TRP:CH2	2.36	0.61
2:G:88:ARG:HB2	2:G:170:THR:HB	1.81	0.61
2:K:167:TYR:CD1	6:K:302:PGT:C34	2.80	0.61
2:G:188:ILE:CD1	6:G:303:PGT:H361	2.11	0.61
4:J:36:PHE:O	4:J:36:PHE:CD1	2.54	0.61
4:B:185:LEU:O	4:B:189:ILE:HG13	2.00	0.61
3:A:334:THR:CA	3:A:335:LYS:CB	2.77	0.60
3:A:218:GLY:O	3:A:219:LYS:HE2	2.02	0.60
3:A:356:ALA:HA	3:A:359:GLU:HB3	1.83	0.60
2:G:128:GLN:O	2:G:131:THR:HG22	2.01	0.60
3:E:352:ALA:O	3:E:354:PRO:HD3	2.01	0.60
4:J:203:ARG:O	4:J:204:MET:HB2	2.02	0.60
3:I:196:ALA:O	3:I:200:PHE:HD1	1.85	0.60
3:A:102:GLY:HA3	3:A:268:LEU:HB3	1.83	0.60
3:E:55:VAL:CG2	3:E:59:GLU:HB3	2.30	0.60
3:E:308:ASN:ND2	3:E:356:ALA:HB3	2.16	0.60
2:K:163:GLY:O	6:K:302:PGT:H361	2.02	0.59
3:E:218:GLY:O	3:E:219:LYS:HE2	2.02	0.59
3:A:137:GLN:HE21	3:A:139:ASN:HD21	1.49	0.59
4:B:55:PHE:O	4:B:124:VAL:HA	2.01	0.59
3:E:274:GLU:H	3:E:275:GLY:CA	2.06	0.59
2:G:92:VAL:O	2:G:95:VAL:HG12	2.01	0.59
4:F:35:PHE:HA	4:F:96:PHE:CZ	2.37	0.59
4:F:36:PHE:O	4:F:36:PHE:HD1	1.86	0.59
2:K:154:TYR:HD1	2:K:157:TYR:HE2	1.50	0.59
4:B:203:ARG:O	4:B:204:MET:HB2	2.03	0.59
4:F:175:ALA:HB1	4:F:182:LEU:HD11	1.84	0.59
3:A:318:GLU:HG3	3:A:327:LEU:CD2	2.32	0.59
2:G:154:TYR:HD1	2:G:157:TYR:CE2	2.20	0.59
3:A:132:TRP:CD1	3:A:155:ILE:HD12	2.38	0.58
2:G:194:ILE:CG2	2:G:195:PRO:HD3	2.31	0.58
2:K:108:VAL:HG12	4:J:29:MET:HE2	1.84	0.58
2:K:47:TRP:HH2	4:J:117:THR:HA	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:57:VAL:HG12	3:A:58:ASN:ND2	2.19	0.58
3:E:356:ALA:CB	3:E:357:PRO:HA	2.32	0.58
2:K:81:ALA:O	6:K:302:PGT:H421	2.03	0.58
2:K:166:PHE:CG	6:K:302:PGT:C39	2.84	0.58
3:A:346:ARG:HB3	3:A:368:GLN:O	2.03	0.58
3:E:318:GLU:HB3	3:E:393:PHE:HB2	1.83	0.58
2:K:84:LEU:CD2	6:K:302:PGT:H321	2.22	0.58
4:B:9:ALA:HA	4:B:14:ASN:O	2.04	0.58
4:B:12:PRO:HB2	2:C:98:ARG:HA	1.86	0.58
3:E:252:SER:C	3:E:253:THR:O	2.43	0.58
3:I:380:LEU:HD11	3:I:387:GLN:H	1.69	0.58
4:F:125:PHE:CZ	4:F:169:ILE:HD12	2.38	0.58
4:F:214:GLY:HA2	4:F:215:LYS:HB2	1.86	0.58
4:F:125:PHE:HZ	4:F:169:ILE:HD12	1.68	0.58
2:K:68:THR:HG21	1:N:8:UNK:HA	1.85	0.58
2:K:54:PHE:HE2	3:I:33:SER:HB3	1.69	0.57
4:J:175:ALA:HB1	4:J:182:LEU:HD11	1.85	0.57
4:B:116:TRP:CD1	2:C:47:TRP:CZ3	2.86	0.57
3:E:33:SER:HB3	2:G:54:PHE:HE2	1.70	0.57
4:B:214:GLY:HA2	4:B:215:LYS:HB2	1.85	0.57
4:F:39:LEU:HD13	4:F:100:GLY:O	2.04	0.57
4:F:129:LEU:C	4:F:132:PRO:HD2	2.30	0.57
2:K:251:VAL:CG1	2:K:252:LYS:N	2.60	0.57
4:J:185:LEU:O	4:J:189:ILE:HG13	2.05	0.57
2:C:119:TYR:C	2:C:119:TYR:CD2	2.83	0.57
2:K:154:TYR:CD1	2:K:157:TYR:HE2	2.21	0.57
2:C:192:MET:HB2	7:C:404:HOH:O	2.02	0.57
2:K:99:GLU:O	2:K:103:ARG:HG3	2.05	0.57
3:E:137:GLN:HE21	3:E:139:ASN:HD21	1.51	0.57
2:K:81:ALA:HB2	6:K:302:PGT:H402	1.83	0.57
2:K:167:TYR:N	6:K:302:PGT:C35	2.65	0.56
3:A:127:ARG:O	3:A:159:MET:HG3	2.05	0.56
2:K:81:ALA:C	6:K:302:PGT:H391	2.30	0.56
2:K:166:PHE:CD1	6:K:302:PGT:H401	2.41	0.56
3:A:372:TRP:HH2	3:A:388:ILE:HD11	1.70	0.56
4:B:129:LEU:O	4:B:132:PRO:HD2	2.05	0.56
3:E:121:SER:HB2	7:E:612:HOH:O	2.04	0.56
3:E:380:LEU:HD11	3:E:387:GLN:H	1.71	0.56
3:A:348:LEU:HB2	3:A:349:SER:HB2	1.87	0.56
3:I:41:ARG:NE	3:I:387:GLN:HG2	2.21	0.56
3:A:46:TYR:CE2	3:A:66:LYS:HD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:356:ALA:HA	3:I:359:GLU:HB3	1.87	0.56
3:E:334:THR:HG21	7:E:602:HOH:O	2.06	0.55
3:E:356:ALA:HB1	3:E:359:GLU:H	1.71	0.55
3:I:51:SER:CB	3:I:62:VAL:H	2.18	0.55
4:F:34:LEU:O	4:F:38:VAL:HG13	2.05	0.55
4:J:36:PHE:O	4:J:36:PHE:HD1	1.88	0.55
2:K:166:PHE:CE1	6:K:302:PGT:H411	2.41	0.55
2:C:154:TYR:HD1	2:C:157:TYR:HE2	1.54	0.55
4:J:35:PHE:HA	4:J:96:PHE:CZ	2.41	0.55
4:J:102:LEU:HD13	4:J:130:ILE:HD12	1.88	0.55
3:E:127:ARG:O	3:E:159:MET:HG3	2.06	0.55
3:A:380:LEU:HD11	3:A:387:GLN:H	1.71	0.55
3:E:356:ALA:CB	3:E:359:GLU:H	2.19	0.55
2:C:154:TYR:CD1	2:C:157:TYR:HE2	2.25	0.55
3:E:58:ASN:OD1	3:E:125:ARG:NH2	2.34	0.55
2:K:84:LEU:HD12	6:K:302:PGT:C36	1.88	0.55
3:I:346:ARG:HB3	3:I:368:GLN:O	2.07	0.55
2:C:154:TYR:HD1	2:C:157:TYR:CE2	2.25	0.55
2:K:166:PHE:CE2	6:K:302:PGT:H411	2.42	0.55
3:E:372:TRP:HH2	3:E:388:ILE:HD11	1.72	0.55
4:J:39:LEU:HD13	4:J:100:GLY:O	2.07	0.55
3:I:260:LEU:HD22	3:I:260:LEU:H	1.70	0.54
3:I:318:GLU:HG3	3:I:327:LEU:HD23	1.89	0.54
3:E:260:LEU:H	3:E:260:LEU:HD22	1.72	0.54
3:I:164:ASP:CB	3:I:165:PRO:HA	2.37	0.54
4:F:116:TRP:CD1	2:G:47:TRP:CZ3	2.92	0.54
3:A:32:LYS:O	3:A:376:ARG:NH1	2.31	0.54
3:A:350:VAL:HG12	3:A:351:ASP:H	1.71	0.54
2:C:19:VAL:HG12	2:C:105:VAL:HG11	1.89	0.54
3:E:68:HIS:HE1	3:E:405:GLU:OE1	1.90	0.54
2:C:16:GLU:N	2:C:16:GLU:OE1	2.40	0.54
3:E:349:SER:HB2	7:E:601:HOH:O	2.07	0.54
3:I:102:GLY:HA3	3:I:268:LEU:HB3	1.90	0.54
4:B:29:MET:CE	2:C:109:GLN:HG3	2.38	0.54
2:K:154:TYR:HD1	2:K:157:TYR:CE2	2.25	0.54
3:A:58:ASN:HD21	3:A:162:PHE:HA	1.73	0.54
3:E:346:ARG:HB3	3:E:368:GLN:O	2.08	0.54
4:F:55:PHE:O	4:F:124:VAL:HA	2.08	0.53
2:K:45:PHE:O	2:K:49:ALA:HB3	2.09	0.53
4:B:29:MET:HE1	2:C:109:GLN:HG3	1.90	0.53
3:I:32:LYS:O	3:I:376:ARG:NH1	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:68:HIS:HD2	3:I:117:ASP:OD1	1.92	0.53
3:I:350:VAL:HG12	3:I:351:ASP:H	1.74	0.53
3:A:207:GLY:HA3	7:A:611:HOH:O	2.08	0.53
3:E:258:ILE:HG13	4:F:184:THR:HG22	1.90	0.53
3:I:132:TRP:CD1	3:I:155:ILE:HD12	2.43	0.53
4:B:116:TRP:C	2:C:47:TRP:CH2	2.87	0.53
3:E:132:TRP:CD1	3:E:155:ILE:HD12	2.43	0.53
2:G:88:ARG:CB	2:G:170:THR:HB	2.39	0.53
2:K:119:TYR:C	2:K:119:TYR:CD2	2.87	0.53
3:E:76:ALA:HB1	4:J:208:GLY:O	2.09	0.53
3:E:350:VAL:HG12	3:E:351:ASP:H	1.74	0.53
3:I:44:ASN:HD21	3:I:70:PHE:HD1	1.57	0.53
4:F:166:TRP:HB3	4:F:167:PRO:CD	2.39	0.53
2:K:128:GLN:O	2:K:131:THR:HG22	2.09	0.53
3:I:348:LEU:HB2	3:I:349:SER:HB2	1.90	0.53
3:A:258:ILE:HG13	4:B:184:THR:HG22	1.91	0.52
4:B:116:TRP:O	2:C:47:TRP:HH2	1.87	0.52
2:K:137:ILE:HG22	2:K:137:ILE:O	2.09	0.52
3:E:32:LYS:O	3:E:376:ARG:NH1	2.31	0.52
3:E:283:ASN:O	3:E:309:ASN:CB	2.50	0.52
4:F:173:HIS:HE1	7:F:310:HOH:O	1.92	0.52
4:J:33:LEU:C	4:J:33:LEU:HD23	2.34	0.52
4:J:174:GLN:HB2	4:J:185:LEU:HD12	1.90	0.52
3:E:41:ARG:NE	3:E:387:GLN:HG2	2.24	0.52
4:B:214:GLY:CA	4:B:215:LYS:HB2	2.39	0.52
2:K:98:ARG:HA	4:J:12:PRO:HB2	1.91	0.52
2:K:102:ARG:NH2	6:K:302:PGT:O1P	2.32	0.52
4:B:150:ALA:O	4:B:154:SER:OG	2.27	0.52
4:B:175:ALA:HB1	4:B:182:LEU:HD11	1.91	0.52
2:K:20:ASP:OD1	2:K:22:ARG:HG2	2.10	0.52
4:B:34:LEU:O	4:B:38:VAL:HG13	2.09	0.52
2:K:88:ARG:HB2	2:K:170:THR:HB	1.92	0.51
3:A:318:GLU:HB3	3:A:393:PHE:HB2	1.91	0.51
3:E:77:VAL:HG13	3:E:143:GLY:HA3	1.91	0.51
4:F:9:ALA:HA	4:F:14:ASN:O	2.10	0.51
4:F:214:GLY:CA	4:F:215:LYS:HB2	2.39	0.51
3:E:100:PHE:HA	3:E:104:GLN:O	2.10	0.51
2:K:81:ALA:CA	6:K:302:PGT:H391	2.40	0.51
3:I:341:TYR:CZ	3:I:342:LEU:HD22	2.46	0.51
6:K:302:PGT:C16	6:K:302:PGT:C12	2.87	0.51
3:E:164:ASP:CB	3:E:165:PRO:HA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:46:TYR:CE2	3:I:66:LYS:HD2	2.46	0.51
3:I:127:ARG:O	3:I:159:MET:HG3	2.11	0.51
2:G:19:VAL:HG12	2:G:105:VAL:HG11	1.93	0.51
2:K:53:SER:OG	2:K:139:ASP:CB	2.59	0.51
2:K:194:ILE:CG2	2:K:195:PRO:HD3	2.39	0.51
3:A:100:PHE:HA	3:A:104:GLN:O	2.11	0.51
3:I:68:HIS:HE1	3:I:405:GLU:OE1	1.93	0.51
3:E:327:LEU:HD11	3:E:343:LEU:HD11	1.94	0.50
4:F:82:ALA:HB1	4:F:241:ARG:HD2	1.93	0.50
4:J:38:VAL:HG22	7:J:301:HOH:O	2.11	0.50
2:K:167:TYR:CD1	6:K:302:PGT:C33	2.72	0.50
3:E:108:ARG:HD3	7:E:620:HOH:O	2.10	0.50
2:K:16:GLU:OE1	2:K:16:GLU:N	2.45	0.50
1:N:7:UNK:O	1:N:8:UNK:C	2.59	0.50
3:E:102:GLY:HA3	3:E:268:LEU:HB3	1.92	0.50
2:K:85:TRP:O	2:K:88:ARG:HB3	2.12	0.50
3:E:196:ALA:O	3:E:200:PHE:HD1	1.95	0.50
4:F:203:ARG:O	4:F:204:MET:HB2	2.12	0.50
4:J:102:LEU:CD1	4:J:130:ILE:HD12	2.41	0.50
4:B:117:THR:HA	2:C:47:TRP:HH2	1.74	0.49
4:B:129:LEU:C	4:B:132:PRO:HD2	2.37	0.49
3:E:356:ALA:HA	3:E:359:GLU:HB3	1.93	0.49
4:F:12:PRO:HB2	2:G:98:ARG:HA	1.93	0.49
4:F:33:LEU:O	4:F:37:ALA:CB	2.59	0.49
2:G:251:VAL:CG1	2:G:252:LYS:N	2.66	0.49
2:K:166:PHE:CB	6:K:302:PGT:C39	2.89	0.49
3:A:252:SER:C	3:A:253:THR:O	2.47	0.49
3:E:276:THR:HG22	3:E:279:VAL:HB	1.94	0.49
4:F:246:THR:HG22	2:G:237:GLN:HG3	1.94	0.49
2:K:83:TYR:HD2	2:K:84:LEU:HG	1.76	0.49
3:E:316:LEU:HB2	3:E:394:PHE:CE2	2.48	0.49
3:E:382:TYR:HB2	4:J:215:LYS:NZ	2.28	0.49
4:F:33:LEU:C	4:F:33:LEU:HD23	2.37	0.49
3:I:307:LYS:HD3	3:I:360:ALA:HB2	1.93	0.49
2:C:114:TYR:CE1	2:C:161:ALA:HB2	2.47	0.49
3:I:50:TRP:O	3:I:51:SER:C	2.56	0.49
3:I:186:ALA:O	3:I:190:PRO:HG2	2.12	0.49
3:E:68:HIS:HD2	3:E:117:ASP:OD1	1.95	0.49
4:F:166:TRP:CE2	4:F:170:ALA:HB2	2.47	0.49
3:A:55:VAL:CG2	3:A:59:GLU:HB3	2.40	0.49
3:A:356:ALA:CB	3:A:357:PRO:HA	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:105:GLU:O	4:B:109:ARG:HG2	2.12	0.49
4:B:116:TRP:C	2:C:47:TRP:HH2	2.21	0.49
3:I:276:THR:HG22	3:I:279:VAL:HB	1.94	0.49
4:F:51:GLY:HA2	4:F:52:ASP:HB2	1.88	0.49
2:C:20:ASP:OD1	2:C:22:ARG:HG2	2.13	0.49
2:K:81:ALA:CA	6:K:302:PGT:C41	2.88	0.48
4:J:114:TRP:CE3	4:J:118:TYR:HA	2.49	0.48
4:J:214:GLY:HA2	4:J:215:LYS:HB2	1.95	0.48
2:C:59:GLN:HA	2:C:63:MET:HB2	1.94	0.48
3:E:57:VAL:O	3:E:58:ASN:HB2	2.13	0.48
2:G:137:ILE:O	2:G:137:ILE:HG22	2.11	0.48
2:C:194:ILE:CG2	2:C:195:PRO:HD3	2.43	0.48
3:A:69:VAL:CG1	3:A:114:ILE:HA	2.44	0.48
3:I:137:GLN:HE21	3:I:139:ASN:HD21	1.60	0.48
3:I:313:PRO:HB2	3:I:354:PRO:HB2	1.96	0.48
2:C:137:ILE:HG22	2:C:137:ILE:O	2.13	0.48
2:K:84:LEU:HB2	6:K:302:PGT:C38	2.43	0.48
3:E:186:ALA:O	3:E:190:PRO:HG2	2.13	0.48
3:I:137:GLN:NE2	3:I:139:ASN:HD21	2.11	0.48
4:J:125:PHE:CZ	4:J:169:ILE:HD12	2.48	0.48
4:F:117:THR:HA	2:G:47:TRP:HH2	1.77	0.48
2:K:19:VAL:HG12	2:K:105:VAL:HG11	1.95	0.48
3:E:382:TYR:CD1	4:J:215:LYS:HD3	2.49	0.48
3:I:356:ALA:CB	3:I:357:PRO:HA	2.41	0.48
4:F:47:MET:SD	2:G:126:THR:HG22	2.53	0.48
3:A:137:GLN:NE2	3:A:139:ASN:HD21	2.11	0.48
4:F:33:LEU:HB2	2:G:112:VAL:HA	1.96	0.48
2:C:100:GLU:OE1	2:C:245:LEU:HD11	2.14	0.48
3:E:33:SER:HG	4:J:213:PHE:HD1	1.58	0.47
4:J:55:PHE:O	4:J:124:VAL:HA	2.13	0.47
2:K:166:PHE:CB	6:K:302:PGT:C38	2.90	0.47
2:K:53:SER:OG	2:K:139:ASP:HB3	2.14	0.47
2:K:84:LEU:HA	2:K:84:LEU:HD23	1.56	0.47
2:K:98:ARG:HG3	4:J:12:PRO:O	2.14	0.47
4:B:213:PHE:CD1	3:I:33:SER:OG	2.66	0.47
3:A:76:ALA:HB1	4:F:208:GLY:O	2.14	0.47
4:B:166:TRP:CE3	4:B:169:ILE:HG22	2.49	0.47
3:E:387:GLN:HG3	3:E:408:GLY:C	2.39	0.47
3:A:186:ALA:O	3:A:190:PRO:HG2	2.14	0.47
3:A:225:GLY:HA2	3:A:229:ARG:NH2	2.30	0.47
4:B:33:LEU:HD23	4:B:33:LEU:C	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:236:TRP:CE2	4:F:239:MET:HE1	2.50	0.47
4:J:59:TRP:CZ3	4:J:203:ARG:O	2.68	0.47
2:K:84:LEU:CD1	6:K:302:PGT:C35	2.53	0.47
2:K:190:PRO:O	2:K:193:ILE:HG22	2.14	0.47
3:A:307:LYS:HD2	3:A:308:ASN:H	1.78	0.47
3:E:35:GLN:HB2	3:E:38:LEU:HD12	1.97	0.47
2:G:20:ASP:OD1	2:G:22:ARG:HG2	2.14	0.47
3:A:196:ALA:O	3:A:200:PHE:HD1	1.97	0.47
3:E:33:SER:OG	4:J:213:PHE:HD1	1.98	0.47
3:I:312:GLN:N	3:I:357:PRO:HG3	2.30	0.47
4:B:208:GLY:O	4:B:209:THR:HG22	2.15	0.47
3:I:100:PHE:HA	3:I:104:GLN:O	2.14	0.47
4:J:51:GLY:HA3	4:J:52:ASP:HB3	1.91	0.47
2:G:35:TYR:CE1	2:G:152:MET:HE3	2.41	0.47
2:K:166:PHE:HB3	6:K:302:PGT:H392	1.94	0.46
4:B:33:LEU:O	4:B:37:ALA:CB	2.62	0.46
2:C:128:GLN:O	2:C:131:THR:HG22	2.14	0.46
3:A:164:ASP:CB	3:A:165:PRO:HA	2.45	0.46
4:J:214:GLY:CA	4:J:215:LYS:HB2	2.44	0.46
4:B:69:VAL:O	4:B:73:GLY:N	2.48	0.46
4:B:162:TYR:HB3	4:B:163:PRO:HD3	1.98	0.46
2:G:188:ILE:O	2:G:189:GLY:C	2.57	0.46
3:A:35:GLN:HB2	3:A:38:LEU:HD12	1.98	0.46
3:I:69:VAL:CG1	3:I:114:ILE:HA	2.45	0.46
4:J:64:MET:HG3	4:J:204:MET:O	2.15	0.46
2:C:157:TYR:CD1	2:C:157:TYR:C	2.93	0.46
3:A:132:TRP:HD1	3:A:155:ILE:HD12	1.80	0.46
4:B:47:MET:O	4:B:51:GLY:HA2	2.16	0.46
4:B:51:GLY:HA3	4:B:52:ASP:HB3	1.90	0.46
2:K:39:ARG:O	2:K:42:GLU:HG2	2.15	0.46
4:J:34:LEU:HD13	4:J:84:TRP:CZ2	2.50	0.46
4:J:125:PHE:HZ	4:J:169:ILE:HD12	1.80	0.46
2:G:111:LEU:O	2:G:114:TYR:HB3	2.16	0.46
3:A:366:LYS:NZ	3:A:368:GLN:HE21	2.14	0.46
3:I:283:ASN:O	3:I:309:ASN:CB	2.62	0.46
4:F:29:MET:O	4:F:33:LEU:HB3	2.15	0.46
4:F:29:MET:HE1	2:G:109:GLN:HG3	1.97	0.46
4:J:82:ALA:HB1	4:J:241:ARG:HD2	1.98	0.46
2:C:84:LEU:HD23	2:C:84:LEU:HA	1.69	0.46
3:A:77:VAL:HG13	3:A:143:GLY:HA3	1.98	0.45
3:E:310:THR:O	3:E:357:PRO:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:356:ALA:HB3	3:E:357:PRO:HA	1.99	0.45
2:C:42:GLU:OE2	2:C:128:GLN:NE2	2.34	0.45
2:G:248:LYS:HG2	2:G:252:LYS:HD2	1.97	0.45
3:A:398:ASP:OD1	3:A:398:ASP:N	2.41	0.45
3:E:382:TYR:CE1	4:J:215:LYS:HA	2.50	0.45
3:I:352:ALA:O	3:I:354:PRO:HD3	2.16	0.45
4:F:117:THR:HG22	2:G:47:TRP:CH2	2.51	0.45
2:K:68:THR:HG21	1:N:8:UNK:CA	2.47	0.45
3:A:341:TYR:CE2	3:A:342:LEU:HD13	2.51	0.45
3:A:58:ASN:OD1	3:A:125:ARG:NH2	2.39	0.45
4:F:125:PHE:CZ	4:F:169:ILE:CD1	2.98	0.45
3:E:80:PRO:HA	3:E:140:VAL:HG13	1.98	0.45
4:J:60:LYS:HD3	4:J:65:TRP:CZ2	2.51	0.45
2:G:187:ALA:C	2:G:188:ILE:HD12	2.41	0.45
4:B:218:VAL:HB	4:B:219:PRO:HD3	1.98	0.45
3:I:55:VAL:CG2	3:I:59:GLU:HB3	2.42	0.45
2:C:53:SER:OG	2:C:139:ASP:CB	2.65	0.45
2:C:248:LYS:HG2	2:C:252:LYS:HD2	1.99	0.45
4:B:212:THR:HG22	4:B:214:GLY:O	2.16	0.45
3:E:107:PRO:HA	4:F:191:PHE:CE1	2.52	0.45
3:E:366:LYS:NZ	3:E:368:GLN:HE21	2.15	0.45
3:E:382:TYR:CZ	4:J:215:LYS:HA	2.52	0.45
2:C:247:GLY:C	2:C:249:GLU:N	2.74	0.45
2:G:169:LYS:HD2	2:G:175:PHE:O	2.17	0.45
2:K:84:LEU:HD12	6:K:302:PGT:C37	2.43	0.45
4:B:125:PHE:CZ	4:B:169:ILE:HD12	2.51	0.45
3:I:113:GLU:HB2	3:I:116:LYS:HG2	1.99	0.45
2:K:241:ARG:HA	2:K:241:ARG:NE	2.32	0.45
3:A:308:ASN:CG	3:A:356:ALA:HB3	2.41	0.45
4:B:43:HIS:HE2	4:B:105:GLU:HG2	1.82	0.45
4:F:44:VAL:HG23	2:G:122:ALA:O	2.16	0.45
2:G:104:LEU:HD23	2:G:172:ILE:HD13	1.97	0.45
2:K:47:TRP:CH2	4:J:116:TRP:C	2.89	0.45
3:E:313:PRO:HB2	3:E:354:PRO:HB2	1.99	0.45
2:G:53:SER:OG	2:G:139:ASP:CB	2.65	0.45
4:B:198:MET:O	4:B:198:MET:HG3	2.17	0.44
2:C:179:TYR:HA	7:C:401:HOH:O	2.16	0.44
3:A:311:SER:C	3:A:357:PRO:HG3	2.41	0.44
4:B:102:LEU:HD23	4:B:102:LEU:HA	1.71	0.44
4:B:215:LYS:HD3	3:I:382:TYR:CD1	2.52	0.44
3:I:356:ALA:HB1	3:I:359:GLU:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:57:VAL:O	3:A:58:ASN:HB2	2.17	0.44
3:A:274:GLU:N	3:A:275:GLY:CA	2.64	0.44
4:F:21:GLY:O	4:F:25:THR:HG23	2.18	0.44
2:K:109:GLN:HG3	4:J:29:MET:CE	2.47	0.44
3:I:272:GLU:O	3:I:279:VAL:HG11	2.17	0.44
2:K:59:GLN:HA	2:K:63:MET:HB2	1.98	0.44
3:I:308:ASN:CG	3:I:356:ALA:HB3	2.42	0.44
2:C:35:TYR:CE1	2:C:152:MET:HE3	2.45	0.44
3:E:225:GLY:HA2	3:E:229:ARG:NH2	2.32	0.44
3:I:258:ILE:HG13	4:J:184:THR:HG22	1.99	0.44
2:C:126:THR:HA	2:C:149:GLU:OE1	2.18	0.44
2:G:119:TYR:CD2	2:G:119:TYR:C	2.95	0.44
2:K:53:SER:OG	2:K:139:ASP:HB2	2.18	0.44
3:E:137:GLN:NE2	3:E:139:ASN:HD21	2.15	0.44
3:E:352:ALA:O	3:E:354:PRO:CD	2.66	0.44
4:F:200:GLU:HG2	4:F:203:ARG:HD2	2.00	0.44
2:C:241:ARG:NE	2:C:241:ARG:HA	2.32	0.44
2:G:169:LYS:NZ	2:G:178:GLY:O	2.51	0.44
2:K:90:ARG:CG	7:K:407:HOH:O	2.61	0.44
3:A:273:THR:CA	3:A:274:GLU:HB2	2.48	0.44
3:E:69:VAL:CG1	3:E:114:ILE:HA	2.48	0.44
3:E:307:LYS:HD3	3:E:360:ALA:HB2	2.00	0.44
2:G:148:ILE:O	2:G:152:MET:HB3	2.17	0.44
2:K:157:TYR:C	2:K:157:TYR:CD1	2.96	0.44
3:A:313:PRO:HB2	3:A:354:PRO:HB2	2.00	0.44
4:B:64:MET:O	4:B:68:VAL:HG13	2.18	0.44
3:E:282:GLU:HB3	3:E:310:THR:HG22	2.00	0.44
3:I:77:VAL:HG13	3:I:143:GLY:HA3	1.99	0.44
4:J:129:LEU:O	4:J:132:PRO:HD2	2.18	0.44
2:C:39:ARG:O	2:C:42:GLU:HG2	2.17	0.44
2:G:85:TRP:O	2:G:88:ARG:HB3	2.18	0.44
2:K:87:THR:HG21	7:K:405:HOH:O	2.18	0.43
3:A:33:SER:HG	4:F:213:PHE:HD1	1.62	0.43
4:B:171:ALA:O	4:B:174:GLN:HG3	2.18	0.43
3:A:393:PHE:CD1	3:A:401:ARG:HD2	2.53	0.43
3:A:272:GLU:O	3:A:279:VAL:HG11	2.18	0.43
3:A:298:ARG:HH11	3:A:370:ALA:HA	1.83	0.43
3:I:164:ASP:CB	3:I:165:PRO:CA	2.96	0.43
3:I:164:ASP:HB3	3:I:165:PRO:CA	2.48	0.43
3:I:372:TRP:HH2	3:I:388:ILE:HD11	1.83	0.43
4:J:49:THR:OG1	4:J:72:LEU:HD22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:114:TYR:HE1	2:C:161:ALA:HB2	1.83	0.43
2:K:166:PHE:CA	6:K:302:PGT:H372	2.39	0.43
2:K:239:LEU:HD23	2:K:239:LEU:HA	1.86	0.43
3:A:324:LEU:HD11	3:A:375:GLU:HG3	2.01	0.43
3:A:352:ALA:O	3:A:354:PRO:CD	2.63	0.43
4:F:64:MET:HG3	4:F:204:MET:O	2.18	0.43
4:J:159:LEU:HD23	4:J:159:LEU:HA	1.79	0.43
3:A:73:TRP:HA	3:A:74:PRO:HD3	1.92	0.43
3:A:293:TYR:CZ	3:A:412:PRO:HB3	2.53	0.43
3:A:308:ASN:HA	3:A:309:ASN:CB	2.41	0.43
4:B:36:PHE:HB3	4:B:39:LEU:HD23	2.00	0.43
3:I:252:SER:C	3:I:253:THR:O	2.55	0.43
4:F:90:LEU:HA	4:F:91:PRO:HD3	1.94	0.43
3:E:316:LEU:HD11	3:E:392:LEU:HD22	2.01	0.43
4:F:59:TRP:O	4:F:61:ASP:N	2.52	0.43
2:G:44:VAL:HG12	2:G:45:PHE:CD1	2.53	0.43
3:E:164:ASP:OD2	3:E:176:LEU:HB2	2.19	0.43
4:F:102:LEU:HD23	4:F:102:LEU:HA	1.85	0.43
2:C:197:VAL:HA	2:C:198:GLY:HA3	1.71	0.43
3:A:355:ILE:CG2	3:A:359:GLU:HG2	2.49	0.43
3:E:46:TYR:CE2	3:E:66:LYS:HD2	2.54	0.43
2:C:138:ARG:HH12	2:C:141:ASP:CA	2.24	0.43
2:G:190:PRO:O	2:G:193:ILE:HG22	2.19	0.43
3:A:212:TYR:CE2	2:C:239:LEU:HB3	2.54	0.43
3:E:137:GLN:HE21	3:E:139:ASN:ND2	2.16	0.43
3:I:113:GLU:HB2	3:I:116:LYS:CG	2.48	0.43
3:I:176:LEU:HD21	4:J:185:LEU:HD22	2.00	0.43
2:G:35:TYR:HE1	2:G:152:MET:CE	2.27	0.43
2:K:248:LYS:HG2	2:K:252:LYS:HD2	2.01	0.43
2:C:83:TYR:CD2	6:C:302:PGT:H391	2.54	0.43
2:C:249:GLU:O	2:C:253:LEU:HB2	2.19	0.43
2:K:166:PHE:HB3	6:K:302:PGT:H371	1.95	0.42
2:K:247:GLY:C	2:K:249:GLU:N	2.74	0.42
3:A:212:TYR:CD2	2:C:239:LEU:HB3	2.54	0.42
3:E:164:ASP:CB	3:E:165:PRO:CA	2.96	0.42
3:I:198:TRP:O	3:I:202:TRP:HD1	2.02	0.42
2:G:16:GLU:N	2:G:16:GLU:OE1	2.52	0.42
2:G:165:PHE:HE2	6:G:303:PGT:H331	1.84	0.42
1:H:13:UNK:C	6:G:302:PGT:H263	2.49	0.42
4:F:129:LEU:O	4:F:132:PRO:CD	2.61	0.42
3:A:273:THR:HA	3:A:274:GLU:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:308:ASN:O	3:I:358:GLY:N	2.52	0.42
4:J:21:GLY:O	4:J:25:THR:HG23	2.20	0.42
2:C:95:VAL:HG23	2:C:99:GLU:HG3	2.01	0.42
2:K:47:TRP:CH2	4:J:117:THR:HG22	2.54	0.42
3:A:283:ASN:O	3:A:309:ASN:CB	2.61	0.42
3:E:96:ARG:HA	3:E:124:LEU:HD23	2.02	0.42
3:I:292:VAL:HA	3:I:411:ILE:O	2.19	0.42
4:F:81:GLN:O	4:F:82:ALA:C	2.61	0.42
2:K:247:GLY:C	2:K:249:GLU:H	2.28	0.42
3:A:141:GLU:HA	4:B:201:TYR:CZ	2.55	0.42
4:J:36:PHE:N	4:J:37:ALA:HB3	2.34	0.42
2:G:53:SER:OG	2:G:139:ASP:HB3	2.19	0.42
2:K:47:TRP:HH2	4:J:116:TRP:C	2.26	0.42
2:G:39:ARG:O	2:G:42:GLU:HG2	2.19	0.42
3:A:348:LEU:HA	3:A:349:SER:HA	1.82	0.42
2:C:32:ASN:O	2:C:36:LEU:HB2	2.20	0.42
2:K:19:VAL:HG23	2:K:19:VAL:O	2.20	0.42
2:K:159:VAL:HG11	6:K:302:PGT:H252	2.01	0.42
4:B:213:PHE:HD1	3:I:33:SER:OG	2.01	0.42
3:E:312:GLN:N	3:E:357:PRO:HG3	2.35	0.42
3:I:260:LEU:H	3:I:260:LEU:CD2	2.31	0.42
4:F:162:TYR:HB3	4:F:163:PRO:HD3	2.02	0.42
3:A:41:ARG:CZ	3:A:387:GLN:HG2	2.50	0.42
3:E:132:TRP:HD1	3:E:155:ILE:HD12	1.83	0.42
2:G:157:TYR:CD1	2:G:157:TYR:C	2.97	0.42
2:G:169:LYS:HE3	6:G:303:PGT:O5	2.19	0.42
2:K:188:ILE:O	2:K:189:GLY:C	2.63	0.41
3:E:185:TYR:HD2	7:E:610:HOH:O	2.03	0.41
3:E:307:LYS:HD2	3:E:308:ASN:H	1.85	0.41
4:J:33:LEU:O	4:J:37:ALA:CB	2.62	0.41
4:J:129:LEU:C	4:J:132:PRO:HD2	2.45	0.41
2:G:247:GLY:C	2:G:249:GLU:N	2.77	0.41
3:A:137:GLN:HE21	3:A:139:ASN:ND2	2.17	0.41
3:E:62:VAL:O	3:E:62:VAL:HG23	2.21	0.41
4:F:29:MET:CE	2:G:109:GLN:HG3	2.50	0.41
4:F:251:THR:HA	2:G:179:TYR:HE2	1.85	0.41
4:J:33:LEU:C	4:J:33:LEU:CD2	2.92	0.41
2:C:48:ARG:O	2:C:49:ALA:HB2	2.19	0.41
3:A:68:HIS:HE1	3:A:405:GLU:OE1	2.03	0.41
4:B:87:ASN:HB2	4:B:88:PHE:CE1	2.55	0.41
4:F:235:LEU:CG	4:F:239:MET:HE2	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:7:UNK:C	1:N:9:UNK:N	2.83	0.41
3:I:311:SER:C	3:I:357:PRO:HG3	2.45	0.41
4:F:234:PHE:O	4:F:235:LEU:C	2.63	0.41
4:J:185:LEU:HA	4:J:185:LEU:HD23	1.90	0.41
2:C:190:PRO:O	2:C:193:ILE:HG22	2.19	0.41
2:K:134:MET:HG3	4:J:56:TRP:CH2	2.55	0.41
2:K:239:LEU:HB3	3:I:212:TYR:CE2	2.55	0.41
2:K:249:GLU:O	2:K:253:LEU:HB2	2.21	0.41
3:E:164:ASP:HB3	3:E:165:PRO:CA	2.51	0.41
4:F:166:TRP:CE3	4:F:169:ILE:HG22	2.54	0.41
4:J:212:THR:HG22	4:J:214:GLY:O	2.21	0.41
2:C:239:LEU:HD23	2:C:239:LEU:HA	1.70	0.41
2:G:22:ARG:HG3	7:G:408:HOH:O	2.19	0.41
2:K:104:LEU:HD23	2:K:172:ILE:HD13	2.02	0.41
3:A:312:GLN:N	3:A:357:PRO:HG3	2.36	0.41
3:I:57:VAL:O	3:I:58:ASN:HB2	2.20	0.41
4:J:29:MET:O	4:J:33:LEU:HB3	2.20	0.41
4:J:81:GLN:O	4:J:82:ALA:C	2.64	0.41
3:E:44:ASN:HD21	3:E:70:PHE:HD1	1.68	0.41
3:I:353:THR:HA	3:I:354:PRO:HD3	1.88	0.41
2:C:247:GLY:C	2:C:249:GLU:H	2.29	0.41
1:H:13:UNK:CB	6:G:302:PGT:C26	2.99	0.41
2:K:109:GLN:HG3	4:J:29:MET:HE3	2.02	0.41
4:B:39:LEU:HD13	4:B:100:GLY:O	2.21	0.41
3:I:137:GLN:HE21	3:I:139:ASN:ND2	2.18	0.41
3:I:356:ALA:HB1	3:I:357:PRO:HA	1.94	0.41
6:C:302:PGT:H322	6:C:302:PGT:H352	1.50	0.41
2:G:21:LEU:HD23	2:G:109:GLN:NE2	2.35	0.41
2:G:25:TRP:O	2:G:26:ILE:C	2.63	0.41
3:A:164:ASP:CB	3:A:165:PRO:CA	2.99	0.41
3:A:282:GLU:HB3	3:A:310:THR:HG22	2.03	0.41
4:B:125:PHE:HZ	4:B:169:ILE:HD12	1.85	0.41
4:B:140:LEU:O	4:B:143:SER:O	2.37	0.41
4:B:178:GLN:O	4:B:179:HIS:C	2.63	0.41
4:B:208:GLY:O	3:I:76:ALA:HB1	2.20	0.41
3:E:257:THR:HB	4:F:173:HIS:HB3	2.02	0.41
3:I:69:VAL:HG12	3:I:114:ILE:HA	2.03	0.41
3:I:356:ALA:CB	3:I:359:GLU:H	2.33	0.41
3:I:398:ASP:HB2	3:I:399:GLY:H	1.75	0.41
4:F:116:TRP:C	2:G:47:TRP:CH2	2.98	0.41
4:F:233:TYR:O	4:F:234:PHE:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:106:TRP:O	4:J:107:ILE:C	2.62	0.41
2:K:100:GLU:OE1	2:K:245:LEU:HD11	2.20	0.41
4:B:36:PHE:HB3	4:B:39:LEU:HB3	2.02	0.41
3:E:170:ASP:OD1	3:E:170:ASP:C	2.64	0.41
3:E:308:ASN:O	3:E:358:GLY:N	2.53	0.41
3:I:41:ARG:CZ	3:I:387:GLN:HG2	2.51	0.41
3:A:236:LEU:HB2	4:B:138:VAL:HG11	2.04	0.40
3:E:341:TYR:CZ	3:E:342:LEU:HD22	2.56	0.40
2:C:41:TYR:CD1	2:C:41:TYR:C	2.99	0.40
2:C:85:TRP:O	2:C:88:ARG:HB3	2.21	0.40
2:G:150:PHE:O	2:G:155:PRO:HD3	2.20	0.40
2:K:121:GLY:HA2	2:K:153:SER:OG	2.21	0.40
3:A:118:TYR:HA	7:A:603:HOH:O	2.20	0.40
4:J:109:ARG:HG3	4:J:126:PRO:HD3	2.04	0.40
2:G:184:LEU:HD12	2:G:184:LEU:HA	1.90	0.40
2:G:249:GLU:O	2:G:253:LEU:HB2	2.21	0.40
2:K:137:ILE:O	2:K:137:ILE:CG2	2.69	0.40
3:A:260:LEU:HD23	4:B:61:ASP:HA	2.03	0.40
2:C:53:SER:OG	2:C:139:ASP:HB3	2.21	0.40
2:C:88:ARG:HB2	2:C:170:THR:HB	2.03	0.40
2:G:121:GLY:HA2	2:G:153:SER:OG	2.22	0.40
2:K:126:THR:HG22	4:J:47:MET:SD	2.62	0.40
6:K:302:PGT:H122	6:K:302:PGT:H161	2.01	0.40
3:E:73:TRP:HA	3:E:74:PRO:HD3	1.94	0.40
4:J:102:LEU:HD23	4:J:102:LEU:HA	1.95	0.40
2:C:73:GLU:OE2	2:C:152:MET:HA	2.22	0.40
2:K:88:ARG:CB	2:K:170:THR:HB	2.51	0.40
3:A:214:ARG:HD3	3:A:222:ASP:CB	2.51	0.40
3:E:311:SER:C	3:E:357:PRO:HG3	2.47	0.40
4:J:92:PHE:O	4:J:96:PHE:HB2	2.22	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	
2	C	210/256 (82%)	180 (86%)	25 (12%)	5 (2%)	4	9
2	G	208/256 (81%)	184 (88%)	21 (10%)	3 (1%)	9	19
2	K	209/256 (82%)	181 (87%)	26 (12%)	2 (1%)	12	28
3	A	386/420 (92%)	339 (88%)	34 (9%)	13 (3%)	3	4
3	E	386/420 (92%)	339 (88%)	32 (8%)	15 (4%)	2	3
3	I	386/420 (92%)	334 (86%)	39 (10%)	13 (3%)	3	4
4	B	242/252 (96%)	212 (88%)	27 (11%)	3 (1%)	10	23
4	F	242/252 (96%)	213 (88%)	25 (10%)	4 (2%)	7	15
4	J	242/252 (96%)	216 (89%)	24 (10%)	2 (1%)	16	34
All	All	2511/2784 (90%)	2198 (88%)	253 (10%)	60 (2%)	4	9

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	251	VAL
3	A	164	ASP
3	A	274	GLU
3	A	335	LYS
3	A	350	VAL
3	A	356	ALA
4	B	37	ALA
4	B	52	ASP
3	E	274	GLU
3	E	335	LYS
3	E	350	VAL
3	E	356	ALA
3	I	335	LYS
3	I	356	ALA
4	F	37	ALA
4	F	52	ASP
4	J	37	ALA
4	J	52	ASP
2	C	251	VAL
2	G	251	VAL
2	K	49	ALA
3	A	220	ALA
3	A	309	ASN

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Mol	Chain	Res	Type
3	A	355	ILE
3	A	358	GLY
3	E	164	ASP
3	E	220	ALA
3	E	309	ASN
3	E	355	ILE
3	I	164	ASP
3	I	220	ALA
3	I	350	VAL
3	I	355	ILE
2	C	49	ALA
2	G	49	ALA
4	B	142	LEU
3	E	76	ALA
3	I	309	ASN
4	F	142	LEU
2	C	196	ASN
2	G	189	GLY
3	A	276	THR
3	A	353	THR
3	A	354	PRO
3	E	276	THR
3	E	353	THR
3	E	358	GLY
3	E	354	PRO
3	I	274	GLU
3	I	353	THR
2	C	149	GLU
3	I	90	PRO
3	I	354	PRO
4	F	86	VAL
3	E	339	PRO
3	I	358	GLY
3	E	90	PRO
3	I	339	PRO
2	C	190	PRO
3	A	339	PRO

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	
2	C	182/213 (85%)	167 (92%)	15 (8%)	10	24
2	G	181/213 (85%)	169 (93%)	12 (7%)	15	34
2	K	182/213 (85%)	168 (92%)	14 (8%)	12	27
3	A	319/336 (95%)	293 (92%)	26 (8%)	10	24
3	E	319/336 (95%)	286 (90%)	33 (10%)	7	15
3	I	319/336 (95%)	288 (90%)	31 (10%)	8	17
4	B	202/208 (97%)	181 (90%)	21 (10%)	7	14
4	F	202/208 (97%)	183 (91%)	19 (9%)	8	18
4	J	202/208 (97%)	184 (91%)	18 (9%)	9	20
All	All	2108/2271 (93%)	1919 (91%)	189 (9%)	9	20

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	36	LEU
2	K	40	ILE
2	K	68	THR
2	K	75	VAL
2	K	116	ILE
2	K	118	ILE
2	K	126	THR
2	K	127	GLU
2	K	157	TYR
2	K	162	VAL
2	K	177	HIS
2	K	197	VAL
2	K	231	VAL
2	K	235	VAL
3	A	29	HIS
3	A	62	VAL
3	A	89	GLU
3	A	97	THR
3	A	116	LYS
3	A	154	GLU
3	A	169	LEU
3	A	173	THR

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Mol	Chain	Res	Type
3	A	182	SER
3	A	204	VAL
3	A	206	LYS
3	A	219	LYS
3	A	234	ILE
3	A	260	LEU
3	A	274	GLU
3	A	276	THR
3	A	279	VAL
3	A	283	ASN
3	A	284	VAL
3	A	299	GLU
3	A	350	VAL
3	A	359	GLU
3	A	363	ILE
3	A	368	GLN
3	A	384	THR
3	A	388	ILE
4	B	15	SER
4	B	16	VAL
4	B	32	VAL
4	B	33	LEU
4	B	36	PHE
4	B	38	VAL
4	B	39	LEU
4	B	48	LEU
4	B	68	VAL
4	B	92	PHE
4	B	130	ILE
4	B	143	SER
4	B	152	VAL
4	B	164	ASN
4	B	169	ILE
4	B	176	THR
4	B	194	VAL
4	B	202	ILE
4	B	209	THR
4	B	234	PHE
4	B	251	THR
3	E	29	HIS
3	E	32	LYS
3	E	61	MET

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Mol	Chain	Res	Type
3	E	62	VAL
3	E	63	LEU
3	E	89	GLU
3	E	94	LEU
3	E	95	VAL
3	E	97	THR
3	E	114	ILE
3	E	116	LYS
3	E	154	GLU
3	E	173	THR
3	E	182	SER
3	E	204	VAL
3	E	206	LYS
3	E	219	LYS
3	E	234	ILE
3	E	253	THR
3	E	274	GLU
3	E	276	THR
3	E	279	VAL
3	E	283	ASN
3	E	284	VAL
3	E	299	GLU
3	E	305	LYS
3	E	350	VAL
3	E	359	GLU
3	E	363	ILE
3	E	366	LYS
3	E	368	GLN
3	E	384	THR
3	E	388	ILE
3	I	29	HIS
3	I	61	MET
3	I	62	VAL
3	I	63	LEU
3	I	89	GLU
3	I	95	VAL
3	I	97	THR
3	I	114	ILE
3	I	116	LYS
3	I	154	GLU
3	I	169	LEU
3	I	173	THR

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Mol	Chain	Res	Type
3	I	182	SER
3	I	204	VAL
3	I	206	LYS
3	I	234	ILE
3	I	253	THR
3	I	256	ARG
3	I	260	LEU
3	I	274	GLU
3	I	276	THR
3	I	279	VAL
3	I	284	VAL
3	I	299	GLU
3	I	305	LYS
3	I	324	LEU
3	I	350	VAL
3	I	359	GLU
3	I	363	ILE
3	I	368	GLN
3	I	388	ILE
4	F	15	SER
4	F	16	VAL
4	F	25	THR
4	F	32	VAL
4	F	33	LEU
4	F	36	PHE
4	F	38	VAL
4	F	39	LEU
4	F	47	MET
4	F	48	LEU
4	F	68	VAL
4	F	92	PHE
4	F	130	ILE
4	F	152	VAL
4	F	164	ASN
4	F	169	ILE
4	F	176	THR
4	F	202	ILE
4	F	251	THR
4	J	15	SER
4	J	16	VAL
4	J	25	THR
4	J	33	LEU

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Mol	Chain	Res	Type
4	J	36	PHE
4	J	38	VAL
4	J	39	LEU
4	J	47	MET
4	J	48	LEU
4	J	68	VAL
4	J	121	ILE
4	J	130	ILE
4	J	152	VAL
4	J	164	ASN
4	J	169	ILE
4	J	176	THR
4	J	202	ILE
4	J	251	THR
2	C	36	LEU
2	C	40	ILE
2	C	68	THR
2	C	75	VAL
2	C	116	ILE
2	C	126	THR
2	C	127	GLU
2	C	157	TYR
2	C	162	VAL
2	C	177	HIS
2	C	183	PHE
2	C	186	VAL
2	C	197	VAL
2	C	231	VAL
2	C	235	VAL
2	G	36	LEU
2	G	40	ILE
2	G	68	THR
2	G	75	VAL
2	G	116	ILE
2	G	118	ILE
2	G	127	GLU
2	G	160	ILE
2	G	162	VAL
2	G	177	HIS
2	G	231	VAL
2	G	235	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29)

such sidechains are listed below:

Mol	Chain	Res	Type
2	K	59	GLN
2	K	91	ASN
2	K	109	GLN
3	A	44	ASN
3	A	68	HIS
3	A	139	ASN
3	A	368	GLN
4	B	45	HIS
4	B	164	ASN
3	E	34	GLN
3	E	44	ASN
3	E	68	HIS
3	E	75	GLN
3	E	104	GLN
3	E	139	ASN
3	E	368	GLN
3	I	34	GLN
3	I	44	ASN
3	I	56	ASN
3	I	68	HIS
3	I	137	GLN
3	I	368	GLN
4	J	45	HIS
4	J	164	ASN
4	J	173	HIS
4	J	179	HIS
2	C	59	GLN
2	G	59	GLN
2	G	128	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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
6	PGT	K	302	-	50,50,50	1.48	5 (10%)	53,56,56	0.98	1 (1%)
6	PGT	G	302	-	50,50,50	1.36	4 (8%)	53,56,56	1.17	2 (3%)
6	PGT	C	302	-	50,50,50	1.25	4 (8%)	53,56,56	1.05	2 (3%)
6	PGT	G	303	-	50,50,50	1.33	4 (8%)	53,56,56	1.08	4 (7%)

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
6	PGT	K	302	-	-	28/55/55/55	-
6	PGT	G	302	-	-	22/55/55/55	-
6	PGT	C	302	-	-	31/55/55/55	-
6	PGT	G	303	-	-	31/55/55/55	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	302	PGT	O3-C11	4.28	1.45	1.33
6	G	303	PGT	O2-C31	3.87	1.45	1.34
6	G	303	PGT	O3-C11	3.83	1.44	1.33
6	C	302	PGT	O3-C11	3.80	1.44	1.33
6	G	302	PGT	O2-C31	3.69	1.44	1.34
6	G	302	PGT	O3-C11	3.67	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	302	PGT	O2-C31	3.55	1.44	1.34
6	C	302	PGT	O2-C31	3.33	1.43	1.34
6	G	302	PGT	O2-C2	-2.95	1.39	1.46
6	C	302	PGT	O2-C2	-2.94	1.39	1.46
6	K	302	PGT	O2-C2	-2.90	1.39	1.46
6	G	303	PGT	O2-C2	-2.82	1.40	1.46
6	G	303	PGT	C12-C11	2.61	1.58	1.50
6	C	302	PGT	C12-C11	2.49	1.57	1.50
6	G	302	PGT	C12-C11	2.49	1.57	1.50
6	K	302	PGT	C12-C11	2.44	1.57	1.50
6	K	302	PGT	C40-C41	2.23	1.62	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	302	PGT	O2-C31-C32	4.67	121.58	111.48
6	G	303	PGT	O2-C31-C32	3.88	119.87	111.48
6	G	302	PGT	O2-C31-O31	-3.69	115.08	123.70
6	K	302	PGT	O2-C31-C32	3.30	118.61	111.48
6	G	303	PGT	O3-C11-C12	3.29	121.86	111.83
6	C	302	PGT	O2-C31-C32	3.25	118.51	111.48
6	C	302	PGT	O3-C11-O11	-2.85	116.51	123.63
6	G	303	PGT	O3-C3-C2	2.50	115.60	108.40
6	G	303	PGT	O3-C11-O11	-2.06	118.48	123.63

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	302	PGT	C32-C31-O2-C2
6	K	302	PGT	O2-C2-C3-O3
6	K	302	PGT	C4-O4P-P-O3P
6	K	302	PGT	C4-O4P-P-O1P
6	K	302	PGT	C4-C5-C6-O6
6	C	302	PGT	C32-C31-O2-C2
6	C	302	PGT	O2-C2-C3-O3
6	C	302	PGT	C1-O3P-P-O1P
6	C	302	PGT	C1-O3P-P-O2P
6	C	302	PGT	C1-O3P-P-O4P
6	G	302	PGT	C32-C31-O2-C2
6	G	302	PGT	O31-C31-O2-C2
6	G	302	PGT	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
6	G	302	PGT	C1-O3P-P-O4P
6	G	302	PGT	C4-O4P-P-O3P
6	G	302	PGT	C4-O4P-P-O2P
6	G	303	PGT	C4-O4P-P-O3P
6	K	302	PGT	O31-C31-O2-C2
6	C	302	PGT	O31-C31-O2-C2
6	G	303	PGT	O31-C31-O2-C2
6	G	303	PGT	C12-C11-O3-C3
6	C	302	PGT	O11-C11-O3-C3
6	G	302	PGT	O11-C11-O3-C3
6	G	303	PGT	O11-C11-O3-C3
6	G	303	PGT	C32-C31-O2-C2
6	C	302	PGT	C12-C11-O3-C3
6	G	302	PGT	C12-C11-O3-C3
6	K	302	PGT	C39-C40-C41-C42
6	K	302	PGT	O5-C5-C6-O6
6	C	302	PGT	C32-C33-C34-C35
6	G	303	PGT	C31-C32-C33-C34
6	K	302	PGT	O11-C11-O3-C3
6	G	302	PGT	C31-C32-C33-C34
6	C	302	PGT	C42-C43-C44-C45
6	G	303	PGT	C4-C5-C6-O6
6	K	302	PGT	C21-C22-C23-C24
6	G	302	PGT	C38-C39-C40-C41
6	K	302	PGT	C44-C45-C46-C47
6	G	302	PGT	C40-C41-C42-C43
6	G	303	PGT	C38-C39-C40-C41
6	K	302	PGT	C34-C35-C36-C37
6	G	303	PGT	C17-C18-C19-C20
6	G	303	PGT	C40-C41-C42-C43
6	G	302	PGT	C42-C43-C44-C45
6	C	302	PGT	C41-C42-C43-C44
6	C	302	PGT	C14-C15-C16-C17
6	K	302	PGT	C42-C43-C44-C45
6	C	302	PGT	C17-C18-C19-C20
6	G	303	PGT	C37-C38-C39-C40
6	C	302	PGT	C37-C38-C39-C40
6	G	303	PGT	C19-C20-C21-C22
6	C	302	PGT	C11-C12-C13-C14
6	G	303	PGT	C11-C12-C13-C14
6	C	302	PGT	C34-C35-C36-C37
6	C	302	PGT	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
6	C	302	PGT	C36-C37-C38-C39
6	G	303	PGT	C13-C14-C15-C16
6	G	303	PGT	C33-C34-C35-C36
6	K	302	PGT	C20-C21-C22-C23
6	G	302	PGT	C36-C37-C38-C39
6	K	302	PGT	C43-C44-C45-C46
6	C	302	PGT	C43-C44-C45-C46
6	C	302	PGT	C1-C2-C3-O3
6	C	302	PGT	C33-C34-C35-C36
6	C	302	PGT	C40-C41-C42-C43
6	G	302	PGT	O2-C2-C3-O3
6	G	303	PGT	C23-C24-C25-C26
6	G	303	PGT	C14-C15-C16-C17
6	G	303	PGT	C15-C16-C17-C18
6	G	303	PGT	C1-C2-C3-O3
6	G	302	PGT	C22-C23-C24-C25
6	G	302	PGT	C18-C19-C20-C21
6	K	302	PGT	C15-C16-C17-C18
6	K	302	PGT	C41-C42-C43-C44
6	G	302	PGT	C21-C22-C23-C24
6	K	302	PGT	C1-C2-O2-C31
6	K	302	PGT	C37-C38-C39-C40
6	K	302	PGT	O3P-C1-C2-O2
6	K	302	PGT	C1-C2-C3-O3
6	G	303	PGT	O2-C2-C3-O3
6	K	302	PGT	C40-C41-C42-C43
6	K	302	PGT	C14-C15-C16-C17
6	G	303	PGT	C12-C13-C14-C15
6	G	302	PGT	C44-C45-C46-C47
6	K	302	PGT	C45-C46-C47-C48
6	G	303	PGT	O5-C5-C6-O6
6	C	302	PGT	C4-O4P-P-O1P
6	G	302	PGT	C1-O3P-P-O2P
6	G	303	PGT	C4-O4P-P-O2P
6	K	302	PGT	C33-C34-C35-C36
6	C	302	PGT	C15-C16-C17-C18
6	G	303	PGT	C35-C36-C37-C38
6	G	302	PGT	C1-C2-C3-O3
6	G	303	PGT	C16-C17-C18-C19
6	G	302	PGT	C34-C35-C36-C37
6	C	302	PGT	C21-C22-C23-C24
6	K	302	PGT	O3P-C1-C2-C3

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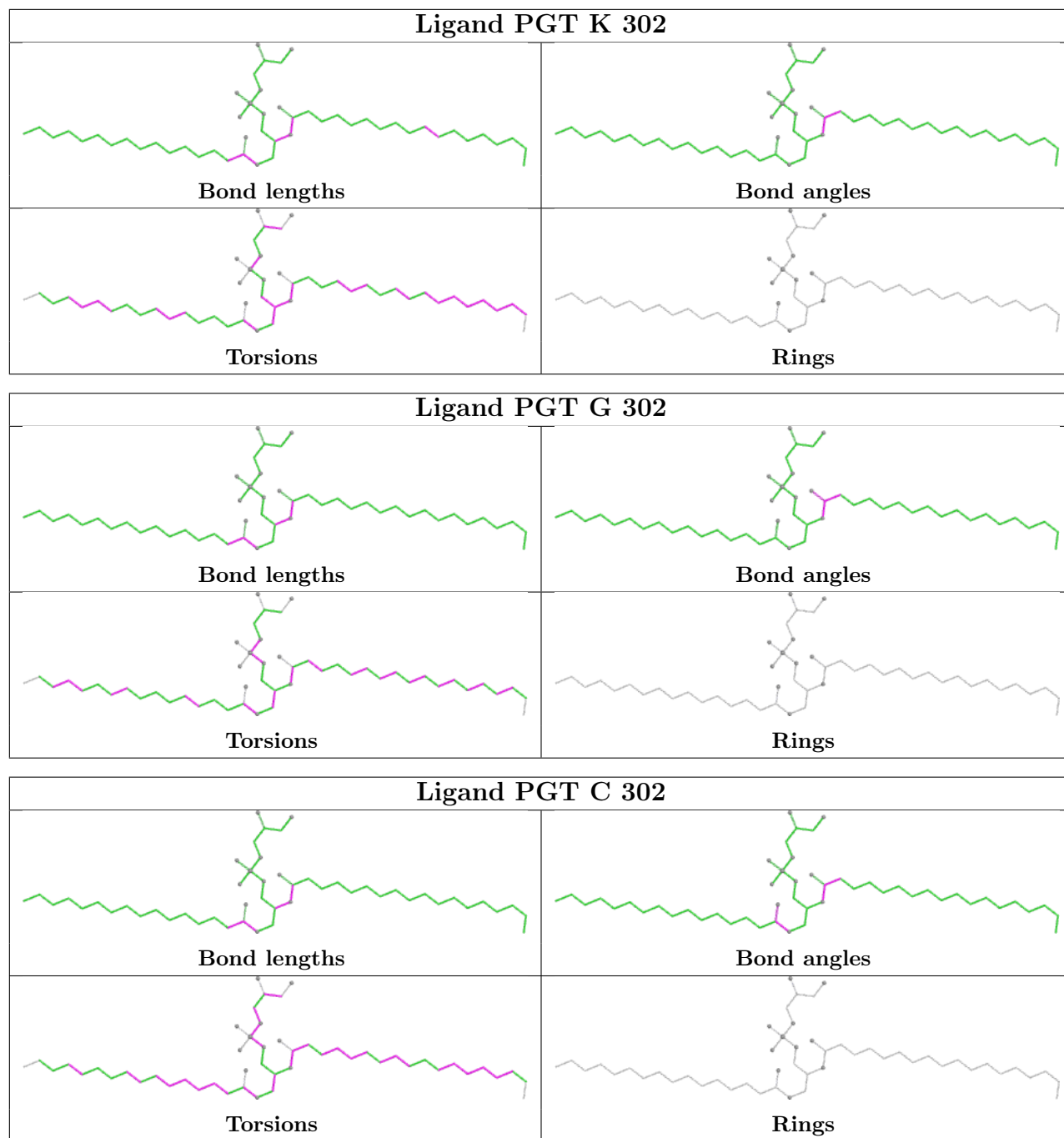
Mol	Chain	Res	Type	Atoms
6	C	302	PGT	C4-C5-C6-O6
6	C	302	PGT	O5-C5-C6-O6
6	C	302	PGT	C13-C14-C15-C16
6	G	303	PGT	C36-C37-C38-C39
6	K	302	PGT	C19-C20-C21-C22
6	K	302	PGT	C12-C11-O3-C3
6	G	303	PGT	C18-C19-C20-C21
6	G	303	PGT	C5-C4-O4P-P
6	G	303	PGT	C43-C44-C45-C46
6	C	302	PGT	C44-C45-C46-C47
6	G	302	PGT	C13-C14-C15-C16
6	C	302	PGT	O2-C31-C32-C33
6	G	303	PGT	O2-C31-C32-C33
6	G	303	PGT	C42-C43-C44-C45
6	C	302	PGT	C5-C4-O4P-P

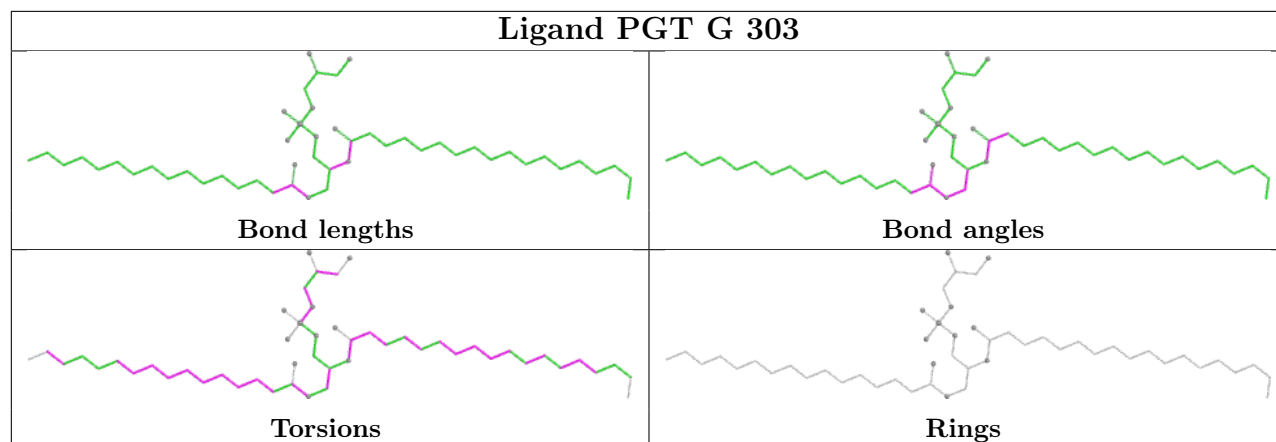
There are no ring outliers.

4 monomers are involved in 105 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	302	PGT	94	0
6	G	302	PGT	2	0
6	C	302	PGT	4	0
6	G	303	PGT	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	D	0/24	-	-	-	-
1	H	0/24	-	-	-	-
1	N	0/24	-	-	-	-
2	C	214/256 (83%)	1.23	47 (21%) 2 2	26, 51, 93, 124	0
2	G	212/256 (82%)	0.95	30 (14%) 6 5	22, 46, 86, 112	0
2	K	213/256 (83%)	0.78	32 (15%) 5 4	14, 37, 92, 120	0
3	A	388/420 (92%)	0.86	51 (13%) 7 5	18, 49, 82, 105	0
3	E	388/420 (92%)	0.22	18 (4%) 37 32	7, 28, 55, 82	0
3	I	388/420 (92%)	0.81	54 (13%) 6 5	18, 43, 83, 141	0
4	B	244/252 (96%)	0.58	21 (8%) 16 12	24, 39, 71, 123	0
4	F	244/252 (96%)	0.16	12 (4%) 35 29	10, 24, 63, 93	0
4	J	244/252 (96%)	0.15	15 (6%) 27 22	11, 24, 52, 88	0
All	All	2535/2856 (88%)	0.62	280 (11%) 10 8	7, 37, 80, 141	0

All (280) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	350	VAL	8.6
3	I	337	ASP	7.4
2	C	47	TRP	7.1
2	G	140	THR	6.8
2	K	252	LYS	6.8
2	C	198	GLY	6.6
2	G	47	TRP	6.6
2	G	194	ILE	6.5
2	K	47	TRP	6.5
3	A	350	VAL	6.4
2	C	48	ARG	6.4
2	G	253	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
3	E	350	VAL	6.1
4	B	10	VAL	6.1
2	K	197	VAL	6.0
2	C	226	TRP	5.9
2	C	197	VAL	5.9
2	G	252	LYS	5.9
3	A	348	LEU	5.8
2	C	17	SER	5.7
2	G	193	ILE	5.7
3	I	319	TYR	5.5
2	G	226	TRP	5.5
4	B	214	GLY	5.5
2	K	194	ILE	5.5
2	K	48	ARG	5.5
2	C	194	ILE	5.4
2	G	48	ARG	5.4
2	C	196	ASN	5.3
2	K	138	ARG	5.3
2	C	193	ILE	5.3
4	F	214	GLY	5.2
4	J	9	ALA	5.2
2	G	255	THR	5.1
3	I	348	LEU	5.0
3	I	416	ALA	4.8
4	F	251	THR	4.8
2	K	253	LEU	4.8
2	K	137	ILE	4.7
3	A	274	GLU	4.7
4	J	227	PHE	4.6
4	B	9	ALA	4.5
2	C	139	ASP	4.5
4	B	252	ILE	4.5
3	A	416	ALA	4.4
2	G	195	PRO	4.4
2	C	227	MET	4.4
3	I	346	ARG	4.3
2	K	191	PHE	4.3
3	I	352	ALA	4.3
2	C	228	ALA	4.2
2	C	252	LYS	4.2
3	I	275	GLY	4.2
2	C	253	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
3	A	60	GLU	4.0
3	A	219	LYS	4.0
2	K	226	TRP	4.0
2	G	138	ARG	3.9
2	C	54	PHE	3.9
3	E	416	ALA	3.9
2	K	193	ILE	3.9
2	C	67	TRP	3.8
2	K	140	THR	3.8
2	C	18	VAL	3.8
3	A	347	GLY	3.8
3	I	316	LEU	3.8
3	A	220	ALA	3.8
3	E	164	ASP	3.8
3	A	132	TRP	3.7
2	C	60	THR	3.7
2	G	196	ASN	3.7
4	J	216	ASP	3.7
2	C	140	THR	3.7
2	G	192	MET	3.7
2	G	139	ASP	3.7
3	I	321	ALA	3.6
4	J	231	MET	3.6
3	I	382	TYR	3.6
2	G	248	LYS	3.6
3	I	367	ILE	3.6
2	G	228	ALA	3.6
3	A	180	GLY	3.6
4	J	214	GLY	3.5
3	E	382	TYR	3.5
2	G	17	SER	3.5
4	B	242	TRP	3.5
4	F	213	PHE	3.5
2	C	52	ASP	3.5
3	I	347	GLY	3.5
4	J	10	VAL	3.4
2	C	195	PRO	3.4
3	A	322	ALA	3.4
2	C	138	ARG	3.4
3	I	355	ILE	3.4
2	K	254	LEU	3.3
3	E	348	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	C	19	VAL	3.3
2	K	139	ASP	3.3
2	K	60	THR	3.2
3	A	399	GLY	3.2
4	B	11	GLY	3.2
2	C	247	GLY	3.2
3	A	170	ASP	3.2
4	J	252	ILE	3.2
4	B	51	GLY	3.2
3	A	169	LEU	3.1
3	E	352	ALA	3.1
4	B	223	PHE	3.1
3	A	227	ASP	3.1
3	I	324	LEU	3.1
3	I	333	THR	3.1
2	K	51	LEU	3.1
4	J	213	PHE	3.1
2	G	227	MET	3.0
3	E	354	PRO	3.0
2	K	17	SER	3.0
2	K	54	PHE	3.0
4	B	215	LYS	3.0
3	I	29	HIS	3.0
3	A	200	PHE	3.0
4	B	36	PHE	3.0
3	I	363	ILE	3.0
3	A	352	ALA	3.0
4	F	9	ALA	3.0
2	G	61	TYR	3.0
3	I	349	SER	3.0
4	F	10	VAL	2.9
4	F	252	ILE	2.9
3	I	354	PRO	2.9
3	A	159	MET	2.9
3	E	355	ILE	2.9
3	A	273	THR	2.9
3	A	281	LYS	2.9
3	E	369	ASP	2.9
2	C	192	MET	2.9
4	B	16	VAL	2.9
3	E	219	LYS	2.9
2	C	53	SER	2.9

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Mol	Chain	Res	Type	RSRZ
4	J	251	THR	2.9
2	K	227	MET	2.9
2	C	59	GLN	2.9
2	G	256	GLU	2.9
2	G	246	VAL	2.8
3	A	397	PRO	2.8
3	A	158	ASP	2.8
3	A	164	ASP	2.8
4	J	242	TRP	2.8
2	K	61	TYR	2.8
4	B	227	PHE	2.8
3	A	335	LYS	2.8
2	K	67	TRP	2.7
3	E	356	ALA	2.7
2	C	90	ARG	2.7
3	A	376	ARG	2.7
4	B	14	ASN	2.7
2	G	141	ASP	2.7
3	E	347	GLY	2.7
4	J	36	PHE	2.7
4	B	219	PRO	2.7
3	E	346	ARG	2.7
3	I	365	VAL	2.7
3	I	220	ALA	2.7
2	K	52	ASP	2.6
3	E	351	ASP	2.6
3	A	157	GLY	2.6
3	I	218	GLY	2.6
3	I	335	LYS	2.6
2	K	19	VAL	2.6
2	K	64	SER	2.6
2	C	61	TYR	2.6
3	A	381	ALA	2.6
3	I	402	TYR	2.6
4	F	243	TYR	2.6
4	J	24	GLN	2.6
2	K	248	LYS	2.6
3	I	370	ALA	2.6
4	F	24	GLN	2.6
3	E	165	PRO	2.6
2	C	97	PRO	2.6
3	A	346	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
3	A	161	ASP	2.5
3	I	222	ASP	2.5
4	B	216	ASP	2.5
3	A	275	GLY	2.5
2	G	251	VAL	2.5
3	I	351	ASP	2.5
3	I	326	PHE	2.5
3	I	395	PHE	2.5
3	I	280	GLY	2.5
2	G	67	TRP	2.5
4	F	242	TRP	2.5
3	E	256	ARG	2.5
3	A	207	GLY	2.4
3	I	376	ARG	2.4
2	C	55	ALA	2.4
2	K	255	THR	2.4
2	K	195	PRO	2.4
4	J	215	LYS	2.4
2	K	59	GLN	2.4
3	I	200	PHE	2.4
4	B	213	PHE	2.4
3	A	334	THR	2.4
3	I	317	GLY	2.4
2	C	254	LEU	2.4
3	A	176	LEU	2.4
3	A	205	ARG	2.4
3	A	380	LEU	2.4
2	K	228	ALA	2.4
4	B	12	PRO	2.3
2	C	20	ASP	2.3
2	G	51	LEU	2.3
2	G	137	ILE	2.3
3	I	256	ARG	2.3
4	J	169	ILE	2.3
3	E	226	ASP	2.3
3	A	184	VAL	2.3
3	I	397	PRO	2.3
3	A	378	SER	2.3
3	I	281	LYS	2.3
3	A	204	VAL	2.3
2	C	57	GLU	2.3
3	I	132	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
3	I	278	GLY	2.3
3	I	366	LYS	2.3
2	C	141	ASP	2.3
3	A	222	ASP	2.3
3	I	334	THR	2.2
2	G	189	GLY	2.2
2	C	248	LYS	2.2
3	A	388	ILE	2.2
3	E	345	ASP	2.2
2	C	16	GLU	2.2
3	I	279	VAL	2.2
3	I	298	ARG	2.2
4	B	38	VAL	2.2
4	J	16	VAL	2.2
3	I	340	ASP	2.2
2	K	196	ASN	2.2
3	I	32	LYS	2.2
2	C	135	THR	2.2
3	I	353	THR	2.2
2	G	249	GLU	2.2
3	A	372	TRP	2.2
3	A	55	VAL	2.2
3	I	129	ALA	2.2
3	I	345	ASP	2.2
3	A	321	ALA	2.1
4	B	50	ALA	2.1
4	F	51	GLY	2.1
2	C	249	GLU	2.1
3	I	219	LYS	2.1
2	C	251	VAL	2.1
3	A	223	VAL	2.1
2	C	36	LEU	2.1
2	K	57	GLU	2.1
4	F	211	ARG	2.1
3	A	162	PHE	2.1
3	A	48	VAL	2.1
3	A	173	THR	2.1
4	B	250	ASP	2.1
2	C	58	PHE	2.1
2	C	150	PHE	2.1
3	I	230	ARG	2.1
3	A	59	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	I	60	GLU	2.1
2	C	86	LYS	2.1
3	A	349	SER	2.1
3	A	313	PRO	2.1
2	C	240	MET	2.1
4	B	231	MET	2.1
2	G	72	LEU	2.0
2	C	46	GLY	2.0
2	C	256	GLU	2.0
2	K	56	PRO	2.0
4	F	231	MET	2.0
2	G	18	VAL	2.0
3	I	332	PHE	2.0
3	I	302	ILE	2.0
3	A	330	ASP	2.0
3	I	226	ASP	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.

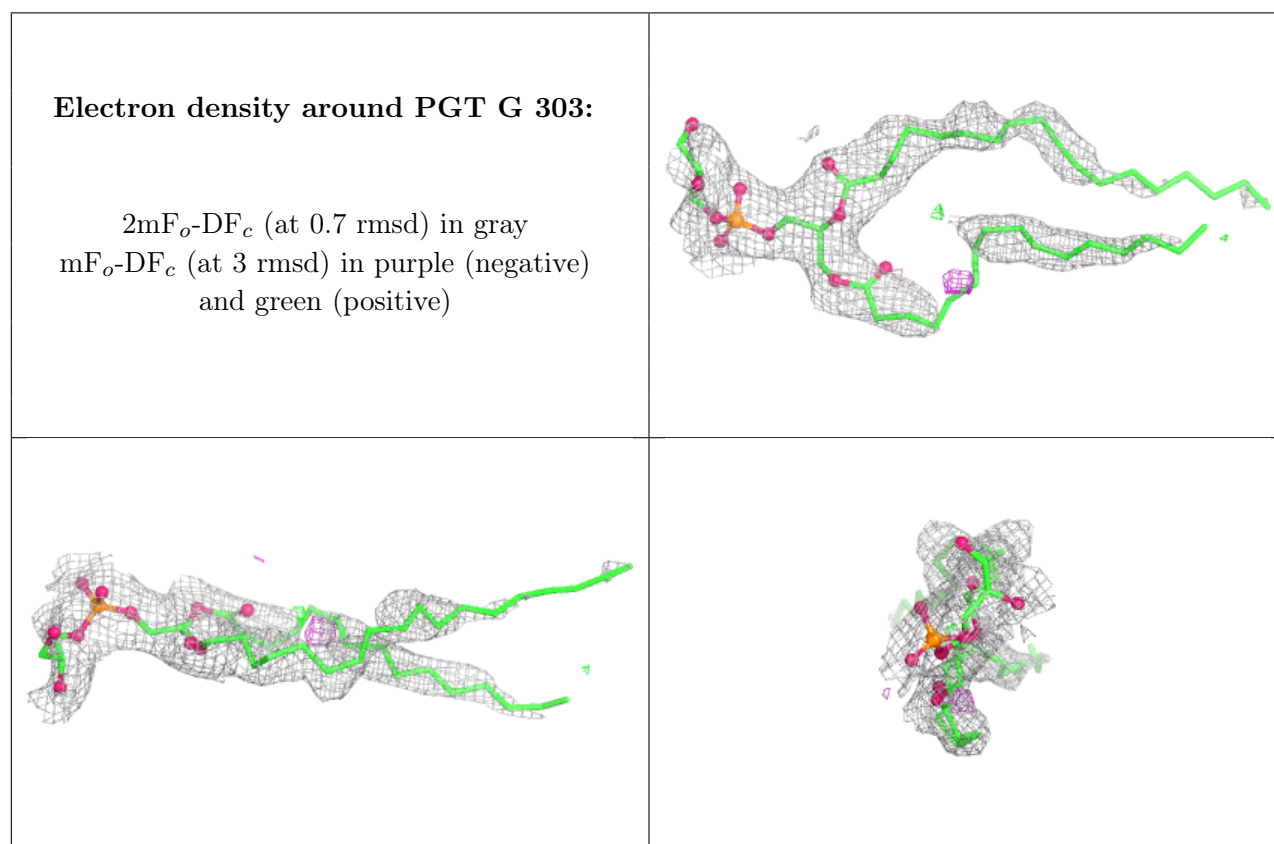
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PGT	G	303	51/51	0.80	0.23	53,71,114,115	0
6	PGT	G	302	51/51	0.86	0.21	45,59,99,106	0
6	PGT	C	302	51/51	0.86	0.21	51,75,90,95	0
6	PGT	K	302	51/51	0.88	0.16	24,39,51,53	0
5	CU	A	501	1/1	0.92	0.15	49,49,49,49	1
5	CU	I	501	1/1	0.95	0.10	60,60,60,60	0
5	CU	C	301	1/1	0.97	0.10	62,62,62,62	1

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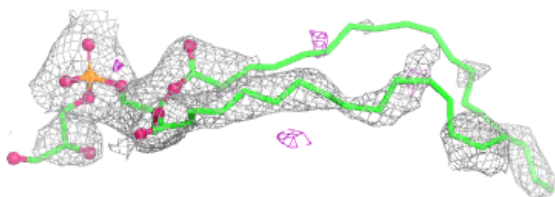
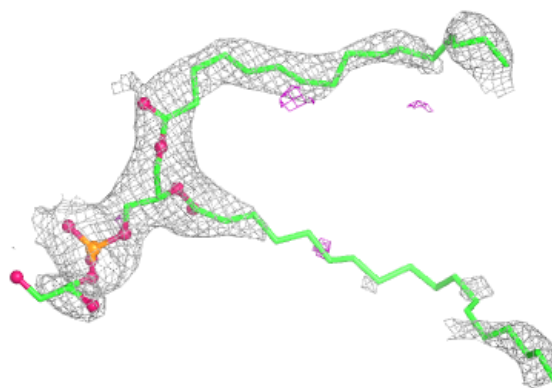
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CU	G	301	1/1	0.97	0.11	70,70,70,70	1
5	CU	E	501	1/1	0.97	0.15	24,24,24,24	1
5	CU	K	301	1/1	0.98	0.10	62,62,62,62	1

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.

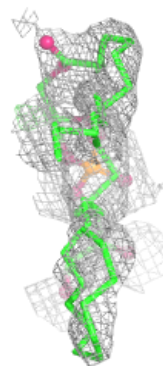
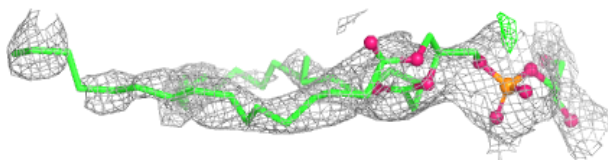
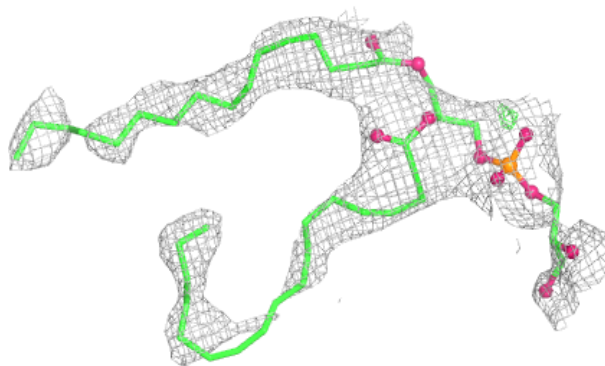


Electron density around PGT G 302:

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

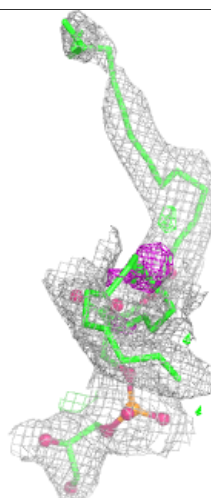
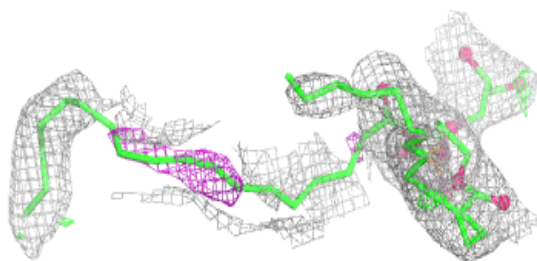
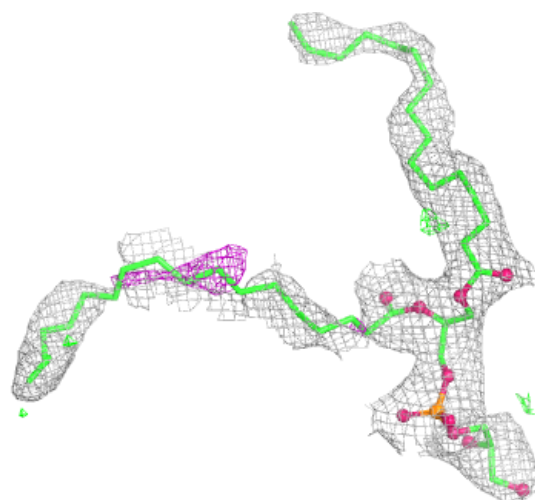
**Electron density around PGT C 302:**

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



Electron density around PGT K 302:

$2mF_o-DF_c$ (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.