



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:18 AM UTC

PDB ID : 5L0G / pdb_00005l0g
Title : Human metavinculin MVt Q971R, R975D, T978R mutant (residues 959-1134)
in complex with PIP2
Authors : Chinthalapudi, K.; Izard, T.
Deposited on : 2016-07-27
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

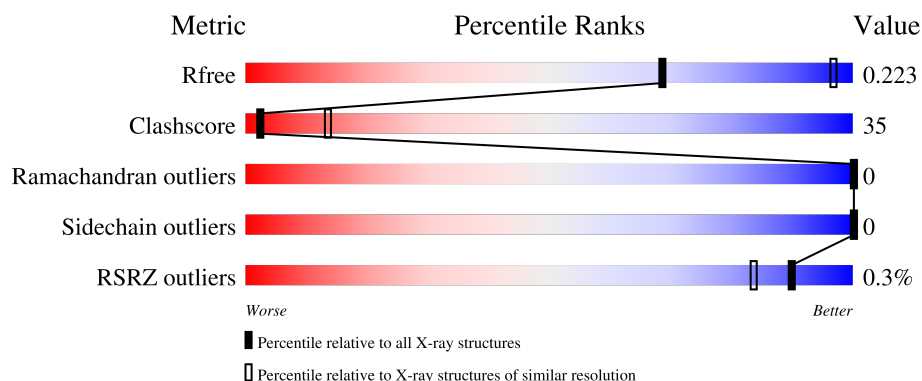
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

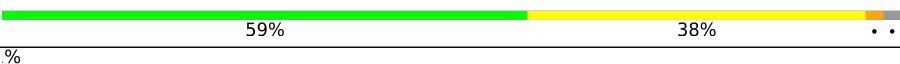
The reported resolution of this entry is 3.40 Å.

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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	176	 69% 28% ..
1	B	176	 59% 38% ..
1	C	176	 59% 37% ..
1	D	176	 58% 35% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5424 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.

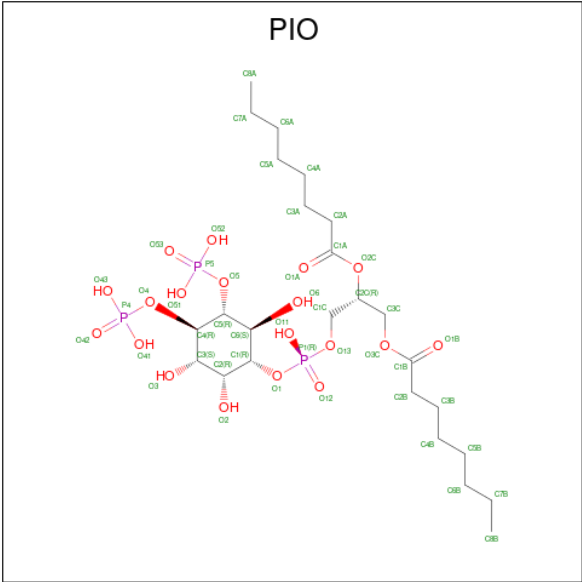
- Molecule 1 is a protein called Vinculin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	1	0
			1328	818	250	251	9			
1	B	172	Total	C	N	O	S	0	0	0
			1330	817	254	250	9			
1	C	171	Total	C	N	O	S	0	2	0
			1337	824	255	249	9			
1	D	170	Total	C	N	O	S	0	1	0
			1327	819	251	248	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	971	ARG	GLN	engineered mutation	UNP P18206
A	975	ASP	ARG	engineered mutation	UNP P18206
A	978	ARG	THR	engineered mutation	UNP P18206
B	971	ARG	GLN	engineered mutation	UNP P18206
B	975	ASP	ARG	engineered mutation	UNP P18206
B	978	ARG	THR	engineered mutation	UNP P18206
C	971	ARG	GLN	engineered mutation	UNP P18206
C	975	ASP	ARG	engineered mutation	UNP P18206
C	978	ARG	THR	engineered mutation	UNP P18206
D	971	ARG	GLN	engineered mutation	UNP P18206
D	975	ASP	ARG	engineered mutation	UNP P18206
D	978	ARG	THR	engineered mutation	UNP P18206

- Molecule 2 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: C₂₅H₄₉O₁₉P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			32	11	18	3		
2	C	1	Total	C	O	P	0	0
			24	6	15	3		

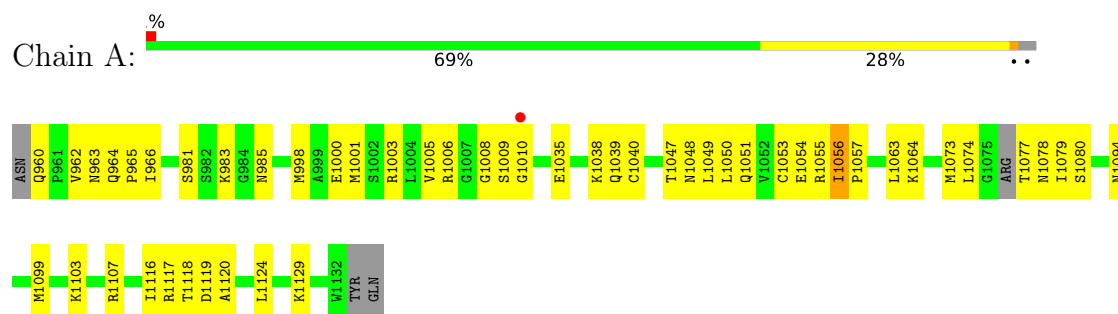
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		
3	B	13	Total	O	0	0
			13	13		
3	C	9	Total	O	0	0
			9	9		
3	D	12	Total	O	0	0
			12	12		

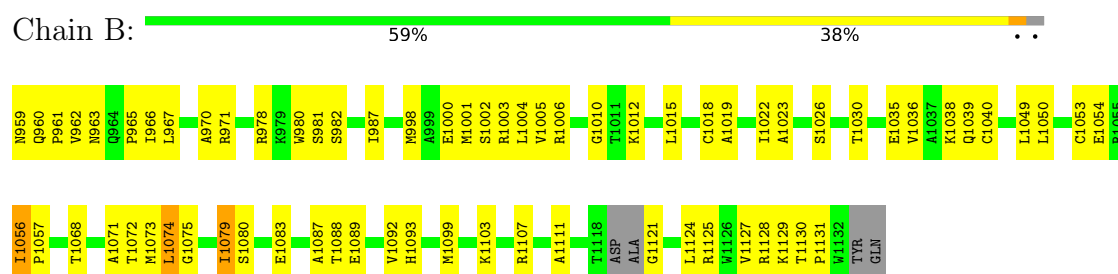
3 Residue-property plots

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.

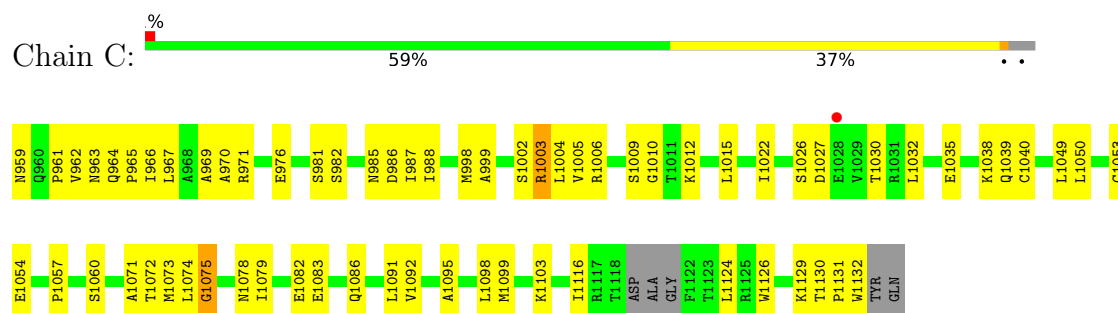
• Molecule 1: Vinculin



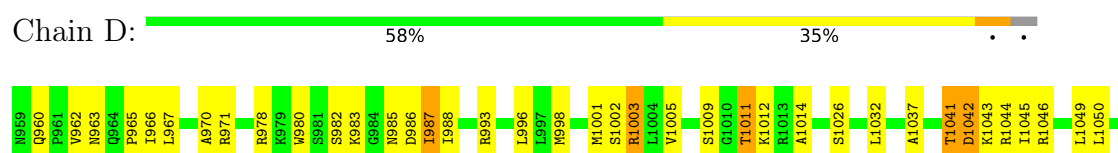
• Molecule 1: Vinculin



• Molecule 1: Vinculin



• Molecule 1: Vinculin



C1053	E1054	R1055	I1056	P1057	T1058	I1059		L1063	K1064		A1071	T1072	M1073	L1074	G1075	ARG	THR	N1078	I1079	S1080		E1083		T1088		V1092	H1093	N1094		L1098	M1099		V1106		S1113	T1114	K1115	I1116	R1117	T1118	ASP	ALA	GLY	F1122	T1123	L1124	R1125	V1126	V1127	R1128	K1129		V1132	V1133	GLN
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4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	56.86Å 56.86Å 193.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.24 – 3.40 49.24 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.24-3.40) 99.9 (49.24-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.180 , 0.221 0.214 , 0.223	Depositor DCC
R_{free} test set	473 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	92.7	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 79.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l 0.145 for h,-h-k,-l 0.053 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5424	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.07% 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: PIO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.84	0/1341	1.38	9/1804 (0.5%)
1	B	0.72	1/1340 (0.1%)	1.37	11/1801 (0.6%)
1	C	0.72	0/1354	1.39	10/1821 (0.5%)
1	D	0.77	0/1341	1.45	16/1802 (0.9%)
All	All	0.77	1/5376 (0.0%)	1.40	46/7228 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	960	GLN	C-N	5.13	1.39	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1056	ILE	CB-CA-C	-10.52	103.71	113.70
1	A	1006	ARG	CA-C-N	9.47	128.71	122.18
1	A	1006	ARG	C-N-CA	9.47	128.71	122.18
1	D	1041	THR	N-CA-C	8.60	120.65	111.28
1	C	1074	LEU	N-CA-C	8.17	119.81	111.07
1	D	1011	THR	N-CA-C	-7.08	102.98	113.61
1	B	1079	ILE	N-CA-C	6.81	119.44	109.63
1	A	1010	GLY	N-CA-C	-6.41	106.23	115.27
1	D	1129	LYS	N-CA-C	-5.95	102.26	110.35
1	A	1040	CYS	CA-C-N	5.89	128.45	120.44
1	A	1040	CYS	C-N-CA	5.89	128.45	120.44
1	C	1075	GLY	N-CA-C	5.80	120.19	112.77
1	B	960	GLN	CA-C-N	-5.74	114.69	120.31
1	B	960	GLN	C-N-CA	-5.74	114.69	120.31
1	C	1040	CYS	CA-C-N	5.71	128.20	120.44
1	C	1040	CYS	C-N-CA	5.71	128.20	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	960	GLN	CA-C-N	-5.70	114.06	119.76
1	A	960	GLN	C-N-CA	-5.70	114.06	119.76
1	B	1074	LEU	N-CA-C	5.67	117.46	111.28
1	B	1010	GLY	N-CA-C	-5.66	107.29	115.27
1	B	1040	CYS	CA-C-N	5.65	128.13	120.44
1	B	1040	CYS	C-N-CA	5.65	128.13	120.44
1	B	1075	GLY	N-CA-C	5.65	120.00	112.77
1	A	1056	ILE	N-CA-C	5.63	119.71	112.67
1	D	970	ALA	CA-C-N	5.62	127.81	120.28
1	D	970	ALA	C-N-CA	5.62	127.81	120.28
1	D	1128	ARG	N-CA-C	-5.58	101.59	109.96
1	C	1003	ARG	CA-C-N	5.58	127.75	120.28
1	C	1003	ARG	C-N-CA	5.58	127.75	120.28
1	C	1130	THR	CA-C-N	-5.54	114.05	119.76
1	C	1130	THR	C-N-CA	-5.54	114.05	119.76
1	B	1056	ILE	CB-CA-C	-5.50	108.52	114.35
1	D	987	ILE	N-CA-C	5.49	116.26	110.72
1	D	993	ARG	CA-C-N	5.49	127.57	120.44
1	D	993	ARG	C-N-CA	5.49	127.57	120.44
1	D	960	GLN	CA-C-N	-5.47	114.29	119.76
1	D	960	GLN	C-N-CA	-5.47	114.29	119.76
1	D	1042	ASP	N-CA-C	5.46	118.45	109.76
1	D	1056	ILE	CB-CA-C	-5.45	108.57	114.35
1	C	1010	GLY	N-CA-C	-5.34	107.31	115.00
1	B	970	ALA	CA-C-N	5.32	127.41	120.28
1	B	970	ALA	C-N-CA	5.32	127.41	120.28
1	D	1056	ILE	O-C-N	5.10	123.69	120.07
1	C	1078	ASN	N-CA-C	5.09	118.59	112.38
1	D	1003	ARG	CA-C-N	5.08	127.09	120.28
1	D	1003	ARG	C-N-CA	5.08	127.09	120.28

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	1328	0	1395	61	3
1	B	1330	0	1396	99	2
1	C	1337	0	1407	122	2
1	D	1327	0	1388	118	3
2	B	32	0	14	5	0
2	C	24	0	9	9	0
3	A	12	0	0	0	0
3	B	13	0	0	0	0
3	C	9	0	0	0	0
3	D	12	0	0	0	0
All	All	5424	0	5609	386	6

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 35.

All (386) 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:D:1041:THR:CG2	1:D:1117:ARG:HB2	1.48	1.43
1:C:1132:TRP:CE3	1:D:996:LEU:HD11	1.57	1.39
1:C:1012:LYS:HE3	1:C:1071:ALA:O	1.13	1.25
1:C:1132:TRP:CZ3	1:D:996:LEU:HD11	1.78	1.17
1:B:981:SER:HA	1:B:1129:LYS:HZ1	0.99	1.15
1:C:962:VAL:CG2	1:C:967:LEU:HD11	1.75	1.14
1:B:966:ILE:CG2	1:B:1002:SER:HB3	1.78	1.13
1:B:961:PRO:HG2	1:B:1006:ARG:HG3	1.31	1.12
1:B:981:SER:HA	1:B:1129:LYS:NZ	1.66	1.10
1:B:998:MET:CE	1:B:1099:MET:HE3	1.81	1.09
1:D:1054:GLU:O	1:D:1057:PRO:HD2	1.50	1.09
1:B:961:PRO:HB2	1:B:1006:ARG:HG2	1.31	1.09
1:A:963:ASN:ND2	1:A:965:PRO:HG2	1.65	1.08
1:C:971:ARG:HG2	1:D:1132:TRP:CE3	1.88	1.08
1:D:980:TRP:HB2	1:D:988:ILE:HD12	1.18	1.08
1:D:1041:THR:HG23	1:D:1117:ARG:HB2	1.29	1.07
1:B:1001:MET:HE1	1:B:1019:ALA:HA	1.34	1.06
1:B:1012:LYS:HG2	1:B:1074:LEU:HD12	1.11	1.06
1:B:980:TRP:C	1:B:1129:LYS:HE2	1.81	1.05
1:B:1012:LYS:HD2	1:B:1071:ALA:O	1.56	1.04
1:C:1012:LYS:CE	1:C:1071:ALA:O	2.04	1.04
1:A:963:ASN:HD21	1:A:965:PRO:HG2	0.87	1.04
1:D:1079:ILE:HG23	1:D:1083:GLU:OE1	1.56	1.04
1:C:1009:SER:HB2	1:C:1075:GLY:HA2	1.34	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:ILE:HD11	1:A:1120:ALA:HB2	1.36	1.02
1:A:963:ASN:HD21	1:A:965:PRO:CG	1.71	1.01
1:D:986:ASP:HB3	1:D:1032:LEU:CD1	1.90	1.01
1:B:998:MET:HE2	1:B:1099:MET:HE3	1.43	1.00
1:C:963:ASN:ND2	1:C:965:PRO:HG2	1.74	1.00
1:C:1009:SER:HB2	1:C:1075:GLY:CA	1.92	1.00
1:C:962:VAL:HG21	1:C:967:LEU:HD11	1.40	0.99
1:B:966:ILE:HG22	1:B:1002:SER:HB3	1.44	0.97
1:B:1073:MET:HG2	1:B:1079:ILE:HD12	1.43	0.97
1:C:1132:TRP:HE3	1:D:996:LEU:HD11	1.16	0.96
1:D:986:ASP:CB	1:D:1032:LEU:HD13	1.95	0.96
1:C:962:VAL:HG23	1:C:967:LEU:HD11	1.48	0.95
1:C:971:ARG:CG	1:D:1132:TRP:CE3	2.48	0.95
1:D:1041:THR:HG22	1:D:1117:ARG:HB2	1.47	0.95
1:D:1041:THR:CG2	1:D:1117:ARG:CB	2.45	0.95
1:C:987:ILE:HD12	1:C:1124:LEU:HD11	1.49	0.94
1:D:980:TRP:HB2	1:D:988:ILE:CD1	1.97	0.94
1:B:961:PRO:CG	1:B:1006:ARG:HG3	1.96	0.94
1:D:1009:SER:HB2	1:D:1074:LEU:C	1.92	0.94
1:D:986:ASP:HB3	1:D:1032:LEU:HD13	1.49	0.94
1:C:1012:LYS:HE3	1:C:1071:ALA:C	1.91	0.94
1:D:980:TRP:CB	1:D:988:ILE:HD12	1.97	0.94
1:C:962:VAL:CG1	1:C:1003:ARG:HG2	1.97	0.93
1:B:1036:VAL:HG21	1:B:1124:LEU:HD11	1.51	0.93
1:B:961:PRO:HG2	1:B:1006:ARG:CG	1.98	0.93
1:D:1045:ILE:HD12	1:D:1115:LYS:HD2	1.49	0.93
1:B:1012:LYS:CD	1:B:1071:ALA:O	2.17	0.92
1:B:961:PRO:CB	1:B:1006:ARG:HG2	2.00	0.92
1:C:1050:LEU:HA	1:C:1053:CYS:SG	2.09	0.92
1:C:988:ILE:HD11	1:C:1126:TRP:CZ3	2.04	0.92
1:B:1073:MET:HG2	1:B:1079:ILE:CD1	1.98	0.91
1:D:985:ASN:HB3	1:D:988:ILE:HG22	1.53	0.91
1:C:962:VAL:HG11	1:C:1003:ARG:HG2	1.52	0.91
1:C:976:GLU:OE1	1:C:1103:LYS:CG	2.19	0.90
1:B:981:SER:CA	1:B:1129:LYS:HZ1	1.82	0.90
1:D:985:ASN:HB3	1:D:988:ILE:CG2	2.03	0.89
1:D:963:ASN:HD22	1:D:966:ILE:HD12	1.38	0.89
1:C:963:ASN:HD21	1:C:965:PRO:HG2	1.36	0.88
1:B:1012:LYS:HG2	1:B:1074:LEU:CD1	2.02	0.88
1:A:983:LYS:HE2	2:B:1201:PIO:O6	1.74	0.88
1:B:966:ILE:HG21	1:B:1002:SER:HB3	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:ILE:HD11	1:A:1120:ALA:CB	2.04	0.86
1:D:985:ASN:HD22	1:D:988:ILE:CG2	1.88	0.86
1:C:963:ASN:HD22	1:C:966:ILE:HG13	1.41	0.86
1:C:998:MET:HE3	1:C:1099:MET:HE3	1.58	0.86
1:C:976:GLU:OE1	1:C:1103:LYS:HG2	1.77	0.85
1:C:1132:TRP:CZ3	1:D:996:LEU:CD1	2.59	0.85
1:D:980:TRP:O	1:D:988:ILE:HD11	1.75	0.85
1:A:1049:LEU:O	1:A:1053:CYS:SG	2.35	0.84
1:B:1080:SER:HB3	1:B:1083:GLU:CG	2.07	0.84
1:B:981:SER:N	1:B:1129:LYS:HE2	1.92	0.84
1:B:1012:LYS:CG	1:B:1074:LEU:HD12	2.05	0.84
1:D:1054:GLU:O	1:D:1057:PRO:CD	2.25	0.83
1:B:1012:LYS:HD3	1:B:1074:LEU:HB2	1.59	0.83
1:B:1036:VAL:CG2	1:B:1124:LEU:HD11	2.09	0.82
1:C:959:ASN:OD1	1:C:959:ASN:O	1.97	0.82
1:C:998:MET:CE	1:C:1099:MET:HE3	2.09	0.82
1:D:1012:LYS:HG2	1:D:1074:LEU:HD12	1.62	0.82
1:A:963:ASN:ND2	1:A:965:PRO:CG	2.38	0.82
1:C:967:LEU:O	1:C:971:ARG:HG3	1.78	0.82
1:B:981:SER:CA	1:B:1129:LYS:NZ	2.40	0.82
1:B:961:PRO:CG	1:B:1006:ARG:CG	2.57	0.81
1:A:1050:LEU:HA	1:A:1053:CYS:SG	2.20	0.81
1:D:1026:SER:OG	1:D:1056:ILE:CG2	2.28	0.81
1:B:998:MET:HE3	1:B:1099:MET:HE3	1.59	0.81
1:B:1001:MET:HE1	1:B:1019:ALA:CA	2.09	0.80
1:D:1050:LEU:HA	1:D:1053:CYS:SG	2.21	0.80
1:C:1073:MET:HA	1:C:1079:ILE:CD1	2.11	0.79
1:B:1073:MET:HE1	1:B:1087:ALA:CB	2.12	0.79
1:D:986:ASP:HB3	1:D:1032:LEU:HD11	1.63	0.79
1:A:1039:GLN:OE1	1:A:1120:ALA:HB1	1.82	0.79
1:B:1001:MET:CE	1:B:1019:ALA:HA	2.13	0.79
1:D:985:ASN:ND2	1:D:988:ILE:HB	1.97	0.79
1:A:1009:SER:HB2	1:A:1074:LEU:C	2.08	0.78
1:B:1039:GLN:NE2	1:B:1121:GLY:HA2	1.98	0.78
1:C:976:GLU:OE1	1:C:1103:LYS:HG3	1.82	0.78
1:C:985:ASN:HA	1:C:1124:LEU:HD22	1.65	0.78
1:C:961:PRO:O	1:C:1006:ARG:HG2	1.83	0.78
1:B:961:PRO:HB2	1:B:1006:ARG:CG	2.11	0.77
1:B:981:SER:HA	1:B:1129:LYS:CE	2.14	0.77
1:B:967:LEU:O	1:B:971:ARG:HG3	1.85	0.77
1:C:982:SER:HB2	2:C:1201:PIO:O43	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:980:TRP:CB	1:D:988:ILE:CD1	2.61	0.76
1:C:985:ASN:OD1	1:C:1124:LEU:HD13	1.86	0.76
2:C:1201:PIO:P1	1:D:983:LYS:HG3	2.25	0.76
1:D:986:ASP:HB2	1:D:1032:LEU:HD13	1.68	0.76
1:A:1039:GLN:CD	1:A:1120:ALA:HB1	2.11	0.75
1:B:1080:SER:HB3	1:B:1083:GLU:HG3	1.67	0.75
1:C:1132:TRP:CE3	1:D:996:LEU:CD1	2.54	0.75
1:C:971:ARG:CG	1:D:1132:TRP:HE3	1.96	0.75
1:D:980:TRP:C	1:D:988:ILE:CD1	2.60	0.74
1:D:1041:THR:HG23	1:D:1117:ARG:CB	2.14	0.74
1:C:1050:LEU:O	1:C:1054:GLU:HG2	1.87	0.74
1:D:1041:THR:HG21	1:D:1117:ARG:HB2	1.68	0.74
1:D:1009:SER:HB2	1:D:1074:LEU:O	1.88	0.74
1:C:987:ILE:HD12	1:C:1124:LEU:CD1	2.17	0.73
1:D:985:ASN:CB	1:D:988:ILE:HG22	2.18	0.73
1:A:1078:ASN:OD1	1:A:1079:ILE:N	2.21	0.73
1:B:1036:VAL:HG21	1:B:1124:LEU:CD1	2.19	0.73
1:D:985:ASN:ND2	1:D:988:ILE:CG2	2.52	0.73
1:B:1001:MET:CE	1:B:1019:ALA:CA	2.67	0.72
1:B:1054:GLU:O	1:B:1057:PRO:HD2	1.88	0.72
1:D:985:ASN:HD22	1:D:988:ILE:HB	1.51	0.72
1:D:1073:MET:HG2	1:D:1079:ILE:CD1	2.20	0.72
2:C:1201:PIO:O11	1:D:983:LYS:CG	2.38	0.72
1:D:967:LEU:O	1:D:971:ARG:HG3	1.89	0.71
1:A:1054:GLU:O	1:A:1057:PRO:HD2	1.90	0.71
1:C:963:ASN:CG	1:C:965:PRO:HD2	2.15	0.71
1:C:962:VAL:HG12	1:C:1003:ARG:HA	1.72	0.71
1:C:963:ASN:OD1	1:C:965:PRO:HD2	1.91	0.71
1:D:980:TRP:C	1:D:988:ILE:HD11	2.15	0.71
1:C:1039:GLN:HB3	1:C:1116:ILE:HD11	1.71	0.70
1:D:962:VAL:HG12	1:D:1003:ARG:HG2	1.70	0.70
1:C:1132:TRP:HE3	1:D:996:LEU:CD1	1.98	0.70
1:C:1050:LEU:HA	1:C:1053:CYS:HG	1.54	0.70
1:B:967:LEU:HD21	1:B:971:ARG:HH21	1.56	0.70
1:C:971:ARG:HG3	1:D:1132:TRP:CE3	2.27	0.70
1:B:1001:MET:CE	1:B:1022:ILE:HD12	2.23	0.69
1:B:1125:ARG:HE	1:B:1127:VAL:HG21	1.57	0.69
1:C:962:VAL:HG23	1:C:967:LEU:CD1	2.22	0.69
1:D:985:ASN:HD22	1:D:988:ILE:CB	2.05	0.69
1:C:1054:GLU:O	1:C:1057:PRO:HD2	1.92	0.69
1:D:1059:ILE:CG2	1:D:1098:LEU:HB2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:985:ASN:HA	1:D:1124:LEU:HD22	1.73	0.69
1:B:961:PRO:CB	1:B:1006:ARG:CG	2.70	0.68
1:B:1001:MET:HE3	1:B:1022:ILE:HD12	1.75	0.68
1:C:987:ILE:HG12	1:C:1032:LEU:HB2	1.74	0.68
1:B:962:VAL:HG12	1:B:1003:ARG:HG2	1.76	0.68
1:C:962:VAL:HG12	1:C:1003:ARG:HG2	1.75	0.68
1:B:1080:SER:HB3	1:B:1083:GLU:CD	2.19	0.68
1:C:1132:TRP:HZ3	1:D:996:LEU:HD11	1.57	0.68
1:C:988:ILE:HD11	1:C:1126:TRP:CH2	2.29	0.68
1:A:1049:LEU:C	1:A:1053:CYS:HG	2.01	0.67
1:A:983:LYS:CE	2:B:1201:PIO:O6	2.42	0.67
1:C:1132:TRP:HZ3	1:D:996:LEU:CD1	2.07	0.67
1:B:1088:THR:O	1:B:1092:VAL:HG23	1.94	0.67
1:D:982:SER:HA	1:D:988:ILE:HG23	1.76	0.67
1:C:1073:MET:HG2	1:C:1079:ILE:HD13	1.77	0.67
1:A:1000:GLU:HG3	1:A:1003:ARG:HH21	1.60	0.66
1:A:1118:THR:HG23	1:A:1119:ASP:H	1.61	0.66
1:D:1073:MET:HG2	1:D:1079:ILE:HD12	1.77	0.66
1:B:980:TRP:O	1:B:1129:LYS:HE2	1.95	0.66
1:D:1054:GLU:C	1:D:1057:PRO:HD2	2.20	0.66
1:D:985:ASN:ND2	1:D:988:ILE:HG22	2.10	0.66
1:C:1009:SER:CB	1:C:1075:GLY:HA2	2.20	0.65
1:C:969:ALA:HB1	1:C:1099:MET:HG3	1.76	0.65
1:D:1050:LEU:O	1:D:1054:GLU:HG3	1.97	0.65
1:D:1012:LYS:HD2	1:D:1071:ALA:O	1.98	0.64
1:A:963:ASN:HD22	1:A:966:ILE:H	1.44	0.63
1:A:1118:THR:HG23	1:A:1119:ASP:N	2.13	0.63
1:A:1078:ASN:OD1	1:A:1079:ILE:HG13	1.99	0.63
1:B:981:SER:CB	1:B:1129:LYS:NZ	2.60	0.63
1:C:966:ILE:CG2	1:C:1002:SER:HB3	2.28	0.63
1:A:963:ASN:ND2	1:A:965:PRO:HD2	2.14	0.62
1:A:963:ASN:ND2	1:A:966:ILE:HG13	2.15	0.62
1:B:1049:LEU:O	1:B:1053:CYS:SG	2.48	0.62
1:D:1059:ILE:HG21	1:D:1098:LEU:HB2	1.82	0.62
1:A:963:ASN:ND2	1:A:965:PRO:CD	2.63	0.62
1:B:981:SER:CA	1:B:1129:LYS:CE	2.78	0.61
1:B:981:SER:CA	1:B:1129:LYS:HE2	2.29	0.61
1:C:963:ASN:ND2	1:C:965:PRO:CG	2.57	0.61
1:B:998:MET:HE2	1:B:1099:MET:CE	2.26	0.60
1:A:1055:ARG:C	1:A:1057:PRO:HD2	2.26	0.60
1:B:1073:MET:HE1	1:B:1087:ALA:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1039:GLN:O	1:C:1116:ILE:HG13	2.01	0.60
1:C:1012:LYS:NZ	1:C:1072:THR:HA	2.16	0.60
1:C:971:ARG:HG2	1:D:1132:TRP:HE3	1.52	0.60
1:C:1073:MET:HA	1:C:1079:ILE:HD11	1.82	0.60
1:C:1057:PRO:HA	1:C:1060:SER:OG	2.01	0.60
2:C:1201:PIO:O11	1:D:983:LYS:HG2	2.00	0.60
1:D:1026:SER:OG	1:D:1056:ILE:HG23	2.02	0.59
1:A:963:ASN:ND2	1:A:966:ILE:H	1.99	0.59
1:B:1001:MET:HB2	1:B:1018:CYS:SG	2.42	0.59
1:C:971:ARG:HG2	1:D:1132:TRP:CD2	2.35	0.59
1:B:1001:MET:CE	1:B:1019:ALA:N	2.65	0.59
1:B:1012:LYS:CD	1:B:1074:LEU:HB2	2.33	0.59
2:C:1201:PIO:H5	2:C:1201:PIO:O42	2.03	0.59
1:D:1012:LYS:CD	1:D:1071:ALA:O	2.51	0.59
1:C:964:GLN:N	1:C:965:PRO:HD2	2.17	0.58
1:D:1059:ILE:CG2	1:D:1098:LEU:HD13	2.33	0.58
1:C:963:ASN:HD21	1:C:965:PRO:CG	2.12	0.58
1:B:967:LEU:HG	1:B:971:ARG:NE	2.18	0.58
1:C:1005[B]:VAL:HG11	1:C:1091:LEU:CD2	2.33	0.58
1:D:1079:ILE:CG2	1:D:1083:GLU:OE1	2.43	0.58
1:A:1117:ARG:O	1:A:1118:THR:HG22	2.03	0.58
1:C:971:ARG:HG3	1:D:1132:TRP:HE3	1.67	0.58
1:D:978:ARG:O	1:D:1129:LYS:HD3	2.04	0.58
1:B:981:SER:CB	1:B:1129:LYS:HZ3	2.18	0.57
1:C:1050:LEU:CA	1:C:1053:CYS:SG	2.90	0.57
1:D:985:ASN:CG	1:D:988:ILE:HG22	2.30	0.57
1:C:998:MET:HE2	1:C:1099:MET:HE3	1.87	0.57
1:A:1054:GLU:O	1:A:1057:PRO:CD	2.53	0.57
1:B:1050:LEU:HA	1:B:1053:CYS:SG	2.45	0.57
1:C:1005[A]:VAL:HG11	1:C:1091:LEU:CD2	2.34	0.57
1:D:985:ASN:ND2	1:D:988:ILE:CB	2.63	0.56
1:A:1073:MET:HG2	1:A:1079:ILE:HD13	1.87	0.56
1:B:982:SER:HB2	2:B:1201:PIO:O3	2.05	0.56
1:B:966:ILE:CG2	1:B:1002:SER:CB	2.71	0.56
1:D:1041:THR:HG22	1:D:1117:ARG:HD3	1.88	0.55
1:B:967:LEU:CD2	1:B:971:ARG:HH21	2.19	0.55
1:D:963:ASN:HD22	1:D:966:ILE:CD1	2.15	0.55
1:A:1047:THR:O	1:A:1051:GLN:HG2	2.05	0.55
1:C:963:ASN:ND2	1:C:966:ILE:HG13	2.18	0.55
1:D:962:VAL:CG1	1:D:1003:ARG:HG2	2.36	0.55
1:D:1088:THR:O	1:D:1092:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1036:VAL:CG2	1:B:1124:LEU:CD1	2.80	0.55
1:C:1027:ASP:O	1:C:1030:THR:OG1	2.22	0.55
1:A:1050:LEU:O	1:A:1054:GLU:HG3	2.06	0.55
1:B:967:LEU:CD2	1:B:971:ARG:NH2	2.70	0.55
1:A:966:ILE:CD1	1:A:1005[B]:VAL:HG21	2.37	0.55
1:A:966:ILE:CD1	1:A:1005[A]:VAL:HG21	2.37	0.55
1:D:1059:ILE:HG21	1:D:1098:LEU:CB	2.37	0.55
1:C:963:ASN:HD22	1:C:966:ILE:CG1	2.17	0.54
1:C:999:ALA:O	1:C:1002:SER:OG	2.19	0.54
2:C:1201:PIO:P1	1:D:983:LYS:CG	2.95	0.54
1:C:1005[B]:VAL:HG11	1:C:1091:LEU:HD21	1.89	0.54
1:B:1068:THR:O	1:B:1072:THR:HG23	2.07	0.54
1:C:966:ILE:HG22	1:C:1002:SER:HB3	1.88	0.54
1:A:1039:GLN:HE22	1:A:1120:ALA:HA	1.72	0.54
1:B:1073:MET:SD	1:B:1079:ILE:HD13	2.48	0.54
1:C:1049:LEU:O	1:C:1053:CYS:SG	2.64	0.54
1:C:1050:LEU:CA	1:C:1053:CYS:HG	2.20	0.54
1:A:966:ILE:HD12	1:A:1005[A]:VAL:HG21	1.90	0.53
1:A:985:ASN:HA	1:A:1124:LEU:HD22	1.90	0.53
1:A:1009:SER:HB2	1:A:1074:LEU:O	2.09	0.53
1:A:966:ILE:HD12	1:A:1005[B]:VAL:HG21	1.90	0.53
1:B:1089:GLU:O	1:B:1093:HIS:CD2	2.62	0.53
1:C:1005[A]:VAL:HG11	1:C:1091:LEU:HD21	1.89	0.53
1:C:965:PRO:HB2	1:C:1092:VAL:HG13	1.90	0.53
1:A:1035:GLU:HA	1:A:1038:LYS:HE3	1.92	0.52
2:C:1201:PIO:O13	1:D:983:LYS:HG3	2.09	0.52
1:C:967:LEU:O	1:C:971:ARG:CG	2.56	0.52
1:B:1125:ARG:HE	1:B:1127:VAL:CG2	2.22	0.52
1:A:998:MET:O	1:A:1001:MET:HB3	2.10	0.52
1:C:971:ARG:N	1:D:1132:TRP:CZ3	2.77	0.52
1:C:969:ALA:C	1:C:1099:MET:HG3	2.35	0.52
1:D:1041:THR:HG22	1:D:1117:ARG:CB	2.24	0.52
1:B:978:ARG:O	1:B:1129:LYS:HG3	2.10	0.51
1:C:966:ILE:HD12	1:C:1002:SER:HA	1.91	0.51
1:C:1073:MET:CA	1:C:1079:ILE:CD1	2.86	0.51
1:D:1049:LEU:O	1:D:1053:CYS:SG	2.65	0.51
1:B:1001:MET:HG3	1:B:1015:LEU:HD12	1.93	0.51
1:A:963:ASN:CG	1:A:965:PRO:HD2	2.36	0.51
1:C:987:ILE:CD1	1:C:1124:LEU:HD11	2.33	0.51
1:D:985:ASN:HB3	1:D:988:ILE:HG21	1.88	0.50
1:D:1042:ASP:OD1	1:D:1043:LYS:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:985:ASN:OD1	1:D:1124:LEU:HD13	2.10	0.50
1:C:1057:PRO:O	1:C:1060:SER:OG	2.28	0.50
1:D:1050:LEU:HA	1:D:1053:CYS:HG	1.73	0.50
1:B:963:ASN:HD21	1:B:965:PRO:HG2	1.76	0.50
1:D:1043:LYS:HG3	1:D:1046:ARG:NH2	2.27	0.50
1:C:1035:GLU:HA	1:C:1038:LYS:HE3	1.93	0.50
1:C:1039:GLN:HB3	1:C:1116:ILE:CD1	2.40	0.50
1:D:1026:SER:HG	1:D:1056:ILE:CG2	2.24	0.50
1:A:1073:MET:HG2	1:A:1079:ILE:CD1	2.42	0.50
1:C:962:VAL:HG12	1:C:1003:ARG:CA	2.41	0.49
1:D:980:TRP:O	1:D:988:ILE:CD1	2.50	0.49
1:D:986:ASP:CB	1:D:1032:LEU:CD1	2.65	0.49
1:C:966:ILE:CD1	1:C:1005[B]:VAL:HG21	2.42	0.49
1:C:966:ILE:CD1	1:C:1005[A]:VAL:HG21	2.42	0.49
1:B:1039:GLN:CD	1:B:1121:GLY:HA2	2.35	0.49
1:B:1035:GLU:HA	1:B:1038:LYS:HE3	1.95	0.49
1:B:987:ILE:HD12	1:B:1124:LEU:CD1	2.42	0.49
1:D:1054:GLU:O	1:D:1057:PRO:CG	2.60	0.49
1:A:983:LYS:NZ	2:B:1201:PIO:O6	2.46	0.48
1:B:1000:GLU:O	1:B:1004:LEU:HG	2.13	0.48
1:C:1082:GLU:O	1:C:1086:GLN:HG2	2.14	0.48
1:D:1059:ILE:HG22	1:D:1098:LEU:HD13	1.95	0.48
1:B:1073:MET:CG	1:B:1079:ILE:CD1	2.83	0.48
1:C:967:LEU:CD2	1:C:1002:SER:OG	2.62	0.48
1:D:1113:SER:O	1:D:1116:ILE:HG23	2.13	0.48
1:C:987:ILE:CG1	1:C:1032:LEU:HB2	2.43	0.48
1:A:1039:GLN:NE2	1:A:1120:ALA:HB1	2.29	0.48
1:B:1073:MET:HE1	1:B:1087:ALA:HB3	1.93	0.48
1:C:966:ILE:CD1	1:C:1002:SER:HA	2.44	0.48
1:A:1056:ILE:N	1:A:1057:PRO:HD2	2.29	0.48
1:A:1079:ILE:HG22	1:A:1080:SER:N	2.28	0.48
1:C:964:GLN:N	1:C:965:PRO:CD	2.77	0.48
1:D:1059:ILE:HG21	1:D:1098:LEU:HA	1.96	0.48
1:D:1125:ARG:HE	1:D:1127:VAL:HG21	1.79	0.47
1:B:1015:LEU:HD23	1:B:1071:ALA:HB2	1.96	0.47
1:D:1079:ILE:CG2	1:D:1083:GLU:HB2	2.45	0.47
1:C:1004:LEU:HD13	1:C:1015:LEU:HA	1.97	0.47
2:C:1201:PIO:O13	2:C:1201:PIO:H6	2.15	0.47
1:D:963:ASN:ND2	1:D:966:ILE:HD12	2.18	0.47
1:D:1059:ILE:HG21	1:D:1098:LEU:CA	2.45	0.47
1:D:1079:ILE:HG22	1:D:1083:GLU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:962:VAL:HG21	1:D:967:LEU:HD22	1.97	0.47
1:B:1001:MET:HE2	1:B:1019:ALA:N	2.29	0.46
1:D:980:TRP:C	1:D:988:ILE:HD13	2.39	0.46
1:D:998:MET:HE3	1:D:1099:MET:HE3	1.97	0.46
1:D:965:PRO:HB2	1:D:1092:VAL:CG1	2.46	0.46
1:D:965:PRO:HB2	1:D:1092:VAL:HG11	1.97	0.46
1:C:1026:SER:O	1:C:1030:THR:HG23	2.16	0.46
1:B:1012:LYS:HD3	1:B:1071:ALA:O	2.10	0.46
1:B:1030:THR:HG22	1:B:1056:ILE:HB	1.98	0.46
1:A:1079:ILE:CG2	1:A:1080:SER:N	2.79	0.46
1:D:982:SER:HA	1:D:988:ILE:CG2	2.44	0.45
1:A:962:VAL:HG12	1:A:1003:ARG:HG2	1.99	0.45
1:B:980:TRP:NE1	1:B:1128:ARG:HD2	2.32	0.45
1:A:1056:ILE:O	1:A:1057:PRO:C	2.59	0.45
1:D:998:MET:CE	1:D:1099:MET:HE3	2.46	0.45
1:C:970:ALA:HB3	1:D:1132:TRP:HZ3	1.82	0.45
1:C:1039:GLN:CB	1:C:1116:ILE:HD11	2.45	0.45
1:D:987:ILE:CG2	1:D:1106:VAL:HG22	2.47	0.45
1:C:1005[A]:VAL:CG1	1:C:1091:LEU:HD21	2.47	0.44
1:C:1054:GLU:O	1:C:1057:PRO:CD	2.65	0.44
1:C:1005[B]:VAL:CG1	1:C:1091:LEU:HD21	2.47	0.44
1:C:1073:MET:CG	1:C:1079:ILE:HD13	2.45	0.44
1:B:987:ILE:HD12	1:B:1124:LEU:HD11	1.99	0.44
1:B:1023:ALA:O	1:B:1026:SER:OG	2.28	0.44
1:A:1063:LEU:HB2	1:A:1094:ASN:HD21	1.83	0.44
1:B:1056:ILE:N	1:B:1057:PRO:HD2	2.31	0.44
1:B:1073:MET:HG2	1:B:1079:ILE:HD13	1.94	0.44
1:B:1030:THR:CG2	1:B:1056:ILE:HB	2.48	0.44
1:C:963:ASN:HD21	1:C:1092:VAL:HG22	1.83	0.44
1:B:1080:SER:CB	1:B:1083:GLU:HG3	2.41	0.43
1:C:969:ALA:CB	1:C:1099:MET:HG3	2.45	0.43
1:D:1001:MET:O	1:D:1005:VAL:HG22	2.18	0.43
1:B:1130:THR:HA	1:B:1131:PRO:HD3	1.79	0.43
1:C:967:LEU:HD21	1:C:1002:SER:OG	2.17	0.43
1:B:1001:MET:O	1:B:1005:VAL:HG23	2.18	0.43
1:A:1048:ASN:OD1	1:C:1131:PRO:HD3	2.18	0.43
1:A:1099:MET:HE2	1:A:1099:MET:HA	1.99	0.43
1:B:1012:LYS:CG	1:B:1074:LEU:HB2	2.48	0.43
1:C:1005[B]:VAL:HG11	1:C:1091:LEU:HD23	1.99	0.43
1:B:959:ASN:OD1	1:B:959:ASN:O	2.36	0.43
2:B:1201:PIO:H2	2:B:1201:PIO:O12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1077:THR:OG1	1:A:1078:ASN:N	2.51	0.42
1:A:1103:LYS:HE2	1:A:1107:ARG:NH2	2.34	0.42
1:A:1050:LEU:CA	1:A:1053:CYS:SG	3.00	0.42
1:C:1095:ALA:O	1:C:1099:MET:HG2	2.20	0.42
1:A:1050:LEU:CA	1:A:1053:CYS:HG	2.33	0.42
1:A:1117:ARG:O	1:A:1118:THR:CG2	2.66	0.42
1:D:1026:SER:HG	1:D:1056:ILE:HG23	1.83	0.42
1:B:1039:GLN:OE1	1:B:1121:GLY:HA3	2.19	0.42
1:C:1005[A]:VAL:HG11	1:C:1091:LEU:HD23	2.00	0.42
1:C:1009:SER:HB2	1:C:1075:GLY:HA3	1.91	0.42
1:A:964:GLN:N	1:A:965:PRO:HD2	2.35	0.41
1:C:966:ILE:HB	1:C:1002:SER:CB	2.50	0.41
1:C:981:SER:HA	1:C:1129:LYS:HE3	2.03	0.41
1:A:1039:GLN:NE2	1:A:1120:ALA:CB	2.83	0.41
1:C:966:ILE:HB	1:C:1002:SER:HB3	2.02	0.41
1:C:1022:ILE:CG2	1:C:1098:LEU:HD21	2.50	0.41
1:A:981:SER:HA	1:A:1129:LYS:HE3	2.03	0.41
1:D:1079:ILE:HG22	1:D:1080:SER:N	2.34	0.41
1:A:1000:GLU:HG3	1:A:1003:ARG:NH2	2.33	0.41
1:B:1103:LYS:HE2	1:B:1107:ARG:NH2	2.36	0.41
2:C:1201:PIO:P1	2:C:1201:PIO:O2	2.79	0.41
1:B:980:TRP:O	1:B:1129:LYS:CE	2.66	0.41
1:B:1054:GLU:O	1:B:1057:PRO:CD	2.65	0.41
1:C:986:ASP:O	1:C:987:ILE:C	2.61	0.41
1:C:1012:LYS:HZ1	1:C:1072:THR:HA	1.86	0.41
1:D:963:ASN:O	1:D:1002:SER:OG	2.33	0.41
1:D:1042:ASP:OD1	1:D:1042:ASP:C	2.64	0.41
1:D:1063:LEU:HB2	1:D:1094:ASN:HD21	1.86	0.41
1:C:987:ILE:CG1	1:C:1032:LEU:CB	2.99	0.41
1:D:1011:THR:O	1:D:1014:ALA:HB3	2.21	0.41
1:D:1037:ALA:O	1:D:1046:ARG:HG3	2.21	0.41
1:D:1009:SER:HB2	1:D:1075:GLY:N	2.33	0.40
1:C:963:ASN:OD1	1:C:965:PRO:CD	2.66	0.40
1:C:1073:MET:CB	1:C:1079:ILE:HD13	2.51	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1083:GLU:OE2	1:D:1064:LYS:NZ[3_675]	1.64	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1083:GLU:OE2	1:D:1064:LYS:CE[3_675]	1.87	0.33
1:A:1008:GLY:CA	1:A:1119:ASP:OD2[1_565]	2.03	0.17
1:A:1008:GLY:N	1:A:1119:ASP:OD2[1_565]	2.08	0.12
1:A:1064:LYS:NZ	1:B:1083:GLU:OE2[2_764]	2.17	0.03
1:B:1111:ALA:CB	1:D:1044:ARG:NH2[3_675]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	169/176 (96%)	167 (99%)	2 (1%)	0	100	100
1	B	168/176 (96%)	166 (99%)	2 (1%)	0	100	100
1	C	169/176 (96%)	166 (98%)	3 (2%)	0	100	100
1	D	165/176 (94%)	164 (99%)	1 (1%)	0	100	100
All	All	671/704 (95%)	663 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	144/148 (97%)	144 (100%)	0	100	100
1	B	144/148 (97%)	144 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	146/148 (99%)	146 (100%)	0	100	100
1	D	144/148 (97%)	144 (100%)	0	100	100
All	All	578/592 (98%)	578 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	963	ASN
1	A	964	GLN
1	A	1039	GLN
1	A	1062	GLN
1	A	1094	ASN
1	A	1097	ASN
1	B	963	ASN
1	B	1017	GLN
1	B	1062	GLN
1	B	1093	HIS
1	B	1094	ASN
1	B	1097	ASN
1	C	959	ASN
1	C	963	ASN
1	C	1062	GLN
1	D	963	ASN
1	D	985	ASN
1	D	1017	GLN
1	D	1062	GLN
1	D	1094	ASN
1	D	1097	ASN

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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PIO	C	1201	-	24,24,47	1.04	1 (4%)	39,39,65	1.39	8 (20%)
2	PIO	B	1201	-	32,32,47	0.42	0	46,49,65	1.06	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PIO	C	1201	-	-	5/15/39/68	0/1/1/1
2	PIO	B	1201	-	-	9/27/51/68	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1201	PIO	P1-O12	3.43	1.61	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1201	PIO	O41-P4-O4	3.08	117.86	105.85
2	C	1201	PIO	O51-P5-O5	2.76	116.61	105.85
2	B	1201	PIO	P4-O4-C4	2.76	130.80	123.43
2	C	1201	PIO	P4-O4-C4	2.76	130.79	123.43
2	C	1201	PIO	O11-P1-O12	-2.72	100.23	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1201	PIO	O13-P1-O11	2.70	117.91	107.80
2	B	1201	PIO	O4-P4-O42	2.38	117.83	109.33
2	B	1201	PIO	O52-P5-O5	-2.17	97.39	105.85
2	B	1201	PIO	P5-O5-C5	2.16	129.21	123.43
2	C	1201	PIO	O52-P5-O5	-2.16	97.44	105.85
2	C	1201	PIO	P5-O5-C5	2.16	129.19	123.43
2	C	1201	PIO	O13-P1-O1	2.12	114.10	105.85
2	B	1201	PIO	O5-P5-O53	2.04	116.60	109.33
2	B	1201	PIO	O11-P1-O1	-2.03	98.43	106.70

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1201	PIO	C2-C1-O1-P1
2	B	1201	PIO	C1C-O13-P1-O1
2	B	1201	PIO	C1C-O13-P1-O12
2	C	1201	PIO	C2-C1-O1-P1
2	C	1201	PIO	C6-C1-O1-P1
2	C	1201	PIO	C3-C4-O4-P4
2	C	1201	PIO	C5-C4-O4-P4
2	C	1201	PIO	C4-C5-O5-P5
2	B	1201	PIO	O13-C1C-C2C-C3C
2	B	1201	PIO	O13-C1C-C2C-O2C
2	B	1201	PIO	C2C-C1C-O13-P1
2	B	1201	PIO	C4-O4-P4-O41
2	B	1201	PIO	C5-O5-P5-O53
2	B	1201	PIO	C5-O5-P5-O52

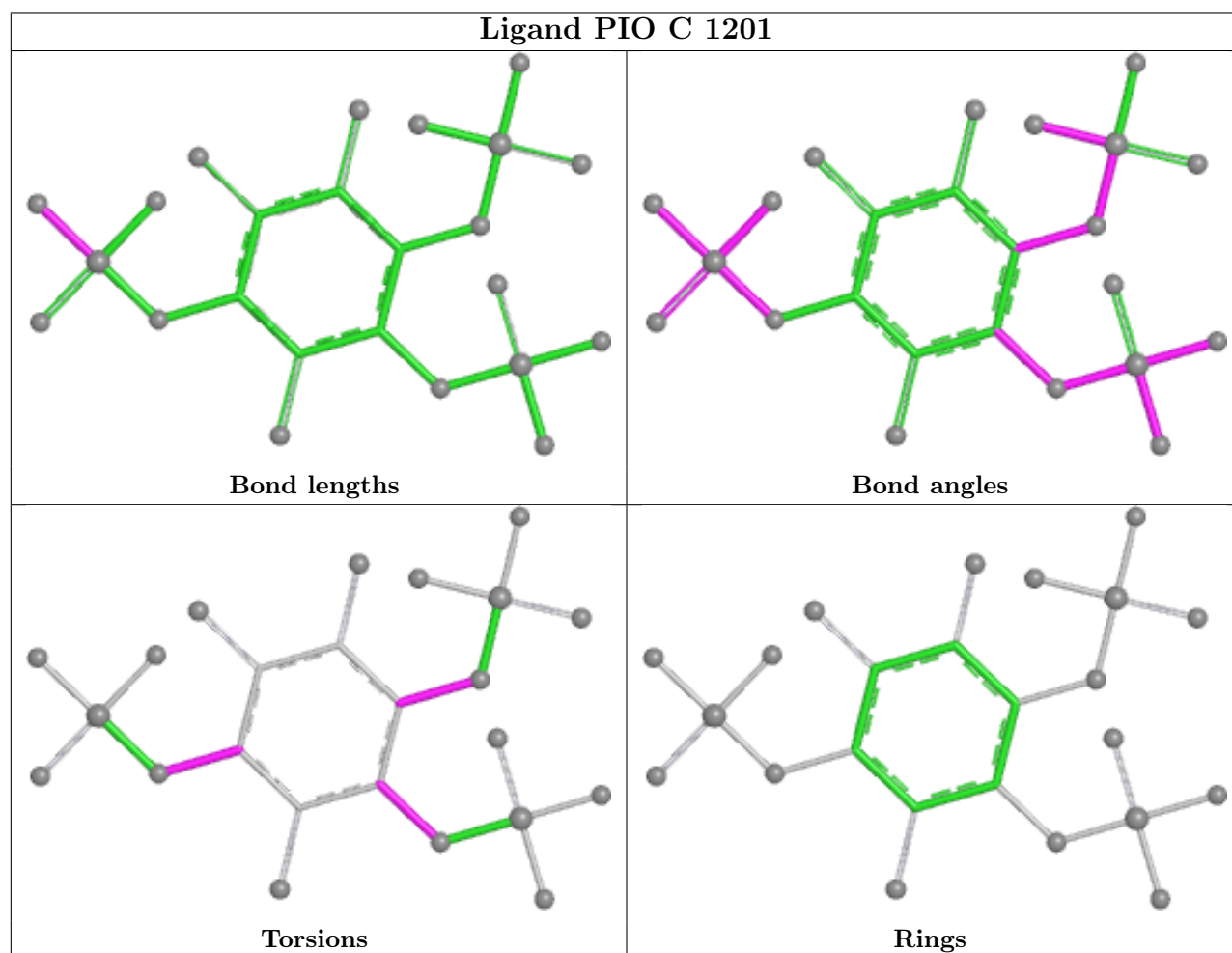
There are no ring outliers.

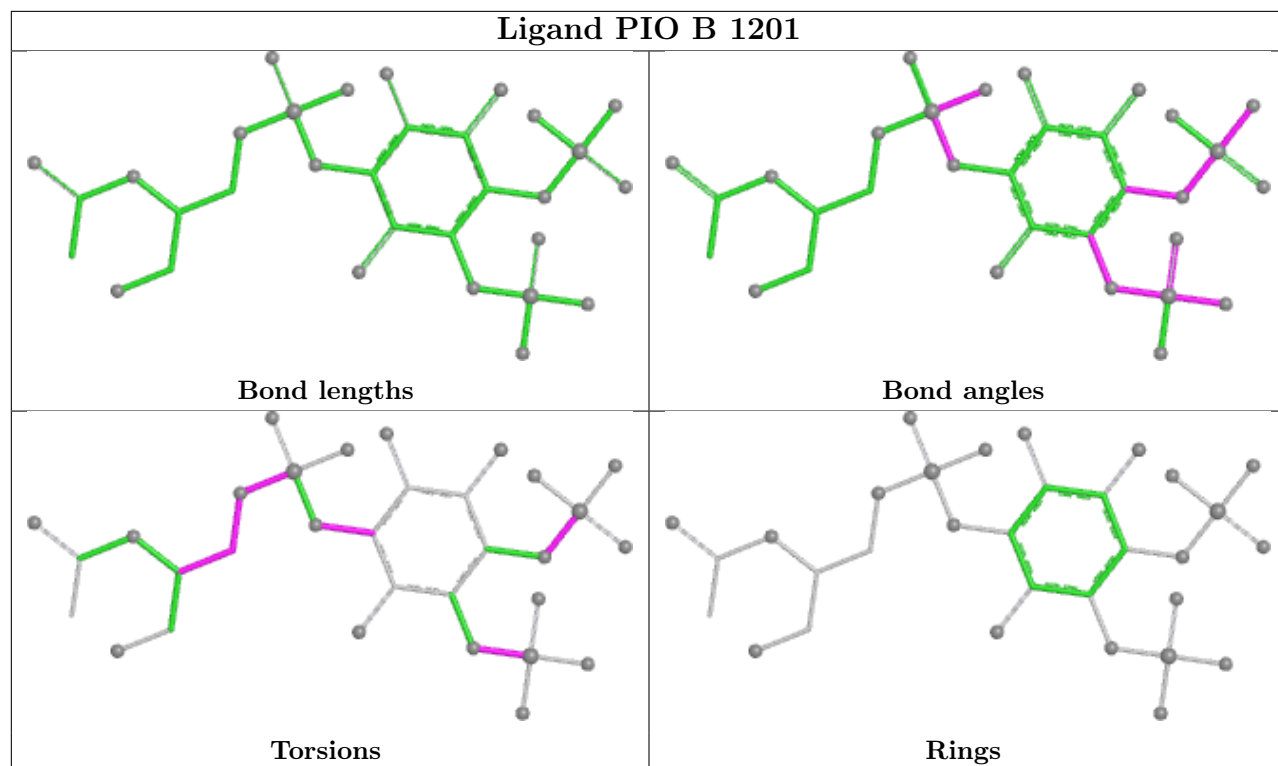
2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1201	PIO	9	0
2	B	1201	PIO	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	172/176 (97%)	-0.15	1 (0%) 85 75	44, 86, 123, 169	1 (0%)
1	B	172/176 (97%)	-0.04	0 100 100	58, 97, 133, 155	0
1	C	171/176 (97%)	0.00	1 (0%) 85 75	33, 88, 136, 164	2 (1%)
1	D	170/176 (96%)	-0.07	0 100 100	41, 96, 128, 145	1 (0%)
All	All	685/704 (97%)	-0.06	2 (0%) 90 84	33, 92, 131, 169	4 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1010	GLY	2.4
1	C	1028	GLU	2.2

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](#)

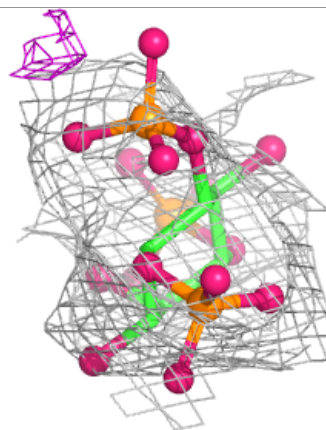
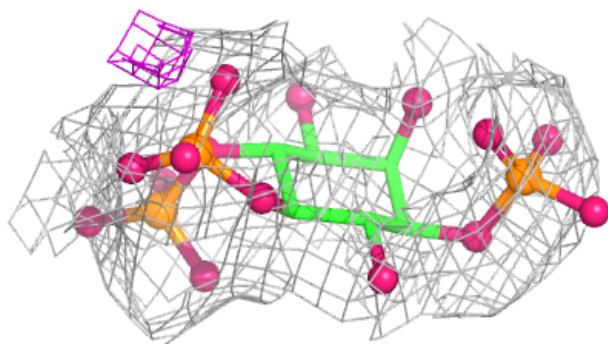
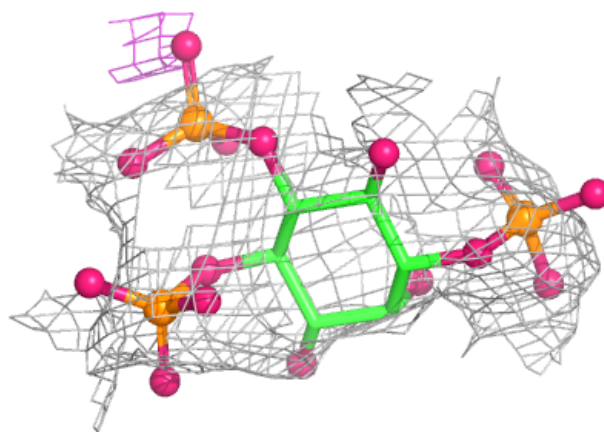
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

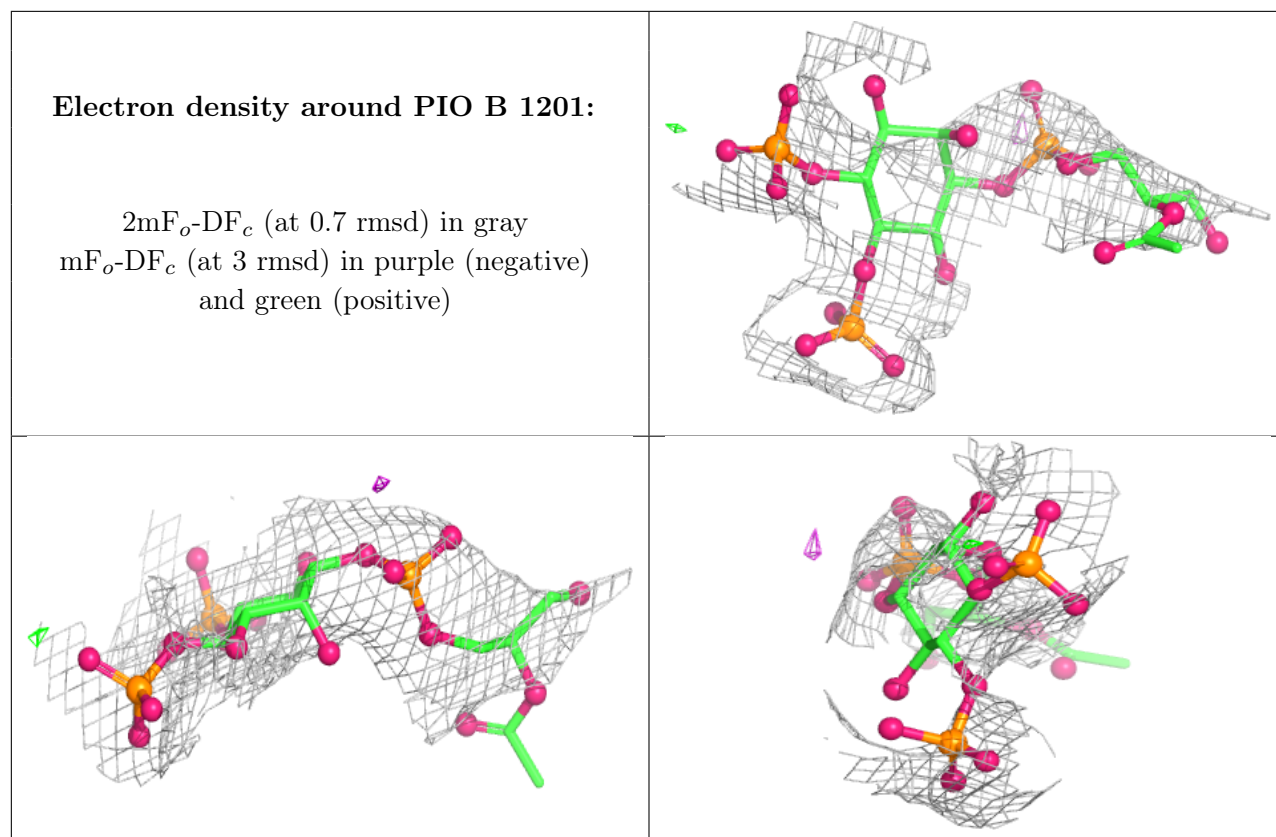
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PIO	C	1201	24/47	0.57	0.08	223,225,226,227	0
2	PIO	B	1201	32/47	0.58	0.10	169,189,192,192	0

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 PIO C 1201:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.