



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:48 pm BST

PDB ID : 6KZ8
Title : Crystal structure of plant Phospholipase D alpha complex with phosphatidic acid
Authors : Li, J.X.; Yu, F.; Zhang, P.
Deposited on : 2019-09-23
Resolution : 2.29 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

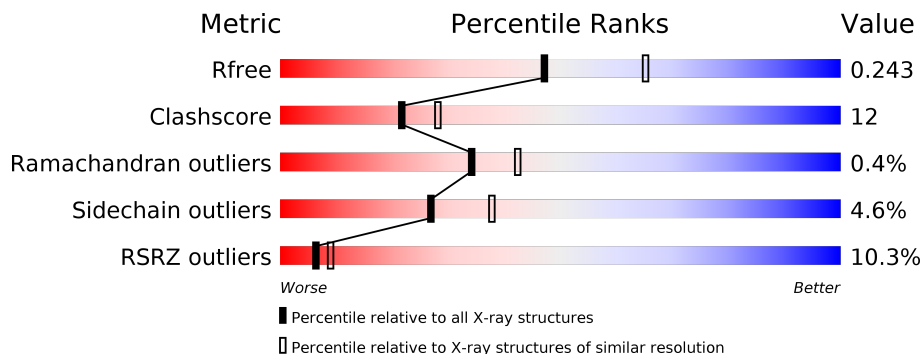
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	810	 13% (red), 72% (green), 21% (yellow), ... (orange, red, grey)
1	B	810	 7% (red), 78% (green), 16% (yellow), ... (orange, red, grey)

2 Entry composition i

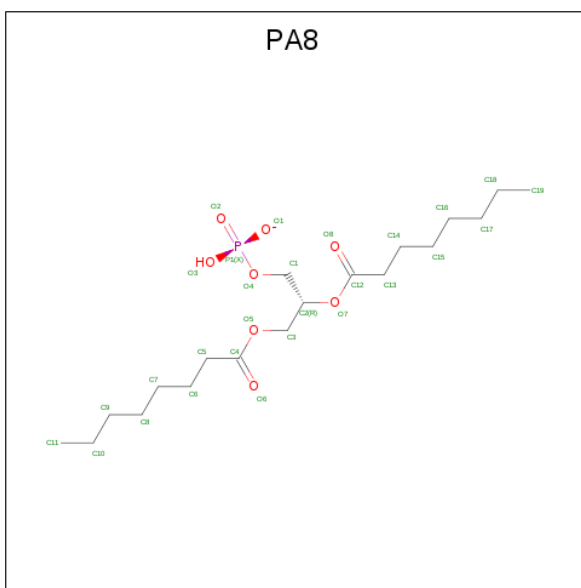
There are 4 unique types of molecules in this entry. The entry contains 13151 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phospholipase D alpha 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	784	Total 6298	4000	1093	1178	27	0	0	0
1	B	784	Total 6298	4000	1093	1178	27	0	0	0

- Molecule 2 is 1,2-DIOCTANOYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PA8) (formula: $C_{19}H_{36}O_8P$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	Total 28	19	8	1	0	0
2	B	1	Total 28	19	8	1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0

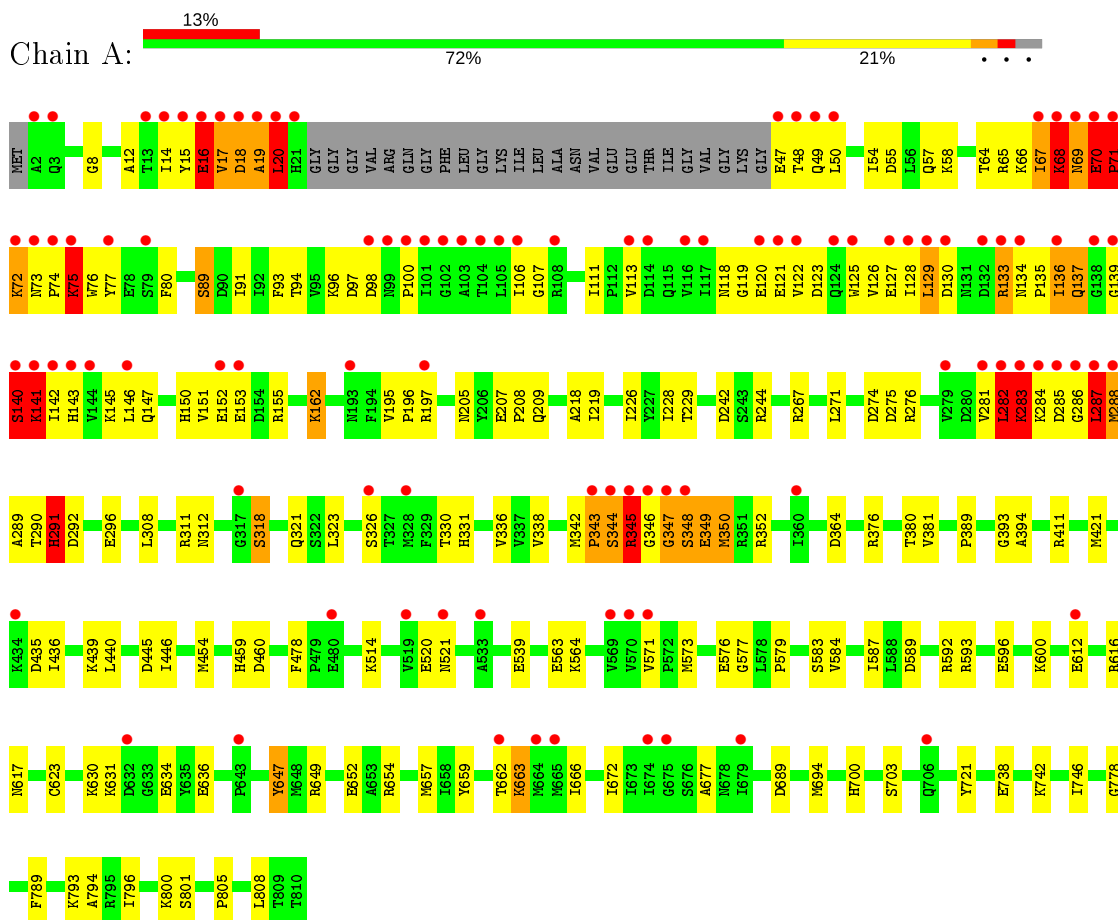
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	227	Total O 227 227	0	0
4	B	270	Total O 270 270	0	0

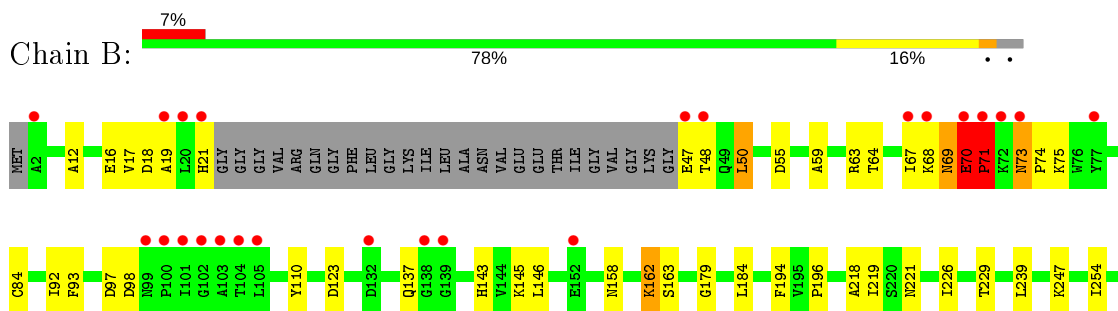
3 Residue-property plots

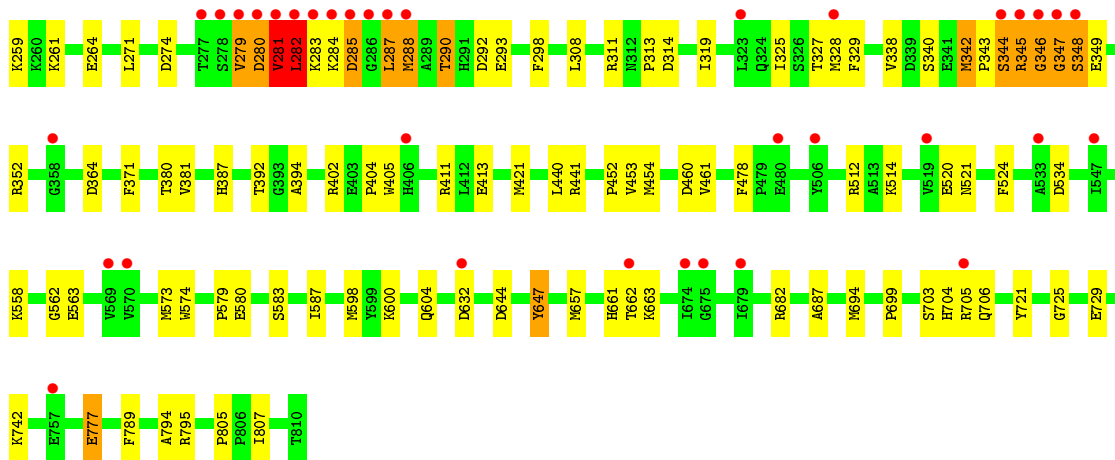
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Phospholipase D alpha 1



- Molecule 1: Phospholipase D alpha 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.04Å 123.03Å 138.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.89 – 2.29 37.89 – 2.29	Depositor EDS
% Data completeness (in resolution range)	68.6 (37.89-2.29) 88.2 (37.89-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.198 , 0.245 0.198 , 0.243	Depositor DCC
R_{free} test set	1999 reflections (2.68%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtrriage
Anisotropy	0.060	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13151	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.3397e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PA8, CA

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	0.66	2/6462 (0.0%)	0.81	17/8760 (0.2%)
1	B	0.57	2/6462 (0.0%)	0.73	12/8760 (0.1%)
All	All	0.62	4/12924 (0.0%)	0.77	29/17520 (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
1	A	0	18
1	B	0	8
All	All	0	26

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	563	GLU	CD-OE2	-6.50	1.18	1.25
1	B	47	GLU	CD-OE1	-5.29	1.19	1.25
1	B	311	ARG	CZ-NH1	-5.13	1.26	1.33
1	A	209	GLN	C-O	-5.02	1.13	1.23

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	GLU	C-N-CD	-13.18	91.61	120.60
1	A	141	LYS	N-CA-C	11.84	142.98	111.00
1	A	71	PRO	CB-CA-C	11.29	140.22	112.00
1	B	69	ASN	N-CA-C	-9.81	84.51	111.00
1	B	163	SER	N-CA-CB	9.32	124.49	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	LYS	N-CA-C	9.07	135.50	111.00
1	A	162	LYS	CB-CA-C	-8.62	93.16	110.40
1	A	141	LYS	CB-CA-C	-8.36	93.69	110.40
1	B	162	LYS	CB-CA-C	-7.60	95.19	110.40
1	B	184	LEU	O-C-N	7.33	134.43	122.70
1	B	380	THR	N-CA-C	7.19	130.42	111.00
1	B	346	GLY	N-CA-C	-7.12	95.31	113.10
1	A	291	HIS	N-CA-C	-7.02	92.04	111.00
1	A	287	LEU	CA-CB-CG	6.94	131.25	115.30
1	B	381	VAL	N-CA-CB	6.89	126.67	111.50
1	A	381	VAL	N-CA-CB	6.87	126.60	111.50
1	A	20	LEU	CB-CG-CD2	-6.66	99.68	111.00
1	B	347	GLY	N-CA-C	-6.36	97.19	113.10
1	A	129	LEU	CA-CB-CG	6.22	129.60	115.30
1	A	380	THR	N-CA-C	6.06	127.36	111.00
1	B	70	GLU	N-CA-CB	-5.71	100.32	110.60
1	A	283	LYS	N-CA-C	5.69	126.37	111.00
1	B	184	LEU	CA-C-N	-5.51	105.08	117.20
1	B	282	LEU	CB-CG-CD2	5.45	120.27	111.00
1	A	69	ASN	N-CA-C	-5.43	96.35	111.00
1	A	76	TRP	N-CA-C	5.41	125.61	111.00
1	A	129	LEU	CB-CG-CD1	-5.25	102.08	111.00
1	A	381	VAL	N-CA-C	-5.22	96.90	111.00
1	B	512	ARG	NE-CZ-NH2	-5.22	117.69	120.30

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	GLY	Peptide
1	A	133	ARG	Peptide
1	A	137	GLN	Peptide
1	A	139	GLY	Peptide
1	A	140	SER	Peptide
1	A	16	GLU	Peptide
1	A	19	ALA	Peptide
1	A	20	LEU	Peptide
1	A	282	LEU	Peptide
1	A	284	LYS	Peptide
1	A	287	LEU	Peptide
1	A	343	PRO	Peptide
1	A	345	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	346	GLY	Peptide
1	A	348	SER	Peptide
1	A	349	GLU	Peptide
1	A	67	ILE	Peptide
1	A	68	LYS	Peptide
1	B	279	VAL	Peptide
1	B	281	VAL	Peptide
1	B	282	LEU	Peptide
1	B	284	LYS	Peptide
1	B	287	LEU	Peptide
1	B	343	PRO	Peptide
1	B	346	GLY	Peptide
1	B	70	GLU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6298	0	6113	184	2
1	B	6298	0	6113	105	3
2	A	28	0	35	11	0
2	B	28	0	36	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	227	0	0	15	1
4	B	270	0	0	16	1
All	All	13151	0	12297	297	4

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 12.

All (297) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:GLU:HB2	1:B:71:PRO:CD	1.38	1.52
1:B:70:GLU:CB	1:B:71:PRO:HD3	1.28	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:MET:O	1:A:344:SER:HB2	1.32	1.29
1:B:70:GLU:CD	1:B:71:PRO:HD2	1.53	1.27
1:A:576:GLU:O	2:A:1101:PA8:H13	1.37	1.23
1:A:20:LEU:CD1	1:A:140:SER:O	1.98	1.11
1:A:129:LEU:HD12	1:A:130:ASP:H	1.15	1.05
1:A:134:ASN:OD1	1:A:135:PRO:HD2	1.56	1.05
1:B:70:GLU:CB	1:B:71:PRO:CD	2.11	1.04
1:A:20:LEU:HD12	1:A:140:SER:O	1.58	1.02
1:B:70:GLU:CD	1:B:71:PRO:CD	2.31	0.97
1:A:20:LEU:HD21	1:A:137:GLN:HB2	1.52	0.91
1:A:657:MET:SD	4:A:1332:HOH:O	2.30	0.88
1:B:349:GLU:OE2	1:B:349:GLU:N	2.06	0.87
1:A:285:ASP:HB2	1:A:393:GLY:HA2	1.56	0.86
1:A:128:ILE:HG13	1:A:142:ILE:H	1.41	0.86
1:A:120:GLU:O	1:A:147:GLN:HG3	1.74	0.85
1:B:345:ARG:HH11	1:B:345:ARG:HB2	1.41	0.85
1:A:18:ASP:HB2	1:A:125:TRP:CZ3	2.11	0.85
1:A:16:GLU:O	1:A:142:ILE:HG13	1.76	0.84
1:A:20:LEU:CD2	1:A:137:GLN:HB2	2.08	0.84
1:A:129:LEU:HD12	1:A:130:ASP:N	1.94	0.82
1:B:574:TRP:H	1:B:657:MET:HE1	1.42	0.81
1:B:70:GLU:OE1	1:B:71:PRO:HD2	1.80	0.81
1:B:704:HIS:O	1:B:705:ARG:NH1	2.13	0.81
1:B:70:GLU:CG	1:B:71:PRO:HD3	2.10	0.81
1:A:584:VAL:HG22	2:A:1101:PA8:H14	1.65	0.78
1:B:344:SER:CB	1:B:347:GLY:HA2	2.13	0.78
1:B:70:GLU:CG	1:B:71:PRO:CD	2.61	0.78
2:A:1101:PA8:H22	4:A:1207:HOH:O	1.84	0.77
1:A:290:THR:O	1:A:292:ASP:N	2.18	0.77
1:A:318:SER:HB2	1:A:321:GLN:H	1.50	0.77
1:A:288:MET:HE2	1:A:289:ALA:H	1.49	0.76
1:A:134:ASN:CG	1:A:135:PRO:HD2	2.05	0.75
1:A:282:LEU:HD12	4:A:1349:HOH:O	1.87	0.75
1:A:47:GLU:OE2	1:A:68:LYS:NZ	2.20	0.73
1:A:111:ILE:HD11	1:A:122:VAL:HG11	1.70	0.73
1:B:344:SER:HB3	1:B:347:GLY:HA2	1.69	0.73
1:A:150:HIS:ND1	1:A:152:GLU:HG2	2.05	0.72
1:A:48:THR:O	1:A:68:LYS:O	2.06	0.72
1:A:454:MET:HE1	1:A:460:ASP:HB2	1.72	0.72
1:B:524:PHE:HE2	1:B:598:MET:HE1	1.55	0.72
1:A:47:GLU:OE1	1:A:69:ASN:ND2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:GLU:O	4:A:1201:HOH:O	2.07	0.71
1:B:16:GLU:HB3	1:B:75:LYS:HG2	1.72	0.71
1:A:20:LEU:HD11	1:A:140:SER:O	1.88	0.71
1:B:274:ASP:OD1	4:B:1001:HOH:O	2.07	0.70
1:B:288:MET:HG3	1:B:387:HIS:HE1	1.56	0.70
1:A:288:MET:CE	1:A:288:MET:HA	2.22	0.70
1:A:14:ILE:HD12	1:A:80:PHE:CE1	2.27	0.70
1:B:55:ASP:OD2	4:B:1002:HOH:O	2.08	0.70
1:A:274:ASP:HB2	1:A:308:LEU:HB3	1.73	0.69
1:A:276:ARG:HH22	1:A:312:ASN:ND2	1.89	0.69
1:A:18:ASP:HB2	1:A:125:TRP:HZ3	1.54	0.69
1:B:293:GLU:OE2	4:B:1001:HOH:O	2.10	0.68
1:A:129:LEU:CD1	1:A:134:ASN:C	2.63	0.67
1:A:195:VAL:O	4:A:1202:HOH:O	2.13	0.67
1:B:48:THR:HG23	1:B:50:LEU:HD13	1.75	0.67
1:A:17:VAL:HG12	1:A:128:ILE:HD11	1.76	0.66
1:A:345:ARG:HG3	1:A:345:ARG:NH1	2.10	0.66
1:B:327:THR:HG23	1:B:328:MET:HG2	1.77	0.66
1:A:16:GLU:O	1:A:142:ILE:CG1	2.43	0.66
1:A:229:THR:HG22	1:A:271:LEU:HB2	1.78	0.66
1:A:197:ARG:HD2	1:A:205:ASN:ND2	2.11	0.65
1:A:288:MET:HE2	1:A:289:ALA:N	2.09	0.65
1:A:288:MET:HA	1:A:288:MET:HE3	1.76	0.65
1:A:276:ARG:HH22	1:A:312:ASN:HD21	1.45	0.64
1:A:350:MET:CE	1:A:445:ASP:O	2.45	0.64
1:A:742:LYS:O	1:A:746:ILE:HD12	1.98	0.64
2:A:1101:PA8:H4	4:A:1207:HOH:O	1.98	0.64
1:B:123:ASP:OD1	1:B:143:HIS:NE2	2.31	0.64
1:B:280:ASP:H	1:B:282:LEU:HB3	1.62	0.63
1:A:275:ASP:OD1	4:A:1203:HOH:O	2.15	0.63
1:A:343:PRO:HD3	1:A:352:ARG:NE	2.13	0.63
1:A:576:GLU:O	2:A:1101:PA8:C8	2.31	0.63
1:B:345:ARG:HH11	1:B:345:ARG:CB	2.09	0.63
1:A:197:ARG:HD2	1:A:205:ASN:HD21	1.64	0.62
1:A:345:ARG:HG3	1:A:345:ARG:HH11	1.64	0.62
1:A:587:ILE:HD11	2:A:1101:PA8:H31	1.81	0.62
1:B:524:PHE:CE2	1:B:598:MET:HE1	2.34	0.62
1:A:123:ASP:OD1	1:A:143:HIS:HE1	1.83	0.61
1:A:91:ILE:HB	1:A:111:ILE:HG23	1.80	0.61
1:B:50:LEU:HD23	1:B:74:PRO:HG3	1.82	0.61
1:B:394:ALA:HA	1:B:647:TYR:CE2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ARG:HD2	4:B:1081:HOH:O	2.01	0.61
1:A:411:ARG:HD2	4:A:1242:HOH:O	2.00	0.61
1:A:67:ILE:O	1:A:67:ILE:HG22	1.99	0.60
1:A:129:LEU:CD1	1:A:134:ASN:O	2.48	0.60
1:B:313:PRO:HG3	1:B:329:PHE:HD2	1.65	0.60
1:B:93:PHE:HZ	1:B:146:LEU:HD21	1.66	0.60
1:A:162:LYS:O	1:A:162:LYS:HG2	2.00	0.60
1:A:805:PRO:HD2	1:A:808:LEU:HD12	1.83	0.60
1:A:345:ARG:HH11	1:A:345:ARG:CG	2.15	0.59
1:A:342:MET:O	1:A:344:SER:CB	2.27	0.59
1:B:345:ARG:HB2	1:B:345:ARG:NH1	2.14	0.59
1:A:49:GLN:HE21	1:A:98:ASP:C	2.07	0.57
1:A:617:ASN:OD1	4:A:1204:HOH:O	2.17	0.57
1:A:126:VAL:O	1:A:141:LYS:C	2.43	0.57
1:A:126:VAL:HG22	1:A:127:GLU:H	1.68	0.57
1:A:126:VAL:O	1:A:142:ILE:O	2.23	0.57
1:A:48:THR:HG23	1:A:97:ASP:OD2	2.04	0.57
1:A:47:GLU:OE2	1:A:68:LYS:HD2	2.05	0.56
1:A:129:LEU:HD11	1:A:134:ASN:N	2.20	0.56
1:A:583:SER:OG	2:A:1101:PA8:H35	2.06	0.56
1:A:577:GLY:HA3	2:A:1101:PA8:H18	1.87	0.56
1:A:376:ARG:NH2	1:A:631:LYS:HE2	2.21	0.56
1:A:19:ALA:HB2	1:A:140:SER:HB2	1.87	0.56
1:A:267:ARG:NH1	1:A:436:ILE:O	2.38	0.56
1:A:596:GLU:O	1:A:600:LYS:HG3	2.06	0.56
1:B:17:VAL:O	1:B:73:ASN:HB3	2.06	0.56
1:A:282:LEU:HA	1:A:283:LYS:HD2	1.88	0.55
1:B:313:PRO:HG3	1:B:329:PHE:CD2	2.41	0.55
1:B:579:PRO:HB2	1:B:794:ALA:CB	2.37	0.55
1:A:636:GLU:OE1	4:A:1205:HOH:O	2.18	0.55
1:B:70:GLU:OE2	1:B:71:PRO:HD2	2.02	0.55
1:B:162:LYS:O	1:B:162:LYS:HG2	2.05	0.55
1:A:573:MET:N	1:A:657:MET:HE1	2.21	0.55
1:A:49:GLN:NE2	1:A:100:PRO:HD3	2.22	0.54
1:A:459:HIS:HA	1:A:700:HIS:CD2	2.43	0.54
1:B:345:ARG:HH11	1:B:345:ARG:CG	2.20	0.54
1:A:89:SER:O	1:A:113:VAL:HG22	2.08	0.54
1:B:285:ASP:N	1:B:285:ASP:OD2	2.38	0.54
1:B:364:ASP:N	1:B:364:ASP:OD1	2.41	0.54
1:B:587:ILE:HD11	2:B:902:PA8:H30	1.88	0.54
1:A:15:TYR:CD2	1:A:77:TYR:CE1	2.96	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:MET:HE1	1:A:445:ASP:O	2.07	0.53
1:B:68:LYS:C	1:B:69:ASN:O	2.39	0.53
1:A:15:TYR:CE2	1:A:77:TYR:CE1	2.97	0.53
1:B:454:MET:HE1	1:B:460:ASP:HB2	1.90	0.53
1:B:63:ARG:HD3	4:B:1025:HOH:O	2.08	0.53
1:B:441:ARG:NH1	4:B:1021:HOH:O	2.42	0.53
1:B:805:PRO:HB2	1:B:807:ILE:HG22	1.91	0.53
1:B:314:ASP:HB3	1:B:687:ALA:HB1	1.91	0.52
1:A:15:TYR:CE2	1:A:77:TYR:CD1	2.98	0.52
1:A:140:SER:HA	1:A:141:LYS:HB2	1.92	0.52
1:B:580:GLU:HG3	4:B:1250:HOH:O	2.09	0.52
1:A:281:VAL:O	1:A:283:LYS:HD2	2.10	0.52
1:A:421:MET:HE1	1:A:440:LEU:HD11	1.92	0.51
1:B:281:VAL:O	1:B:281:VAL:HG22	2.10	0.51
1:A:242:ASP:OD2	1:A:244:ARG:NH2	2.43	0.51
1:A:218:ALA:HB1	1:A:338:VAL:HG21	1.93	0.51
1:A:326:SER:O	4:A:1206:HOH:O	2.19	0.51
2:B:902:PA8:H4	4:B:1040:HOH:O	2.11	0.51
1:A:421:MET:CE	1:A:440:LEU:HD11	2.41	0.51
1:A:64:THR:HG22	1:A:80:PHE:HZ	1.75	0.51
1:A:107:GLY:HA3	1:A:128:ILE:HG23	1.93	0.50
1:A:19:ALA:CB	1:A:140:SER:HB2	2.41	0.50
1:B:524:PHE:HE2	1:B:598:MET:CE	2.23	0.50
1:B:196:PRO:HD3	1:B:721:TYR:CD2	2.46	0.50
1:B:261:LYS:O	1:B:264:GLU:HG2	2.11	0.50
1:A:129:LEU:HD11	1:A:133:ARG:HA	1.92	0.50
1:B:196:PRO:HD3	1:B:721:TYR:CE2	2.46	0.50
1:A:128:ILE:O	1:A:136:ILE:HG22	2.12	0.50
1:A:589:ASP:OD2	1:A:592:ARG:NH1	2.45	0.50
1:A:125:TRP:CE3	1:A:143:HIS:HB2	2.47	0.49
1:A:286:GLY:HA3	1:A:389:PRO:HA	1.93	0.49
1:A:649:ARG:HD3	4:A:1390:HOH:O	2.12	0.49
1:B:703:SER:HA	1:B:706:GLN:O	2.13	0.49
1:A:15:TYR:HE2	1:A:77:TYR:CD1	2.30	0.49
1:A:514:LYS:NZ	1:A:703:SER:O	2.42	0.49
1:A:17:VAL:CG1	1:A:128:ILE:HD11	2.40	0.49
1:A:657:MET:HE2	1:A:659:TYR:HD2	1.78	0.49
1:B:70:GLU:OE1	1:B:71:PRO:CD	2.52	0.49
1:A:18:ASP:CB	1:A:125:TRP:HZ3	2.22	0.48
1:B:682:ARG:NE	2:B:902:PA8:H24	2.28	0.48
1:A:290:THR:O	1:A:291:HIS:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PHE:HZ	1:A:146:LEU:HD21	1.78	0.48
1:B:562:GLY:HA2	4:B:1254:HOH:O	2.14	0.48
1:A:14:ILE:HD11	1:A:54:ILE:HD11	1.95	0.48
1:B:219:ILE:HG23	1:B:226:ILE:HD13	1.96	0.48
1:A:129:LEU:HD13	1:A:134:ASN:C	2.34	0.47
1:A:15:TYR:HB2	1:A:143:HIS:O	2.14	0.47
1:B:18:ASP:OD1	1:B:19:ALA:N	2.42	0.47
1:B:795:ARG:HG3	4:B:1232:HOH:O	2.15	0.47
1:A:394:ALA:HA	1:A:647:TYR:CE2	2.50	0.47
1:A:521:ASN:HA	1:A:662:THR:O	2.13	0.47
1:B:521:ASN:HA	1:B:662:THR:O	2.15	0.47
1:A:129:LEU:HD12	1:A:134:ASN:O	2.14	0.47
1:B:583:SER:HB3	2:B:902:PA8:H16	1.97	0.47
2:A:1101:PA8:H22	2:A:1101:PA8:H4	1.70	0.47
1:A:50:LEU:HD11	1:A:106:ILE:HD11	1.97	0.46
1:A:127:GLU:HA	1:A:141:LYS:HA	1.97	0.46
1:A:350:MET:HE1	1:A:445:ASP:C	2.36	0.46
1:B:194:PHE:CD1	1:B:371:PHE:CE1	3.03	0.46
1:A:296:GLU:HB2	1:A:308:LEU:HD21	1.97	0.46
1:A:107:GLY:HA3	1:A:128:ILE:CG2	2.45	0.46
1:A:64:THR:HG22	1:A:80:PHE:CZ	2.51	0.46
1:A:125:TRP:O	1:A:141:LYS:HG2	2.16	0.46
1:A:350:MET:CE	1:A:446:ILE:HA	2.45	0.46
1:A:77:TYR:CD2	1:A:77:TYR:N	2.83	0.46
1:B:461:VAL:O	1:B:699:PRO:HD2	2.15	0.46
2:B:902:PA8:H14	2:B:902:PA8:H7	1.54	0.46
1:B:534:ASP:O	1:B:534:ASP:OD1	2.33	0.46
2:A:1101:PA8:H29	4:A:1338:HOH:O	2.16	0.46
1:A:126:VAL:HG22	1:A:127:GLU:N	2.29	0.46
1:A:130:ASP:HB2	1:A:136:ILE:HD12	1.98	0.45
1:B:239:LEU:HD11	1:B:254:ILE:HD13	1.98	0.45
1:B:229:THR:HG22	1:B:271:LEU:HB2	1.98	0.45
1:A:49:GLN:HB2	1:A:66:LYS:HG2	1.98	0.45
1:A:634:GLU:OE1	1:A:654:ARG:NH2	2.48	0.45
1:A:70:GLU:HA	1:A:71:PRO:HD3	1.11	0.45
1:A:127:GLU:OE2	1:A:129:LEU:HB2	2.15	0.45
1:A:330:THR:OG1	1:A:689:ASP:OD2	2.19	0.45
1:B:218:ALA:HB1	1:B:338:VAL:HG21	1.98	0.45
1:A:571:VAL:O	1:A:623:CYS:HA	2.16	0.45
1:B:453:VAL:O	1:B:454:MET:HG3	2.17	0.45
1:A:125:TRP:CD2	1:A:143:HIS:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ALA:HA	1:A:145:LYS:O	2.17	0.45
1:A:219:ILE:HG23	1:A:226:ILE:HD13	1.99	0.45
1:B:194:PHE:CD1	1:B:371:PHE:HE1	2.35	0.45
1:B:520:GLU:HB2	1:B:662:THR:HG21	1.99	0.45
1:A:129:LEU:HD11	1:A:133:ARG:C	2.36	0.45
1:B:179:GLY:HA3	1:B:452:PRO:HB3	1.98	0.45
1:A:14:ILE:HD12	1:A:80:PHE:HE1	1.77	0.45
1:A:666:ILE:HG12	1:A:672:ILE:HG13	1.98	0.45
1:B:441:ARG:HG2	1:B:441:ARG:H	1.61	0.45
1:B:574:TRP:N	1:B:657:MET:HE1	2.22	0.45
1:B:682:ARG:CZ	2:B:902:PA8:H24	2.47	0.45
1:B:92:ILE:HG12	1:B:110:TYR:CD2	2.53	0.45
1:A:196:PRO:HD3	1:A:721:TYR:CE2	2.51	0.44
1:A:793:LYS:HB3	1:A:793:LYS:HE3	1.86	0.44
1:A:579:PRO:HB2	1:A:794:ALA:CB	2.48	0.44
1:A:285:ASP:HB2	1:A:393:GLY:CA	2.39	0.44
1:A:520:GLU:HB2	1:A:662:THR:HG21	1.99	0.44
1:A:49:GLN:NE2	1:A:98:ASP:O	2.46	0.44
1:B:405:TRP:CZ2	1:B:661:HIS:CG	3.05	0.44
1:B:725:GLY:HA2	4:B:1165:HOH:O	2.17	0.44
1:B:221:ASN:HB2	4:B:1188:HOH:O	2.17	0.44
1:B:50:LEU:O	1:B:67:ILE:HG22	2.18	0.44
1:B:573:MET:HG2	1:B:789:PHE:CE1	2.52	0.44
1:A:616:ARG:NE	4:A:1215:HOH:O	2.37	0.44
1:A:20:LEU:HD23	1:A:137:GLN:HB2	1.97	0.44
1:A:600:LYS:HG2	1:A:778:GLY:HA3	2.00	0.44
1:B:342:MET:HE3	1:B:342:MET:HB3	1.90	0.44
1:A:311:ARG:HB2	1:A:331:HIS:CD2	2.53	0.44
1:B:558:LYS:HE3	1:B:563:GLU:HB2	2.00	0.43
1:A:228:ILE:HG12	1:A:336:VAL:HG22	2.00	0.43
1:A:800:LYS:HD2	1:A:801:SER:N	2.33	0.43
1:B:290:THR:HG22	1:B:292:ASP:N	2.33	0.43
1:A:539:GLU:CD	1:A:539:GLU:H	2.21	0.43
1:A:16:GLU:HB3	1:A:75:LYS:HD2	2.01	0.43
1:A:126:VAL:CG2	1:A:127:GLU:H	2.29	0.43
1:A:343:PRO:HD3	1:A:352:ARG:CD	2.49	0.43
1:B:59:ALA:HB1	4:B:1089:HOH:O	2.18	0.43
1:B:158:ASN:OD1	1:B:558:LYS:NZ	2.47	0.43
1:A:142:ILE:HG12	1:A:143:HIS:N	2.34	0.43
1:A:55:ASP:HB3	1:A:57:GLN:O	2.18	0.42
1:A:57:GLN:HB3	1:A:58:LYS:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ASP:OD2	1:B:98:ASP:N	2.52	0.42
1:A:573:MET:H	1:A:657:MET:HE1	1.84	0.42
1:A:657:MET:HE2	1:A:659:TYR:CD2	2.52	0.42
1:A:323:LEU:HD23	1:A:323:LEU:HA	1.88	0.42
1:A:196:PRO:HD3	1:A:721:TYR:CD2	2.54	0.42
1:B:12:ALA:HA	1:B:145:LYS:O	2.20	0.42
1:B:325:ILE:HD12	1:B:329:PHE:HE2	1.83	0.42
1:A:288:MET:CE	1:A:288:MET:CA	2.96	0.42
1:B:259:LYS:HD2	1:B:298:PHE:CE2	2.55	0.42
1:B:600:LYS:O	1:B:604:GLN:HG3	2.19	0.42
1:B:352:ARG:HD2	4:B:1149:HOH:O	2.20	0.42
1:A:663:LYS:HB3	1:A:677:ALA:O	2.20	0.42
2:A:1101:PA8:H30	2:A:1101:PA8:H9	2.01	0.42
1:A:347:GLY:HA2	1:A:348:SER:HA	1.38	0.42
1:A:73:ASN:HA	1:A:74:PRO:HD2	1.77	0.42
1:B:137:GLN:HG2	4:B:1148:HOH:O	2.19	0.42
1:B:17:VAL:HG22	1:B:74:PRO:HD2	2.02	0.42
1:B:352:ARG:HH12	1:B:413:GLU:HB3	1.85	0.42
1:B:421:MET:HE1	1:B:440:LEU:HD11	2.00	0.42
1:A:350:MET:HE1	1:A:446:ILE:HA	2.01	0.42
1:B:421:MET:CE	1:B:440:LEU:HD11	2.50	0.42
1:A:8:GLY:HA2	1:A:151:VAL:HG13	2.00	0.41
1:A:155:ARG:HG2	1:A:155:ARG:O	2.19	0.41
1:A:94:THR:HG22	1:A:96:LYS:HG3	2.01	0.41
1:A:350:MET:HE3	1:A:445:ASP:O	2.17	0.41
1:A:789:PHE:CE1	1:A:796:ILE:HA	2.55	0.41
1:A:134:ASN:HA	1:A:135:PRO:HD3	1.79	0.41
1:A:195:VAL:CG1	1:A:208:PRO:HG3	2.50	0.41
1:B:63:ARG:HG2	1:B:64:THR:O	2.21	0.41
1:A:128:ILE:HD11	1:A:142:ILE:HB	2.02	0.41
1:B:247:LYS:HE3	1:B:247:LYS:HB3	1.89	0.41
1:B:402:ARG:O	1:B:404:PRO:HD3	2.20	0.41
1:A:129:LEU:HD11	1:A:133:ARG:CA	2.51	0.41
1:A:282:LEU:H	1:A:282:LEU:HG	1.79	0.41
1:A:288:MET:HA	1:A:288:MET:HE2	2.00	0.41
1:A:439:LYS:HA	1:A:439:LYS:HD3	1.91	0.41
1:B:705:ARG:HD3	1:B:705:ARG:HA	1.92	0.41
1:B:194:PHE:HD1	1:B:371:PHE:CE1	2.38	0.41
1:B:514:LYS:NZ	1:B:703:SER:O	2.39	0.41
1:A:364:ASP:HB3	4:A:1284:HOH:O	2.21	0.41
1:A:126:VAL:O	1:A:141:LYS:O	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:ASP:O	1:A:593:ARG:HG3	2.21	0.40
1:A:72:LYS:CG	1:A:72:LYS:O	2.69	0.40
1:A:800:LYS:HD2	1:A:801:SER:H	1.86	0.40
1:A:121:GLU:O	1:A:122:VAL:C	2.60	0.40
1:A:68:LYS:HA	1:A:68:LYS:HD3	1.82	0.40
2:B:902:PA8:H22	4:B:1040:HOH:O	2.21	0.40
1:B:274:ASP:HB2	1:B:308:LEU:HB3	2.03	0.40
1:B:16:GLU:CB	1:B:75:LYS:HG2	2.47	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:GLU:OE2	1:B:281:VAL:CG1[4_548]	2.10	0.10
1:A:349:GLU:OE2	1:B:348:SER:OG[3_448]	2.11	0.09
1:B:348:SER:CA	1:B:777:GLU:OE2[3_448]	2.12	0.08
4:A:1349:HOH:O	4:B:1180:HOH:O[4_448]	2.14	0.06

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	780/810 (96%)	712 (91%)	63 (8%)	5 (1%)	25 31
1	B	780/810 (96%)	737 (94%)	41 (5%)	2 (0%)	41 50
All	All	1560/1620 (96%)	1449 (93%)	104 (7%)	7 (0%)	34 42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	PRO
1	A	347	GLY

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Mol	Chain	Res	Type
1	B	70	GLU
1	B	71	PRO
1	A	291	HIS
1	A	435	ASP
1	A	318	SER

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	680/697 (98%)	649 (95%)	31 (5%)	27	38
1	B	680/697 (98%)	649 (95%)	31 (5%)	27	38
All	All	1360/1394 (98%)	1298 (95%)	62 (5%)	27	38

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	17	VAL
1	A	18	ASP
1	A	20	LEU
1	A	65	ARG
1	A	68	LYS
1	A	70	GLU
1	A	72	LYS
1	A	75	LYS
1	A	89	SER
1	A	118	ASN
1	A	136	ILE
1	A	140	SER
1	A	141	LYS
1	A	153	GLU
1	A	207	GLU
1	A	282	LEU
1	A	283	LYS

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Mol	Chain	Res	Type
1	A	287	LEU
1	A	288	MET
1	A	344	SER
1	A	345	ARG
1	A	350	MET
1	A	478	PHE
1	A	564	LYS
1	A	612	GLU
1	A	630	LYS
1	A	647	TYR
1	A	652	GLU
1	A	663	LYS
1	A	694	MET
1	B	21	HIS
1	B	50	LEU
1	B	70	GLU
1	B	71	PRO
1	B	73	ASN
1	B	84	CYS
1	B	279	VAL
1	B	280	ASP
1	B	281	VAL
1	B	282	LEU
1	B	283	LYS
1	B	285	ASP
1	B	287	LEU
1	B	288	MET
1	B	290	THR
1	B	319	ILE
1	B	340	SER
1	B	342	MET
1	B	344	SER
1	B	345	ARG
1	B	348	SER
1	B	392	THR
1	B	478	PHE
1	B	632	ASP
1	B	644	ASP
1	B	647	TYR
1	B	663	LYS
1	B	694	MET
1	B	729	GLU

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Mol	Chain	Res	Type
1	B	742	LYS
1	B	777	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	69	ASN
1	A	118	ASN
1	A	312	ASN
1	B	209	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
2	PA8	B	902	-	27,27,27	1.14	4 (14%)	31,32,32	1.00	2 (6%)
2	PA8	A	1101	-	27,27,27	1.49	5 (18%)	31,32,32	1.73	6 (19%)

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	PA8	B	902	-	-	19/29/29/29	-
2	PA8	A	1101	-	-	15/29/29/29	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	PA8	O5-C4	3.51	1.43	1.33
2	A	1101	PA8	O7-C2	-3.20	1.38	1.46
2	A	1101	PA8	O7-C12	3.13	1.43	1.34
2	B	902	PA8	O5-C4	2.79	1.41	1.33
2	A	1101	PA8	P1-O1	-2.71	1.44	1.54
2	B	902	PA8	O7-C2	-2.67	1.39	1.46
2	B	902	PA8	O7-C12	2.24	1.40	1.34
2	A	1101	PA8	P1-O3	-2.17	1.46	1.54
2	B	902	PA8	O5-C3	-2.04	1.40	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	PA8	C2-O7-C12	-4.69	106.24	117.79
2	A	1101	PA8	O7-C12-C13	4.33	120.83	111.50
2	B	902	PA8	O7-C12-C13	3.75	119.59	111.50
2	A	1101	PA8	O1-P1-O4	-3.48	97.47	106.73
2	A	1101	PA8	O3-P1-O1	3.20	119.88	107.64
2	A	1101	PA8	O7-C12-O8	-3.03	116.37	123.70
2	A	1101	PA8	C3-O5-C4	2.43	126.11	117.12
2	B	902	PA8	C2-O7-C12	-2.26	112.23	117.79

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	902	PA8	O8-C12-O7-C2
2	A	1101	PA8	O8-C12-O7-C2
2	B	902	PA8	C13-C12-O7-C2
2	A	1101	PA8	C13-C12-O7-C2
2	B	902	PA8	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	A	1101	PA8	C14-C15-C16-C17
2	B	902	PA8	C4-C5-C6-C7
2	B	902	PA8	C6-C7-C8-C9
2	B	902	PA8	C14-C15-C16-C17
2	B	902	PA8	C13-C14-C15-C16
2	B	902	PA8	C15-C16-C17-C18
2	A	1101	PA8	C7-C8-C9-C10
2	A	1101	PA8	C16-C17-C18-C19
2	B	902	PA8	C7-C8-C9-C10
2	A	1101	PA8	C2-C1-O4-P1
2	B	902	PA8	C1-C2-C3-O5
2	B	902	PA8	C12-C13-C14-C15
2	A	1101	PA8	C6-C7-C8-C9
2	A	1101	PA8	C15-C16-C17-C18
2	B	902	PA8	O7-C2-C3-O5
2	A	1101	PA8	O7-C2-C3-O5
2	A	1101	PA8	C11-C10-C9-C8
2	B	902	PA8	C2-C1-O4-P1
2	B	902	PA8	C16-C17-C18-C19
2	A	1101	PA8	C1-C2-C3-O5
2	B	902	PA8	O4-C1-C2-C3
2	B	902	PA8	C11-C10-C9-C8
2	B	902	PA8	O4-C1-C2-O7
2	A	1101	PA8	O4-C1-C2-O7
2	A	1101	PA8	O7-C12-C13-C14
2	A	1101	PA8	O4-C1-C2-C3
2	A	1101	PA8	O8-C12-C13-C14
2	B	902	PA8	O5-C4-C5-C6
2	B	902	PA8	O6-C4-C5-C6

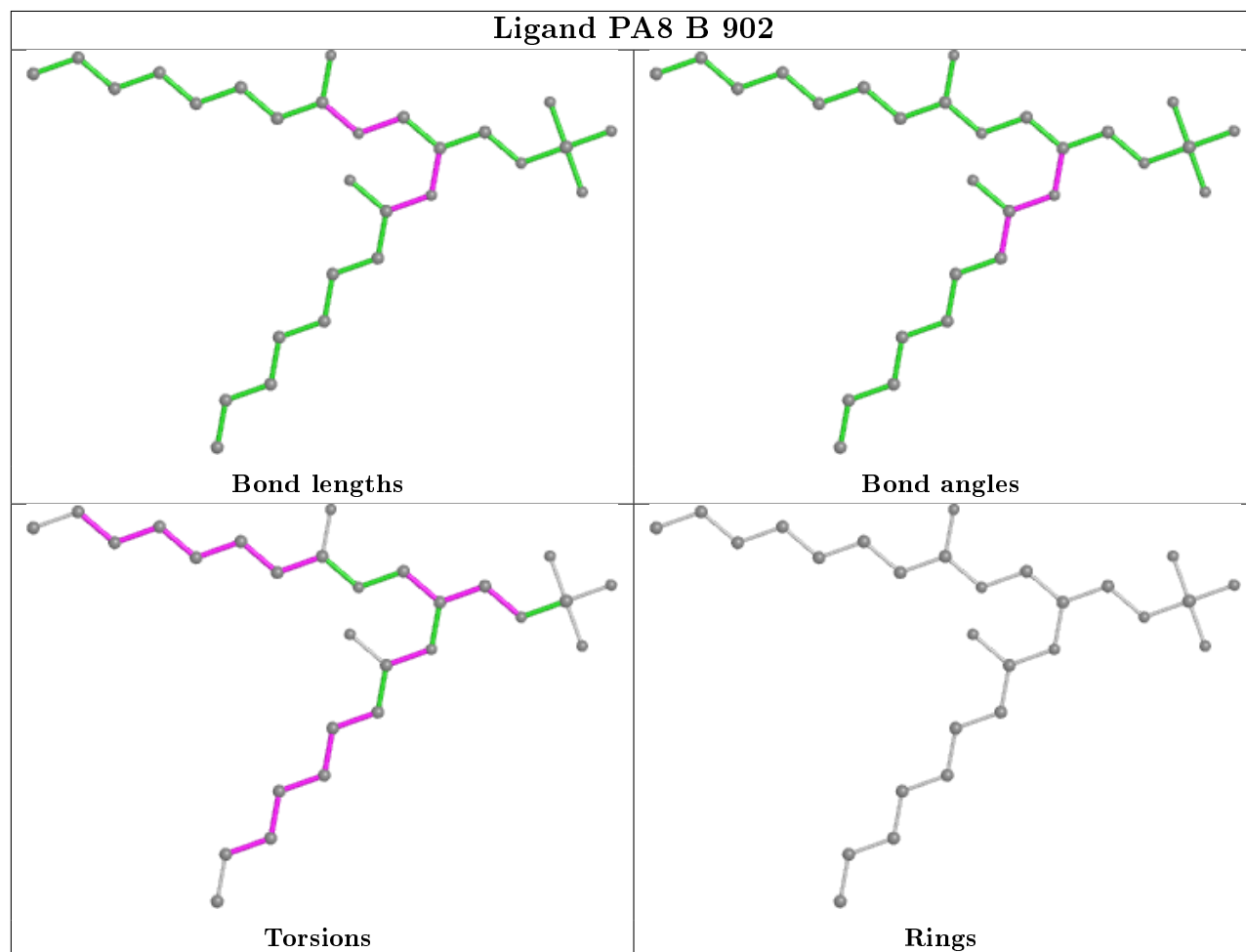
There are no ring outliers.

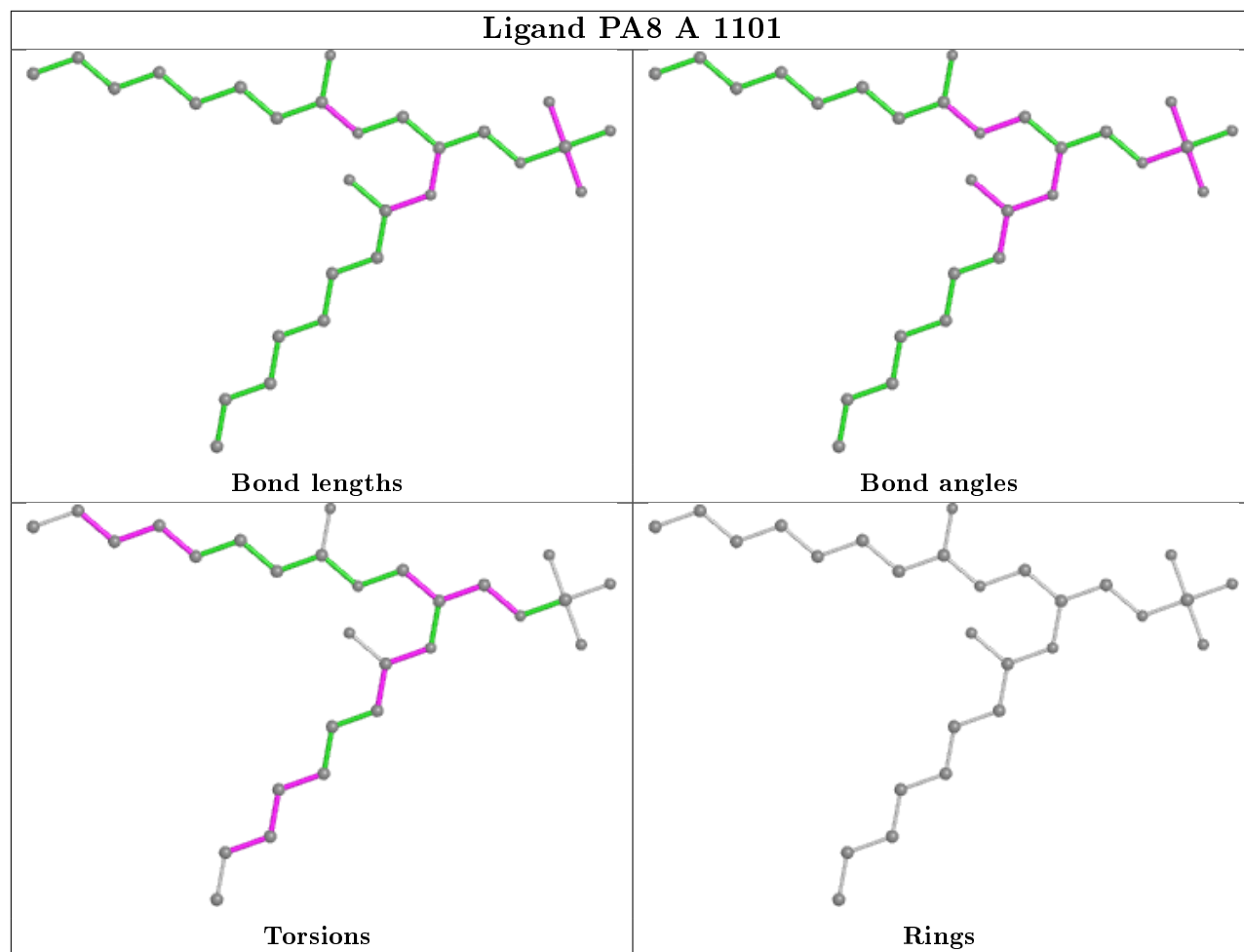
2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	902	PA8	7	0
2	A	1101	PA8	11	0

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

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	784/810 (96%)	0.55	102 (13%) 3 4	5, 14, 42, 53	0
1	B	784/810 (96%)	0.28	59 (7%) 14 19	4, 12, 32, 54	0
All	All	1568/1620 (96%)	0.42	161 (10%) 6 9	4, 13, 37, 54	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	VAL	9.7
1	A	346	GLY	9.7
1	A	100	PRO	8.5
1	A	19	ALA	8.3
1	B	348	SER	7.5
1	A	105	LEU	7.5
1	A	286	GLY	7.4
1	A	103	ALA	7.2
1	A	284	LYS	7.2
1	A	101	ILE	7.1
1	B	100	PRO	6.7
1	B	285	ASP	6.6
1	A	345	ARG	6.6
1	A	17	VAL	6.6
1	A	348	SER	6.5
1	A	104	THR	6.4
1	B	347	GLY	6.4
1	A	102	GLY	6.4
1	B	346	GLY	6.3
1	A	347	GLY	5.8
1	A	344	SER	5.5
1	B	48	THR	5.4
1	A	18	ASP	5.1
1	A	128	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	20	LEU	5.1
1	A	69	ASN	5.1
1	A	287	LEU	5.1
1	B	101	ILE	5.1
1	B	21	HIS	5.0
1	B	99	ASN	4.7
1	A	343	PRO	4.7
1	B	287	LEU	4.7
1	A	285	ASP	4.6
1	A	132	ASP	4.5
1	A	48	THR	4.3
1	B	280	ASP	4.3
1	A	138	GLY	4.3
1	A	279	VAL	4.2
1	A	117	ILE	4.2
1	A	72	LYS	4.2
1	B	20	LEU	4.1
1	B	77	TYR	4.1
1	A	77	TYR	4.0
1	A	21	HIS	4.0
1	A	130	ASP	4.0
1	A	13	THR	4.0
1	B	519	VAL	4.0
1	A	533	ALA	3.9
1	B	344	SER	3.8
1	A	519	VAL	3.8
1	A	125	TRP	3.8
1	B	103	ALA	3.8
1	B	102	GLY	3.7
1	A	153	GLU	3.7
1	A	129	LEU	3.6
1	A	283	LYS	3.5
1	A	73	ASN	3.5
1	A	139	GLY	3.5
1	A	47	GLU	3.4
1	A	74	PRO	3.4
1	B	104	THR	3.4
1	B	68	LYS	3.3
1	A	612	GLU	3.3
1	A	632	ASP	3.3
1	B	138	GLY	3.3
1	B	71	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	662	THR	3.3
1	A	2	ALA	3.2
1	B	70	GLU	3.2
1	B	279	VAL	3.2
1	A	68	LYS	3.2
1	A	281	VAL	3.2
1	A	152	GLU	3.1
1	A	140	SER	3.1
1	B	533	ALA	3.1
1	B	282	LEU	3.1
1	B	705	ARG	3.1
1	A	99	ASN	3.1
1	B	345	ARG	3.1
1	B	286	GLY	3.0
1	B	19	ALA	3.0
1	A	282	LEU	3.0
1	A	288	MET	3.0
1	B	284	LYS	3.0
1	B	278	SER	2.9
1	B	73	ASN	2.9
1	A	134	ASN	2.9
1	B	283	LYS	2.9
1	B	480	GLU	2.9
1	B	632	ASP	2.9
1	A	133	ARG	2.9
1	A	15	TYR	2.9
1	A	71	PRO	2.8
1	A	146	LEU	2.8
1	B	152	GLU	2.8
1	A	122	VAL	2.8
1	A	67	ILE	2.7
1	A	326	SER	2.7
1	A	643	PRO	2.7
1	A	70	GLU	2.7
1	A	124	GLN	2.7
1	A	16	GLU	2.7
1	B	139	GLY	2.6
1	B	569	VAL	2.6
1	A	114	ASP	2.6
1	B	675	GLY	2.6
1	B	72	LYS	2.5
1	A	79	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	674	ILE	2.5
1	B	67	ILE	2.5
1	A	116	VAL	2.5
1	A	49	GLN	2.5
1	A	360	ILE	2.5
1	A	328	MET	2.4
1	A	193	ASN	2.4
1	B	570	VAL	2.4
1	A	106	ILE	2.4
1	A	317	GLY	2.4
1	B	547	ILE	2.4
1	B	757	GLU	2.3
1	B	132	ASP	2.3
1	B	328	MET	2.3
1	A	120	GLU	2.3
1	B	277	THR	2.3
1	A	98	ASP	2.3
1	A	113	VAL	2.3
1	A	570	VAL	2.3
1	A	142	ILE	2.3
1	A	480	GLU	2.2
1	B	2	ALA	2.2
1	B	323	LEU	2.2
1	B	288	MET	2.2
1	A	675	GLY	2.2
1	B	662	THR	2.2
1	B	679	ILE	2.2
1	A	197	ARG	2.2
1	A	121	GLU	2.2
1	A	569	VAL	2.2
1	A	571	VAL	2.2
1	A	75	LYS	2.2
1	A	679	ILE	2.2
1	B	674	ILE	2.1
1	A	143	HIS	2.1
1	A	434	LYS	2.1
1	A	3	GLN	2.1
1	A	665	MET	2.1
1	A	136	ILE	2.1
1	A	144	VAL	2.1
1	B	506	TYR	2.1
1	A	706	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	406	HIS	2.1
1	A	664	MET	2.1
1	A	14	ILE	2.0
1	A	141	LYS	2.0
1	A	521	ASN	2.0
1	A	127	GLU	2.0
1	B	47	GLU	2.0
1	A	50	LEU	2.0
1	A	108	ARG	2.0
1	B	105	LEU	2.0
1	B	358	GLY	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 carbohydrates in this entry.

6.4 Ligands [i](#)

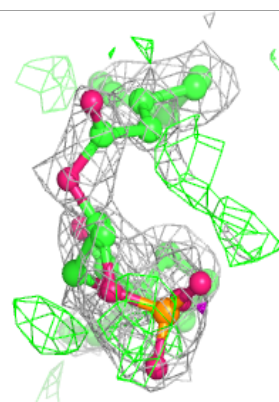
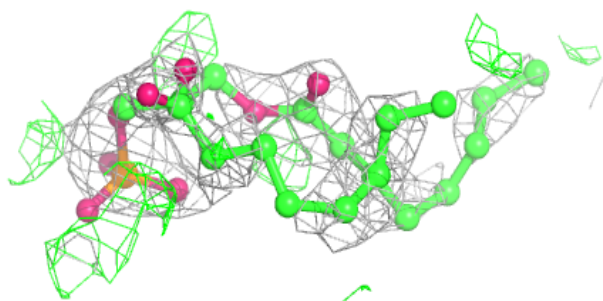
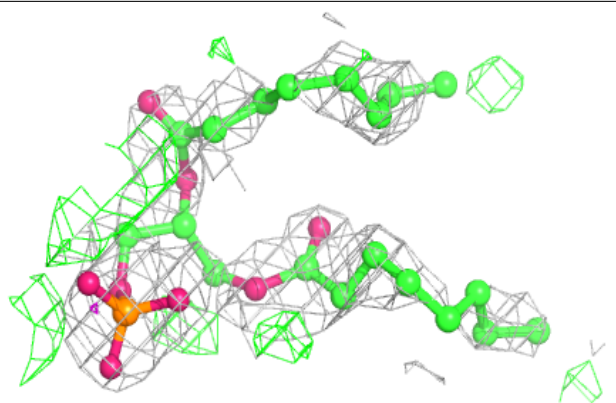
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PA8	A	1101	28/28	0.82	0.35	7,15,21,21	28
2	PA8	B	902	28/28	0.83	0.39	4,16,22,24	28
3	CA	A	1102	1/1	0.97	0.20	4,4,4,4	0
3	CA	B	901	1/1	0.99	0.26	5,5,5,5	0

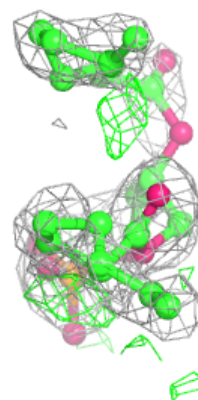
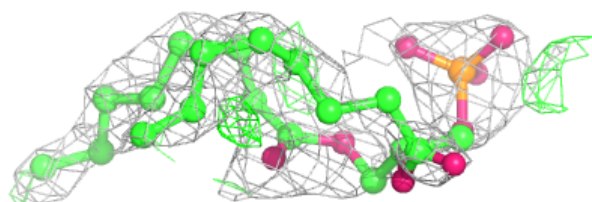
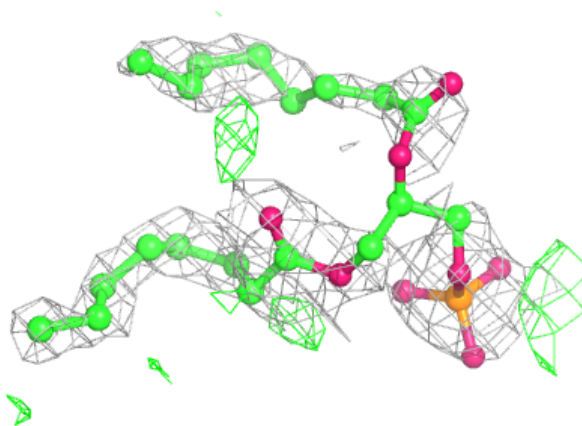
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PA8 A 1101:

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

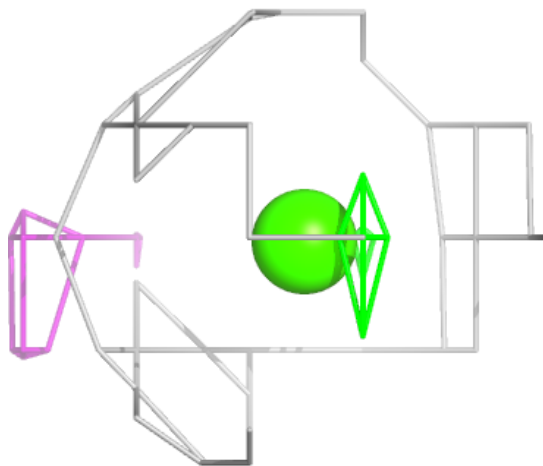
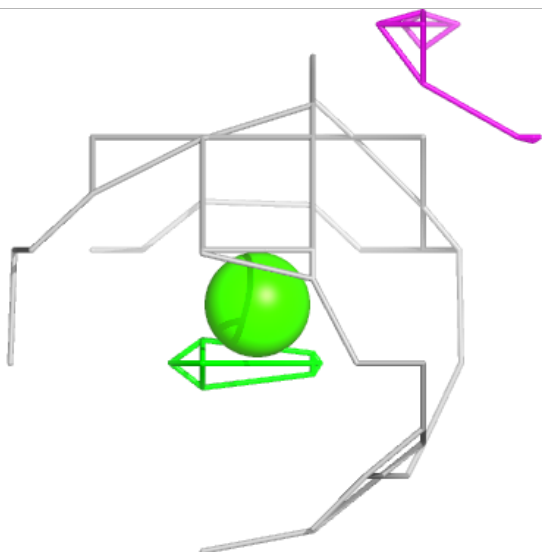
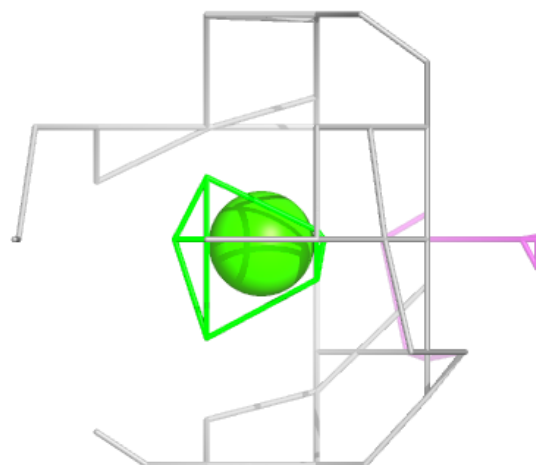
**Electron density around PA8 B 902:**

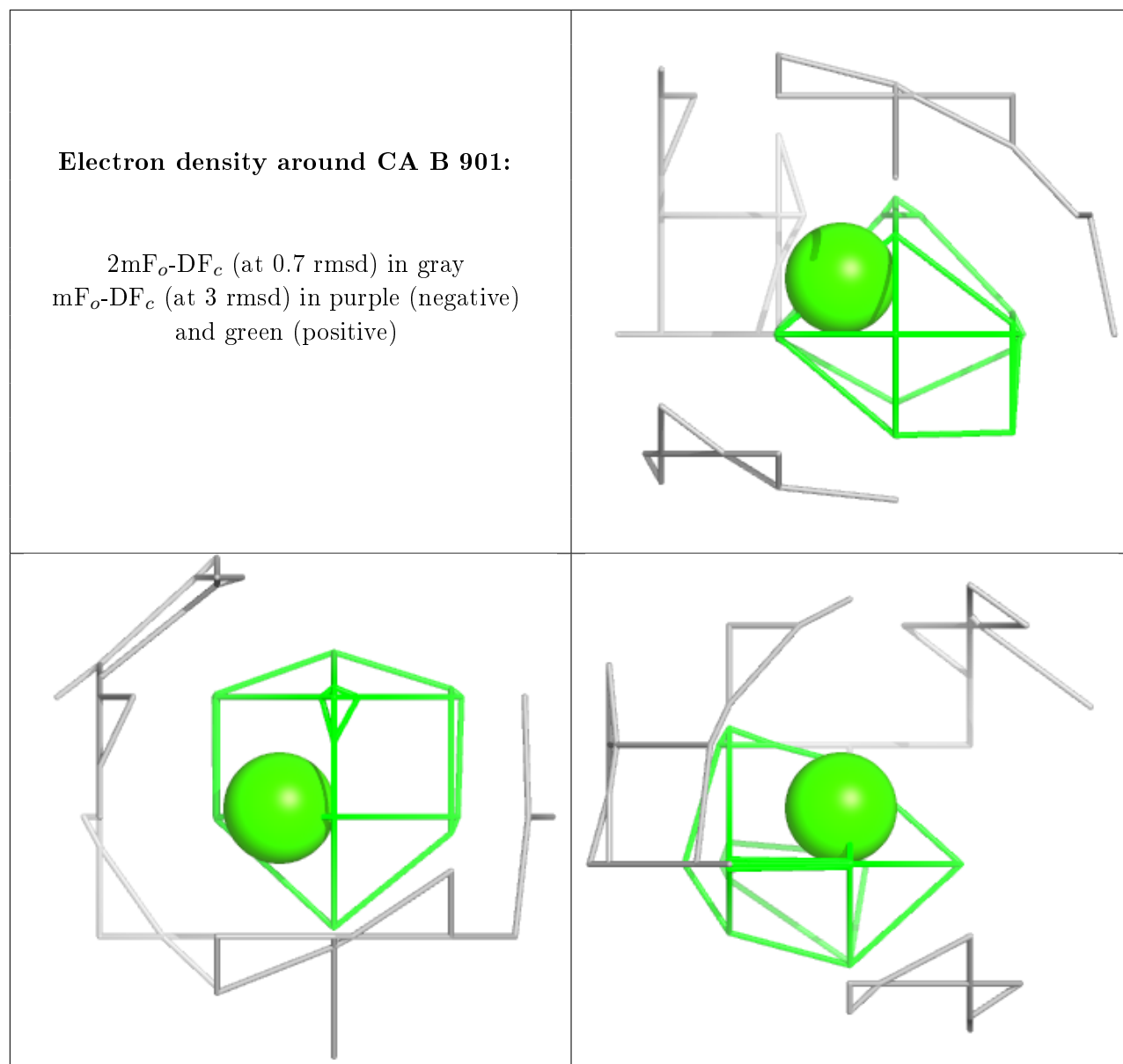
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA A 1102:

$2mF_o-DF_c$ (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.