



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:13 PM UTC

PDB ID : 2XEL / pdb_00002xel
Title : Molecular Mechanism of Pentachloropseudilin Mediated Inhibition of Myosin Motor Activity
Authors : Chinthalapudi, K.; Taft, M.H.; Martin, R.; Hartmann, F.K.; Heissler, S.M.; Tsiavalariis, G.; Gutzeit, H.O.; Knoelker, H.J.; Coluccio, L.M.; Fedorov, R.; Manstein, D.J.
Deposited on : 2010-05-16
Resolution : 2.50 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](#) ①) 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

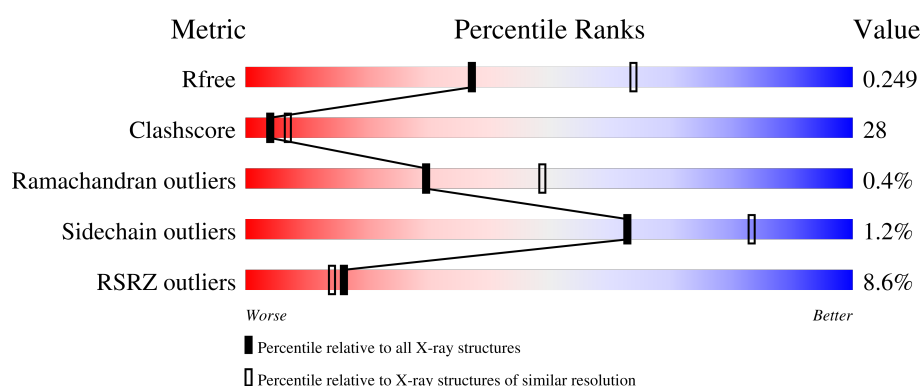
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	776	9% 62% 33% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6746 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.

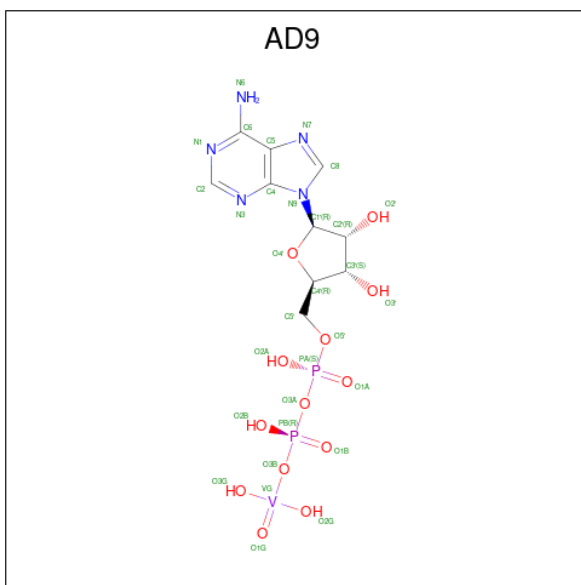
- Molecule 1 is a protein called MYOSIN-2 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	776	6239	3961	1076	1185	17	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	762	LEU	-	expression tag	UNP P08799
A	763	GLU	-	expression tag	UNP P08799
A	764	SER	-	expression tag	UNP P08799
A	765	ASN	-	expression tag	UNP P08799
A	766	GLU	-	expression tag	UNP P08799
A	767	PRO	-	expression tag	UNP P08799
A	768	PRO	-	expression tag	UNP P08799
A	769	MET	-	expression tag	UNP P08799
A	770	ASP	-	expression tag	UNP P08799
A	771	PHE	-	expression tag	UNP P08799
A	772	ASP	-	expression tag	UNP P08799
A	773	ASP	-	expression tag	UNP P08799
A	774	ASP	-	expression tag	UNP P08799
A	775	ILE	-	expression tag	UNP P08799
A	776	PRO	-	expression tag	UNP P08799
A	777	PHE	-	expression tag	UNP P08799

- Molecule 2 is ADP METAVANADATE (CCD ID: AD9) (formula: $C_{10}H_{16}N_5O_{13}P_2V$).

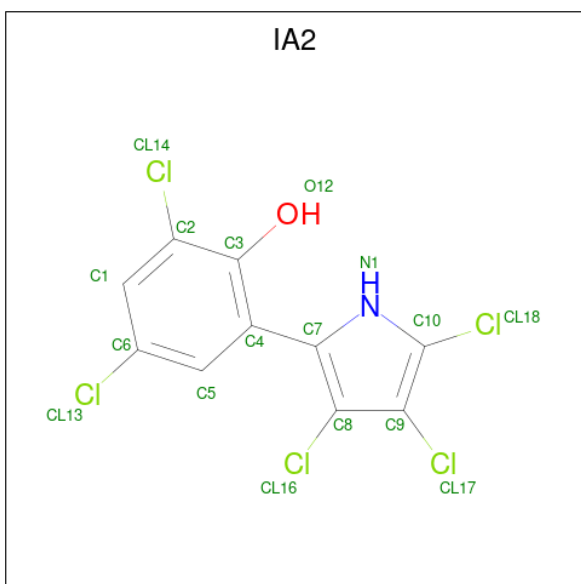


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	V	0	0
			31	10	5	13	2	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2,4-DICHLORO-6-(3,4,5-TRICHLORO-1H-PYRROL-2YL)PHENOL (CCD ID: IA2) (formula: C₁₀H₄Cl₅NO).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			17	10	5	1	1		

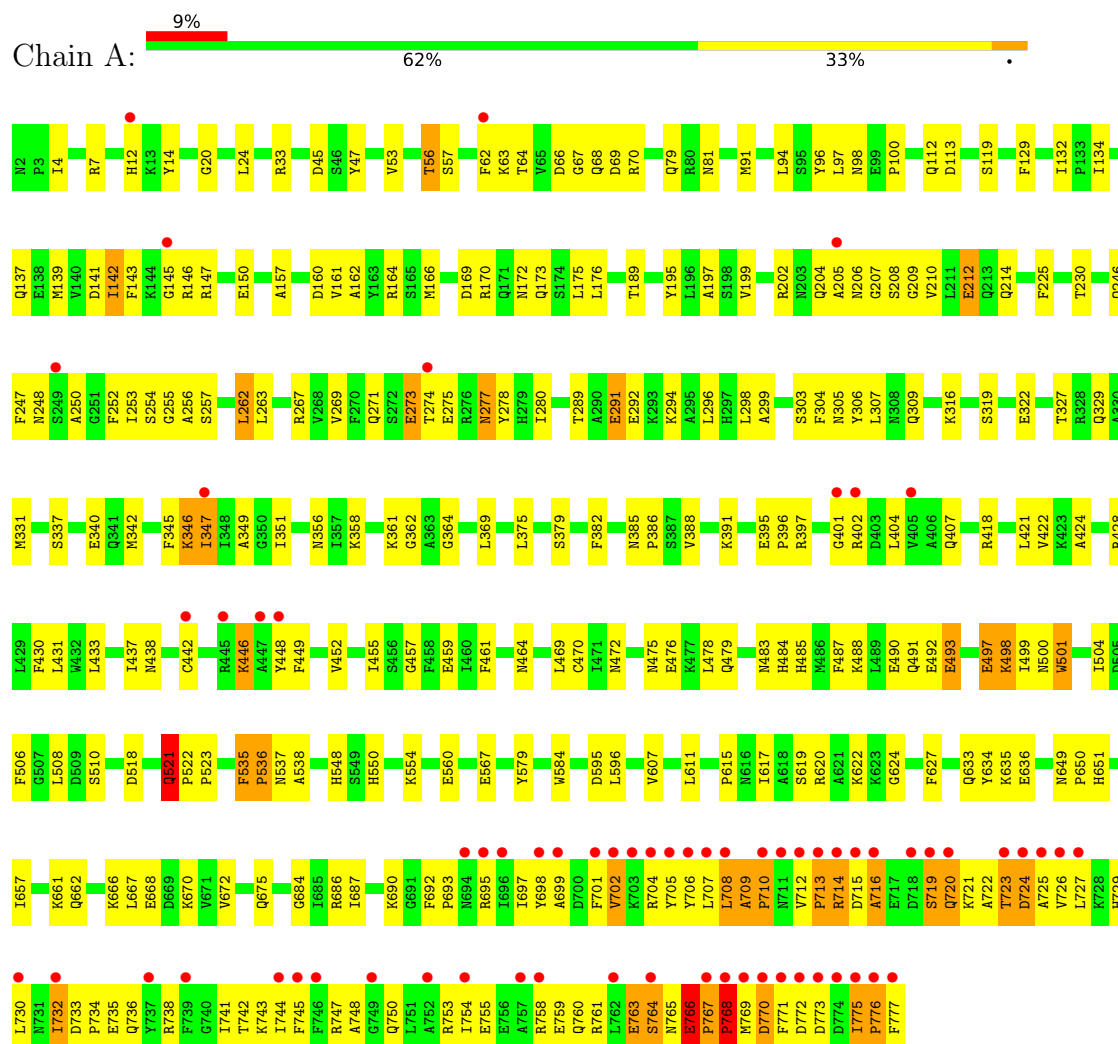
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	458	Total	O	0	0
			458	458		

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: MYOSIN-2 HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	89.53Å 147.49Å 153.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.59 – 2.50 24.59 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.59-2.50) 99.9 (24.59-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 2.50Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.229 , 0.253 0.222 , 0.249	Depositor DCC
R_{free} test set	1777 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.031 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6746	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: IA2, AD9, MG

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	0.53	12/6364 (0.2%)	1.14	69/8590 (0.8%)

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	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	PHE	C-O	-12.57	1.07	1.24
1	A	536	PRO	N-CD	-8.55	1.35	1.47
1	A	776	PRO	N-CD	-8.55	1.35	1.47
1	A	143	PHE	CE1-CZ	-7.96	1.14	1.38
1	A	768	PRO	CA-C	7.56	1.61	1.52
1	A	713	PRO	N-CD	7.11	1.57	1.47
1	A	143	PHE	CE2-CZ	-7.00	1.17	1.38
1	A	143	PHE	CA-C	-6.98	1.43	1.52
1	A	143	PHE	CD1-CE1	-6.70	1.18	1.38
1	A	143	PHE	CD2-CE2	-6.09	1.20	1.38
1	A	143	PHE	C-N	-6.00	1.24	1.33
1	A	767	PRO	CA-CB	-5.87	1.46	1.54

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	764	SER	N-CA-C	22.83	140.78	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	768	PRO	CA-N-CD	-17.43	87.60	112.00
1	A	767	PRO	CA-N-CD	-15.97	89.64	112.00
1	A	347	ILE	N-CA-C	-15.27	99.53	111.90
1	A	763	GLU	N-CA-C	-14.20	88.84	108.86
1	A	725	ALA	N-CA-C	11.79	128.84	112.45
1	A	713	PRO	CA-N-CD	-10.65	97.09	112.00
1	A	770	ASP	N-CA-C	10.09	125.33	112.92
1	A	725	ALA	CB-CA-C	-9.69	91.80	110.11
1	A	521	GLN	N-CA-C	9.17	127.65	108.39
1	A	716	ALA	CB-CA-C	9.04	125.61	110.43
1	A	764	SER	N-CA-CB	-8.95	98.95	112.28
1	A	535	PHE	N-CA-C	-8.87	98.64	109.72
1	A	716	ALA	N-CA-C	-8.84	94.81	108.42
1	A	763	GLU	CB-CA-C	8.58	132.23	111.65
1	A	773	ASP	N-CA-C	8.57	120.32	110.97
1	A	767	PRO	C-N-CD	-8.47	90.28	125.00
1	A	723	THR	N-CA-C	8.29	121.88	111.69
1	A	346	LYS	CB-CA-C	-7.81	96.47	110.37
1	A	535	PHE	CB-CA-C	7.79	120.69	109.08
1	A	766	GLU	C-N-CD	-7.69	93.47	125.00
1	A	273	GLU	CB-CA-C	7.54	121.85	109.70
1	A	775	ILE	N-CA-C	7.31	124.68	108.88
1	A	720	GLN	N-CA-C	-7.26	103.37	111.28
1	A	501	TRP	N-CA-C	7.24	121.05	109.24
1	A	716	ALA	N-CA-CB	-7.20	100.62	111.56
1	A	775	ILE	N-CA-CB	-6.89	101.56	111.21
1	A	764	SER	CB-CA-C	-6.85	100.59	111.48
1	A	273	GLU	N-CA-C	-6.83	100.60	110.24
1	A	734	PRO	CB-CA-C	-6.82	102.16	112.11
1	A	768	PRO	CB-CA-C	6.81	121.18	110.49
1	A	768	PRO	N-CA-C	-6.80	103.18	114.75
1	A	706	TYR	N-CA-C	-6.80	98.24	109.80
1	A	500	ASN	N-CA-C	6.79	121.02	111.92
1	A	735	GLU	N-CA-C	-6.65	105.06	112.57
1	A	262	LEU	N-CA-C	6.56	120.29	111.24
1	A	535	PHE	CA-C-N	6.49	127.95	119.84
1	A	535	PHE	C-N-CA	6.49	127.95	119.84
1	A	706	TYR	CB-CA-C	-6.48	102.93	113.37
1	A	724	ASP	N-CA-C	-6.45	105.71	112.93
1	A	501	TRP	N-CA-CB	-6.42	99.97	110.43
1	A	768	PRO	N-CA-CB	6.38	109.91	102.76
1	A	766	GLU	CB-CA-C	-6.37	97.62	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	PHE	CA-C-N	6.26	130.29	121.02
1	A	143	PHE	C-N-CA	6.26	130.29	121.02
1	A	537	ASN	N-CA-C	6.16	120.42	113.02
1	A	143	PHE	CB-CA-C	-5.99	99.23	109.65
1	A	769	MET	N-CA-C	5.96	122.41	114.12
1	A	723	THR	CB-CA-C	-5.95	99.81	110.70
1	A	493	GLU	N-CA-C	-5.93	104.45	111.03
1	A	721	LYS	N-CA-C	5.90	117.51	111.14
1	A	732	ILE	CB-CA-C	5.84	119.67	111.08
1	A	523	PRO	N-CA-C	5.79	119.95	111.03
1	A	277	ASN	N-CA-C	-5.75	100.82	109.79
1	A	719	SER	N-CA-C	5.70	118.71	111.69
1	A	714	ARG	CB-CA-C	5.58	121.52	110.42
1	A	145	GLY	N-CA-C	5.56	122.76	115.36
1	A	14	TYR	N-CA-C	5.49	120.09	113.17
1	A	708	LEU	N-CA-C	-5.48	104.85	112.30
1	A	455	ILE	CB-CA-C	-5.33	104.14	111.49
1	A	521	GLN	CB-CA-C	-5.32	101.07	111.29
1	A	492	GLU	N-CA-C	-5.31	106.31	112.89
1	A	56	THR	N-CA-C	-5.28	102.08	109.69
1	A	704	ARG	N-CA-C	-5.25	106.56	113.17
1	A	724	ASP	CB-CA-C	-5.17	101.87	110.81
1	A	710	PRO	N-CA-C	-5.15	102.87	111.26
1	A	767	PRO	N-CA-CB	5.14	108.07	103.08
1	A	650	PRO	N-CA-C	5.05	118.43	110.80
1	A	770	ASP	N-CA-CB	-5.00	103.25	110.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	521	GLN	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	A	6239	0	6175	346	1
2	A	31	0	14	0	0
3	A	1	0	0	0	0
4	A	17	0	3	4	0
5	A	458	0	0	9	0
All	All	6746	0	6192	346	1

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 28.

All (346) 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:A:431:LEU:HD22	4:A:999:IA2:CL17	1.53	1.43
1:A:289:THR:CG2	1:A:292:GLU:HG3	1.54	1.36
1:A:707:LEU:HD11	1:A:713:PRO:CD	1.56	1.35
1:A:707:LEU:CD1	1:A:713:PRO:HD3	1.59	1.31
1:A:289:THR:HG22	1:A:292:GLU:OE2	1.30	1.24
1:A:761:ARG:HD3	1:A:763:GLU:O	1.21	1.24
1:A:64:THR:HG1	1:A:68:GLN:HB2	1.07	1.15
1:A:289:THR:HG23	1:A:292:GLU:HG3	1.18	1.11
1:A:431:LEU:CD2	4:A:999:IA2:CL17	2.35	1.10
1:A:64:THR:OG1	1:A:68:GLN:HB2	1.53	1.08
1:A:289:THR:CG2	1:A:292:GLU:CG	2.32	1.06
1:A:289:THR:HG22	1:A:292:GLU:CD	1.81	1.04
1:A:767:PRO:HB2	1:A:768:PRO:HD2	1.40	1.03
1:A:246:GLN:HG2	1:A:446:LYS:HG2	1.45	0.99
1:A:657:ILE:H	1:A:675:GLN:HE22	1.02	0.98
1:A:342:MET:HG3	1:A:346:LYS:HE3	1.43	0.97
1:A:709:ALA:HB1	1:A:710:PRO:CD	1.94	0.96
1:A:499:ILE:HG21	1:A:745:PHE:CE2	2.02	0.94
1:A:761:ARG:CD	1:A:763:GLU:O	2.16	0.93
1:A:246:GLN:HB3	1:A:446:LYS:HG2	1.50	0.93
1:A:289:THR:CG2	1:A:292:GLU:OE2	2.17	0.91
1:A:461:PHE:H	1:A:464:ASN:HD21	1.19	0.91
1:A:246:GLN:CG	1:A:446:LYS:HG2	2.01	0.90
1:A:385:ASN:HD22	1:A:388:VAL:HG23	1.36	0.90
1:A:693:PRO:O	1:A:695:ARG:NH2	2.04	0.90
1:A:275:GLU:OE1	5:A:2220:HOH:O	1.90	0.90
1:A:697:ILE:HD13	1:A:743:LYS:HG2	1.55	0.89
1:A:709:ALA:HB1	1:A:710:PRO:HD2	1.52	0.89
1:A:63:LYS:HG2	1:A:69:ASP:OD1	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLN:CB	1:A:446:LYS:HG2	2.02	0.88
1:A:764:SER:HA	1:A:768:PRO:HG2	1.55	0.88
1:A:498:LYS:HG3	1:A:741:ILE:HD11	1.55	0.87
1:A:491:GLN:HE22	1:A:504:ILE:H	1.19	0.85
1:A:246:GLN:HG2	1:A:446:LYS:CG	2.08	0.84
1:A:491:GLN:HE21	1:A:501:TRP:HE1	1.22	0.83
1:A:736:GLN:HG3	1:A:750:GLN:NE2	1.94	0.82
1:A:289:THR:HG23	1:A:292:GLU:CG	2.04	0.81
1:A:205:ALA:HB3	1:A:208:SER:HB2	1.63	0.81
1:A:741:ILE:HG22	1:A:742:THR:HG23	1.64	0.80
1:A:397:ARG:N	1:A:595:ASP:OD2	2.15	0.78
1:A:719:SER:O	1:A:723:THR:HG23	1.83	0.78
1:A:81:ASN:HD22	1:A:94:LEU:HD22	1.47	0.78
1:A:327:THR:HG22	1:A:331:MET:HE2	1.65	0.78
1:A:661:LYS:HE3	1:A:666:LYS:HE2	1.64	0.78
1:A:767:PRO:HB2	1:A:768:PRO:CD	2.11	0.78
1:A:64:THR:OG1	1:A:68:GLN:CB	2.32	0.78
1:A:246:GLN:HB3	1:A:446:LYS:CG	2.13	0.78
1:A:289:THR:HG22	1:A:292:GLU:CG	2.04	0.77
1:A:705:TYR:CD1	1:A:726:VAL:HG11	2.20	0.76
1:A:736:GLN:OE1	1:A:747:ARG:HD2	1.86	0.75
1:A:497:GLU:HB3	1:A:499:ILE:HG23	1.67	0.74
1:A:707:LEU:CG	1:A:713:PRO:HD3	2.18	0.73
1:A:709:ALA:CB	1:A:710:PRO:CD	2.66	0.73
1:A:397:ARG:HB3	1:A:404:LEU:HD11	1.69	0.73
1:A:499:ILE:CG2	1:A:745:PHE:CE2	2.71	0.73
1:A:291:GLU:HA	1:A:294:LYS:HE2	1.71	0.72
1:A:497:GLU:OE2	1:A:497:GLU:HA	1.88	0.72
1:A:693:PRO:C	1:A:695:ARG:HH21	1.97	0.72
1:A:499:ILE:HG21	1:A:745:PHE:CD2	2.23	0.72
1:A:342:MET:O	1:A:346:LYS:HG3	1.90	0.72
1:A:712:VAL:O	1:A:712:VAL:HG13	1.89	0.71
1:A:469:LEU:HD22	1:A:584:TRP:CH2	2.25	0.71
1:A:491:GLN:NE2	1:A:504:ILE:H	1.88	0.71
1:A:497:GLU:HG3	1:A:745:PHE:CZ	2.26	0.70
1:A:707:LEU:HD11	1:A:713:PRO:HD3	0.78	0.70
1:A:204:GLN:HA	1:A:209:GLY:HA3	1.73	0.70
1:A:697:ILE:CD1	1:A:743:LYS:HE2	2.20	0.70
1:A:764:SER:O	1:A:764:SER:OG	2.03	0.70
1:A:772:ASP:HB3	1:A:776:PRO:HG3	1.74	0.69
1:A:697:ILE:HD11	1:A:743:LYS:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:GLN:O	1:A:723:THR:OG1	2.09	0.69
1:A:173:GLN:NE2	1:A:649:ASN:HB3	2.07	0.69
1:A:485:HIS:HB3	5:A:2322:HOH:O	1.92	0.69
1:A:661:LYS:NZ	1:A:668:GLU:OE1	2.25	0.69
1:A:275:GLU:OE2	5:A:2219:HOH:O	2.11	0.68
1:A:499:ILE:HD11	1:A:501:TRP:HB2	1.74	0.68
1:A:535:PHE:CD1	1:A:536:PRO:HD2	2.28	0.68
1:A:661:LYS:CE	1:A:666:LYS:HE2	2.22	0.68
1:A:723:THR:O	1:A:727:LEU:HD13	1.93	0.68
1:A:479:GLN:HE21	1:A:483:ASN:HD21	1.42	0.67
1:A:81:ASN:ND2	1:A:94:LEU:HD22	2.09	0.67
1:A:748:ALA:HB3	1:A:753:ARG:NH2	2.09	0.67
1:A:147:ARG:HB2	1:A:150:GLU:HG3	1.77	0.67
1:A:738:ARG:O	1:A:744:ILE:HD12	1.95	0.67
1:A:176:LEU:HD23	1:A:478:LEU:HD11	1.77	0.66
1:A:385:ASN:ND2	1:A:388:VAL:HG23	2.09	0.66
1:A:748:ALA:HB3	1:A:753:ARG:CZ	2.26	0.66
1:A:230:THR:HA	1:A:275:GLU:HG2	1.78	0.66
1:A:770:ASP:CG	1:A:770:ASP:O	2.38	0.65
1:A:697:ILE:HD13	1:A:743:LYS:CG	2.26	0.65
1:A:498:LYS:HG3	1:A:741:ILE:CD1	2.24	0.65
1:A:550:HIS:O	1:A:554:LYS:HE3	1.97	0.65
1:A:56:THR:HG22	1:A:57:SER:H	1.59	0.65
1:A:47:TYR:CZ	1:A:100:PRO:HG3	2.32	0.64
1:A:469:LEU:HD22	1:A:584:TRP:HH2	1.61	0.64
1:A:361:LYS:HD3	1:A:362:GLY:O	1.97	0.64
1:A:289:THR:HG23	1:A:292:GLU:H	1.63	0.64
1:A:273:GLU:O	1:A:274:THR:HB	1.98	0.63
1:A:709:ALA:CB	1:A:710:PRO:HD2	2.26	0.63
1:A:712:VAL:HG23	5:A:2443:HOH:O	1.98	0.63
1:A:761:ARG:NH1	1:A:765:ASN:HB2	2.14	0.63
1:A:274:THR:HG22	1:A:274:THR:O	1.99	0.62
1:A:56:THR:HG22	1:A:57:SER:N	2.15	0.62
1:A:459:GLU:H	1:A:472:ASN:HD21	1.48	0.62
1:A:369:LEU:HD23	1:A:375:LEU:HD22	1.81	0.62
1:A:62:PHE:CZ	1:A:70:ARG:HB2	2.34	0.62
1:A:446:LYS:CD	1:A:446:LYS:C	2.72	0.61
1:A:657:ILE:N	1:A:675:GLN:HE22	1.85	0.61
1:A:497:GLU:CG	1:A:745:PHE:HZ	2.13	0.61
1:A:518:ASP:HB2	1:A:635:LYS:HE3	1.83	0.61
1:A:724:ASP:CG	1:A:724:ASP:O	2.42	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:HD12	1:A:146:ARG:NH2	2.16	0.61
1:A:147:ARG:HB2	1:A:150:GLU:CG	2.31	0.61
1:A:709:ALA:HB1	1:A:710:PRO:HD3	1.80	0.61
1:A:246:GLN:HG2	1:A:446:LYS:HE3	1.83	0.60
1:A:160:ASP:OD1	1:A:164:ARG:NE	2.31	0.60
1:A:337:SER:HB3	1:A:340:GLU:HG3	1.81	0.60
1:A:491:GLN:HE22	1:A:504:ILE:N	1.96	0.60
1:A:766:GLU:HB2	1:A:767:PRO:HD2	1.83	0.60
1:A:64:THR:N	1:A:68:GLN:O	2.32	0.60
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.84	0.60
1:A:726:VAL:HG13	1:A:727:LEU:HD12	1.82	0.60
1:A:197:ALA:HA	1:A:253:ILE:CD1	2.31	0.60
1:A:736:GLN:HG3	1:A:750:GLN:CD	2.27	0.60
1:A:709:ALA:HA	1:A:729:HIS:HD2	1.65	0.59
1:A:212:GLU:H	1:A:212:GLU:CD	2.11	0.59
1:A:395:GLU:HA	1:A:407:GLN:O	2.02	0.59
1:A:7:ARG:HG2	1:A:12:HIS:CE1	2.38	0.58
1:A:617:ILE:O	4:A:999:IA2:C10	2.52	0.58
1:A:707:LEU:CD1	1:A:713:PRO:HA	2.33	0.58
1:A:248:ASN:HD21	1:A:252:PHE:HB2	1.69	0.58
1:A:733:ASP:HB3	1:A:736:GLN:HB2	1.85	0.58
1:A:173:GLN:HE22	1:A:649:ASN:HD22	1.49	0.58
1:A:761:ARG:HH12	1:A:765:ASN:HB2	1.68	0.58
1:A:497:GLU:HG3	1:A:745:PHE:CE2	2.40	0.57
1:A:709:ALA:CB	1:A:726:VAL:HA	2.34	0.57
1:A:289:THR:HG21	1:A:292:GLU:HG3	1.74	0.57
1:A:306:TYR:O	1:A:307:LEU:HD23	2.05	0.57
1:A:707:LEU:HD11	1:A:713:PRO:CA	2.34	0.57
1:A:709:ALA:HB2	1:A:726:VAL:HA	1.87	0.57
1:A:497:GLU:CG	1:A:745:PHE:CZ	2.88	0.57
1:A:727:LEU:HB3	1:A:732:ILE:HD11	1.85	0.57
1:A:262:LEU:HD11	1:A:470:CYS:CB	2.35	0.56
1:A:446:LYS:C	1:A:446:LYS:HD3	2.30	0.56
1:A:697:ILE:CD1	1:A:743:LYS:CE	2.83	0.56
1:A:64:THR:O	1:A:67:GLY:N	2.30	0.56
1:A:535:PHE:HD1	1:A:536:PRO:HD2	1.68	0.56
1:A:707:LEU:HD11	1:A:713:PRO:CG	2.33	0.56
1:A:479:GLN:NE2	1:A:483:ASN:HD21	2.03	0.56
1:A:68:GLN:HG2	5:A:2072:HOH:O	2.05	0.56
1:A:304:PHE:HA	1:A:356:ASN:HD21	1.71	0.56
1:A:697:ILE:HD11	1:A:743:LYS:CE	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:ARG:C	1:A:761:ARG:HD2	2.32	0.55
1:A:33:ARG:HH21	1:A:79:GLN:HE22	1.53	0.55
1:A:361:LYS:HE2	1:A:364:GLY:O	2.07	0.55
1:A:289:THR:HG23	1:A:291:GLU:HG3	1.87	0.55
1:A:20:GLY:HA3	1:A:24:LEU:HD23	1.89	0.54
1:A:81:ASN:HD21	1:A:94:LEU:HB3	1.72	0.54
1:A:98:ASN:OD1	1:A:100:PRO:HD2	2.08	0.54
1:A:693:PRO:HA	1:A:695:ARG:HH21	1.73	0.54
1:A:761:ARG:CD	1:A:764:SER:HB3	2.38	0.54
1:A:139:MET:O	1:A:142:ILE:HB	2.08	0.54
1:A:246:GLN:HB3	1:A:446:LYS:CB	2.38	0.54
1:A:401:GLY:O	1:A:402:ARG:HB2	2.08	0.54
1:A:202:ARG:HG2	1:A:252:PHE:HD2	1.73	0.53
1:A:262:LEU:HG	1:A:634:TYR:CE1	2.43	0.53
1:A:271:GLN:NE2	1:A:277:ASN:HB2	2.24	0.53
1:A:289:THR:CG2	1:A:291:GLU:HG3	2.38	0.53
1:A:497:GLU:OE2	1:A:497:GLU:CA	2.55	0.53
1:A:53:VAL:HG11	1:A:63:LYS:HD2	1.88	0.53
1:A:176:LEU:HD23	1:A:478:LEU:CD1	2.37	0.53
1:A:777:PHE:HD1	1:A:777:PHE:H	1.55	0.53
1:A:761:ARG:HD2	1:A:761:ARG:O	2.08	0.53
1:A:476:GLU:OE1	1:A:510:SER:HB2	2.08	0.53
1:A:246:GLN:OE1	1:A:255:GLY:C	2.52	0.53
1:A:701:PHE:HZ	1:A:727:LEU:HD11	1.74	0.53
1:A:7:ARG:HA	1:A:12:HIS:CG	2.44	0.52
1:A:446:LYS:HD2	1:A:446:LYS:O	2.09	0.52
1:A:693:PRO:O	1:A:695:ARG:CZ	2.57	0.52
1:A:298:LEU:HD21	1:A:349:ALA:HB1	1.91	0.52
1:A:129:PHE:CZ	1:A:662:GLN:HA	2.44	0.52
1:A:319:SER:HB3	1:A:322:GLU:HB2	1.91	0.52
1:A:484:HIS:HD2	1:A:488:LYS:HD3	1.75	0.52
1:A:262:LEU:HD11	1:A:470:CYS:HB3	1.92	0.52
1:A:461:PHE:H	1:A:464:ASN:ND2	1.99	0.52
1:A:705:TYR:CD1	1:A:726:VAL:CG1	2.92	0.52
1:A:172:ASN:OD1	1:A:448:TYR:HA	2.09	0.52
1:A:730:LEU:H	1:A:758:ARG:HH22	1.57	0.52
1:A:273:GLU:O	1:A:274:THR:CB	2.57	0.51
1:A:761:ARG:NH2	1:A:765:ASN:HB2	2.25	0.51
1:A:730:LEU:HB3	1:A:758:ARG:HH22	1.74	0.51
1:A:7:ARG:HG2	1:A:12:HIS:NE2	2.25	0.51
1:A:4:ILE:HD12	1:A:146:ARG:HH22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLY:H	1:A:210:VAL:HG23	1.76	0.51
1:A:747:ARG:HG3	1:A:747:ARG:HH11	1.76	0.50
1:A:499:ILE:CD1	1:A:501:TRP:HB2	2.41	0.50
1:A:697:ILE:HD13	1:A:743:LYS:HE2	1.92	0.50
1:A:730:LEU:H	1:A:758:ARG:NH2	2.08	0.50
1:A:64:THR:HG1	1:A:68:GLN:CB	1.99	0.50
1:A:189:THR:HG23	1:A:452:VAL:HG11	1.93	0.50
1:A:254:SER:OG	1:A:446:LYS:HB3	2.11	0.50
1:A:342:MET:O	1:A:342:MET:HE3	2.11	0.50
1:A:291:GLU:HA	1:A:294:LYS:HG2	1.93	0.50
1:A:195:TYR:CZ	1:A:199:VAL:HG11	2.47	0.50
1:A:421:LEU:HB2	1:A:596:LEU:HD13	1.94	0.50
1:A:257:SER:HB3	1:A:442:CYS:SG	2.51	0.50
1:A:693:PRO:O	1:A:695:ARG:NE	2.45	0.49
1:A:750:GLN:NE2	1:A:753:ARG:HH21	2.10	0.49
1:A:207:GLY:H	1:A:210:VAL:CG2	2.24	0.49
1:A:715:ASP:O	1:A:716:ALA:HB2	2.12	0.49
1:A:615:PRO:O	1:A:619:SER:HB2	2.11	0.49
1:A:369:LEU:CD2	1:A:375:LEU:HD22	2.41	0.49
1:A:137:GLN:NE2	1:A:141:ASP:OD2	2.44	0.49
1:A:248:ASN:ND2	1:A:252:PHE:HB2	2.28	0.49
1:A:705:TYR:HD1	1:A:726:VAL:HG11	1.73	0.49
1:A:761:ARG:CZ	1:A:765:ASN:HB2	2.42	0.49
1:A:296:LEU:HD11	1:A:342:MET:HE1	1.95	0.49
1:A:421:LEU:HD22	1:A:596:LEU:HD22	1.95	0.49
1:A:709:ALA:HA	1:A:729:HIS:CD2	2.47	0.48
1:A:331:MET:HE1	1:A:345:PHE:CZ	2.48	0.48
1:A:331:MET:HE1	1:A:345:PHE:HZ	1.78	0.48
1:A:81:ASN:OD1	1:A:96:TYR:HB2	2.12	0.48
1:A:91:MET:HE3	1:A:119:SER:OG	2.12	0.48
1:A:147:ARG:HD2	1:A:150:GLU:OE1	2.14	0.48
1:A:316:LYS:HD3	1:A:316:LYS:C	2.38	0.48
1:A:708:LEU:HD13	1:A:758:ARG:HB3	1.94	0.48
1:A:347:ILE:HA	1:A:382:PHE:CE1	2.49	0.48
1:A:457:GLY:HA2	1:A:475:ASN:HD21	1.79	0.48
1:A:763:GLU:O	1:A:764:SER:HB3	2.11	0.48
1:A:693:PRO:HA	1:A:695:ARG:NH2	2.29	0.48
1:A:766:GLU:HB2	1:A:767:PRO:CD	2.44	0.48
1:A:173:GLN:HE22	1:A:649:ASN:HB3	1.79	0.48
1:A:418:ARG:C	1:A:418:ARG:HD2	2.39	0.47
1:A:712:VAL:O	1:A:712:VAL:CG1	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:ILE:HG23	1:A:755:GLU:N	2.28	0.47
1:A:97:LEU:HD23	1:A:686:ARG:HG2	1.96	0.47
1:A:262:LEU:HD11	1:A:470:CYS:HB2	1.95	0.47
1:A:147:ARG:HB2	1:A:150:GLU:CD	2.39	0.47
1:A:160:ASP:HB2	1:A:195:TYR:OH	2.15	0.47
1:A:289:THR:CG2	1:A:292:GLU:CD	2.60	0.47
1:A:708:LEU:HD13	1:A:758:ARG:CB	2.45	0.47
1:A:716:ALA:HB1	1:A:722:ALA:HB2	1.97	0.47
1:A:33:ARG:HB3	5:A:2086:HOH:O	2.15	0.47
1:A:147:ARG:HH21	1:A:760:GLN:HE21	1.63	0.47
1:A:397:ARG:HB3	1:A:404:LEU:CD1	2.42	0.47
1:A:438:ASN:O	1:A:442:CYS:HB2	2.15	0.46
1:A:296:LEU:HB2	1:A:298:LEU:HG	1.97	0.46
1:A:431:LEU:HD23	4:A:999:IA2:CL17	2.46	0.46
1:A:277:ASN:OD1	1:A:278:TYR:N	2.44	0.46
1:A:775:ILE:N	1:A:776:PRO:CD	2.78	0.46
1:A:205:ALA:HB2	5:A:2188:HOH:O	2.16	0.46
1:A:708:LEU:CD1	1:A:758:ARG:HB3	2.45	0.46
1:A:169:ASP:O	1:A:170:ARG:HB2	2.16	0.46
1:A:693:PRO:CA	1:A:695:ARG:HH21	2.28	0.46
1:A:246:GLN:OE1	1:A:256:ALA:N	2.49	0.46
1:A:157:ALA:O	1:A:161:VAL:HG23	2.16	0.46
1:A:707:LEU:CD1	1:A:713:PRO:CD	2.48	0.46
1:A:63:LYS:HA	1:A:68:GLN:O	2.17	0.45
1:A:206:ASN:C	1:A:208:SER:H	2.24	0.45
1:A:759:GLU:HG2	1:A:760:GLN:H	1.81	0.45
1:A:535:PHE:HA	1:A:536:PRO:HD2	1.72	0.45
1:A:775:ILE:N	1:A:776:PRO:HD3	2.31	0.45
1:A:535:PHE:HD2	1:A:538:ALA:HB2	1.80	0.45
1:A:81:ASN:ND2	1:A:94:LEU:HB3	2.31	0.45
1:A:521:GLN:HA	1:A:522:PRO:C	2.40	0.45
1:A:205:ALA:H	1:A:209:GLY:HA3	1.81	0.45
1:A:461:PHE:N	1:A:464:ASN:HD21	2.00	0.45
1:A:506:PHE:CE2	1:A:687:ILE:HD13	2.52	0.45
1:A:299:ALA:HB3	1:A:303:SER:OG	2.16	0.45
1:A:622:LYS:HE2	1:A:624:GLY:O	2.17	0.45
1:A:379:SER:CB	1:A:386:PRO:HG3	2.47	0.45
1:A:767:PRO:CB	1:A:768:PRO:HD2	2.19	0.45
1:A:225:PHE:CE2	1:A:280:ILE:HG12	2.52	0.44
1:A:391:LYS:O	1:A:395:GLU:N	2.45	0.44
1:A:263:LEU:HD22	1:A:430:PHE:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:PRO:HA	1:A:595:ASP:OD2	2.18	0.44
1:A:548:HIS:CE1	1:A:560:GLU:HG3	2.53	0.44
1:A:684:GLY:O	1:A:687:ILE:HG22	2.18	0.44
1:A:744:ILE:O	1:A:744:ILE:HG23	2.17	0.44
1:A:269:VAL:HG12	1:A:306:TYR:CZ	2.52	0.44
1:A:497:GLU:O	1:A:498:LYS:C	2.60	0.44
1:A:305:ASN:ND2	1:A:356:ASN:HA	2.32	0.44
1:A:490:GLU:HA	1:A:490:GLU:OE1	2.18	0.44
1:A:686:ARG:HG2	1:A:686:ARG:HH11	1.83	0.44
1:A:761:ARG:HH22	1:A:765:ASN:HB2	1.82	0.44
1:A:493:GLU:OE2	1:A:493:GLU:HA	2.18	0.43
1:A:692:PHE:CB	1:A:745:PHE:HB3	2.48	0.43
1:A:697:ILE:HD13	1:A:743:LYS:CE	2.48	0.43
1:A:667:LEU:HD11	1:A:672:VAL:HG21	2.00	0.43
1:A:695:ARG:HD3	1:A:745:PHE:HE1	1.84	0.43
1:A:197:ALA:HA	1:A:253:ILE:HD11	2.00	0.43
1:A:162:ALA:O	1:A:173:GLN:HG3	2.18	0.43
1:A:759:GLU:HB3	1:A:760:GLN:OE1	2.19	0.43
1:A:47:TYR:CE1	1:A:100:PRO:HG3	2.54	0.43
1:A:202:ARG:HH21	1:A:248:ASN:HD22	1.65	0.43
1:A:274:THR:O	1:A:274:THR:CG2	2.66	0.43
1:A:385:ASN:HA	1:A:386:PRO:HD3	1.92	0.43
1:A:247:PHE:HA	1:A:252:PHE:O	2.19	0.43
1:A:329:GLN:HE21	1:A:329:GLN:HB2	1.61	0.43
1:A:64:THR:OG1	1:A:68:GLN:CA	2.67	0.43
1:A:66:ASP:OD1	1:A:68:GLN:HB2	2.18	0.43
1:A:291:GLU:HG3	1:A:292:GLU:H	1.84	0.43
1:A:501:TRP:HZ3	1:A:690:LYS:O	2.01	0.43
1:A:506:PHE:CZ	1:A:687:ILE:HD13	2.53	0.43
1:A:767:PRO:O	1:A:771:PHE:HE1	2.02	0.43
1:A:449:PHE:CD2	1:A:449:PHE:C	2.97	0.42
1:A:607:VAL:O	1:A:611:LEU:HG	2.18	0.42
1:A:210:VAL:O	1:A:214:GLN:HG3	2.19	0.42
1:A:699:ALA:C	1:A:701:PHE:H	2.28	0.42
1:A:202:ARG:NH2	1:A:248:ASN:HD22	2.18	0.42
1:A:230:THR:HG22	1:A:267:ARG:NH2	2.34	0.42
1:A:433:LEU:O	1:A:437:ILE:HG13	2.19	0.42
1:A:62:PHE:CD1	1:A:62:PHE:N	2.87	0.42
1:A:695:ARG:HB3	1:A:745:PHE:CD1	2.55	0.42
1:A:697:ILE:HG22	1:A:698:TYR:N	2.35	0.42
1:A:633:GLN:O	1:A:636:GLU:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ASN:OD1	1:A:250:ALA:HB3	2.20	0.42
1:A:567:GLU:HA	1:A:579:TYR:O	2.19	0.42
1:A:730:LEU:HB3	1:A:758:ARG:HH12	1.85	0.42
1:A:761:ARG:NE	1:A:764:SER:HB3	2.34	0.42
1:A:424:ALA:O	1:A:428:ARG:HG3	2.19	0.41
1:A:730:LEU:CB	1:A:758:ARG:HH22	2.33	0.41
1:A:535:PHE:CD2	1:A:538:ALA:HB2	2.55	0.41
1:A:702:VAL:HG11	1:A:714:ARG:O	2.20	0.41
1:A:707:LEU:CD1	1:A:713:PRO:CA	2.96	0.41
1:A:132:ILE:HG22	1:A:134:ILE:HG23	2.02	0.41
1:A:727:LEU:HD12	1:A:727:LEU:N	2.34	0.41
1:A:166:MET:HE1	1:A:247:PHE:CD1	2.55	0.41
1:A:172:ASN:OD1	1:A:449:PHE:N	2.52	0.41
1:A:4:ILE:HD12	1:A:146:ARG:CZ	2.49	0.41
1:A:147:ARG:NH2	1:A:760:GLN:HE21	2.19	0.41
1:A:358:LYS:HD2	5:A:2128:HOH:O	2.20	0.41
1:A:478:LEU:HB3	5:A:2317:HOH:O	2.20	0.41
1:A:484:HIS:CD2	1:A:488:LYS:HD3	2.55	0.41
1:A:499:ILE:CG2	1:A:745:PHE:HE2	2.30	0.41
1:A:112:GLN:O	1:A:113:ASP:HB2	2.20	0.41
1:A:761:ARG:CD	1:A:761:ARG:C	2.94	0.41
1:A:175:LEU:HD13	1:A:651:HIS:HB2	2.02	0.41
1:A:205:ALA:H	1:A:209:GLY:N	2.19	0.41
1:A:491:GLN:HE21	1:A:501:TRP:NE1	2.03	0.41
1:A:692:PHE:HB3	1:A:745:PHE:HB3	2.02	0.41
1:A:446:LYS:CD	1:A:446:LYS:O	2.67	0.40
1:A:45:ASP:OD2	1:A:670:LYS:HD2	2.21	0.40
1:A:620:ARG:HG2	1:A:627:PHE:HB3	2.03	0.40
1:A:705:TYR:HB3	1:A:726:VAL:HG11	2.04	0.40
1:A:487:PHE:CE2	1:A:508:LEU:HD12	2.57	0.40

All (1) 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:24:LEU:CD2	1:A:402:ARG:NH1[6_555]	2.07	0.13

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	774/776 (100%)	714 (92%)	57 (7%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	709	ALA
1	A	766	GLU
1	A	702	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	680/680 (100%)	672 (99%)	8 (1%)	63	83

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	ILE
1	A	212	GLU
1	A	291	GLU
1	A	309	GLN
1	A	446	LYS
1	A	497	GLU
1	A	498	LYS
1	A	768	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	71	GLN
1	A	79	GLN
1	A	111	ASN
1	A	171	GLN
1	A	173	GLN
1	A	305	ASN
1	A	309	GLN
1	A	329	GLN
1	A	356	ASN
1	A	376	ASN
1	A	385	ASN
1	A	439	ASN
1	A	464	ASN
1	A	472	ASN
1	A	475	ASN
1	A	483	ASN
1	A	484	HIS
1	A	491	GLN
1	A	500	ASN
1	A	550	HIS
1	A	613	ASN
1	A	637	GLN
1	A	662	GLN
1	A	675	GLN
1	A	679	ASN
1	A	729	HIS
1	A	750	GLN
1	A	760	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 3 ligands modelled in this entry, 1 is 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	$\# Z > 2$
4	IA2	A	999	-	17,18,18	3.05	8 (47%)	25,27,27	1.93	5 (20%)
2	AD9	A	900	3	29,33,33	2.03	5 (17%)	42,52,52	1.09	5 (11%)

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
4	IA2	A	999	-	-	3/4/4/4	0/2/2/2
2	AD9	A	900	3	-	1/16/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	AD9	PA-O3A	6.83	1.66	1.59
4	A	999	IA2	C5-C4	5.32	1.48	1.39
4	A	999	IA2	C4-C3	5.17	1.49	1.41
4	A	999	IA2	C3-C2	4.90	1.47	1.39
4	A	999	IA2	C4-C7	4.43	1.54	1.48
2	A	900	AD9	PB-O3A	4.39	1.64	1.59
4	A	999	IA2	C5-C6	4.23	1.45	1.38
4	A	999	IA2	C1-C6	3.65	1.44	1.38
4	A	999	IA2	C1-C2	3.55	1.44	1.38
2	A	900	AD9	PB-O2B	3.14	1.69	1.55
2	A	900	AD9	PA-O2A	2.98	1.69	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	IA2	C7-C8	2.76	1.45	1.38
2	A	900	AD9	O4'-C1'	2.56	1.47	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	IA2	C7-N1-C10	5.76	114.01	109.27
4	A	999	IA2	C4-C7-C8	4.01	136.72	129.94
4	A	999	IA2	C5-C4-C7	-3.20	114.95	119.35
2	A	900	AD9	O2B-PB-O3A	-3.04	99.06	107.27
4	A	999	IA2	C3-C4-C7	3.04	127.06	122.09
2	A	900	AD9	O2A-PA-O3A	-2.71	99.94	107.27
4	A	999	IA2	C8-C7-N1	-2.51	103.64	106.64
2	A	900	AD9	O5'-PA-O1A	2.17	117.54	108.94
2	A	900	AD9	O2B-PB-O3B	-2.12	100.58	107.59
2	A	900	AD9	O3A-PA-O1A	2.05	116.88	110.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	999	IA2	C5-C4-C7-C8
4	A	999	IA2	C3-C4-C7-C8
4	A	999	IA2	C5-C4-C7-N1
2	A	900	AD9	PA-O3A-PB-O2B

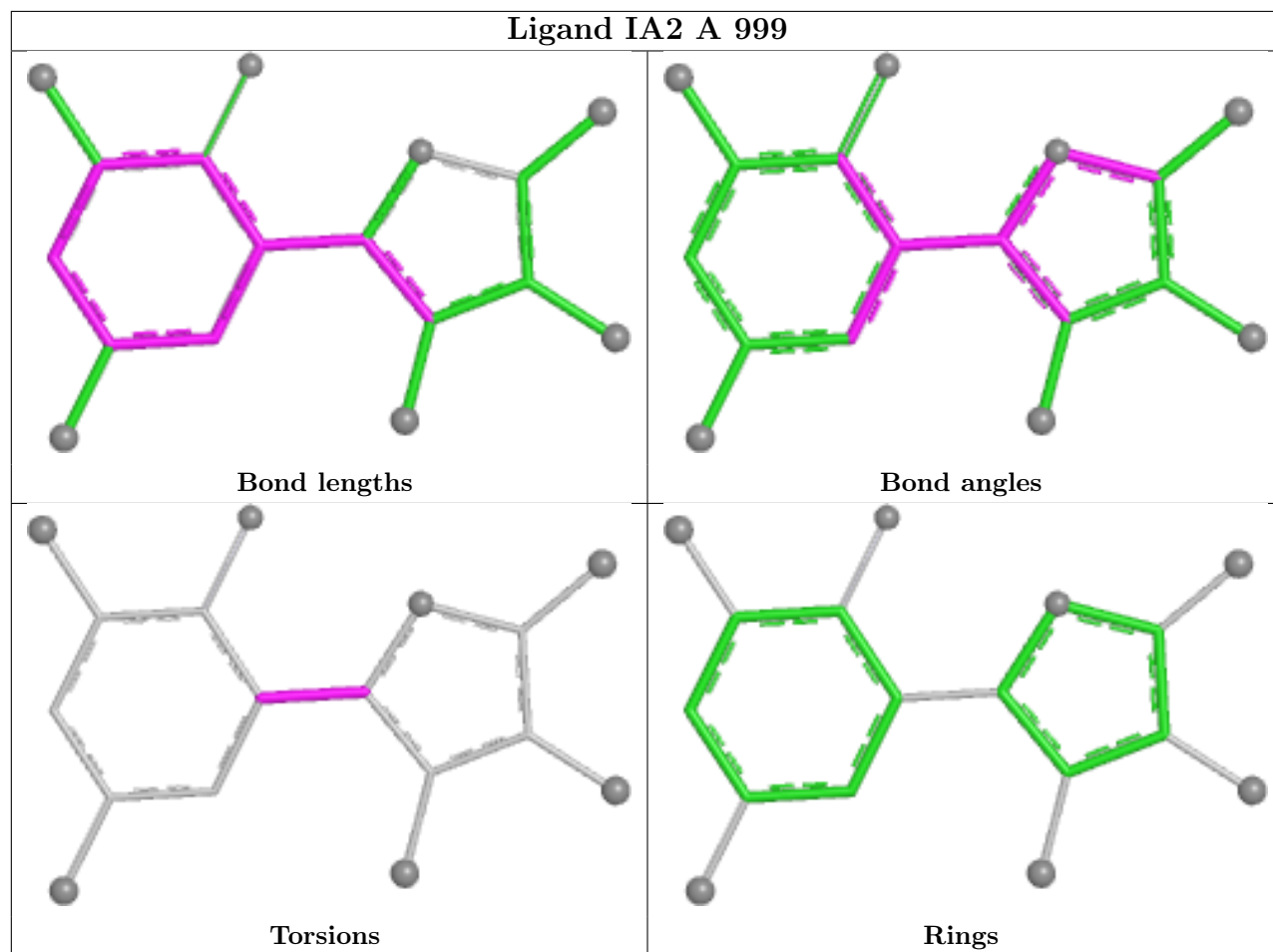
There are no ring outliers.

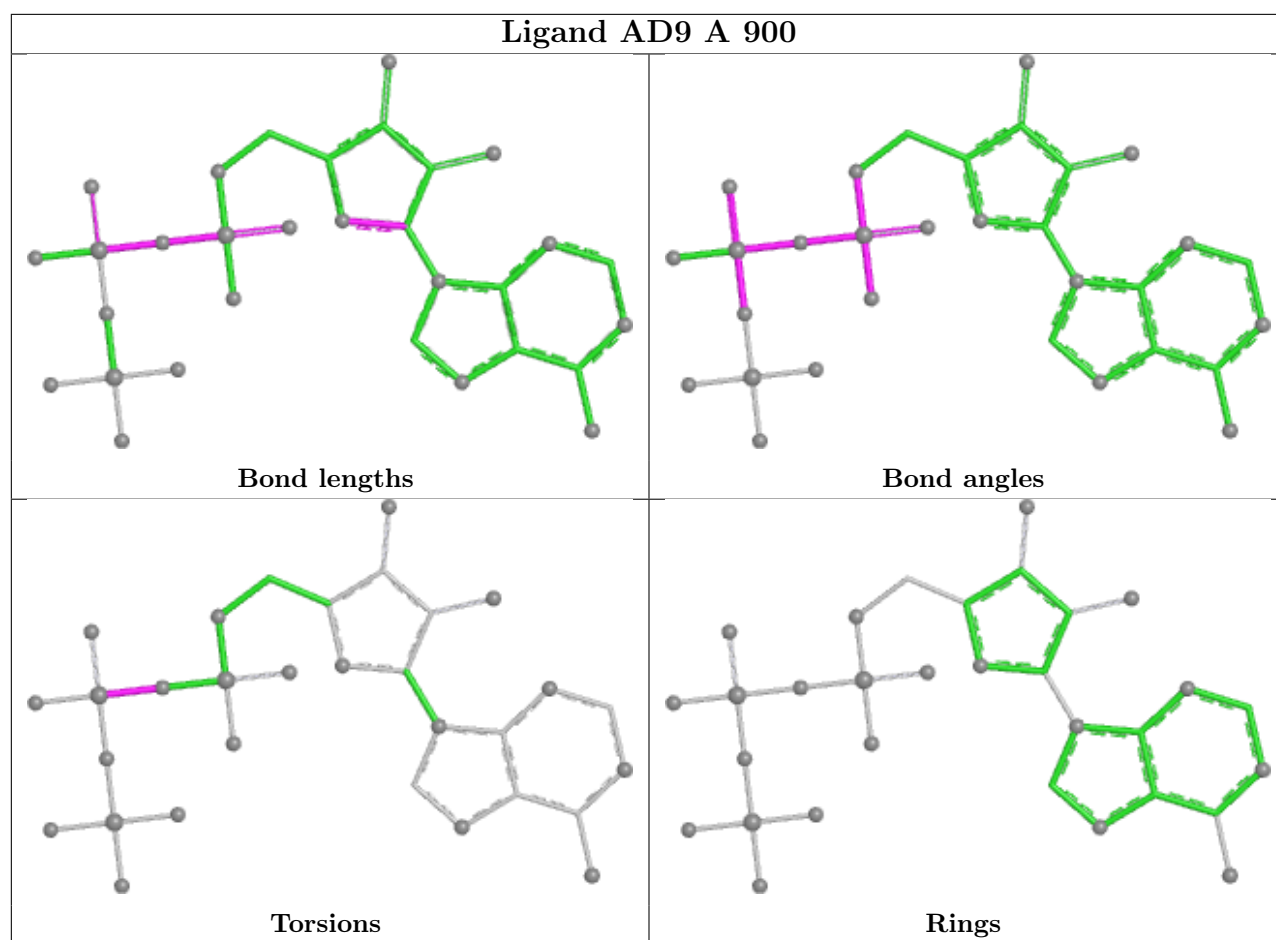
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	IA2	4	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	776/776 (100%)	0.27	67 (8%)	16 14	19, 45, 104, 150	20 (2%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	705	TYR	6.6
1	A	706	TYR	6.5
1	A	401	GLY	6.4
1	A	710	PRO	5.9
1	A	708	LEU	5.2
1	A	757	ALA	4.8
1	A	702	VAL	4.8
1	A	720	GLN	4.7
1	A	402	ARG	4.5
1	A	716	ALA	4.5
1	A	707	LEU	4.4
1	A	274	THR	4.3
1	A	12	HIS	4.1
1	A	725	ALA	4.1
1	A	718	ASP	4.0
1	A	719	SER	3.7
1	A	772	ASP	3.7
1	A	771	PHE	3.4
1	A	696	ILE	3.4
1	A	758	ARG	3.4
1	A	754	ILE	3.3
1	A	774	ASP	3.3
1	A	704	ARG	3.3
1	A	447	ALA	3.3
1	A	713	PRO	3.2
1	A	732	ILE	3.2
1	A	698	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	145	GLY	3.0
1	A	712	VAL	3.0
1	A	694	ASN	3.0
1	A	775	ILE	3.0
1	A	730	LEU	3.0
1	A	723	THR	2.9
1	A	770	ASP	2.9
1	A	703	LYS	2.8
1	A	727	LEU	2.8
1	A	711	ASN	2.8
1	A	764	SER	2.8
1	A	768	PRO	2.7
1	A	776	PRO	2.7
1	A	405	VAL	2.7
1	A	726	VAL	2.7
1	A	749	GLY	2.6
1	A	739	PHE	2.6
1	A	744	ILE	2.6
1	A	762	LEU	2.6
1	A	445	ARG	2.4
1	A	769	MET	2.4
1	A	695	ARG	2.4
1	A	752	ALA	2.4
1	A	62	PHE	2.3
1	A	701	PHE	2.3
1	A	737	TYR	2.3
1	A	699	ALA	2.3
1	A	777	PHE	2.3
1	A	249	SER	2.3
1	A	715	ASP	2.2
1	A	767	PRO	2.2
1	A	724	ASP	2.1
1	A	746	PHE	2.1
1	A	773	ASP	2.1
1	A	714	ARG	2.1
1	A	442	CYS	2.1
1	A	205	ALA	2.0
1	A	347	ILE	2.0
1	A	448	TYR	2.0
1	A	745	PHE	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](#)

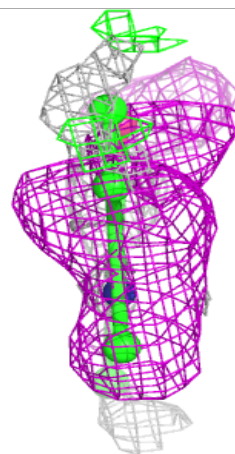
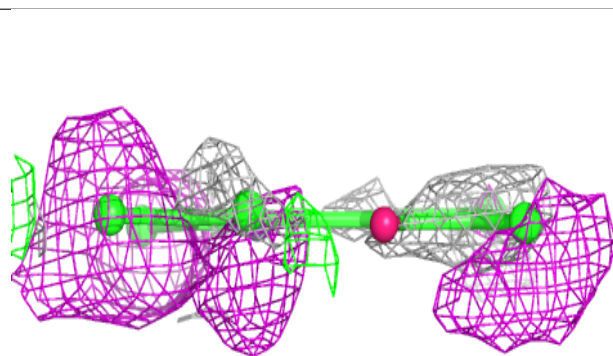
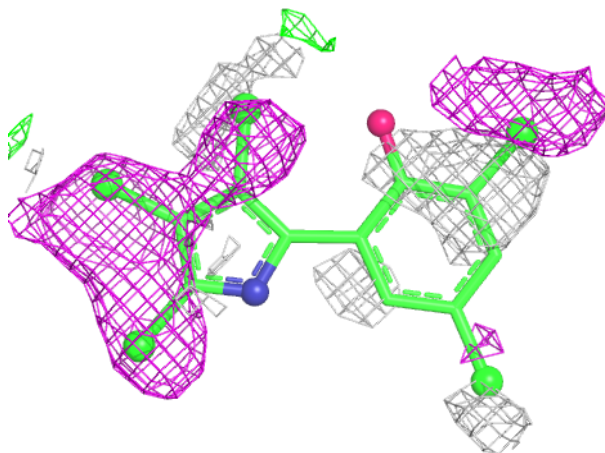
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

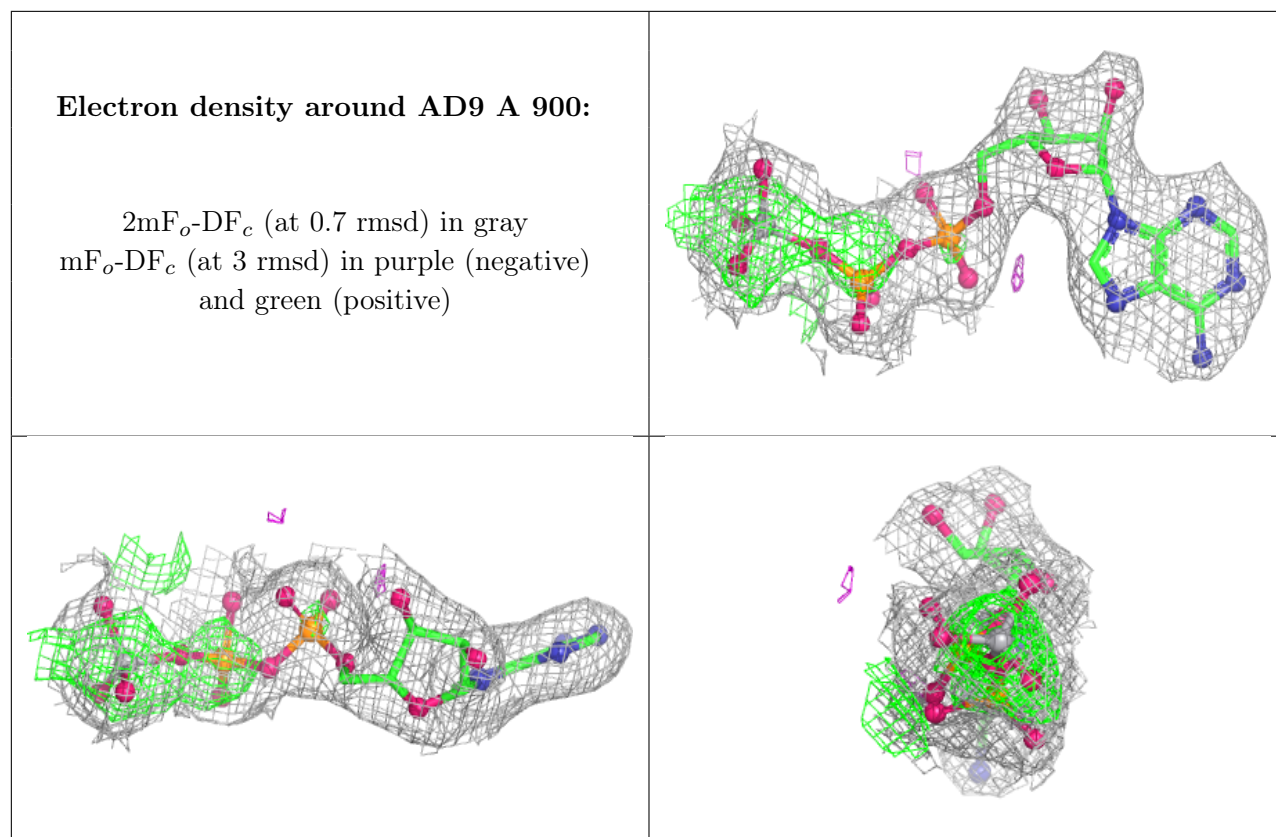
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	IA2	A	999	17/17	0.39	0.24	86,88,91,91	17
3	MG	A	901	1/1	0.94	0.15	31,31,31,31	0
2	AD9	A	900	31/31	0.97	0.10	38,41,43,45	0

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 IA2 A 999:

$2mF_o-DF_c$ (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.