



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:21 PM UTC

PDB ID : 1ASL / pdb_00001asl
Title : CRYSTAL STRUCTURES OF ESCHERICHIA COLI ASPARTATE AMINO-TRANSFERASE IN TWO CONFORMATIONS: COMPARISON OF AN UNLIGANDED OPEN AND TWO LIGANDED CLOSED FORMS
Authors : Jaeger, J.; Jansonius, J.N.
Deposited on : 1993-09-16
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

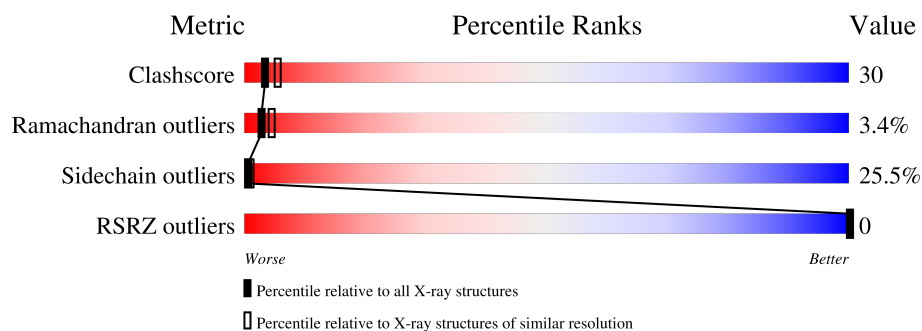
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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

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

Mol	Chain	Length	Quality of chain
1	A	396	
1	B	396	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLA	B	410	-	-	X	-

2 Entry composition [i](#)

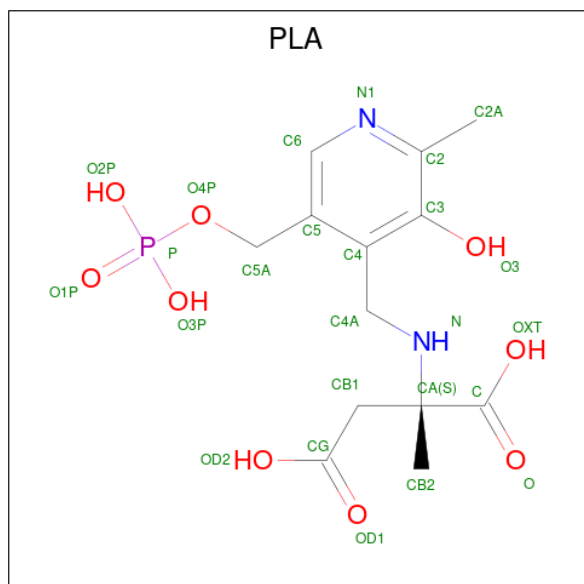
There are 3 unique types of molecules in this entry. The entry contains 6407 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3069	1936	536	584	13			
1	B	396	Total	C	N	O	S	0	0	0
			3069	1936	536	584	13			

- Molecule 2 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL)-AMINO]-2-METHYL-SUCCINIC ACID (CCD ID: PLA) (formula: C₁₃H₁₉N₂O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	B	1	Total	C	N	O	P	0	0
			25	13	2	9	1		

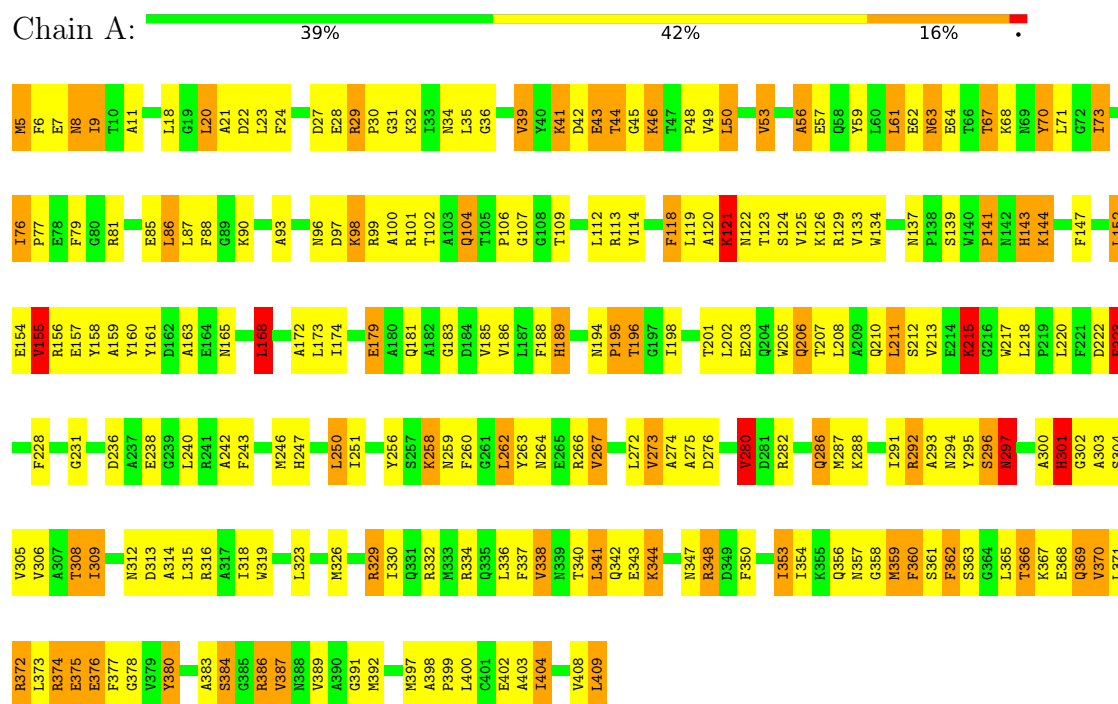
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	113	Total 113	O 113	0	0
3	B	106	Total 106	O 106	0	0

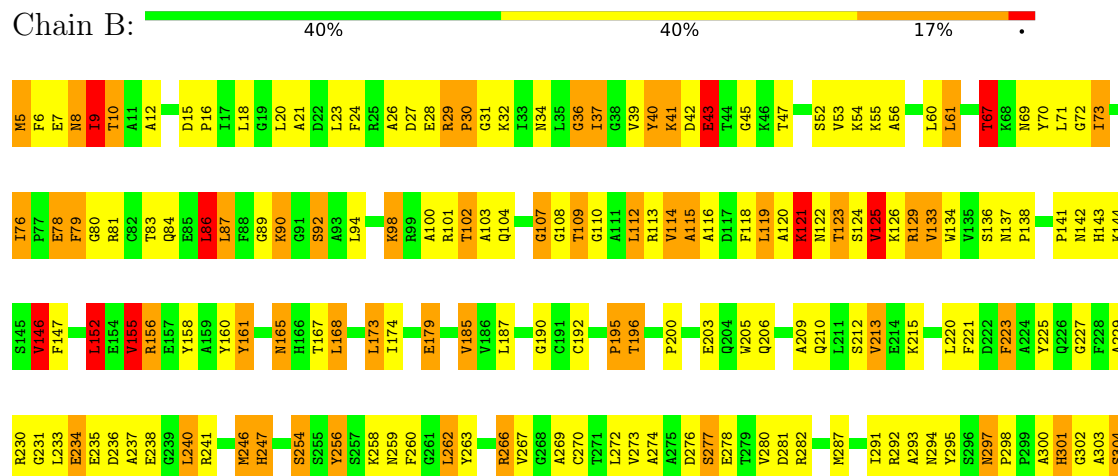
3 Residue-property plots

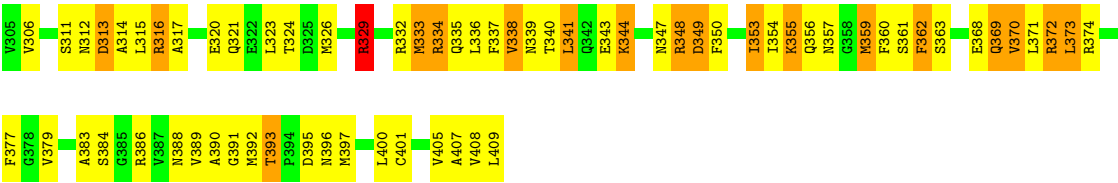
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: ASPARTATE AMINOTRANSFERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.60Å 78.80Å 89.60Å 90.00° 118.60° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60 10.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.60) 94.5 (10.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.51Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.183 , (Not available) 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h-l 0.000 for -h-l,k,h 0.457 for h,-k,-h-l 0.000 for l,-k,h 0.000 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6407	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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: PLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.10	6/3130 (0.2%)	1.49	49/4240 (1.2%)
1	B	1.11	5/3130 (0.2%)	1.47	38/4240 (0.9%)
All	All	1.11	11/6260 (0.2%)	1.48	87/8480 (1.0%)

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	B	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	VAL	CA-CB	-6.69	1.46	1.54
1	A	56	ALA	CA-CB	-6.50	1.42	1.53
1	A	196	THR	CA-CB	6.26	1.64	1.53
1	B	196	THR	CA-CB	6.08	1.63	1.53
1	B	146	VAL	CA-CB	5.98	1.62	1.54
1	A	293	ALA	CA-C	-5.62	1.45	1.52
1	A	53	VAL	CA-CB	5.51	1.61	1.54
1	B	303	ALA	CA-CB	-5.45	1.45	1.53
1	B	56	ALA	CA-CB	-5.13	1.44	1.53
1	B	293	ALA	CA-C	-5.07	1.46	1.52
1	A	155	VAL	CA-CB	5.06	1.60	1.54

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	ALA	N-CA-C	10.60	122.41	111.07
1	A	29	ARG	CA-C-N	9.85	129.21	118.97
1	A	29	ARG	C-N-CA	9.85	129.21	118.97
1	B	115	ALA	N-CA-C	-9.01	101.41	111.14
1	B	27	ASP	N-CA-C	-8.77	96.70	109.59
1	A	20	LEU	N-CA-C	-8.57	101.15	111.69
1	A	344	LYS	N-CA-C	-8.37	102.08	112.88
1	B	304	SER	N-CA-C	-8.26	102.28	111.28
1	B	89	GLY	N-CA-C	7.99	132.11	113.18
1	B	363	SER	N-CA-C	7.97	120.05	111.36
1	B	369	GLN	N-CA-C	-7.95	102.21	111.03
1	A	76	ILE	CA-C-N	7.72	127.27	119.24
1	A	76	ILE	C-N-CA	7.72	127.27	119.24
1	B	377	PHE	N-CA-C	7.71	125.17	113.61
1	B	300	ALA	N-CA-C	7.70	119.75	111.36
1	A	360	PHE	N-CA-C	7.37	121.50	109.85
1	A	63	ASN	N-CA-C	7.11	121.79	113.18
1	A	67	THR	N-CA-C	7.09	119.85	109.07
1	A	402	GLU	N-CA-C	-7.06	104.29	113.12
1	B	298	PRO	N-CA-C	7.04	119.28	110.70
1	B	313	ASP	N-CA-C	7.00	119.76	111.71
1	A	88	PHE	N-CA-C	6.97	122.08	112.04
1	B	108	GLY	N-CA-C	-6.92	103.48	113.86
1	B	126	LYS	N-CA-C	-6.90	106.76	114.62
1	A	163	ALA	N-CA-C	6.85	121.63	113.28
1	A	157	GLU	N-CA-C	6.72	120.59	108.69
1	B	107	GLY	CA-C-O	-6.72	117.85	122.22
1	B	9	ILE	N-CA-C	6.66	117.63	109.30
1	B	234	GLU	N-CA-C	-6.63	105.18	113.20
1	A	161	TYR	N-CA-C	6.61	119.05	108.41
1	A	247	HIS	N-CA-C	6.60	119.47	110.55
1	B	67	THR	N-CA-C	6.50	118.73	108.79
1	A	368	GLU	N-CA-C	-6.46	104.44	112.90
1	A	359	MET	N-CA-C	6.42	119.09	111.71
1	B	94	LEU	N-CA-C	-6.32	104.39	111.28
1	A	369	GLN	N-CA-C	-6.27	104.37	111.14
1	B	102	THR	N-CA-C	6.24	119.41	109.24
1	A	76	ILE	N-CA-C	6.15	113.97	107.76
1	A	275	ALA	N-CA-C	6.13	119.60	111.75
1	B	247	HIS	N-CA-C	6.00	118.44	110.53
1	A	386	ARG	N-CA-C	-5.96	101.02	109.96
1	A	297	ASN	CA-C-N	-5.88	114.33	120.38
1	A	297	ASN	C-N-CA	-5.88	114.33	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	VAL	N-CA-C	5.86	116.38	108.17
1	B	103	ALA	N-CA-C	-5.86	99.85	109.40
1	A	409	LEU	CA-CB-CG	5.82	136.66	116.30
1	B	360	PHE	N-CA-C	5.76	118.24	109.95
1	A	156	ARG	N-CA-C	-5.76	101.68	110.14
1	A	309	ILE	CB-CA-C	-5.76	104.37	112.14
1	B	86	LEU	N-CA-C	-5.69	105.16	111.36
1	A	330	ILE	N-CA-C	-5.63	105.36	110.82
1	B	161	TYR	N-CA-C	5.61	117.87	108.73
1	A	280	VAL	CB-CA-C	-5.60	104.70	112.04
1	B	76	ILE	N-CA-C	5.52	113.33	107.76
1	A	168	LEU	CA-CB-CG	5.51	135.57	116.30
1	A	22	ASP	N-CA-C	-5.48	104.95	111.69
1	A	363	SER	N-CA-C	5.46	119.21	112.54
1	A	102	THR	N-CA-C	5.46	118.38	109.59
1	B	87	LEU	N-CA-C	5.43	117.06	111.03
1	B	29	ARG	CA-C-N	5.40	126.59	119.84
1	B	29	ARG	C-N-CA	5.40	126.59	119.84
1	B	349	ASP	N-CA-C	-5.39	101.67	109.59
1	B	76	ILE	CA-C-O	5.38	122.33	119.15
1	A	228	PHE	N-CA-C	5.38	119.83	113.16
1	A	71	LEU	N-CA-C	-5.37	102.94	110.35
1	B	125	VAL	N-CA-C	5.35	116.26	110.21
1	A	85	GLU	N-CA-C	-5.35	106.26	112.89
1	A	223	PHE	CA-C-N	-5.34	114.14	122.37
1	A	223	PHE	C-N-CA	-5.34	114.14	122.37
1	A	303	ALA	N-CA-C	-5.30	105.17	111.69
1	A	70	TYR	N-CA-C	5.27	117.98	110.24
1	B	359	MET	N-CA-C	5.25	118.94	112.54
1	B	79	PHE	N-CA-C	-5.23	105.49	111.14
1	A	242	ALA	N-CA-C	-5.21	105.68	111.36
1	B	72	GLY	N-CA-C	-5.20	104.64	112.60
1	A	141	PRO	N-CA-C	5.15	123.08	112.47
1	A	183	GLY	N-CA-C	-5.14	108.14	115.64
1	B	92	SER	N-CA-C	5.13	121.72	110.80
1	A	143	HIS	N-CA-C	-5.12	105.78	111.36
1	A	189	HIS	N-CA-C	-5.11	100.39	108.73
1	A	63	ASN	CA-C-N	-5.09	115.42	122.30
1	A	63	ASN	C-N-CA	-5.09	115.42	122.30
1	B	40	TYR	N-CA-C	5.08	117.09	110.43
1	B	329	ARG	N-CA-C	-5.08	106.34	112.54
1	A	301	HIS	N-CA-C	5.06	121.57	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	359	MET	CG-SD-CE	-5.02	89.86	100.90
1	A	380	TYR	N-CA-C	5.00	116.84	107.99

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	256	TYR	Sidechain

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	3069	0	3018	179	0
1	B	3069	0	3018	213	0
2	A	25	0	14	4	0
2	B	25	0	14	9	0
3	A	113	0	0	9	0
3	B	106	0	0	15	0
All	All	6407	0	6064	370	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (370) 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:260:PHE:HB3	1:B:262:LEU:HD22	1.34	1.07
1:A:39:VAL:HG21	1:B:69:ASN:HD22	1.21	1.03
1:A:260:PHE:HB3	1:A:262:LEU:HD22	1.44	1.00
1:A:196:THR:HA	1:A:362:PHE:HB2	1.43	1.00
1:B:8:ASN:HD22	1:B:8:ASN:H	1.12	0.98
1:A:39:VAL:HG21	1:B:69:ASN:ND2	1.82	0.94
1:A:294:ASN:HD21	1:B:294:ASN:HD21	0.95	0.94
1:A:61:LEU:HD12	1:B:61:LEU:HD12	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LYS:HG2	1:A:359:MET:HE1	1.52	0.90
1:A:210:GLN:O	1:A:213:VAL:HG12	1.73	0.89
1:B:258:LYS:NZ	2:B:410:PLA:H4A2	1.88	0.88
1:A:196:THR:HG22	1:A:362:PHE:CD2	2.09	0.87
1:B:123:THR:CG2	1:B:125:VAL:HG13	2.07	0.85
1:A:8:ASN:H	1:A:8:ASN:HD22	1.23	0.84
1:A:296:SER:HB2	1:B:109:THR:HG21	1.59	0.83
1:B:107:GLY:HA3	1:B:266:ARG:NH1	1.92	0.83
1:B:323:LEU:HD12	1:B:326:MET:HE3	1.60	0.83
1:A:294:ASN:ND2	1:B:294:ASN:HD21	1.77	0.81
1:A:6:PHE:HD1	1:A:9:ILE:HD11	1.46	0.81
1:A:276:ASP:O	1:A:280:VAL:HG23	1.81	0.80
1:B:258:LYS:HZ1	2:B:410:PLA:H4A2	1.43	0.80
1:B:8:ASN:H	1:B:8:ASN:ND2	1.75	0.80
1:A:294:ASN:HD21	1:B:294:ASN:ND2	1.79	0.80
1:B:129:ARG:HD2	1:B:134:TRP:HE1	1.47	0.80
1:B:121:LYS:O	1:B:121:LYS:HD3	1.83	0.79
1:A:350:PHE:HB3	1:A:353:ILE:HD13	1.66	0.78
1:B:338:VAL:HG11	1:B:354:ILE:CD1	2.14	0.78
1:B:209:ALA:O	1:B:213:VAL:HG23	1.83	0.78
1:A:6:PHE:O	1:A:9:ILE:HG13	1.84	0.78
1:A:120:ALA:HB2	1:A:152:LEU:HD13	1.65	0.78
1:A:107:GLY:HA3	1:A:266:ARG:NH1	2.01	0.76
1:A:366:THR:HG22	1:A:369:GLN:H	1.48	0.76
1:A:122:ASN:OD1	1:A:286:GLN:HG2	1.85	0.76
1:A:274:ALA:HB3	1:A:280:VAL:HG22	1.66	0.76
1:A:258:LYS:CG	1:A:359:MET:HE1	2.16	0.75
1:B:40:TYR:CE2	1:B:326:MET:HG2	2.20	0.75
1:B:18:LEU:HD21	3:B:515:HOH:O	1.86	0.74
2:B:410:PLA:H4A1	3:B:509:HOH:O	1.87	0.74
1:A:129:ARG:NH2	1:A:181:GLN:HG3	2.03	0.73
1:B:110:GLY:O	1:B:114:VAL:HG13	1.87	0.73
1:B:355:LYS:O	1:B:355:LYS:HD3	1.89	0.73
1:B:227:GLY:HA2	1:B:231:GLY:O	1.88	0.72
1:B:338:VAL:HG11	1:B:354:ILE:HD11	1.72	0.72
1:A:77:PRO:O	1:A:81:ARG:HG3	1.90	0.71
1:A:212:SER:HB3	1:A:217:TRP:HE3	1.56	0.70
1:A:120:ALA:HB2	1:A:152:LEU:CD1	2.21	0.70
1:B:223:PHE:CE2	1:B:240:LEU:HD12	2.27	0.70
1:A:99:ARG:O	1:A:280:VAL:HG21	1.91	0.70
1:B:274:ALA:HB3	1:B:280:VAL:HB	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLN:OE1	1:B:12:ALA:HB2	1.92	0.69
1:B:165:ASN:HD21	1:B:167:THR:HG22	1.57	0.69
1:A:123:THR:OG1	1:A:125:VAL:HG23	1.92	0.68
1:A:11:ALA:HB2	1:B:282:ARG:HG2	1.75	0.68
1:A:159:ALA:O	1:A:173:LEU:HD23	1.94	0.68
1:A:374:ARG:HG3	1:A:375:GLU:N	2.05	0.68
1:B:8:ASN:HD22	1:B:8:ASN:N	1.90	0.68
1:B:350:PHE:HB3	1:B:353:ILE:HD13	1.74	0.68
1:A:266:ARG:HD2	1:B:297:ASN:O	1.94	0.68
1:B:76:ILE:O	1:B:79:PHE:HB3	1.94	0.67
1:B:195:PRO:HB3	1:B:386:ARG:HG3	1.77	0.67
1:B:129:ARG:NH1	1:B:129:ARG:HB3	2.09	0.67
1:B:142:ASN:O	1:B:146:VAL:HG13	1.95	0.67
1:B:165:ASN:ND2	1:B:167:THR:HG22	2.10	0.66
1:B:67:THR:HG21	3:B:516:HOH:O	1.94	0.65
1:A:329:ARG:NH2	1:A:392:MET:O	2.29	0.65
1:A:168:LEU:HD13	1:A:168:LEU:O	1.95	0.65
1:A:297:ASN:O	1:B:266:ARG:HD2	1.97	0.65
1:B:98:LYS:O	1:B:101:ARG:NH1	2.30	0.64
1:B:133:VAL:HB	1:B:185:VAL:HG22	1.78	0.64
1:B:329:ARG:NH2	1:B:392:MET:O	2.30	0.63
1:A:266:ARG:NH2	2:A:410:PLA:O1P	2.32	0.63
1:A:356:GLN:C	1:A:357:ASN:HD22	2.07	0.63
1:A:73:ILE:CG2	1:A:288:LYS:HG2	2.28	0.63
1:B:260:PHE:HB3	1:B:262:LEU:CD2	2.21	0.63
1:A:24:PHE:CE1	1:A:34:ASN:HB2	2.33	0.63
1:B:40:TYR:OH	1:B:326:MET:HA	1.99	0.63
1:B:258:LYS:HG2	1:B:359:MET:HE1	1.80	0.63
1:A:220:LEU:HD12	1:A:251:ILE:HB	1.80	0.63
1:B:374:ARG:HD3	3:B:490:HOH:O	1.99	0.63
1:A:398:ALA:H	1:A:399:PRO:HD2	1.64	0.62
1:A:109:THR:HG22	1:A:109:THR:O	1.98	0.62
1:A:134:TRP:HH2	1:A:179:GLU:HG2	1.64	0.62
1:A:46:LYS:O	1:A:48:PRO:HD3	1.99	0.62
1:A:286:GLN:NE2	1:B:10:THR:O	2.32	0.62
1:B:6:PHE:O	1:B:9:ILE:HG13	1.99	0.62
1:A:238:GLU:HB2	3:A:413:HOH:O	2.00	0.62
1:B:266:ARG:HH22	2:B:410:PLA:P	2.21	0.62
1:A:42:ASP:O	1:A:45:GLY:N	2.31	0.62
1:A:76:ILE:O	1:A:79:PHE:HB3	1.99	0.62
1:A:212:SER:HB3	1:A:217:TRP:CE3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:VAL:HG11	1:B:354:ILE:HD12	1.81	0.61
1:B:333:MET:CE	1:B:336:LEU:HD23	2.30	0.61
1:B:137:ASN:O	1:B:160:TYR:HB3	2.01	0.61
1:A:179:GLU:HG3	1:A:179:GLU:O	1.99	0.61
1:A:101:ARG:HD3	3:A:491:HOH:O	2.00	0.61
1:A:70:TYR:HE1	1:B:266:ARG:HH21	1.48	0.61
1:B:323:LEU:HA	1:B:326:MET:CE	2.31	0.60
2:B:410:PLA:O3	2:B:410:PLA:N	2.29	0.60
1:B:24:PHE:CZ	1:B:32:LYS:HG3	2.37	0.59
1:B:348:ARG:NH1	1:B:409:LEU:HB3	2.17	0.59
1:A:334:ARG:NH2	3:A:513:HOH:O	2.34	0.59
1:B:196:THR:HA	1:B:362:PHE:HB2	1.85	0.59
1:B:123:THR:HG22	1:B:125:VAL:H	1.67	0.59
1:A:73:ILE:HD11	1:B:18:LEU:HD12	1.84	0.59
1:B:254:SER:HB2	3:B:492:HOH:O	2.02	0.59
1:B:258:LYS:HG2	1:B:359:MET:CE	2.33	0.59
1:A:348:ARG:HB3	1:A:350:PHE:CE1	2.38	0.58
1:A:250:LEU:HB3	1:A:273:VAL:HG13	1.86	0.58
1:A:366:THR:HB	1:A:369:GLN:CD	2.28	0.58
1:B:40:TYR:CZ	1:B:326:MET:HA	2.38	0.58
1:B:338:VAL:HG21	1:B:354:ILE:HD11	1.86	0.58
1:A:340:THR:O	1:A:344:LYS:HB2	2.03	0.58
1:B:270:CYS:SG	1:B:287:MET:HE1	2.43	0.58
1:A:57:GLU:OE2	1:A:301:HIS:HE1	1.85	0.58
1:A:286:GLN:CD	1:B:12:ALA:HB2	2.28	0.58
1:B:334:ARG:HG3	1:B:353:ILE:HG22	1.86	0.57
1:A:211:LEU:HD22	1:A:215:LYS:HD3	1.85	0.57
1:B:323:LEU:HD12	1:B:326:MET:CE	2.34	0.57
1:A:158:TYR:CD1	1:A:173:LEU:CD2	2.88	0.57
1:A:336:LEU:HG	1:A:397:MET:HG2	1.85	0.57
1:B:24:PHE:CE2	1:B:32:LYS:HE3	2.39	0.57
1:B:100:ALA:O	1:B:101:ARG:HD2	2.03	0.57
1:B:129:ARG:HD2	1:B:134:TRP:NE1	2.18	0.57
1:B:156:ARG:HD3	3:B:439:HOH:O	2.04	0.57
1:B:107:GLY:HA3	1:B:266:ARG:HH12	1.67	0.57
1:B:333:MET:HE3	1:B:336:LEU:HD23	1.87	0.57
1:A:8:ASN:H	1:A:8:ASN:ND2	1.97	0.56
1:B:258:LYS:NZ	2:B:410:PLA:HB22	2.20	0.56
1:B:356:GLN:OE1	1:B:361:SER:HA	2.05	0.56
1:A:373:LEU:HA	1:A:377:PHE:HD2	1.71	0.56
1:A:337:PHE:O	1:A:341:LEU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:GLU:HG2	3:B:428:HOH:O	2.05	0.56
1:B:389:VAL:O	1:B:392:MET:HB2	2.05	0.56
1:A:159:ALA:HB3	1:A:172:ALA:O	2.06	0.56
1:A:338:VAL:HG21	1:A:354:ILE:HD11	1.88	0.56
1:A:361:SER:OG	1:A:387:VAL:HG23	2.06	0.55
1:A:370:VAL:HG21	1:A:383:ALA:HA	1.88	0.55
1:A:366:THR:HG22	1:A:369:GLN:N	2.20	0.55
1:B:321:GLN:HG3	3:B:430:HOH:O	2.06	0.55
1:A:134:TRP:CH2	1:A:179:GLU:HG2	2.41	0.55
1:B:187:LEU:CD1	1:B:220:LEU:HG	2.37	0.55
1:A:215:LYS:HG2	3:A:510:HOH:O	2.05	0.55
1:A:56:ALA:HB1	1:A:308:THR:HG21	1.89	0.55
1:B:160:TYR:O	1:B:168:LEU:HD23	2.07	0.55
1:B:24:PHE:CE1	1:B:34:ASN:HB2	2.42	0.54
1:B:40:TYR:CZ	1:B:326:MET:HG2	2.42	0.54
1:A:18:LEU:HD23	1:B:73:ILE:HD11	1.89	0.54
1:A:86:LEU:HD12	1:A:256:TYR:HE1	1.72	0.54
1:B:143:HIS:O	1:B:147:PHE:CD2	2.60	0.54
1:B:152:LEU:HD13	1:B:152:LEU:H	1.73	0.54
1:B:323:LEU:HA	1:B:326:MET:HE2	1.88	0.54
1:A:143:HIS:O	1:A:147:PHE:CD2	2.61	0.54
1:A:21:ALA:HB1	3:A:509:HOH:O	2.08	0.54
1:A:292:ARG:HD2	1:A:292:ARG:O	2.07	0.54
2:A:410:PLA:N	2:A:410:PLA:O3	2.40	0.53
1:A:125:VAL:HG11	1:A:185:VAL:HG23	1.90	0.53
1:A:266:ARG:HH22	2:A:410:PLA:P	2.30	0.53
1:B:165:ASN:HD21	1:B:167:THR:CG2	2.20	0.53
1:B:206:GLN:O	1:B:209:ALA:HB3	2.08	0.53
1:A:129:ARG:HH22	1:A:181:GLN:HG3	1.71	0.53
1:A:258:LYS:HD3	1:A:263:TYR:CE1	2.43	0.53
1:B:123:THR:HG21	1:B:125:VAL:HG13	1.86	0.53
1:B:370:VAL:HG21	1:B:383:ALA:HA	1.91	0.52
1:B:332:ARG:HB2	1:B:332:ARG:CZ	2.39	0.52
1:A:189:HIS:CD2	1:A:194:ASN:H	2.27	0.52
1:A:129:ARG:HE	1:A:134:TRP:HE1	1.58	0.52
1:B:291:ILE:HG23	1:B:295:TYR:CZ	2.45	0.52
1:B:86:LEU:HD12	1:B:256:TYR:HE1	1.73	0.52
1:A:122:ASN:CG	1:A:286:GLN:HG2	2.35	0.52
1:B:344:LYS:O	1:B:344:LYS:HD3	2.09	0.52
1:A:59:TYR:O	1:A:63:ASN:ND2	2.42	0.51
1:A:334:ARG:HD3	1:A:353:ILE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LEU:HD12	1:B:220:LEU:HG	1.91	0.51
1:A:9:ILE:CG2	1:B:122:ASN:HB3	2.40	0.51
1:A:195:PRO:HB3	1:A:386:ARG:HG3	1.91	0.51
1:B:237:ALA:HB3	1:B:241:ARG:HH21	1.75	0.51
1:B:8:ASN:HB3	3:B:461:HOH:O	2.10	0.51
1:B:29:ARG:HD2	3:B:414:HOH:O	2.10	0.51
1:B:392:MET:HE3	1:B:397:MET:HE1	1.92	0.51
1:A:73:ILE:HG21	1:A:288:LYS:HG2	1.92	0.51
1:B:5:MET:C	1:B:8:ASN:HD21	2.18	0.51
1:A:319:TRP:CZ2	1:A:323:LEU:HD22	2.46	0.51
1:B:15:ASP:CG	1:B:16:PRO:HD2	2.35	0.51
1:A:5:MET:N	1:A:7:GLU:OE1	2.44	0.51
1:A:106:PRO:HD2	1:A:295:TYR:CZ	2.46	0.51
1:A:403:ALA:O	1:A:404:ILE:C	2.54	0.51
1:B:316:ARG:HD2	1:B:320:GLU:OE2	2.11	0.51
1:B:258:LYS:HZ3	2:B:410:PLA:H4A2	1.73	0.51
1:B:355:LYS:HD3	1:B:355:LYS:C	2.36	0.50
1:B:37:ILE:O	1:B:388:ASN:ND2	2.44	0.50
1:B:102:THR:CG2	1:B:269:ALA:HB1	2.42	0.50
1:A:168:LEU:HB3	1:A:198:ILE:HG21	1.92	0.50
1:A:369:GLN:HG2	1:A:408:VAL:O	2.11	0.50
1:B:71:LEU:HB2	3:B:411:HOH:O	2.11	0.50
1:A:314:ALA:O	1:A:318:ILE:HG12	2.12	0.50
1:B:393:THR:HG22	1:B:396:ASN:H	1.76	0.50
1:B:36:GLY:HA3	3:B:511:HOH:O	2.10	0.50
1:B:229:ALA:O	1:B:236:ASP:OD1	2.30	0.50
1:A:53:VAL:O	1:A:57:GLU:HG3	2.11	0.50
1:B:123:THR:CG2	1:B:125:VAL:H	2.24	0.50
1:A:133:VAL:HG22	1:A:185:VAL:HB	1.94	0.49
1:B:158:TYR:HD1	1:B:173:LEU:HD22	1.77	0.49
1:B:79:PHE:CD2	1:B:104:GLN:HG3	2.47	0.49
1:A:334:ARG:NH2	1:A:358:GLY:O	2.45	0.49
1:A:398:ALA:N	1:A:399:PRO:HD2	2.26	0.49
1:B:123:THR:HG23	1:B:124:SER:N	2.27	0.49
1:B:200:PRO:HG2	1:B:205:TRP:CE2	2.47	0.49
1:B:277:SER:O	1:B:280:VAL:HG12	2.13	0.49
1:B:41:LYS:O	1:B:329:ARG:NH1	2.45	0.49
1:B:179:GLU:O	1:B:179:GLU:HG3	2.11	0.49
1:A:67:THR:OG1	1:B:47:THR:O	2.22	0.49
1:B:80:GLY:O	1:B:83:THR:HB	2.12	0.49
1:A:44:THR:OG1	1:A:46:LYS:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:PHE:CD2	1:B:240:LEU:HD12	2.47	0.49
1:B:212:SER:HG	1:B:247:HIS:CE1	2.31	0.48
1:A:139:SER:N	3:A:477:HOH:O	2.38	0.48
1:A:61:LEU:CD1	1:B:61:LEU:HD12	2.34	0.48
1:A:97:ASP:O	1:A:98:LYS:HB2	2.14	0.48
1:B:129:ARG:HB3	1:B:129:ARG:CZ	2.43	0.48
1:A:205:TRP:HE3	1:A:243:PHE:HE1	1.61	0.48
1:A:260:PHE:HB3	1:A:262:LEU:CD2	2.29	0.48
1:B:121:LYS:HD3	1:B:121:LYS:C	2.39	0.48
1:B:348:ARG:NH2	1:B:369:GLN:HE22	2.11	0.48
1:B:372:ARG:HG2	1:B:408:VAL:CG1	2.42	0.48
1:A:100:ALA:C	1:A:101:ARG:HG2	2.39	0.48
1:A:188:PHE:CE1	1:A:208:LEU:HD13	2.49	0.48
1:B:393:THR:CG2	1:B:395:ASP:H	2.27	0.48
1:A:231:GLY:O	1:A:236:ASP:HB2	2.13	0.47
1:A:312:ASN:OD1	1:A:315:LEU:HB2	2.14	0.47
1:A:350:PHE:HB3	1:A:353:ILE:CD1	2.42	0.47
1:B:78:GLU:CD	1:B:78:GLU:H	2.22	0.47
1:B:229:ALA:HB2	1:B:357:ASN:HB3	1.95	0.47
1:A:366:THR:HB	1:A:369:GLN:OE1	2.14	0.47
1:B:5:MET:N	1:B:7:GLU:OE1	2.47	0.47
1:A:144:LYS:HG2	1:A:155:VAL:HG21	1.96	0.47
1:A:362:PHE:HE1	1:A:384:SER:HB2	1.79	0.47
1:A:258:LYS:HD3	1:A:263:TYR:HE1	1.78	0.47
1:B:29:ARG:HB3	1:B:30:PRO:HD2	1.96	0.47
1:A:222:ASP:OD2	2:A:410:PLA:N1	2.48	0.47
1:A:291:ILE:HG23	1:A:295:TYR:CZ	2.50	0.47
1:B:272:LEU:HD12	1:B:287:MET:SD	2.55	0.47
1:B:276:ASP:O	1:B:280:VAL:HG12	2.15	0.47
1:B:362:PHE:HD1	1:B:362:PHE:HA	1.62	0.47
1:B:270:CYS:SG	1:B:287:MET:CE	3.03	0.47
1:A:93:ALA:O	1:A:97:ASP:HB2	2.15	0.47
1:A:359:MET:N	3:A:465:HOH:O	2.41	0.47
1:B:120:ALA:O	1:B:121:LYS:HB2	2.15	0.47
1:A:104:GLN:NE2	3:A:495:HOH:O	2.43	0.46
1:B:133:VAL:CB	1:B:185:VAL:HG22	2.43	0.46
1:B:372:ARG:CZ	1:B:408:VAL:HG12	2.46	0.46
1:B:133:VAL:HA	1:B:185:VAL:O	2.15	0.46
1:B:335:GLN:O	1:B:338:VAL:HG22	2.16	0.46
1:B:372:ARG:HG2	1:B:408:VAL:HG11	1.98	0.46
1:B:401:CYS:O	1:B:405:VAL:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:GLY:O	1:A:306:VAL:HG23	2.15	0.46
1:A:20:LEU:HA	1:A:20:LEU:HD23	1.67	0.45
1:B:229:ALA:O	1:B:230:ARG:HB2	2.16	0.45
1:B:340:THR:O	1:B:344:LYS:HB2	2.16	0.45
1:B:79:PHE:CE2	1:B:104:GLN:HG3	2.51	0.45
1:B:370:VAL:O	1:B:370:VAL:HG23	2.16	0.45
1:B:266:ARG:NH2	2:B:410:PLA:O1P	2.45	0.45
1:B:137:ASN:HD22	1:B:138:PRO:HA	1.81	0.45
1:B:192:CYS:SG	1:B:229:ALA:HB2	2.57	0.45
1:B:338:VAL:CG1	1:B:354:ILE:HD11	2.45	0.45
1:A:68:LYS:HB2	3:B:424:HOH:O	2.16	0.45
1:B:209:ALA:HB3	1:B:246:MET:HE3	1.98	0.45
1:B:323:LEU:HA	1:B:326:MET:HE3	1.98	0.45
1:A:35:LEU:HD11	1:A:400:LEU:HD13	1.99	0.45
1:A:137:ASN:O	1:A:160:TYR:HB3	2.17	0.45
1:B:115:ALA:O	1:B:118:PHE:HB3	2.17	0.45
1:B:373:LEU:HD12	1:B:373:LEU:HA	1.71	0.45
1:B:237:ALA:HB3	1:B:241:ARG:HE	1.82	0.45
1:A:158:TYR:HD1	1:A:173:LEU:CD2	2.30	0.44
1:A:372:ARG:O	1:A:376:GLU:HB2	2.16	0.44
1:A:338:VAL:HG21	1:A:354:ILE:CD1	2.47	0.44
1:A:373:LEU:HD23	1:A:377:PHE:CD2	2.52	0.44
1:A:377:PHE:HE2	1:A:408:VAL:CG1	2.30	0.44
1:B:43:GLU:CD	1:B:43:GLU:H	2.25	0.44
1:B:40:TYR:CG	1:B:41:LYS:N	2.85	0.44
1:A:24:PHE:CZ	1:A:34:ASN:HB2	2.51	0.44
1:A:41:LYS:O	1:A:329:ARG:NH1	2.49	0.44
1:A:61:LEU:O	1:B:54:LYS:NZ	2.49	0.44
1:B:123:THR:CG2	1:B:124:SER:N	2.80	0.44
1:B:190:GLY:HA2	1:B:221:PHE:CE1	2.53	0.44
1:B:373:LEU:HG	1:B:379:VAL:HB	1.99	0.44
1:A:220:LEU:HD11	1:A:251:ILE:HG21	2.00	0.44
1:A:305:VAL:O	1:A:308:THR:HB	2.17	0.44
1:B:113:ARG:O	1:B:116:ALA:HB3	2.17	0.44
1:B:119:LEU:O	1:B:123:THR:HB	2.18	0.44
1:B:314:ALA:O	1:B:317:ALA:HB3	2.17	0.44
1:B:133:VAL:O	1:B:155:VAL:HA	2.17	0.44
1:A:27:ASP:O	1:A:32:LYS:NZ	2.38	0.44
1:A:334:ARG:NH1	3:A:513:HOH:O	2.51	0.44
1:A:118:PHE:CE1	1:A:119:LEU:HD23	2.53	0.44
1:B:237:ALA:CB	1:B:241:ARG:HE	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:HH22	1:A:369:GLN:HE22	1.66	0.43
1:B:348:ARG:HH22	1:B:369:GLN:HE22	1.65	0.43
1:B:41:LYS:HG2	1:B:45:GLY:HA2	2.00	0.43
1:B:158:TYR:CD1	1:B:173:LEU:HD22	2.53	0.43
1:A:76:ILE:HA	1:A:77:PRO:HD3	1.89	0.43
1:A:397:MET:HG3	1:A:397:MET:O	2.18	0.43
1:A:109:THR:O	1:B:294:ASN:O	2.37	0.43
1:B:337:PHE:HB2	1:B:392:MET:HE1	2.00	0.43
1:A:126:LYS:HD2	1:A:126:LYS:HA	1.69	0.43
1:B:20:LEU:O	1:B:21:ALA:C	2.61	0.43
1:B:39:VAL:HG23	1:B:263:TYR:CE1	2.54	0.43
1:B:42:ASP:HB2	1:B:43:GLU:OE2	2.18	0.43
1:A:34:ASN:HA	1:A:380:TYR:HB2	2.01	0.43
1:B:53:VAL:HG21	3:B:443:HOH:O	2.18	0.43
1:A:350:PHE:HZ	1:A:409:LEU:HD21	1.83	0.42
1:B:229:ALA:CB	1:B:357:ASN:HB3	2.49	0.42
1:A:113:ARG:O	1:A:113:ARG:HG3	2.18	0.42
1:A:308:THR:HG22	1:A:309:ILE:N	2.33	0.42
1:B:101:ARG:NH2	1:B:281:ASP:OD1	2.53	0.42
1:A:46:LYS:C	1:A:48:PRO:HD3	2.44	0.42
1:B:5:MET:HB2	1:B:5:MET:HE2	1.51	0.42
1:B:292:ARG:O	1:B:292:ARG:HG3	2.19	0.42
1:B:324:THR:HG22	1:B:324:THR:O	2.18	0.42
1:B:354:ILE:O	1:B:354:ILE:HG22	2.19	0.42
1:B:372:ARG:NH2	1:B:407:ALA:O	2.53	0.42
1:B:389:VAL:C	1:B:391:GLY:H	2.28	0.42
1:A:35:LEU:HD11	1:A:400:LEU:CD1	2.50	0.42
1:A:202:LEU:O	1:A:203:GLU:C	2.61	0.42
1:A:202:LEU:HD22	1:A:206:GLN:NE2	2.35	0.42
1:A:223:PHE:HD1	1:A:223:PHE:HA	1.73	0.42
1:B:6:PHE:HD1	1:B:9:ILE:HD11	1.84	0.42
1:B:30:PRO:HG2	1:B:31:GLY:H	1.84	0.42
1:B:240:LEU:HD23	1:B:240:LEU:O	2.20	0.42
1:B:348:ARG:O	1:B:350:PHE:CD1	2.72	0.42
1:B:152:LEU:HD13	1:B:152:LEU:N	2.35	0.42
1:A:344:LYS:HD2	1:A:344:LYS:HA	1.86	0.42
1:A:389:VAL:C	1:A:391:GLY:H	2.28	0.42
1:B:195:PRO:HB3	1:B:386:ARG:CG	2.48	0.42
1:A:6:PHE:C	1:A:9:ILE:HG13	2.44	0.42
1:A:24:PHE:CD1	1:A:34:ASN:HB2	2.54	0.42
1:A:256:TYR:HB2	1:A:267:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:THR:OG1	1:A:68:LYS:N	2.54	0.41
1:A:9:ILE:HG23	1:B:122:ASN:HB3	2.00	0.41
1:A:109:THR:O	1:A:109:THR:CG2	2.67	0.41
1:A:119:LEU:C	1:A:121:LYS:H	2.27	0.41
1:A:373:LEU:HA	1:A:373:LEU:HD23	1.80	0.41
1:B:112:LEU:HB3	1:B:146:VAL:HG21	2.02	0.41
1:A:305:VAL:HG12	1:A:306:VAL:N	2.32	0.41
1:B:341:LEU:HD12	1:B:405:VAL:HG23	2.02	0.41
1:A:49:VAL:O	1:A:50:LEU:C	2.62	0.41
1:B:123:THR:HG23	1:B:125:VAL:HG13	1.93	0.41
1:B:392:MET:HG2	1:B:400:LEU:CD2	2.50	0.41
1:A:133:VAL:O	1:A:155:VAL:HA	2.21	0.41
1:A:264:ASN:HB2	1:B:71:LEU:HG	2.02	0.41
1:B:6:PHE:HA	1:B:9:ILE:HG13	2.02	0.41
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.83	0.41
1:A:5:MET:HE2	1:B:123:THR:HG23	2.03	0.41
1:A:272:LEU:HD12	1:A:287:MET:SD	2.61	0.41
1:B:225:TYR:OH	2:B:410:PLA:HB23	2.21	0.41
1:B:338:VAL:CG2	1:B:339:ASN:N	2.84	0.41
1:B:393:THR:HG23	1:B:395:ASP:H	1.85	0.41
1:B:260:PHE:CD2	1:B:306:VAL:HG22	2.56	0.41
1:B:359:MET:HB3	1:B:388:ASN:OD1	2.21	0.41
1:B:383:ALA:HB2	3:B:467:HOH:O	2.21	0.40
1:A:205:TRP:HE3	1:A:243:PHE:CE1	2.39	0.40
1:B:209:ALA:O	1:B:213:VAL:CG2	2.62	0.40
1:B:280:VAL:HG13	1:B:281:ASP:N	2.35	0.40
1:B:225:TYR:HE1	1:B:359:MET:HE3	1.85	0.40
1:A:18:LEU:HD13	1:B:292:ARG:NH2	2.36	0.40
1:A:30:PRO:HG2	1:A:31:GLY:H	1.86	0.40
1:A:39:VAL:HG23	1:A:263:TYR:CE1	2.57	0.40
1:A:301:HIS:O	1:A:304:SER:HB2	2.21	0.40
1:B:161:TYR:CE2	1:B:362:PHE:HD2	2.39	0.40
1:B:301:HIS:HB3	1:B:302:GLY:H	1.78	0.40
1:B:312:ASN:OD1	1:B:315:LEU:HG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	394/396 (100%)	345 (88%)	37 (9%)	12 (3%)	3	6
1	B	394/396 (100%)	335 (85%)	44 (11%)	15 (4%)	2	3
All	All	788/792 (100%)	680 (86%)	81 (10%)	27 (3%)	3	4

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	92	SER
1	B	136	SER
1	B	152	LEU
1	B	301	HIS
1	A	36	GLY
1	A	50	LEU
1	A	121	LYS
1	A	301	HIS
1	B	26	ALA
1	B	30	PRO
1	B	121	LYS
1	B	390	ALA
1	A	141	PRO
1	A	215	LYS
1	A	338	VAL
1	A	378	GLY
1	B	36	GLY
1	B	37	ILE
1	B	43	GLU
1	B	70	TYR
1	B	141	PRO
1	A	43	GLU
1	A	201	THR
1	B	90	LYS
1	A	404	ILE

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Mol	Chain	Res	Type
1	B	195	PRO
1	A	195	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/320 (100%)	241 (75%)	79 (25%)	1	1
1	B	320/320 (100%)	236 (74%)	84 (26%)	0	1
All	All	640/640 (100%)	477 (74%)	163 (26%)	0	1

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	8	ASN
1	A	9	ILE
1	A	23	LEU
1	A	28	GLU
1	A	29	ARG
1	A	39	VAL
1	A	41	LYS
1	A	43	GLU
1	A	44	THR
1	A	46	LYS
1	A	61	LEU
1	A	62	GLU
1	A	64	GLU
1	A	73	ILE
1	A	86	LEU
1	A	87	LEU
1	A	90	LYS
1	A	96	ASN
1	A	98	LYS
1	A	104	GLN

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Mol	Chain	Res	Type
1	A	112	LEU
1	A	114	VAL
1	A	118	PHE
1	A	121	LYS
1	A	124	SER
1	A	144	LYS
1	A	152	LEU
1	A	154	GLU
1	A	155	VAL
1	A	165	ASN
1	A	168	LEU
1	A	174	ILE
1	A	179	GLU
1	A	206	GLN
1	A	207	THR
1	A	211	LEU
1	A	215	LYS
1	A	218	LEU
1	A	223	PHE
1	A	240	LEU
1	A	246	MET
1	A	250	LEU
1	A	258	LYS
1	A	259	ASN
1	A	262	LEU
1	A	267	VAL
1	A	273	VAL
1	A	280	VAL
1	A	282	ARG
1	A	286	GLN
1	A	292	ARG
1	A	296	SER
1	A	297	ASN
1	A	308	THR
1	A	313	ASP
1	A	316	ARG
1	A	326	MET
1	A	329	ARG
1	A	332	ARG
1	A	341	LEU
1	A	342	GLN
1	A	343	GLU

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Mol	Chain	Res	Type
1	A	347	ASN
1	A	348	ARG
1	A	353	ILE
1	A	360	PHE
1	A	362	PHE
1	A	365	LEU
1	A	366	THR
1	A	367	LYS
1	A	370	VAL
1	A	371	LEU
1	A	372	ARG
1	A	374	ARG
1	A	375	GLU
1	A	376	GLU
1	A	384	SER
1	A	387	VAL
1	B	5	MET
1	B	8	ASN
1	B	9	ILE
1	B	10	THR
1	B	23	LEU
1	B	28	GLU
1	B	41	LYS
1	B	43	GLU
1	B	52	SER
1	B	55	LYS
1	B	60	LEU
1	B	61	LEU
1	B	67	THR
1	B	73	ILE
1	B	78	GLU
1	B	81	ARG
1	B	84	GLN
1	B	86	LEU
1	B	87	LEU
1	B	90	LYS
1	B	98	LYS
1	B	109	THR
1	B	112	LEU
1	B	114	VAL
1	B	119	LEU
1	B	121	LYS

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Mol	Chain	Res	Type
1	B	123	THR
1	B	125	VAL
1	B	129	ARG
1	B	133	VAL
1	B	144	LYS
1	B	146	VAL
1	B	152	LEU
1	B	155	VAL
1	B	156	ARG
1	B	165	ASN
1	B	168	LEU
1	B	173	LEU
1	B	174	ILE
1	B	179	GLU
1	B	185	VAL
1	B	210	GLN
1	B	213	VAL
1	B	215	LYS
1	B	223	PHE
1	B	233	LEU
1	B	234	GLU
1	B	235	GLU
1	B	238	GLU
1	B	240	LEU
1	B	246	MET
1	B	254	SER
1	B	259	ASN
1	B	262	LEU
1	B	266	ARG
1	B	267	VAL
1	B	273	VAL
1	B	277	SER
1	B	278	GLU
1	B	297	ASN
1	B	304	SER
1	B	311	SER
1	B	313	ASP
1	B	316	ARG
1	B	329	ARG
1	B	333	MET
1	B	334	ARG
1	B	338	VAL

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Mol	Chain	Res	Type
1	B	341	LEU
1	B	343	GLU
1	B	344	LYS
1	B	347	ASN
1	B	348	ARG
1	B	349	ASP
1	B	353	ILE
1	B	355	LYS
1	B	362	PHE
1	B	368	GLU
1	B	370	VAL
1	B	371	LEU
1	B	372	ARG
1	B	373	LEU
1	B	384	SER
1	B	393	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	58	GLN
1	A	63	ASN
1	A	104	GLN
1	A	137	ASN
1	A	181	GLN
1	A	189	HIS
1	A	226	GLN
1	A	247	HIS
1	A	259	ASN
1	A	301	HIS
1	A	331	GLN
1	A	339	ASN
1	A	357	ASN
1	B	8	ASN
1	B	69	ASN
1	B	104	GLN
1	B	137	ASN
1	B	165	ASN
1	B	226	GLN
1	B	259	ASN
1	B	294	ASN

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Mol	Chain	Res	Type
1	B	301	HIS
1	B	331	GLN
1	B	339	ASN
1	B	342	GLN
1	B	357	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	PLA	B	410	-	25,25,25	2.04	4 (16%)	34,37,37	2.74	14 (41%)
2	PLA	A	410	-	25,25,25	1.86	3 (12%)	34,37,37	2.89	15 (44%)

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	PLA	B	410	-	-	8/23/23/23	0/1/1/1
2	PLA	A	410	-	-	9/23/23/23	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	410	PLA	C4A-C4	-5.92	1.43	1.52
2	A	410	PLA	C4A-C4	-5.14	1.44	1.52
2	A	410	PLA	CB1-CA	-4.57	1.50	1.55
2	B	410	PLA	CB1-CA	-4.43	1.50	1.55
2	B	410	PLA	C3-C4	-4.02	1.34	1.40
2	A	410	PLA	C3-C4	-2.73	1.36	1.40
2	B	410	PLA	C5-C4	2.37	1.43	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	410	PLA	C4A-C4-C5	6.46	126.78	119.75
2	A	410	PLA	C2A-C2-C3	5.81	127.59	120.80
2	B	410	PLA	C2A-C2-C3	5.78	127.56	120.80
2	A	410	PLA	C4A-C4-C5	5.47	125.71	119.75
2	B	410	PLA	O2P-P-O4P	5.04	119.80	106.67
2	A	410	PLA	O2P-P-O4P	4.98	119.65	106.67
2	A	410	PLA	C6-C5-C4	4.90	121.77	118.06
2	A	410	PLA	CB2-CA-CB1	-4.84	104.00	110.76
2	B	410	PLA	C3-C2-N1	-4.65	115.09	120.96
2	A	410	PLA	O4P-C5A-C5	4.64	118.05	109.36
2	A	410	PLA	C3-C2-N1	-4.62	115.14	120.96
2	B	410	PLA	C5-C6-N1	-4.41	116.65	123.83
2	B	410	PLA	C4A-C4-C3	-4.27	114.31	119.98
2	A	410	PLA	C5-C6-N1	-4.26	116.91	123.83
2	A	410	PLA	O3P-P-O1P	4.25	127.40	110.83
2	B	410	PLA	C6-N1-C2	4.12	126.67	119.20
2	A	410	PLA	C6-N1-C2	4.05	126.55	119.20
2	B	410	PLA	C6-C5-C4	4.01	121.09	118.06
2	B	410	PLA	O3P-P-O1P	3.81	125.66	110.83
2	A	410	PLA	O4P-P-O1P	-2.99	98.35	106.44
2	B	410	PLA	CB2-CA-CB1	2.82	114.71	110.76
2	B	410	PLA	O-C-CA	-2.54	118.23	122.78
2	A	410	PLA	C-CA-N	2.31	113.93	107.83
2	A	410	PLA	C5A-C5-C6	-2.30	115.62	119.36
2	B	410	PLA	O3P-P-O4P	-2.19	100.96	106.67
2	A	410	PLA	C3-C4-C5	-2.17	116.77	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	410	PLA	C4A-C4-C3	-2.14	117.14	119.98
2	B	410	PLA	CA-CB1-CG	-2.11	109.01	113.22
2	B	410	PLA	O4P-P-O1P	-2.02	100.99	106.44

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	410	PLA	C4-C5-C5A-O4P
2	A	410	PLA	C6-C5-C5A-O4P
2	A	410	PLA	O-C-CA-CB1
2	B	410	PLA	C4-C5-C5A-O4P
2	B	410	PLA	C6-C5-C5A-O4P
2	B	410	PLA	O-C-CA-CB1
2	B	410	PLA	OXT-C-CA-CB1
2	A	410	PLA	C5-C4-C4A-N
2	B	410	PLA	C5-C4-C4A-N
2	A	410	PLA	C5A-O4P-P-O1P
2	B	410	PLA	C5A-O4P-P-O1P
2	A	410	PLA	C3-C4-C4A-N
2	B	410	PLA	C3-C4-C4A-N
2	A	410	PLA	OXT-C-CA-CB1
2	B	410	PLA	C5A-O4P-P-O2P
2	A	410	PLA	CB2-CA-N-C4A
2	A	410	PLA	C5A-O4P-P-O2P

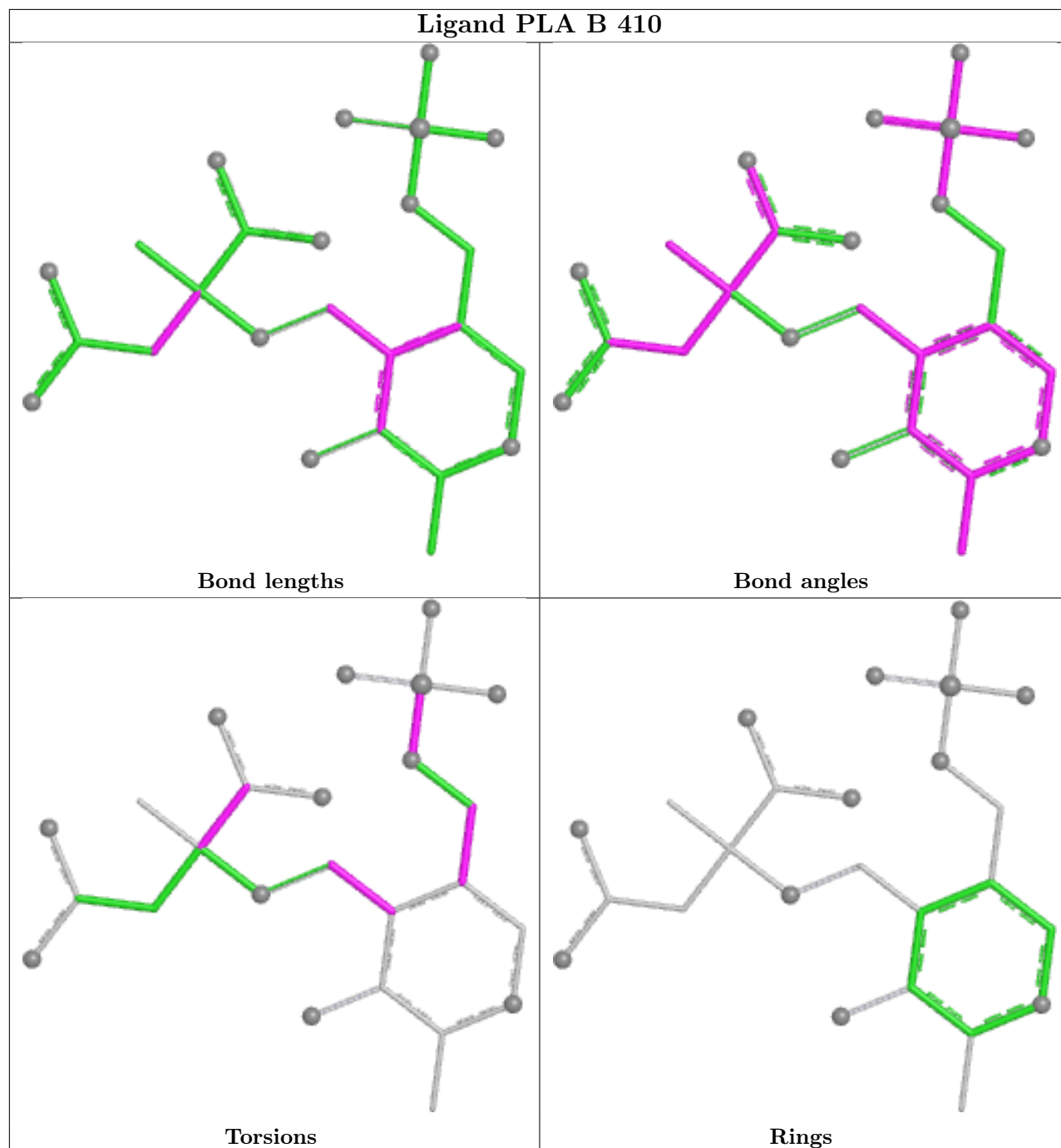
There are no ring outliers.

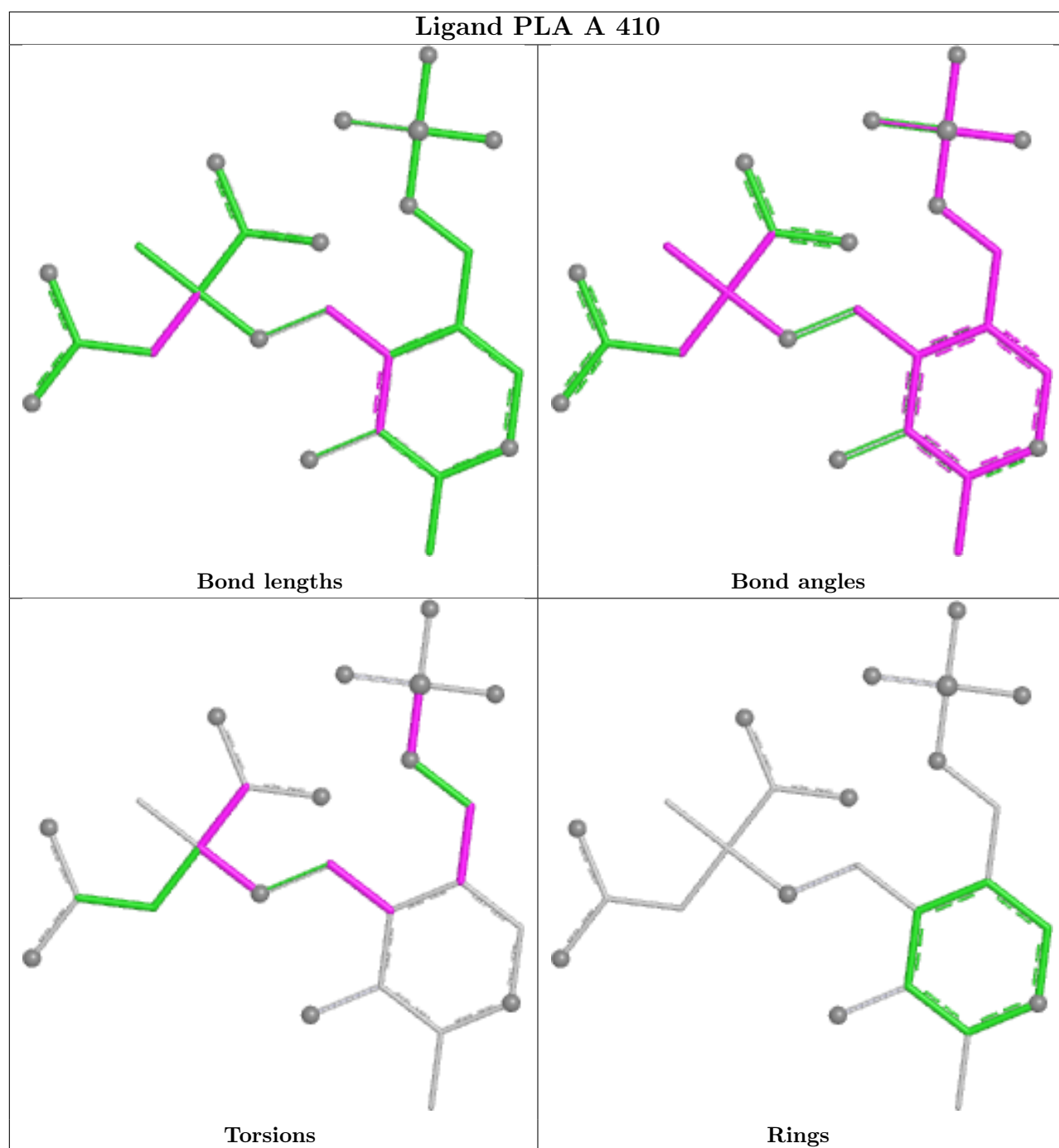
2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	410	PLA	9	0
2	A	410	PLA	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 [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	396/396 (100%)	-1.92	0 100 100	8, 30, 67, 86	0
1	B	396/396 (100%)	-1.92	0 100 100	4, 31, 67, 81	0
All	All	792/792 (100%)	-1.92	0 100 100	4, 31, 67, 86	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

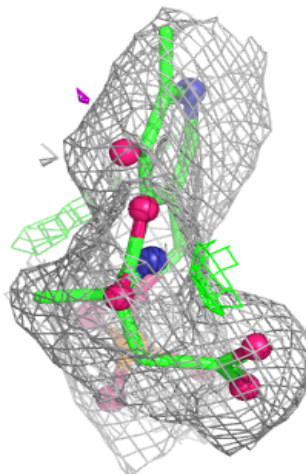
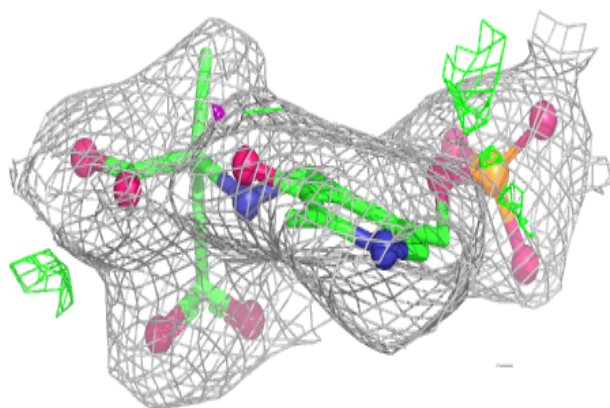
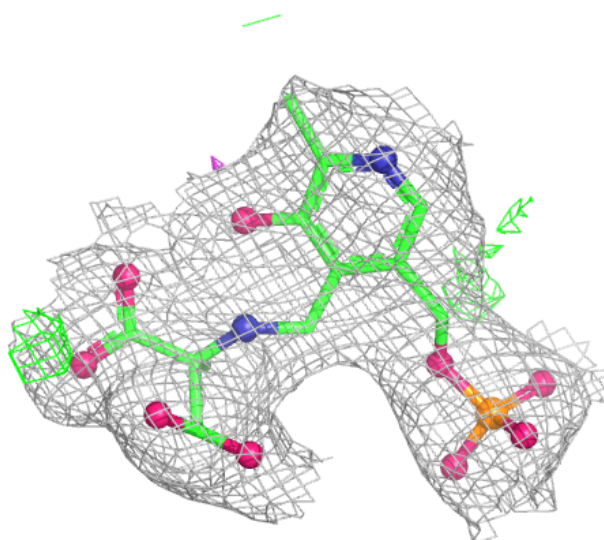
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

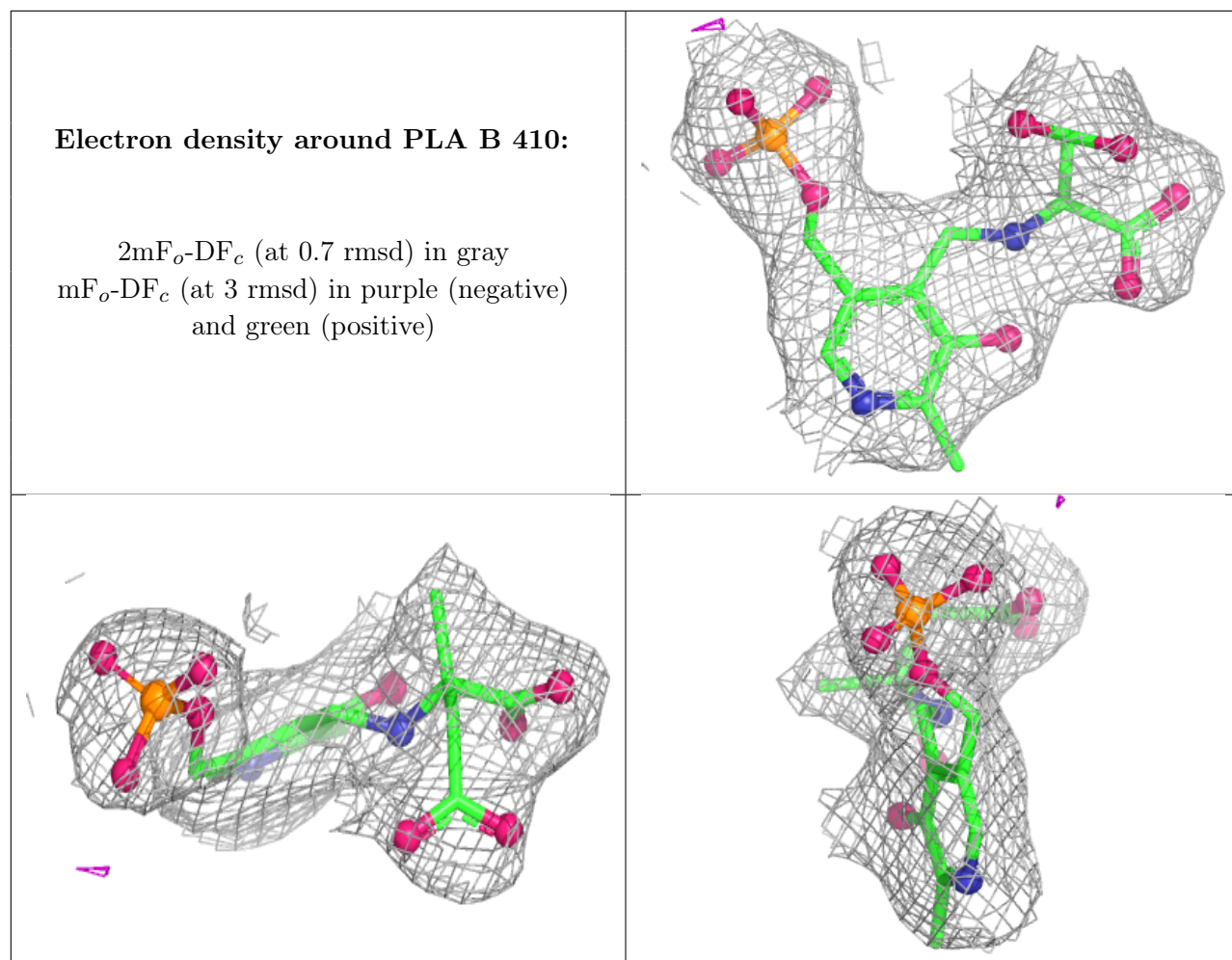
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PLA	A	410	25/25	1.00	0.02	7,22,40,49	0
2	PLA	B	410	25/25	1.00	0.01	9,20,48,76	0

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 PLA A 410:

$2mF_o-DF_c$ (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.