



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:36 AM UTC

PDB ID : 3PYB / pdb_00003pyb
Title : Crystal structure of ent-copalyl diphosphate synthase from *Arabidopsis thaliana* in complex with 13-aza-13,14-dihydrocopalyl diphosphate
Authors : Koksai, M.; Christianson, D.W.
Deposited on : 2010-12-12
Resolution : 2.76 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

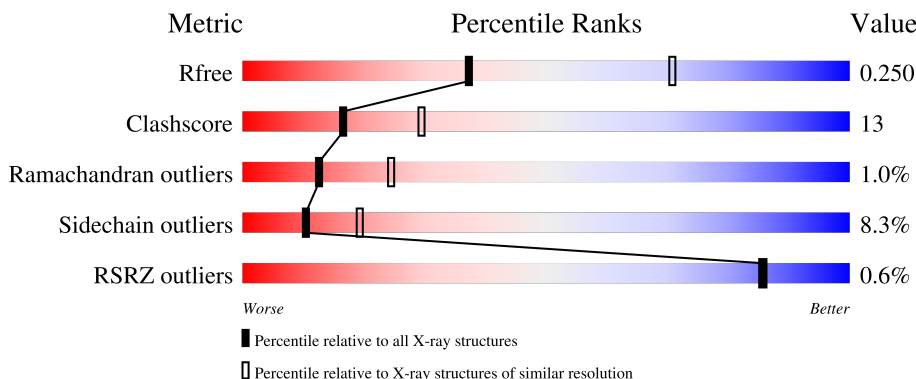
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	727	
1	B	727	
1	C	727	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17263 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 Ent-copalyl diphosphate synthase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	685	Total	C	N	O	S	0	4	0
			5633	3618	948	1038	29			
1	B	689	Total	C	N	O	S	0	1	0
			5649	3622	952	1046	29			
1	C	685	Total	C	N	O	S	0	0	0
			5607	3598	943	1037	29			

There are 27 discrepancies between the modelled and reference sequences:

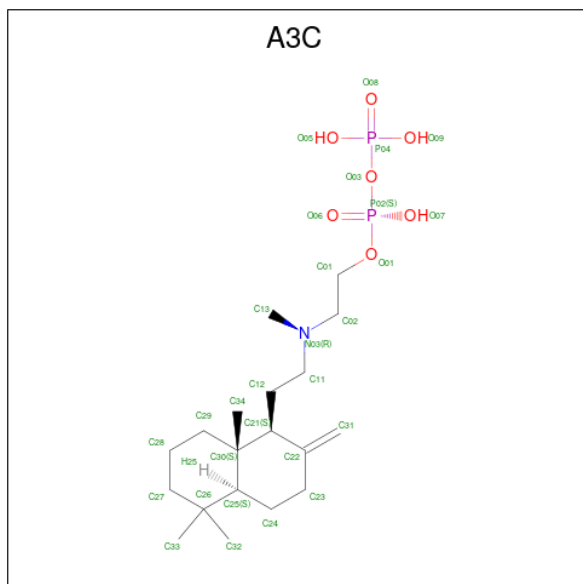
Chain	Residue	Modelled	Actual	Comment	Reference
A	84	MET	-	expression tag	UNP Q38802
A	803	GLY	-	expression tag	UNP Q38802
A	804	SER	-	expression tag	UNP Q38802
A	805	HIS	-	expression tag	UNP Q38802
A	806	HIS	-	expression tag	UNP Q38802
A	807	HIS	-	expression tag	UNP Q38802
A	808	HIS	-	expression tag	UNP Q38802
A	809	HIS	-	expression tag	UNP Q38802
A	810	HIS	-	expression tag	UNP Q38802
B	84	MET	-	expression tag	UNP Q38802
B	803	GLY	-	expression tag	UNP Q38802
B	804	SER	-	expression tag	UNP Q38802
B	805	HIS	-	expression tag	UNP Q38802
B	806	HIS	-	expression tag	UNP Q38802
B	807	HIS	-	expression tag	UNP Q38802
B	808	HIS	-	expression tag	UNP Q38802
B	809	HIS	-	expression tag	UNP Q38802
B	810	HIS	-	expression tag	UNP Q38802
C	84	MET	-	expression tag	UNP Q38802
C	803	GLY	-	expression tag	UNP Q38802
C	804	SER	-	expression tag	UNP Q38802
C	805	HIS	-	expression tag	UNP Q38802
C	806	HIS	-	expression tag	UNP Q38802

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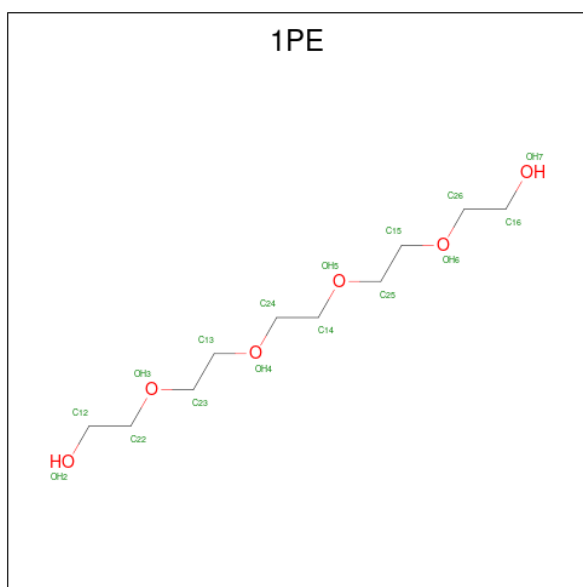
Chain	Residue	Modelled	Actual	Comment	Reference
C	807	HIS	-	expression tag	UNP Q38802
C	808	HIS	-	expression tag	UNP Q38802
C	809	HIS	-	expression tag	UNP Q38802
C	810	HIS	-	expression tag	UNP Q38802

- Molecule 2 is 2-(methyl{2-[(1S,4aS,8aS)-5,5,8a-trimethyl-2-methylidenedecahydronaphthalen-1-yl]ethyl}amino)ethyl trihydrogen diphosphate (CCD ID: A3C) (formula: C₁₉H₃₇NO₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	19	1	7	2		

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	A	1	Total	C	O	0	0
			16	10	6		
3	A	1	Total	C	O	0	0
			16	10	6		
3	A	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	0
			16	10	6		

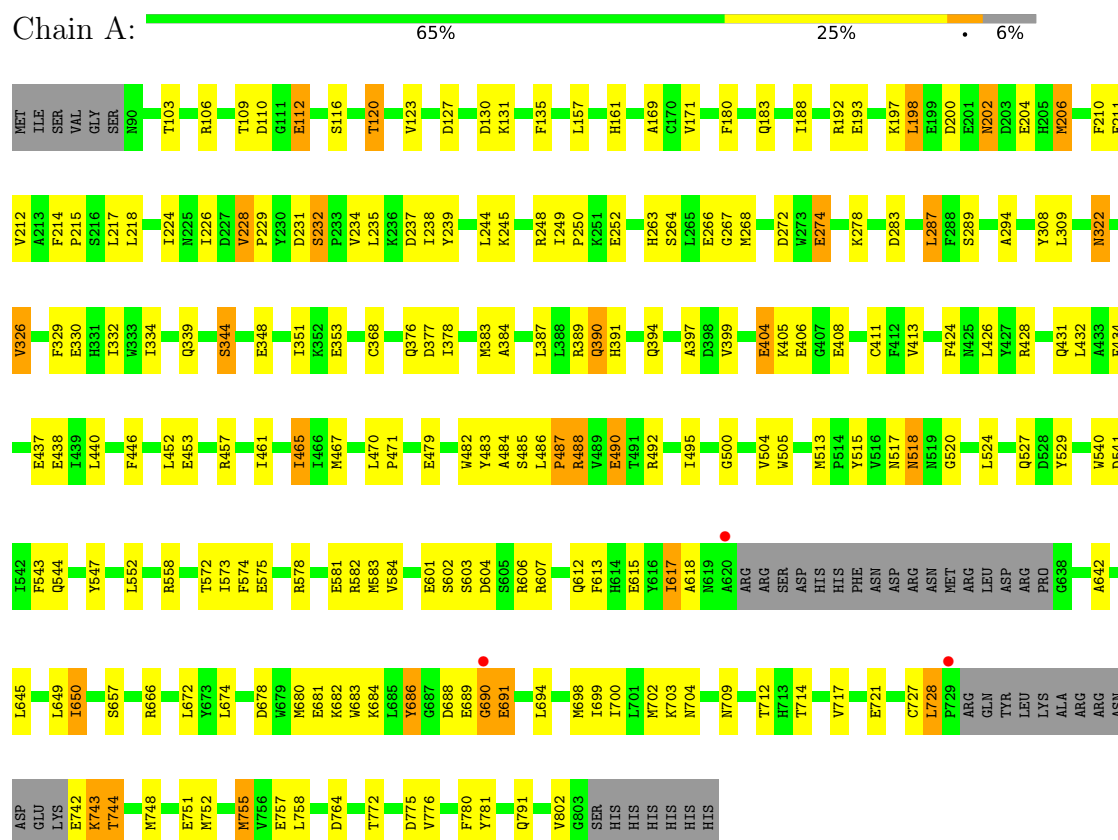
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	84	Total	O	0	0
			84	84		
4	B	68	Total	O	0	0
			68	68		
4	C	49	Total	O	0	0
			49	49		

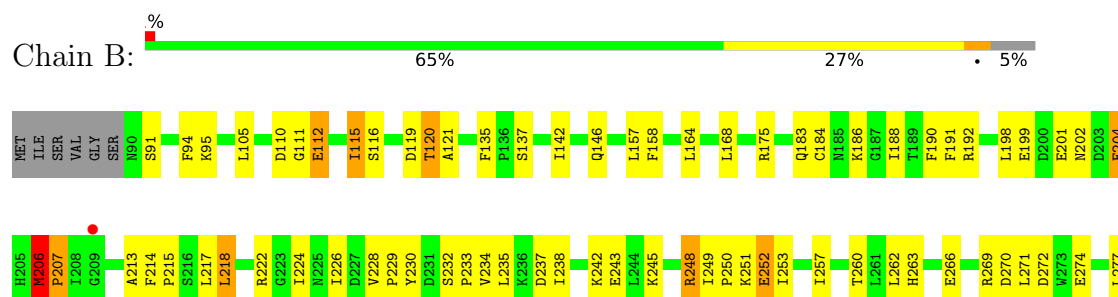
3 Residue-property plots

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: Ent-copalyl diphosphate synthase, chloroplastic



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.74Å 188.55Å 229.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.52 – 2.76 44.52 – 2.76	Depositor EDS
% Data completeness (in resolution range)	86.1 (44.52-2.76) 86.1 (44.52-2.76)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.177 , 0.257 0.170 , 0.250	Depositor DCC
R_{free} test set	2000 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.741	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17263	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: A3C, 1PE

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	0.36	0/5785	0.73	3/7817 (0.0%)
1	B	0.34	0/5790	0.72	4/7823 (0.1%)
1	C	0.32	0/5745	0.73	7/7764 (0.1%)
All	All	0.34	0/17320	0.73	14/23404 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	MET	CA-C-N	6.20	127.59	119.84
1	B	206	MET	C-N-CA	6.20	127.59	119.84
1	C	546	TRP	N-CA-C	-6.16	106.74	114.56
1	C	616	TYR	N-CA-C	-6.14	106.12	113.97
1	C	747	SER	N-CA-C	-5.97	107.82	114.62
1	A	743	LYS	N-CA-C	-5.82	106.34	113.50
1	C	206	MET	CA-C-N	5.57	125.88	119.92
1	C	206	MET	C-N-CA	5.57	125.88	119.92
1	B	135	PHE	CA-C-N	5.29	125.60	119.47
1	B	135	PHE	C-N-CA	5.29	125.60	119.47
1	A	180	PHE	CA-C-N	5.25	124.57	118.85
1	A	180	PHE	C-N-CA	5.25	124.57	118.85
1	C	135	PHE	CA-C-N	5.05	124.66	119.05
1	C	135	PHE	C-N-CA	5.05	124.66	119.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5633	0	5486	140	0
1	B	5649	0	5494	148	0
1	C	5607	0	5452	143	0
2	A	29	0	34	6	0
3	A	64	0	88	2	0
3	B	48	0	66	2	0
3	C	32	0	44	4	0
4	A	84	0	0	0	0
4	B	68	0	0	0	0
4	C	49	0	0	1	0
All	All	17263	0	16664	436	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 13.

All (436) 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:C:163:ARG:HG2	1:C:163:ARG:HH11	1.23	1.04
1:C:431:GLN:HE22	1:C:482:TRP:H	1.10	0.98
1:B:728:LEU:HB3	1:B:729:PRO:HD2	1.44	0.97
1:C:453:GLU:HB3	1:C:457:ARG:HH12	1.27	0.94
1:A:431:GLN:HE22	1:A:482:TRP:H	1.17	0.90
1:B:215:PRO:HB2	1:B:242:LYS:HD2	1.54	0.88
1:B:504:VAL:HG22	1:B:512:ARG:HH12	1.38	0.88
1:C:163:ARG:HH11	1:C:163:ARG:CG	1.88	0.86
1:C:431:GLN:NE2	1:C:482:TRP:H	1.71	0.86
1:A:206:MET:HE3	1:A:210:PHE:HB3	1.58	0.85
1:A:431:GLN:NE2	1:A:482:TRP:H	1.81	0.79
1:A:686:TYR:HD2	1:A:689:GLU:HG3	1.48	0.78
1:B:518:ASN:ND2	1:B:520:GLY:H	1.81	0.77
1:C:253:ILE:HG23	1:C:257:ILE:HD11	1.66	0.77
1:C:452:LEU:O	1:C:456:GLU:HG2	1.84	0.77
1:A:601:GLU:HG2	1:A:602:SER:H	1.49	0.76
1:A:103:THR:HG22	1:A:106[A]:ARG:HH22	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:THR:HG22	1:B:320:VAL:H	1.52	0.74
1:B:728:LEU:HB3	1:B:729:PRO:CD	2.17	0.73
1:C:698:MET:HA	1:C:698:MET:HE2	1.69	0.73
1:C:562:LEU:HD12	1:C:590:VAL:HG21	1.71	0.72
1:C:453:GLU:HB3	1:C:457:ARG:NH1	2.05	0.71
1:A:112:GLU:HG3	1:A:515:TYR:CE1	2.25	0.71
1:C:215:PRO:HB2	1:C:242:LYS:HD2	1.71	0.71
1:C:195:ILE:HD11	1:C:235:LEU:HD21	1.71	0.71
1:A:272:ASP:OD1	1:A:274:GLU:HB3	1.92	0.70
1:C:169:ALA:HB2	1:C:217:LEU:HD21	1.74	0.70
1:A:206:MET:HE1	1:A:211:GLU:HG3	1.73	0.70
1:A:518:ASN:ND2	1:A:520:GLY:H	1.90	0.69
1:A:518:ASN:HD22	1:A:520:GLY:N	1.89	0.69
2:A:901:A3C:H31	2:A:901:A3C:H11	1.73	0.68
1:B:683:TRP:HD1	1:B:688:ASP:HA	1.58	0.68
1:C:112:GLU:HG3	1:C:515:TYR:CE1	2.28	0.68
1:C:111:GLY:HA3	1:C:326:VAL:HG12	1.75	0.68
1:A:666:ARG:HG2	1:A:666:ARG:HH11	1.57	0.68
1:C:90:ASN:O	1:C:91:SER:HB2	1.94	0.68
1:A:212:VAL:HG12	1:A:267:GLY:HA3	1.74	0.67
1:B:698:MET:HE2	1:B:698:MET:HA	1.76	0.67
1:B:512:ARG:HG2	1:B:512:ARG:HH11	1.60	0.67
1:C:431:GLN:HE22	1:C:482:TRP:N	1.88	0.67
1:B:207:PRO:HB3	1:B:508:LYS:O	1.94	0.66
1:C:362:TRP:CZ2	1:C:399:VAL:HG21	2.30	0.66
1:A:390:GLN:HG2	1:A:391:HIS:CD2	2.31	0.66
1:A:405:LYS:HG2	1:A:406:GLU:HG2	1.77	0.66
1:B:116:SER:O	1:B:120:THR:HG23	1.96	0.66
1:B:500:GLY:O	1:B:517:ASN:HB3	1.96	0.65
1:C:163:ARG:HG2	1:C:163:ARG:NH1	2.00	0.65
1:A:244:LEU:HD21	1:A:248:ARG:NH2	2.12	0.65
1:B:726:ILE:HG23	1:B:748:MET:HG2	1.78	0.65
1:C:652:THR:HG22	1:C:656:MET:HE2	1.79	0.64
1:C:131:LYS:HD2	1:C:131:LYS:N	2.13	0.64
1:B:418:GLN:HG2	1:B:423:MET:HE3	1.80	0.64
1:A:329:PHE:HE2	1:A:513:MET:HE2	1.63	0.63
1:C:190:PHE:O	1:C:194:ASN:HB2	1.99	0.62
1:C:362:TRP:HZ2	1:C:399:VAL:HG21	1.64	0.62
1:B:431:GLN:NE2	1:B:482:TRP:H	1.97	0.62
1:A:601:GLU:HG2	1:A:602:SER:N	2.14	0.62
1:A:431:GLN:HE22	1:A:482:TRP:N	1.95	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:GLU:O	1:B:695:MET:HG2	2.00	0.62
1:B:430:SER:HA	1:B:440:LEU:HD22	1.81	0.62
1:A:214:PHE:HB3	1:A:215:PRO:HD3	1.80	0.61
1:B:105:LEU:HD21	1:B:334:ILE:HG21	1.81	0.61
1:A:202:ASN:H	1:A:202:ASN:ND2	1.98	0.61
1:A:229:PRO:O	1:A:235:LEU:HD12	1.99	0.61
1:B:326:VAL:HG13	1:B:326:VAL:O	1.99	0.61
1:C:238:ILE:HD12	1:C:239:TYR:N	2.16	0.61
1:A:465:ILE:HD13	1:A:505:TRP:CD2	2.36	0.61
1:B:111:GLY:HA3	1:B:326:VAL:HG12	1.82	0.61
1:C:285:SER:HB3	1:C:308:TYR:CE2	2.36	0.61
1:A:294:ALA:HA	1:A:309:LEU:HD11	1.82	0.60
1:A:518:ASN:ND2	1:A:520:GLY:N	2.49	0.60
1:B:199:GLU:HB2	1:B:234:VAL:HB	1.81	0.60
1:B:518:ASN:HD22	1:B:520:GLY:N	1.99	0.60
1:A:603:SER:HA	1:A:606:ARG:NH2	2.16	0.60
1:B:489:VAL:HG22	1:B:797:VAL:HG21	1.83	0.60
1:C:401:LYS:HG2	1:C:439:ILE:HD12	1.83	0.60
1:A:326:VAL:O	1:A:326:VAL:HG13	2.01	0.60
1:B:431:GLN:HE22	1:B:482:TRP:H	1.50	0.60
1:C:378:ILE:HG22	1:C:411:CYS:HA	1.83	0.60
1:B:518:ASN:HD22	1:B:520:GLY:H	1.46	0.59
1:C:266:GLU:OE2	1:C:508:LYS:HE2	2.02	0.59
1:C:657:SER:HB2	1:C:672:LEU:HD12	1.84	0.59
1:B:332:ILE:HG21	1:B:383:MET:HB3	1.84	0.59
1:B:518:ASN:ND2	1:B:520:GLY:N	2.50	0.59
1:A:453:GLU:O	1:A:457:ARG:HG3	2.03	0.59
1:C:218:LEU:HD21	1:C:235:LEU:HD13	1.85	0.59
1:B:232:SER:OG	1:B:233:PRO:HD2	2.03	0.59
1:B:601:GLU:CD	1:B:601:GLU:H	2.11	0.59
1:B:213:ALA:O	1:B:217:LEU:HB2	2.03	0.58
1:A:116:SER:O	1:A:120:THR:HG23	2.03	0.58
1:B:336:ASP:O	1:B:340:ARG:HG3	2.03	0.58
1:C:322:ASN:C	1:C:322:ASN:HD22	2.11	0.58
1:A:518:ASN:HD22	1:A:520:GLY:H	1.49	0.58
1:B:533:GLN:O	1:B:537:GLN:HG3	2.03	0.58
1:C:326:VAL:HG13	1:C:326:VAL:O	2.02	0.58
1:A:686:TYR:HB2	1:A:689:GLU:OE1	2.03	0.58
1:C:500:GLY:O	1:C:517:ASN:HB3	2.04	0.58
1:C:646:ALA:O	1:C:650:ILE:HD13	2.02	0.58
1:B:601:GLU:HG2	1:B:602:SER:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:GLU:OE1	1:A:578:ARG:HD3	2.04	0.57
2:A:901:A3C:H13B	2:A:901:A3C:O01	2.03	0.57
1:C:752:MET:O	1:C:755:MET:HB3	2.04	0.57
1:A:329:PHE:CE2	1:A:513:MET:HE2	2.40	0.57
1:B:465:ILE:HG13	1:B:467:MET:HG3	1.85	0.57
1:C:492:ARG:HD3	1:C:529:TYR:CE2	2.39	0.57
1:A:192:ARG:HG2	1:A:229:PRO:HD3	1.87	0.57
1:A:483:TYR:CE1	3:A:911:1PE:H162	2.40	0.57
1:B:404:GLU:HG2	1:B:405:LYS:N	2.19	0.57
1:C:514:PRO:O	1:C:518:ASN:HB2	2.05	0.57
1:A:330:GLU:O	1:A:334:ILE:HG13	2.03	0.57
1:B:214:PHE:HB3	1:B:215:PRO:HD3	1.86	0.57
1:A:263:HIS:CE1	1:A:289:SER:HB2	2.40	0.56
1:C:420:VAL:HG23	4:C:826:HOH:O	2.06	0.56
1:A:617:ILE:HG22	1:A:618:ALA:N	2.19	0.56
1:A:408:GLU:HG2	1:A:446:PHE:CE1	2.40	0.56
1:A:500:GLY:O	1:A:517:ASN:HB3	2.05	0.56
1:B:495:ILE:HG21	1:B:802:VAL:HG11	1.87	0.56
1:C:285:SER:HB3	1:C:308:TYR:CD2	2.41	0.56
1:C:198:LEU:HD22	1:C:198:LEU:O	2.06	0.56
1:C:215:PRO:O	1:C:219:GLU:HG2	2.05	0.56
1:C:718:ARG:O	1:C:722:ILE:HG13	2.05	0.55
1:B:424:PHE:CZ	1:B:428:ARG:HD2	2.41	0.55
1:A:467:MET:HE1	1:A:470:LEU:HD13	1.87	0.55
1:B:687:GLY:O	1:B:689:GLU:HG2	2.05	0.55
1:A:484:ALA:HB2	1:A:781:TYR:HD2	1.71	0.55
1:B:479:GLU:HG2	1:B:480:ILE:HG12	1.88	0.55
1:C:402:ASN:ND2	1:C:402:ASN:H	2.03	0.55
1:B:657:SER:HB3	1:B:672:LEU:HD12	1.87	0.55
1:C:90:ASN:O	1:C:91:SER:CB	2.55	0.55
1:B:329:PHE:CE2	1:B:513:MET:HE2	2.42	0.54
1:B:573:ILE:HG23	1:B:578:ARG:NH1	2.22	0.54
1:C:390:GLN:HG2	1:C:391:HIS:CD2	2.42	0.54
1:B:269:ARG:O	1:B:271:LEU:HG	2.06	0.54
1:B:683:TRP:CD1	1:B:688:ASP:HA	2.39	0.54
1:A:212:VAL:CG1	1:A:267:GLY:HA3	2.37	0.54
1:A:657:SER:HB3	1:A:672:LEU:HD12	1.88	0.54
2:A:901:A3C:H31	2:A:901:A3C:C11	2.36	0.54
1:B:424:PHE:HA	1:B:451:LEU:HD11	1.89	0.54
1:A:112:GLU:HG3	1:A:515:TYR:CZ	2.43	0.54
1:A:322:ASN:H	1:A:322:ASN:HD22	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PRO:HG3	1:A:238:ILE:HD13	1.90	0.54
1:A:404:GLU:HG2	1:A:408:GLU:O	2.08	0.54
1:A:465:ILE:HD12	1:A:504:VAL:O	2.07	0.54
1:B:444:LYS:HE2	3:B:911:1PE:OH6	2.08	0.54
1:C:115:ILE:HD11	1:C:316:PHE:HB3	1.89	0.54
1:C:672:LEU:HD23	1:C:698:MET:HE1	1.90	0.53
1:A:686:TYR:CD2	1:A:689:GLU:HG3	2.37	0.53
1:A:717:VAL:O	1:A:721:GLU:HG3	2.07	0.53
1:B:168:LEU:HD21	1:B:218:LEU:HD13	1.90	0.53
1:C:271:LEU:HD22	1:C:276:LEU:HD11	1.89	0.53
1:C:390:GLN:HG2	1:C:391:HIS:HD2	1.73	0.53
1:B:285:SER:HB3	1:B:308:TYR:CE2	2.43	0.53
1:A:744:THR:O	1:A:748:MET:HG3	2.09	0.53
1:A:540:TRP:O	1:A:544:GLN:HG3	2.08	0.53
1:B:228:VAL:O	1:B:230:TYR:N	2.43	0.52
1:C:488:ARG:HD3	1:C:574:PHE:CG	2.45	0.52
1:B:404:GLU:HG2	1:B:405:LYS:H	1.75	0.52
1:C:158:PHE:C	1:C:158:PHE:CD2	2.88	0.52
1:C:483:TYR:CE1	3:C:911:1PE:H262	2.43	0.52
1:A:332:ILE:HG22	1:A:383:MET:HE3	1.90	0.52
1:B:506:ILE:HG13	1:B:510:LEU:CD2	2.39	0.52
1:C:288:PHE:HB3	1:C:324:PHE:O	2.08	0.52
1:A:378:ILE:HG22	1:A:411:CYS:HA	1.91	0.52
1:C:444:LYS:HE2	3:C:911:1PE:H241	1.92	0.52
1:A:700:ILE:O	1:A:703:LYS:HG3	2.10	0.52
1:B:518:ASN:HD22	1:B:518:ASN:C	2.18	0.52
1:B:726:ILE:O	1:B:728:LEU:HG	2.10	0.52
1:A:202:ASN:H	1:A:202:ASN:HD22	1.58	0.51
1:B:115:ILE:HD11	1:B:316:PHE:HB3	1.91	0.51
1:C:255:HIS:C	1:C:256:LYS:HD2	2.36	0.51
1:C:405:LYS:HG2	1:C:406:GLU:HG3	1.92	0.51
1:B:146:GLN:OE1	1:B:186:LYS:HE2	2.10	0.51
1:A:575:GLU:CD	1:A:575:GLU:H	2.17	0.51
1:A:397:ALA:HB3	1:A:437:GLU:HG2	1.91	0.51
1:A:484:ALA:HB2	1:A:781:TYR:CD2	2.45	0.51
1:B:672:LEU:HD23	1:B:701:LEU:CD1	2.41	0.51
1:C:99:LYS:O	1:C:103:THR:HG23	2.11	0.51
1:C:589:SER:HA	1:C:695:MET:HE1	1.92	0.51
1:C:163:ARG:CG	1:C:163:ARG:NH1	2.58	0.51
1:A:283:ASP:O	1:A:308:TYR:HB2	2.11	0.50
1:B:462:ASP:HB3	1:B:465:ILE:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:GLU:OE1	1:C:578:ARG:HD3	2.11	0.50
1:B:603:SER:O	1:B:607:ARG:HG3	2.12	0.50
1:C:322:ASN:HD22	1:C:323:VAL:N	2.10	0.50
1:C:378:ILE:CG2	1:C:411:CYS:HA	2.40	0.50
1:A:378:ILE:HD11	1:A:426:LEU:HD13	1.93	0.50
1:A:700:ILE:HA	1:A:703:LYS:HG3	1.94	0.50
1:B:476:PHE:CE2	1:B:490:GLU:HG2	2.46	0.50
1:B:716:PHE:C	1:B:716:PHE:CD2	2.89	0.50
1:C:791:GLN:HA	1:C:791:GLN:HE21	1.76	0.50
1:B:759:ALA:HA	1:B:770:SER:HB2	1.92	0.50
2:A:901:A3C:C11	2:A:901:A3C:C31	2.89	0.50
1:A:198:LEU:HD22	1:A:198:LEU:O	2.12	0.50
1:B:672:LEU:HD23	1:B:701:LEU:HD13	1.94	0.50
1:B:512:ARG:HG2	1:B:512:ARG:NH1	2.25	0.49
1:C:612:GLN:O	1:C:616:TYR:HB2	2.12	0.49
1:B:368:CYS:HA	1:B:377:ASP:OD1	2.11	0.49
1:B:783:PHE:O	1:B:787:GLY:HA3	2.12	0.49
1:C:723:ILE:C	1:C:725:ARG:H	2.19	0.49
1:A:171:VAL:HG11	1:A:188:ILE:HG12	1.92	0.49
1:B:164:LEU:CD1	1:B:198:LEU:HB2	2.42	0.49
1:C:332:ILE:HG21	1:C:383:MET:HB3	1.93	0.49
1:A:492:ARG:HD3	1:A:529:TYR:CZ	2.47	0.49
1:B:544:GLN:HE21	1:B:559:ARG:HE	1.60	0.49
1:B:451:LEU:HD22	1:B:474:ILE:HG21	1.93	0.49
1:C:748:MET:O	1:C:752:MET:HB2	2.13	0.49
1:A:206:MET:HE1	1:A:211:GLU:CG	2.42	0.49
1:C:465:ILE:O	1:C:465:ILE:HG13	2.12	0.49
1:A:495:ILE:HG21	1:A:802:VAL:HG11	1.95	0.48
1:C:463:LYS:HE3	1:C:464:TRP:CZ2	2.48	0.48
1:C:791:GLN:HE21	1:C:791:GLN:CA	2.26	0.48
1:B:91:SER:O	1:B:95:LYS:HG3	2.12	0.48
1:A:485:SER:OG	1:A:490:GLU:HG3	2.13	0.48
1:B:224:ILE:HD11	1:B:226:ILE:HD11	1.95	0.48
1:B:332:ILE:CG2	1:B:383:MET:HB3	2.43	0.48
1:C:260:THR:HG23	1:C:415:GLN:HE22	1.78	0.48
1:C:591:LEU:HD13	1:C:649:LEU:HD23	1.95	0.48
1:A:424:PHE:CZ	1:A:428:ARG:HD2	2.49	0.48
1:A:581:GLU:HB3	1:A:699:ILE:HG23	1.95	0.48
1:A:686:TYR:HD2	1:A:689:GLU:CG	2.25	0.48
1:B:158:PHE:C	1:B:158:PHE:CD2	2.91	0.48
1:B:607:ARG:HG2	1:B:684:LYS:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ILE:CD1	1:A:384:ALA:HB2	2.44	0.48
1:B:266:GLU:HA	1:B:295:PHE:CG	2.49	0.48
1:C:184:CYS:O	1:C:188:ILE:HG13	2.14	0.48
1:C:613:PHE:CE1	1:C:650:ILE:HD11	2.49	0.48
1:A:689:GLU:O	1:A:691:GLU:N	2.44	0.47
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.69	0.47
1:B:728:LEU:CB	1:B:729:PRO:CD	2.89	0.47
1:C:424:PHE:CZ	1:C:428:ARG:HD2	2.49	0.47
1:C:544:GLN:O	1:C:548:GLU:HG3	2.14	0.47
1:A:683:TRP:HD1	1:A:688:ASP:HA	1.80	0.47
1:C:177:TRP:O	1:C:179:LEU:HG	2.14	0.47
1:B:112:GLU:O	1:B:514:PRO:HD2	2.14	0.47
1:C:764:ASP:O	1:C:767:ARG:HB3	2.15	0.47
1:B:198:LEU:C	1:B:198:LEU:HD13	2.40	0.47
1:A:215:PRO:HG3	1:A:238:ILE:CD1	2.45	0.47
1:A:434:PHE:CE1	1:A:757:GLU:HA	2.49	0.47
1:A:666:ARG:HG2	1:A:666:ARG:NH1	2.29	0.47
1:B:466:ILE:HG13	1:B:506:ILE:HD11	1.96	0.47
1:B:488:ARG:HD2	1:B:488:ARG:HA	1.49	0.47
1:B:689:GLU:O	1:B:691:GLU:N	2.35	0.47
1:C:698:MET:HE2	1:C:698:MET:CA	2.43	0.47
1:A:109:THR:OG1	1:A:110:ASP:N	2.47	0.47
1:A:231:ASP:O	1:A:232:SER:C	2.58	0.47
1:A:332:ILE:HG23	1:A:387:LEU:HD12	1.97	0.47
1:B:252:GLU:HG3	1:B:253:ILE:N	2.29	0.47
1:B:332:ILE:HG23	1:B:387:LEU:HD12	1.95	0.47
1:B:691:GLU:HG3	1:B:695:MET:HE3	1.96	0.47
1:A:389:ARG:HG2	1:A:432:LEU:HD23	1.97	0.46
1:B:222:ARG:NH2	1:B:230:TYR:HB3	2.30	0.46
1:B:290:PRO:HG2	1:B:321:PRO:O	2.15	0.46
1:C:210:PHE:CD2	1:C:210:PHE:C	2.93	0.46
1:B:110:ASP:HB3	1:B:325:PRO:HB3	1.97	0.46
1:B:120:THR:CG2	1:B:320:VAL:H	2.24	0.46
1:B:585:TRP:CD1	1:B:585:TRP:C	2.92	0.46
1:C:368:CYS:HA	1:C:377:ASP:OD1	2.15	0.46
1:C:651:GLY:O	1:C:655:GLN:HG3	2.15	0.46
1:A:244:LEU:C	1:A:244:LEU:HD23	2.40	0.46
1:A:584:VAL:HG11	1:A:702:MET:HG3	1.97	0.46
1:B:470:LEU:N	1:B:471:PRO:CD	2.78	0.46
1:B:119:ASP:OD2	1:B:291:SER:HB3	2.15	0.46
1:B:584:VAL:HB	1:B:702:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:691:GLU:HG3	1:C:695:MET:HE2	1.97	0.46
1:C:698:MET:HA	1:C:698:MET:CE	2.44	0.46
1:B:234:VAL:O	1:B:237:ASP:HB3	2.16	0.46
1:B:546:TRP:CE2	1:B:587:LYS:HE2	2.51	0.46
1:C:196:GLY:C	1:C:198:LEU:H	2.24	0.46
1:A:470:LEU:N	1:A:471:PRO:CD	2.79	0.46
1:A:488:ARG:HD3	1:A:574:PHE:CD2	2.50	0.46
1:C:131:LYS:HD2	1:C:131:LYS:H	1.79	0.46
1:C:513:MET:HE3	1:C:513:MET:HB3	1.77	0.46
1:A:390:GLN:HG2	1:A:391:HIS:HD2	1.77	0.46
1:B:365:ASN:HD22	1:B:402:ASN:HD21	1.63	0.46
1:C:190:PHE:CD2	1:C:190:PHE:C	2.94	0.46
1:C:198:LEU:HB3	1:C:234:VAL:HG21	1.98	0.46
1:C:215:PRO:CB	1:C:242:LYS:HD2	2.41	0.46
1:C:469:ASP:O	1:C:473:GLU:HG3	2.16	0.46
1:A:235:LEU:HD23	1:A:235:LEU:HA	1.68	0.45
1:A:714:THR:HG23	1:B:204:GLU:OE1	2.16	0.45
1:A:465:ILE:HD13	1:A:505:TRP:CE3	2.51	0.45
1:B:201:GLU:HG2	1:B:202:ASN:N	2.31	0.45
2:A:901:A3C:H01	2:A:901:A3C:H11A	1.64	0.45
1:C:409:PHE:CE2	1:C:443:ALA:HA	2.51	0.45
1:C:704:ASN:HD22	1:C:704:ASN:N	2.14	0.45
1:B:263:HIS:CE1	1:B:289:SER:HB2	2.52	0.45
1:A:607:ARG:HG2	1:A:684:LYS:HD3	1.98	0.45
1:B:546:TRP:CZ2	1:B:587:LYS:HG2	2.51	0.45
1:C:786:CYS:HB3	1:C:789:HIS:CE1	2.52	0.45
1:C:116:SER:O	1:C:120:THR:HG23	2.16	0.45
1:A:332:ILE:HD13	1:A:384:ALA:HB2	1.99	0.45
1:B:272:ASP:OD1	1:B:274:GLU:HB3	2.17	0.45
1:B:492:ARG:HD3	1:B:529:TYR:CZ	2.51	0.45
1:A:488:ARG:HD2	1:A:488:ARG:HA	1.54	0.45
1:B:184:CYS:O	1:B:188:ILE:HG13	2.16	0.45
1:B:728:LEU:CB	1:B:729:PRO:HD2	2.31	0.45
1:B:269:ARG:HG2	1:B:269:ARG:HH11	1.82	0.45
1:C:613:PHE:CD1	1:C:650:ILE:HD11	2.53	0.44
1:A:169:ALA:HB2	1:A:217:LEU:HD21	1.99	0.44
1:A:368:CYS:HA	1:A:377:ASP:OD1	2.18	0.44
1:A:682:LYS:HD2	1:A:690:GLY:H	1.83	0.44
1:C:98:VAL:O	1:C:102:LYS:HB2	2.17	0.44
1:C:199:GLU:OE2	1:C:234:VAL:HA	2.17	0.44
1:C:214:PHE:HB3	1:C:215:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:686:TYR:HB3	1:C:687:GLY:H	1.49	0.44
1:A:492:ARG:HD3	1:A:529:TYR:CE2	2.52	0.44
1:A:776:VAL:O	1:A:780[B]:PHE:HD2	2.01	0.44
1:B:202:ASN:HB2	1:B:204:GLU:CD	2.42	0.44
1:C:287:LEU:HD23	1:C:287:LEU:HA	1.57	0.44
3:C:931:1PE:H231	3:C:931:1PE:H241	1.79	0.44
1:A:326:VAL:O	1:A:326:VAL:CG1	2.66	0.44
1:B:285:SER:HB3	1:B:308:TYR:CD2	2.52	0.44
1:C:229:PRO:O	1:C:235:LEU:HD12	2.17	0.44
1:C:434:PHE:HB3	1:C:435:PRO:HD2	2.00	0.44
1:C:460:LEU:HD23	1:C:460:LEU:HA	1.74	0.44
1:B:168:LEU:CD2	1:B:218:LEU:HD13	2.48	0.44
1:C:506:ILE:HG12	1:C:510:LEU:CD2	2.48	0.44
1:A:672:LEU:HD23	1:A:698:MET:HE1	2.00	0.44
1:B:235:LEU:C	1:B:237:ASP:H	2.26	0.44
1:C:121:ALA:HA	1:C:142:ILE:HD11	1.98	0.44
1:C:748:MET:O	1:C:752:MET:N	2.51	0.44
1:B:201:GLU:HG2	1:B:202:ASN:ND2	2.33	0.43
1:C:328:LEU:HD13	1:C:367:ILE:HD12	2.00	0.43
1:A:657:SER:HB3	1:A:672:LEU:CD1	2.47	0.43
1:A:228:VAL:HG22	1:A:229:PRO:HD2	2.00	0.43
1:B:206:MET:O	1:B:206:MET:HG3	2.18	0.43
1:B:661:PHE:HA	1:B:666:ARG:H	1.83	0.43
1:C:460:LEU:HD22	1:C:474:ILE:HD12	1.99	0.43
1:B:191:PHE:C	1:B:191:PHE:CD2	2.97	0.43
1:B:396:SER:O	1:B:399:VAL:HG23	2.18	0.43
1:A:249:ILE:HA	1:A:250:PRO:HD3	1.80	0.43
1:A:613:PHE:CE1	1:A:650:ILE:HD11	2.53	0.43
1:B:121:ALA:HA	1:B:142:ILE:HD11	2.00	0.43
1:B:215:PRO:CB	1:B:242:LYS:HD2	2.37	0.43
1:B:245:LYS:O	1:B:249:ILE:HG12	2.18	0.43
1:C:332:ILE:CG2	1:C:383:MET:HB3	2.49	0.43
1:C:470:LEU:N	1:C:471:PRO:CD	2.81	0.43
1:C:488:ARG:HD3	1:C:574:PHE:CD2	2.54	0.43
1:C:710:PHE:CD1	1:C:766:PHE:HD2	2.37	0.43
1:A:440:LEU:HD23	1:A:440:LEU:HA	1.83	0.43
1:B:250:PRO:O	1:B:251:LYS:C	2.62	0.43
1:B:277:LEU:HD23	1:B:286:PHE:HZ	1.84	0.43
1:B:329:PHE:HE2	1:B:513:MET:HE2	1.82	0.43
1:C:492:ARG:HD3	1:C:529:TYR:CZ	2.54	0.43
1:B:698:MET:HE2	1:B:698:MET:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:911:1PE:H262	3:B:911:1PE:H252	1.61	0.43
1:C:613:PHE:O	1:C:617:ILE:HG13	2.18	0.43
1:B:262:LEU:HD11	1:B:279:LEU:HB3	2.00	0.43
1:C:440:LEU:HD23	1:C:440:LEU:HA	1.83	0.43
1:C:540:TRP:O	1:C:544:GLN:HG3	2.19	0.43
1:A:612:GLN:HG3	1:A:642:ALA:HB3	1.99	0.42
1:A:742:GLU:HG2	1:A:743:LYS:N	2.33	0.42
1:B:339:GLN:NE2	1:B:391:HIS:NE2	2.63	0.42
1:C:786:CYS:O	1:C:788:ASP:N	2.51	0.42
1:A:339:GLN:HA	1:A:344:SER:HB3	2.02	0.42
1:A:483:TYR:CZ	3:A:911:1PE:H162	2.55	0.42
1:A:704:ASN:N	1:A:704:ASN:HD22	2.17	0.42
2:A:901:A3C:H02	2:A:901:A3C:H12	1.79	0.42
1:A:224:ILE:HG13	1:A:226:ILE:HG13	2.01	0.42
1:B:601:GLU:HG2	1:B:602:SER:N	2.35	0.42
1:A:755:MET:HE2	1:A:755:MET:HB2	1.79	0.42
1:C:573:ILE:O	1:C:582:ARG:HD3	2.20	0.42
1:A:584:VAL:HG22	1:A:698:MET:HB3	2.02	0.42
1:B:105:LEU:CD2	1:B:334:ILE:HG21	2.50	0.42
1:C:116:SER:O	1:C:120:THR:CG2	2.67	0.42
1:C:228:VAL:HG13	1:C:229:PRO:HD2	2.01	0.42
1:B:105:LEU:HD21	1:B:334:ILE:CG2	2.49	0.42
1:A:698:MET:HE2	1:A:698:MET:HA	2.01	0.42
1:B:215:PRO:HG2	1:B:242:LYS:HB2	2.02	0.42
1:C:766:PHE:O	1:C:767:ARG:C	2.61	0.42
1:A:572:THR:HG21	1:A:775:ASP:HB3	2.01	0.42
1:A:604:ASP:OD1	1:A:604:ASP:C	2.63	0.41
1:A:742:GLU:OE1	1:A:742:GLU:N	2.53	0.41
1:B:112:GLU:OE2	1:B:112:GLU:HA	2.20	0.41
1:B:738:ASN:O	1:B:741:LYS:HB3	2.19	0.41
1:C:123:VAL:HG22	1:C:309:LEU:HD22	2.02	0.41
1:C:329:PHE:CE2	1:C:513:MET:HE2	2.55	0.41
1:C:595:ILE:HG12	1:C:645:LEU:HD11	2.02	0.41
1:C:231:ASP:O	1:C:232:SER:C	2.63	0.41
1:C:257:ILE:HD13	1:C:257:ILE:N	2.35	0.41
1:A:127:ASP:OD1	1:A:131:LYS:HD3	2.19	0.41
1:A:238:ILE:HD12	1:A:239:TYR:N	2.35	0.41
1:C:589:SER:HA	1:C:695:MET:CE	2.51	0.41
1:C:694:LEU:O	1:C:698:MET:HG2	2.20	0.41
1:A:674:LEU:HD13	1:B:457:ARG:HG3	2.02	0.41
1:A:513:MET:HE3	1:A:513:MET:HB3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:MET:O	1:A:681:GLU:C	2.63	0.41
1:B:340:ARG:HD2	1:B:428:ARG:NH2	2.35	0.41
1:B:612:GLN:O	1:B:616:TYR:HB2	2.20	0.41
1:C:326:VAL:O	1:C:326:VAL:CG1	2.68	0.41
1:A:694:LEU:O	1:A:698:MET:HG2	2.21	0.41
1:C:252:GLU:OE1	1:C:252:GLU:HA	2.21	0.41
1:C:655:GLN:O	1:C:659:ASP:HB2	2.20	0.41
1:A:130:ASP:OD1	1:A:130:ASP:N	2.54	0.41
1:A:547:TYR:HA	1:A:552:LEU:HD12	2.02	0.41
1:A:748:MET:CE	1:A:780[A]:PHE:HE1	2.33	0.41
1:C:202:ASN:OD1	1:C:204:GLU:HB2	2.21	0.41
1:C:660:LEU:O	1:C:660:LEU:HG	2.20	0.41
1:A:573:ILE:O	1:A:582:ARG:HD3	2.20	0.41
1:B:249:ILE:HA	1:B:250:PRO:HD3	1.87	0.41
1:B:269:ARG:HG2	1:B:269:ARG:NH1	2.35	0.41
1:B:581:GLU:O	1:B:584:VAL:HG12	2.21	0.41
1:C:386:ARG:NH2	1:C:428:ARG:NH2	2.69	0.41
1:A:235:LEU:C	1:A:237:ASP:N	2.77	0.41
1:A:332:ILE:HG21	1:A:383:MET:HB3	2.02	0.41
1:A:486:LEU:O	1:A:487:PRO:C	2.63	0.41
1:A:543:PHE:HD1	1:A:583:MET:HE3	1.85	0.41
1:B:188:ILE:O	1:B:192:ARG:HB2	2.21	0.41
1:B:362:TRP:CZ2	1:B:399:VAL:HG21	2.56	0.41
1:B:774:LEU:HD23	1:B:774:LEU:HA	1.83	0.41
1:C:294:ALA:HA	1:C:309:LEU:HD11	2.01	0.41
1:A:488:ARG:HD3	1:A:574:PHE:CG	2.56	0.41
1:A:123:VAL:HG13	1:A:135:PHE:CD2	2.57	0.40
1:A:727:CYS:C	1:A:728:LEU:HG	2.46	0.40
1:B:190:PHE:CD2	1:B:190:PHE:C	2.99	0.40
1:B:518:ASN:ND2	1:B:518:ASN:C	2.80	0.40
1:B:591:LEU:O	1:B:595:ILE:HG13	2.21	0.40
1:B:691:GLU:CG	1:B:695:MET:HE3	2.51	0.40
1:C:444:LYS:NZ	3:C:911:1PE:H122	2.35	0.40
1:A:772:THR:O	1:A:776:VAL:HG23	2.21	0.40
1:B:248:ARG:HD2	1:B:248:ARG:HA	1.95	0.40
1:C:601:GLU:HG2	1:C:605:SER:OG	2.21	0.40
1:A:161:HIS:CD2	1:A:198:LEU:HD21	2.56	0.40
1:A:678:ASP:OD2	1:B:457:ARG:NH2	2.55	0.40
1:B:175:ARG:O	1:B:175:ARG:HD3	2.22	0.40
1:B:758:LEU:HD23	1:B:758:LEU:HA	1.87	0.40
1:B:762:GLU:CD	1:B:762:GLU:N	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ASP:O	1:A:232:SER:O	2.40	0.40
1:A:368:CYS:HB3	1:A:376:GLN:HA	2.03	0.40
1:B:115:ILE:CD1	1:B:316:PHE:HB3	2.51	0.40
1:C:581:GLU:OE2	1:C:703:LYS:HG2	2.22	0.40
1:B:94:PHE:CE2	1:B:524:LEU:CD2	3.05	0.40
1:C:262:LEU:HD11	1:C:279:LEU:HB3	2.04	0.40
1:C:645:LEU:O	1:C:645:LEU:HD22	2.22	0.40
1:C:649:LEU:O	1:C:653:LEU:HG	2.21	0.40
1:C:758:LEU:O	1:C:762:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

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	683/727 (94%)	651 (95%)	29 (4%)	3 (0%)	30	50
1	B	684/727 (94%)	628 (92%)	50 (7%)	6 (1%)	14	28
1	C	679/727 (93%)	615 (91%)	52 (8%)	12 (2%)	6	13
All	All	2046/2181 (94%)	1894 (93%)	131 (6%)	21 (1%)	12	24

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	SER
1	B	601	GLU
1	C	91	SER
1	C	763	SER
1	A	690	GLY
1	B	229	PRO
1	B	690	GLY
1	B	728	LEU

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Mol	Chain	Res	Type
1	C	194	ASN
1	C	326	VAL
1	C	229	PRO
1	C	787	GLY
1	C	197	LYS
1	C	399	VAL
1	B	207	PRO
1	B	711	PHE
1	C	232	SER
1	C	266	GLU
1	C	688	ASP
1	C	250	PRO
1	A	487	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	608/644 (94%)	546 (90%)	62 (10%)	7	14
1	B	609/644 (95%)	558 (92%)	51 (8%)	10	19
1	C	604/644 (94%)	567 (94%)	37 (6%)	17	31
All	All	1821/1932 (94%)	1671 (92%)	150 (8%)	10	20

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	GLU
1	A	120	THR
1	A	157	LEU
1	A	183	GLN
1	A	193	GLU
1	A	197	LYS
1	A	198	LEU
1	A	200	ASP
1	A	202	ASN

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Mol	Chain	Res	Type
1	A	204	GLU
1	A	206	MET
1	A	218	LEU
1	A	228	VAL
1	A	234	VAL
1	A	245	LYS
1	A	252	GLU
1	A	264	SER
1	A	266	GLU
1	A	268	MET
1	A	274	GLU
1	A	278	LYS
1	A	287	LEU
1	A	322	ASN
1	A	326	VAL
1	A	344	SER
1	A	348	GLU
1	A	351	ILE
1	A	353	GLU
1	A	390	GLN
1	A	394	GLN
1	A	399	VAL
1	A	404	GLU
1	A	413	VAL
1	A	438	GLU
1	A	452	LEU
1	A	461	ILE
1	A	465	ILE
1	A	479	GLU
1	A	488	ARG
1	A	490	GLU
1	A	518	ASN
1	A	524	LEU
1	A	527	GLN
1	A	541	ASP
1	A	558	ARG
1	A	615	GLU
1	A	617	ILE
1	A	645	LEU
1	A	649	LEU
1	A	650	ILE
1	A	686	TYR

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Mol	Chain	Res	Type
1	A	691	GLU
1	A	709	ASN
1	A	712	THR
1	A	728	LEU
1	A	744	THR
1	A	751	GLU
1	A	752	MET
1	A	755	MET
1	A	758	LEU
1	A	764	ASP
1	A	791	GLN
1	B	112	GLU
1	B	115	ILE
1	B	120	THR
1	B	137	SER
1	B	157	LEU
1	B	183	GLN
1	B	204	GLU
1	B	206	MET
1	B	218	LEU
1	B	238	ILE
1	B	243	GLU
1	B	248	ARG
1	B	252	GLU
1	B	257	ILE
1	B	260	THR
1	B	270	ASP
1	B	287	LEU
1	B	292	SER
1	B	303	SER
1	B	322	ASN
1	B	326	VAL
1	B	378	ILE
1	B	390	GLN
1	B	465	ILE
1	B	479	GLU
1	B	488	ARG
1	B	490	GLU
1	B	504	VAL
1	B	518	ASN
1	B	523	GLU
1	B	524	LEU

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Mol	Chain	Res	Type
1	B	553	SER
1	B	560	SER
1	B	615	GLU
1	B	639	SER
1	B	645	LEU
1	B	649	LEU
1	B	650	ILE
1	B	671	LEU
1	B	674	LEU
1	B	685	LEU
1	B	708	THR
1	B	718	ARG
1	B	723	ILE
1	B	738	ASN
1	B	744	THR
1	B	746	LYS
1	B	752	MET
1	B	762	GLU
1	B	789	HIS
1	B	792	THR
1	C	99	LYS
1	C	120	THR
1	C	163	ARG
1	C	178	ASN
1	C	183	GLN
1	C	198	LEU
1	C	212	VAL
1	C	228	VAL
1	C	234	VAL
1	C	247	THR
1	C	257	ILE
1	C	269	ARG
1	C	274	GLU
1	C	287	LEU
1	C	322	ASN
1	C	326	VAL
1	C	390	GLN
1	C	401	LYS
1	C	402	ASN
1	C	461	ILE
1	C	465	ILE
1	C	467	MET

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Mol	Chain	Res	Type
1	C	488	ARG
1	C	490	GLU
1	C	538	LEU
1	C	577	GLU
1	C	590	VAL
1	C	596	SER
1	C	619	ASN
1	C	669	ASN
1	C	671	LEU
1	C	672	LEU
1	C	758	LEU
1	C	765	THR
1	C	767	ARG
1	C	768	ASP
1	C	791	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	280	GLN
1	A	339	GLN
1	A	391	HIS
1	A	394	GLN
1	A	431	GLN
1	A	449	ASN
1	A	502	ASN
1	A	518	ASN
1	A	527	GLN
1	A	535	GLN
1	A	655	GLN
1	A	664	HIS
1	A	670	ASN
1	A	704	ASN
1	B	182	HIS
1	B	185	ASN
1	B	280	GLN
1	B	359	HIS
1	B	365	ASN
1	B	390	GLN
1	B	417	ASN
1	B	431	GLN

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Mol	Chain	Res	Type
1	B	449	ASN
1	B	502	ASN
1	B	518	ASN
1	B	527	GLN
1	B	535	GLN
1	B	544	GLN
1	B	550	ASN
1	B	580	HIS
1	B	612	GLN
1	B	655	GLN
1	B	791	GLN
1	C	280	GLN
1	C	299	GLN
1	C	322	ASN
1	C	390	GLN
1	C	402	ASN
1	C	415	GLN
1	C	431	GLN
1	C	449	ASN
1	C	502	ASN
1	C	518	ASN
1	C	544	GLN
1	C	612	GLN
1	C	614	HIS
1	C	655	GLN
1	C	669	ASN
1	C	704	ASN
1	C	789	HIS
1	C	791	GLN
1	C	800	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](#)

10 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
3	1PE	C	911	-	15,15,15	0.57	0	14,14,14	0.73	0
3	1PE	A	921	-	15,15,15	0.57	0	14,14,14	0.76	0
3	1PE	B	931	-	15,15,15	0.61	0	14,14,14	0.68	0
3	1PE	C	931	-	15,15,15	0.55	0	14,14,14	0.80	0
3	1PE	B	921	-	15,15,15	0.56	0	14,14,14	0.72	0
3	1PE	B	911	-	15,15,15	0.56	0	14,14,14	0.79	0
2	A3C	A	901	-	29,30,30	1.04	1 (3%)	44,47,47	2.71	12 (27%)
3	1PE	A	811	-	15,15,15	0.54	0	14,14,14	0.76	0
3	1PE	A	931	-	15,15,15	0.62	0	14,14,14	0.60	0
3	1PE	A	911	-	15,15,15	0.57	0	14,14,14	0.75	0

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
3	1PE	C	911	-	-	4/13/13/13	-
3	1PE	A	921	-	-	4/13/13/13	-
3	1PE	B	931	-	-	6/13/13/13	-
3	1PE	C	931	-	-	8/13/13/13	-
3	1PE	B	921	-	-	4/13/13/13	-
3	1PE	B	911	-	-	9/13/13/13	-
2	A3C	A	901	-	-	2/18/53/53	0/2/2/2
3	1PE	A	811	-	-	2/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	A	931	-	-	6/13/13/13	-
3	1PE	A	911	-	-	8/13/13/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	A3C	P02-O03	2.66	1.62	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	A3C	C21-C22-C31	10.23	139.63	124.60
2	A	901	A3C	C23-C22-C21	-6.68	104.85	113.35
2	A	901	A3C	C24-C23-C22	5.57	119.03	110.98
2	A	901	A3C	C34-C30-C25	4.79	121.78	112.94
2	A	901	A3C	C23-C22-C31	-4.45	115.48	122.15
2	A	901	A3C	C34-C30-C29	-3.89	102.13	108.31
2	A	901	A3C	C12-C11-N03	-3.24	105.28	113.69
2	A	901	A3C	C29-C30-C25	3.20	111.80	108.02
2	A	901	A3C	C28-C29-C30	-3.11	109.54	113.19
2	A	901	A3C	C23-C24-C25	2.98	115.63	110.89
2	A	901	A3C	C30-C21-C22	2.58	112.93	109.95
2	A	901	A3C	C24-C25-C26	-2.28	111.27	114.27

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	A3C	P04-O03-P02-O01
2	A	901	A3C	C11-C12-C21-C22
3	A	921	1PE	OH4-C13-C23-OH3
3	C	931	1PE	OH5-C14-C24-OH4
3	B	921	1PE	OH4-C13-C23-OH3
3	B	931	1PE	OH6-C15-C25-OH5
3	C	911	1PE	OH5-C14-C24-OH4
3	B	931	1PE	OH5-C14-C24-OH4
3	B	911	1PE	OH2-C12-C22-OH3
3	C	931	1PE	OH2-C12-C22-OH3
3	A	931	1PE	OH7-C16-C26-OH6
3	A	921	1PE	OH5-C14-C24-OH4
3	A	911	1PE	OH7-C16-C26-OH6

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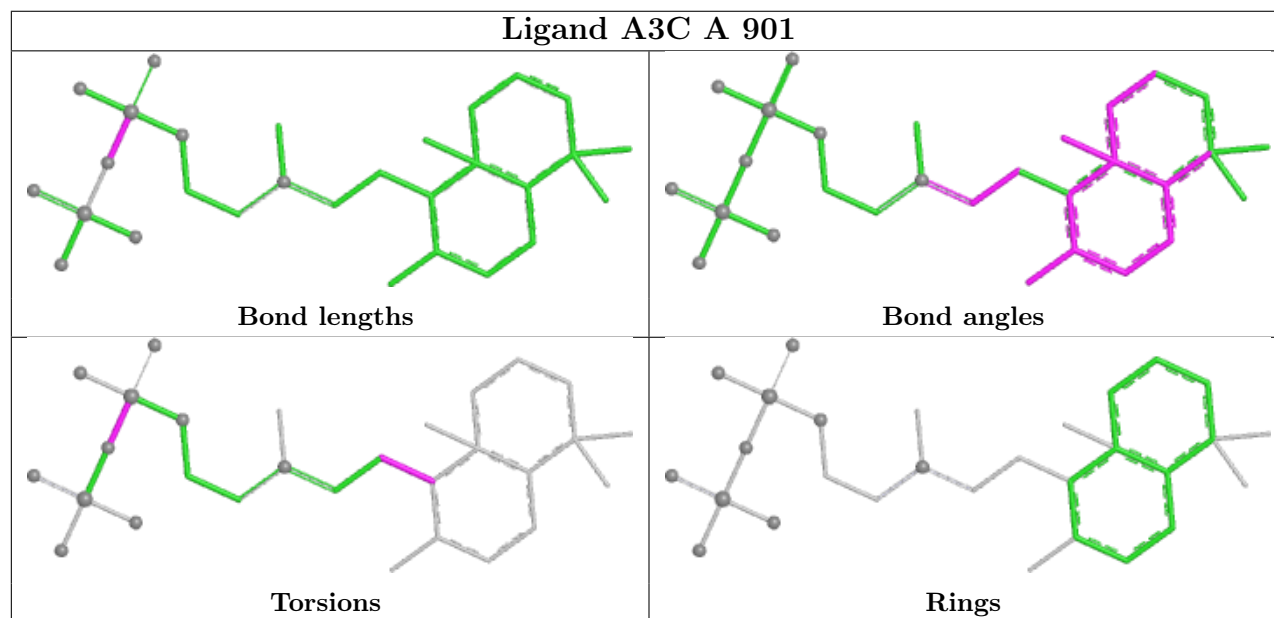
Mol	Chain	Res	Type	Atoms
3	A	931	1PE	OH2-C12-C22-OH3
3	B	931	1PE	OH7-C16-C26-OH6
3	C	931	1PE	C24-C14-OH5-C25
3	A	911	1PE	OH2-C12-C22-OH3
3	B	911	1PE	OH4-C13-C23-OH3
3	B	911	1PE	C25-C15-OH6-C26
3	B	911	1PE	OH6-C15-C25-OH5
3	A	921	1PE	OH2-C12-C22-OH3
3	A	931	1PE	OH6-C15-C25-OH5
3	B	921	1PE	OH6-C15-C25-OH5
3	A	911	1PE	C25-C15-OH6-C26
3	C	911	1PE	C25-C15-OH6-C26
3	A	931	1PE	C13-C23-OH3-C22
3	B	921	1PE	C25-C15-OH6-C26
3	A	911	1PE	C13-C23-OH3-C22
3	B	921	1PE	C13-C23-OH3-C22
3	B	911	1PE	C15-C25-OH5-C14
3	C	911	1PE	C13-C23-OH3-C22
3	A	911	1PE	C23-C13-OH4-C24
3	A	911	1PE	OH6-C15-C25-OH5
3	C	911	1PE	C24-C14-OH5-C25
3	A	931	1PE	C23-C13-OH4-C24
3	A	811	1PE	C12-C22-OH3-C23
3	C	931	1PE	C16-C26-OH6-C15
3	B	911	1PE	OH5-C14-C24-OH4
3	B	911	1PE	C23-C13-OH4-C24
3	A	811	1PE	OH7-C16-C26-OH6
3	B	931	1PE	C12-C22-OH3-C23
3	A	911	1PE	C14-C24-OH4-C13
3	C	931	1PE	C12-C22-OH3-C23
3	A	921	1PE	C12-C22-OH3-C23
3	A	911	1PE	C24-C14-OH5-C25
3	B	931	1PE	C23-C13-OH4-C24
3	B	911	1PE	C12-C22-OH3-C23
3	A	931	1PE	C12-C22-OH3-C23
3	B	911	1PE	OH7-C16-C26-OH6
3	B	931	1PE	OH2-C12-C22-OH3
3	C	931	1PE	C14-C24-OH4-C13
3	C	931	1PE	C23-C13-OH4-C24
3	C	931	1PE	OH4-C13-C23-OH3

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	911	1PE	3	0
3	C	931	1PE	1	0
3	B	911	1PE	2	0
2	A	901	A3C	6	0
3	A	911	1PE	2	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 ⓘ

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	685/727 (94%)	-0.50	3 (0%) 88 89	22, 46, 94, 133	4 (0%)
1	B	689/727 (94%)	-0.36	4 (0%) 85 86	28, 55, 100, 177	1 (0%)
1	C	685/727 (94%)	-0.36	5 (0%) 84 84	30, 57, 106, 173	0
All	All	2059/2181 (94%)	-0.41	12 (0%) 85 86	22, 53, 101, 177	5 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	729	PRO	3.5
1	A	729	PRO	3.0
1	B	715	HIS	2.9
1	A	620	ALA	2.9
1	B	209	GLY	2.7
1	C	690	GLY	2.7
1	A	690	GLY	2.6
1	B	803	GLY	2.5
1	C	620	ALA	2.4
1	C	689	GLU	2.3
1	C	803	GLY	2.1
1	C	688	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

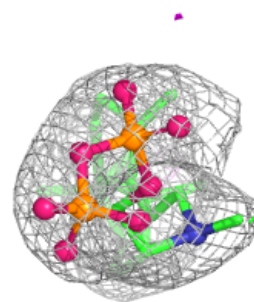
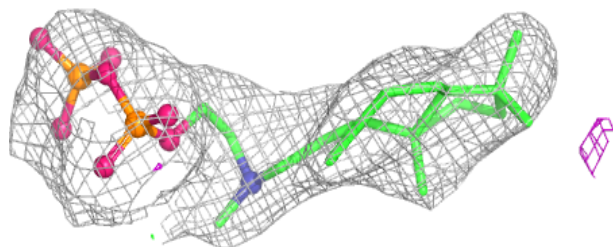
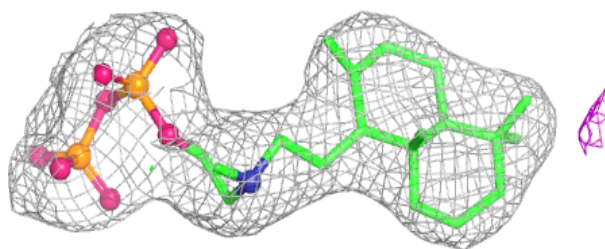
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	1PE	C	911	16/16	0.87	0.14	54,79,93,95	0
3	1PE	C	931	16/16	0.88	0.17	61,80,95,97	0
3	1PE	B	931	16/16	0.90	0.14	55,77,98,102	0
3	1PE	A	931	16/16	0.90	0.17	61,78,96,98	0
3	1PE	B	911	16/16	0.90	0.14	61,72,95,96	0
3	1PE	A	921	16/16	0.91	0.11	42,58,77,92	0
3	1PE	A	811	16/16	0.91	0.11	41,60,79,87	0
3	1PE	A	911	16/16	0.93	0.11	60,72,90,90	0
2	A3C	A	901	29/29	0.94	0.07	39,52,112,143	0
3	1PE	B	921	16/16	0.94	0.09	54,69,89,97	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 A3C A 901:

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.