WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2025 – 03:17 pm GMT

PDB ID	:	9GRN
Title	:	Crystal structure of the engineered C-terminal phosphatase domain from Saccharomyces cerevisiae Vip1 (apo, loop deletion residues 848-918)
Authors	:	Raia, P.; Lee, K.; Hothorn, M.
Deposited on	:	2024-09-11
Resolution	:	3.40 Å(reported)

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

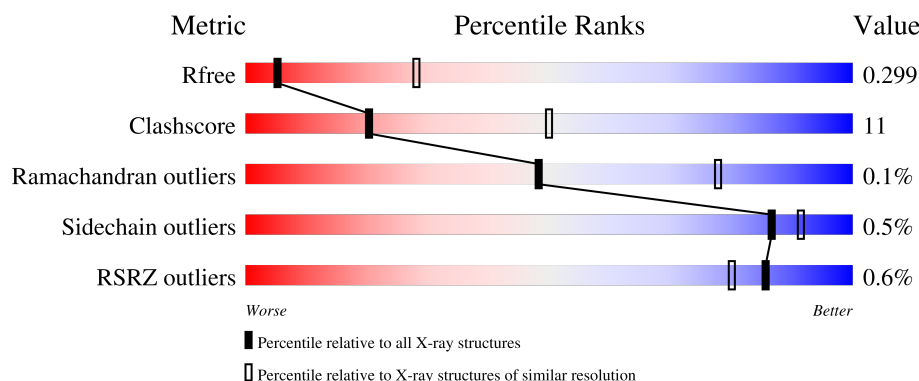|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.299
Clashscore		11
Ramachandran outliers		0.1%
Sidechain outliers		0.5%
RSRZ outliers		0.6%

Worse *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)

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 <=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	507	71% 21% · 7%
1	B	507	72% 22% 6%
1	C	507	69% 26% 5%
1	D	507	66% 24% · 9%

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
5	ACT	C	1111	-	-	X	-

2 Entity composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 31764 atoms, of which 16038 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 Inositol hexakisphosphate and diphosphoinositol-pentakisphosphate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	470	Total	C	H	N	O	S	0	0	0
			7785	2474	3936	660	698	17			
1	B	479	Total	C	H	N	O	S	0	0	0
			7909	2509	3995	674	714	17			
1	C	484	Total	C	H	N	O	S	0	0	0
			7946	2524	4006	677	722	17			
1	D	462	Total	C	H	N	O	S	0	0	0
			7626	2418	3854	648	689	17			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	534	GLY	-	expression tag	UNP Q06685
A	535	ALA	-	expression tag	UNP Q06685
A	848	GLY	-	linker	UNP Q06685
A	849	SER	-	linker	UNP Q06685
A	850	SER	-	linker	UNP Q06685
A	851	GLY	-	linker	UNP Q06685
B	534	GLY	-	expression tag	UNP Q06685
B	535	ALA	-	expression tag	UNP Q06685
B	848	GLY	-	linker	UNP Q06685
B	849	SER	-	linker	UNP Q06685
B	850	SER	-	linker	UNP Q06685
B	851	GLY	-	linker	UNP Q06685
C	534	GLY	-	expression tag	UNP Q06685
C	535	ALA	-	expression tag	UNP Q06685
C	848	GLY	-	linker	UNP Q06685
C	849	SER	-	linker	UNP Q06685
C	850	SER	-	linker	UNP Q06685
C	851	GLY	-	linker	UNP Q06685
D	534	GLY	-	expression tag	UNP Q06685
D	535	ALA	-	expression tag	UNP Q06685

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Chain	Residue	Modelled	Actual	Comment	Reference
D	848	GLY	-	linker	UNP Q06685
D	849	SER	-	linker	UNP Q06685
D	850	SER	-	linker	UNP Q06685
D	851	GLY	-	linker	UNP Q06685

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 14	C 3	H 8	O 3	0	0
2	B	1	Total 14	C 3	H 8	O 3	0	0
2	B	1	Total 14	C 3	H 8	O 3	0	0
2	B	1	Total 14	C 3	H 8	O 3	0	0
2	B	1	Total 14	C 3	H 8	O 3	0	0
2	B	1	Total 14	C 3	H 8	O 3	0	0
2	C	1	Total 14	C 3	H 8	O 3	0	0
2	C	1	Total 14	C 3	H 8	O 3	0	0
2	C	1	Total 14	C 3	H 8	O 3	0	0
2	C	1	Total 14	C 3	H 8	O 3	0	0
2	C	1	Total 14	C 3	H 8	O 3	0	0
2	D	1	Total 14	C 3	H 8	O 3	0	0
2	D	1	Total 14	C 3	H 8	O 3	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Zn 2	0	0
3	B	2	Total 2	Zn 2	0	0
3	C	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0

- Molecule 4 is [1-MYRISTOYL-GLYCEROL-3-YL]PHOSPHONYLCHOLINE (three-letter code: LPC) (formula: $C_{22}H_{47}NO_7P$).

LPC
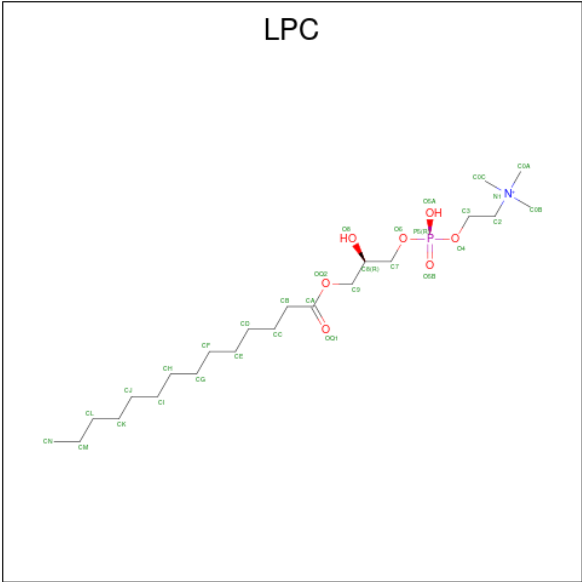
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	P	0	0
			74	21	44	1	7	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT
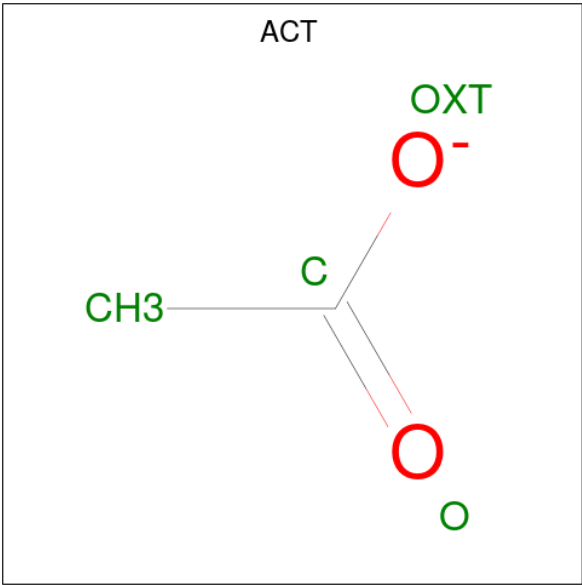
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	H	O	0	0
			7	2	3	2		
5	C	1	Total	C	H	O	0	0
			7	2	3	2		
5	C	1	Total	C	H	O	0	0
			7	2	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total 7	C 2	H 3	O 2	0	0
5	C	1	Total 7	C 2	H 3	O 2	0	0
5	C	1	Total 7	C 2	H 3	O 2	0	0
5	D	1	Total 7	C 2	H 3	O 2	0	0
5	D	1	Total 7	C 2	H 3	O 2	0	0
5	D	1	Total 7	C 2	H 3	O 2	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total 11	O 11	0	0
6	B	11	Total 11	O 11	0	0
6	C	10	Total 10	O 10	0	0
6	D	15	Total 15	O 15	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: Inositol hexakisphosphate and diphosphoinositol-pentakisphosphate kinase

Chain A:

• Molecule 1: Inositol hexakisphosphate and diphosphoinositol-pentakisphosphate kinase

Chain B:

• Molecule 1: Inositol hexakisphosphate and diphosphoinositol-pentakisphosphate kinase

Chain C:

• Molecule 1: Inositol hexakisphosphate and diphosphoinositol-pentakisphosphate kinase

Chain D:
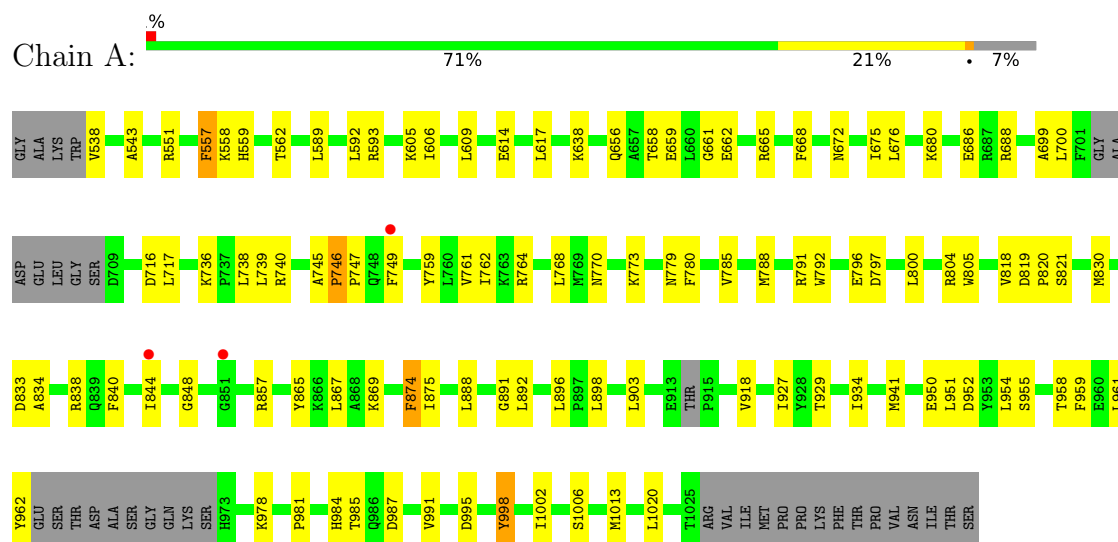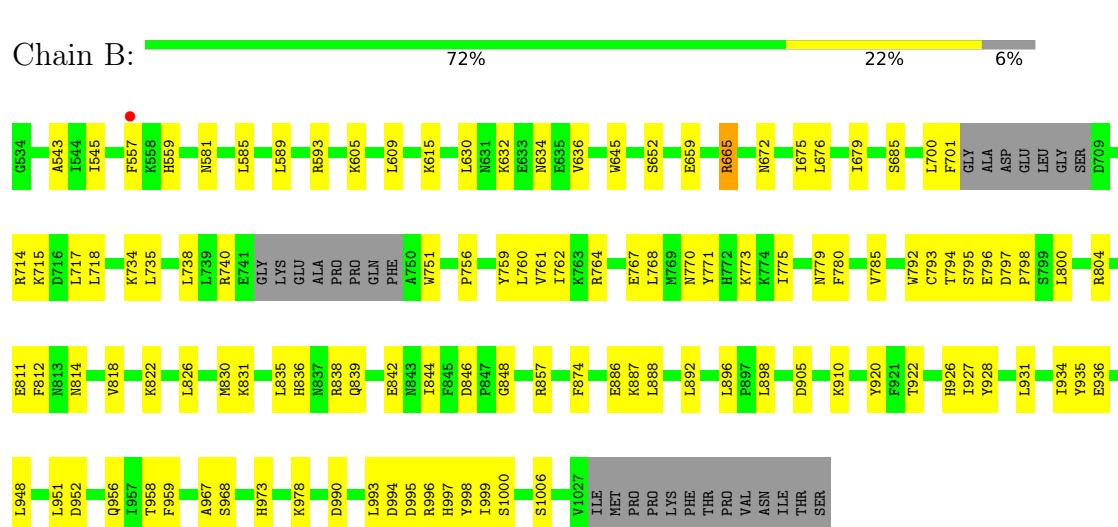
4　Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	249.47Å　90.52Å　200.90Å 90.00°　126.91°　90.00°	Depositor
Resolution (Å)	45.26　–　3.40	Depositor
	45.26　–　3.40	EDS
% Data completeness (in resolution range)	99.2 (45.26-3.40)	Depositor
	99.4 (45.26-3.40)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, R_{free}	0.244　,　0.294	Depositor
	0.249　,　0.299	DCC
R_{free} test set	2468 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	102.3	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 80.6	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.41, < L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	31764	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: LPC, ZN, ACT, GOL

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	0.26	0/3929	0.52	0/5287
1	B	0.26	0/3994	0.53	0/5376
1	C	0.27	0/4023	0.55	0/5418
1	D	0.26	0/3849	0.54	1/5183 (0.0%)
All	All	0.26	0/15795	0.53	1/21264 (0.0%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	542	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	665	ARG	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	3849	3936	3935	74	0
1	B	3914	3995	3998	82	1
1	C	3940	4006	4014	103	0
1	D	3772	3854	3855	96	1
2	A	60	80	80	2	0
2	B	30	40	40	1	0
2	C	30	40	40	0	0
2	D	12	16	16	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	30	44	41	0	0
5	C	24	18	18	2	0
5	D	12	9	9	0	0
6	A	11	0	0	1	0
6	B	11	0	0	0	0
6	C	10	0	0	2	0
6	D	15	0	0	1	0
All	All	15726	16038	16046	353	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 11.

All (353) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:936:LYS:NZ	1:D:1017:GLU:OE1	2.02	0.92
1:D:762:ILE:HD11	1:D:818:VAL:HG11	1.55	0.87
1:A:869:LYS:NZ	1:A:950:GLU:OE1	2.08	0.86
1:B:831:LYS:NZ	1:B:952:ASP:OD1	2.09	0.85
1:D:690:LEU:HD13	1:D:713:ILE:HD11	1.61	0.83
1:C:605:LYS:O	1:C:609:LEU:HD13	1.79	0.81
1:A:716:ASP:OD1	1:A:717:LEU:HD12	1.80	0.81
1:B:735:LEU:HA	1:B:738:LEU:HD13	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:ILE:HD11	1:A:818:VAL:HG11	1.64	0.79
1:D:563:SER:OG	1:D:600:ALA:O	2.01	0.79
1:C:716:ASP:OD1	1:C:717:LEU:HD12	1.82	0.77
1:A:592:LEU:HD12	1:A:606:ILE:HG23	1.66	0.77
1:C:764:ARG:O	1:C:768:LEU:HD23	1.84	0.77
1:C:595:ALA:O	1:C:600:ALA:HB2	1.85	0.77
1:D:605:LYS:O	1:D:609:LEU:HD13	1.86	0.75
1:C:665:ARG:NH1	1:C:700:LEU:O	2.20	0.74
1:B:780:PHE:CD1	1:B:785:VAL:HG11	2.23	0.74
1:D:542:LEU:HD21	1:D:1027:GLU:HA	1.68	0.73
1:A:780:PHE:CD1	1:A:785:VAL:HG11	2.25	0.72
1:C:869:LYS:NZ	1:C:950:GLU:OE1	2.22	0.72
1:C:576:GLU:OE2	1:C:625:GLN:NE2	2.23	0.71
1:C:927:ILE:HG22	1:C:951:LEU:HD13	1.73	0.70
1:A:888:LEU:O	1:A:892:LEU:HD23	1.90	0.70
1:A:903:LEU:HD21	1:A:1020:LEU:HD13	1.73	0.70
1:B:605:LYS:O	1:B:609:LEU:HD23	1.90	0.70
1:D:802:LYS:NZ	1:D:806:ASP:OD2	2.19	0.70
1:C:762:ILE:HD11	1:C:818:VAL:HG11	1.72	0.70
1:B:679:ILE:HD13	1:B:700:LEU:HD21	1.72	0.70
1:D:820:PRO:HB3	1:D:942:ILE:HG21	1.72	0.70
1:A:688:ARG:NH2	2:A:2008:GOL:O2	2.25	0.69
1:C:688:ARG:NH2	6:C:1201:HOH:O	2.24	0.68
1:C:835:LEU:HD21	1:C:999:ILE:CD1	2.24	0.67
1:C:812:PHE:CE2	1:C:826:LEU:HD22	2.30	0.67
1:A:605:LYS:NZ	2:A:2001:GOL:O2	2.28	0.67
1:C:812:PHE:HE2	1:C:826:LEU:HD22	1.60	0.66
1:D:839:GLN:OE1	1:D:839:GLN:N	2.27	0.66
1:D:565:ILE:HD11	1:D:598:GLU:OE1	1.96	0.65
1:C:735:LEU:HA	1:C:738:LEU:HD13	1.79	0.65
1:C:750:ALA:O	1:C:874:PHE:CD1	2.51	0.64
1:A:927:ILE:HG22	1:A:951:LEU:HD13	1.81	0.63
1:C:838:ARG:HD2	1:C:993:LEU:HD12	1.80	0.63
1:B:764:ARG:O	1:B:768:LEU:HD23	1.98	0.63
1:B:887:LYS:HB3	1:B:887:LYS:HZ3	1.63	0.63
1:D:689:VAL:O	1:D:692:THR:HG22	1.99	0.63
1:D:780:PHE:HD1	1:D:785:VAL:HG21	1.65	0.62
1:C:835:LEU:HD21	1:C:999:ILE:HD11	1.80	0.62
1:B:935:TYR:OH	1:B:948:LEU:HD11	1.99	0.62
1:C:595:ALA:C	1:C:600:ALA:HB2	2.20	0.62
1:A:739:LEU:HD12	1:A:820:PRO:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:780:PHE:CD1	1:C:785:VAL:HG11	2.36	0.61
1:A:665:ARG:HD3	1:A:700:LEU:O	2.00	0.60
1:C:826:LEU:HD11	1:C:830:MET:HE3	1.82	0.60
1:A:538:VAL:HG23	1:A:962:TYR:HB3	1.82	0.60
1:B:796:GLU:OE1	1:B:804:ARG:NH2	2.33	0.60
1:B:812:PHE:CE1	1:B:818:VAL:HG13	2.36	0.60
1:C:838:ARG:NH1	1:C:991:VAL:O	2.34	0.60
1:B:762:ILE:HD11	1:B:818:VAL:HG11	1.83	0.60
1:C:1021:ARG:HH12	5:C:1111:ACT:H1	1.66	0.59
1:A:961:LEU:HD11	1:A:1013:MET:CE	2.33	0.59
1:D:542:LEU:HG	1:D:543:ALA:H	1.68	0.59
1:C:714:ARG:HB3	1:C:717:LEU:HD13	1.85	0.58
1:C:609:LEU:HD23	1:C:641:PHE:CD1	2.38	0.58
1:C:739:LEU:HD12	1:C:820:PRO:HG3	1.85	0.58
1:D:548:HIS:HA	1:D:692:THR:HG21	1.86	0.58
1:A:759:TYR:O	1:A:762:ILE:HG22	2.04	0.57
1:C:551:ARG:NH1	1:C:828:ASP:OD2	2.32	0.57
1:C:738:LEU:HD12	1:C:738:LEU:H	1.68	0.57
1:D:581:ASN:O	1:D:585:LEU:HD12	2.03	0.57
1:B:589:LEU:HD21	1:B:593:ARG:HE	1.69	0.57
1:C:870:VAL:HG13	1:C:874:PHE:CE2	2.40	0.57
1:B:826:LEU:HD11	1:B:830:MET:HE3	1.86	0.57
1:C:888:LEU:O	1:C:892:LEU:HD13	2.05	0.57
1:D:720:ASP:OD2	1:D:990:LYS:NZ	2.35	0.57
1:C:994:ASP:OD2	1:C:996:ARG:NE	2.37	0.57
1:D:679:ILE:HD13	1:D:700:LEU:HD21	1.86	0.57
1:A:952:ASP:O	1:A:955:SER:OG	2.14	0.56
1:B:888:LEU:O	1:B:892:LEU:HD13	2.05	0.56
1:B:928:TYR:CD1	1:B:951:LEU:HD12	2.40	0.56
1:D:807:LYS:NZ	1:D:825:GLU:OE1	2.38	0.56
1:A:562:THR:HG22	1:A:638:LYS:HB3	1.87	0.56
1:C:656:GLN:HB3	1:C:954:LEU:HD12	1.88	0.56
1:D:609:LEU:HD23	1:D:641:PHE:CD1	2.41	0.56
1:B:756:PRO:HB2	1:B:760:LEU:HD12	1.88	0.56
1:A:746:PRO:CB	1:A:747:PRO:HD2	2.34	0.56
1:D:679:ILE:HD13	1:D:700:LEU:CD2	2.35	0.56
1:D:723:ALA:HB1	1:D:960:LEU:HD22	1.88	0.56
1:C:913:GLU:OE1	1:C:913:GLU:N	2.33	0.55
1:B:812:PHE:CE2	1:B:826:LEU:HD22	2.42	0.55
1:D:679:ILE:HD12	1:D:701:PHE:CZ	2.42	0.55
1:B:994:ASP:OD1	1:B:995:ASP:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:549:ALA:HB3	1:C:653:ALA:HB1	1.89	0.54
1:B:759:TYR:O	1:B:762:ILE:HG22	2.07	0.54
1:D:826:LEU:HD11	1:D:830:MET:HE3	1.89	0.54
1:B:581:ASN:O	1:B:585:LEU:HD12	2.06	0.54
1:C:835:LEU:HD21	1:C:999:ILE:HG13	1.90	0.54
1:A:746:PRO:HB3	1:A:747:PRO:HD2	1.89	0.54
1:B:931:LEU:HD11	1:B:948:LEU:CD2	2.36	0.54
1:D:780:PHE:CD1	1:D:785:VAL:HG21	2.43	0.54
1:D:718:LEU:HD22	1:D:989:THR:HB	1.90	0.54
1:C:707:GLY:N	6:C:1202:HOH:O	2.39	0.54
1:C:791:ARG:NH1	1:C:995:ASP:O	2.40	0.54
1:D:759:TYR:O	1:D:762:ILE:HG22	2.08	0.54
1:B:665:ARG:HD2	1:B:700:LEU:O	2.08	0.53
1:D:1001:ILE:HG22	1:D:1008:MET:HE3	1.91	0.53
1:B:888:LEU:HD21	1:B:936:GLU:CB	2.39	0.53
1:C:965:THR:HG22	1:C:971:LYS:HD2	1.91	0.53
1:D:780:PHE:CD1	1:D:844:ILE:HD11	2.44	0.53
1:B:543:ALA:HB3	1:B:959:PHE:HB2	1.91	0.53
1:D:679:ILE:HG22	1:D:681:ILE:HD11	1.89	0.53
1:A:978:LYS:NZ	1:A:1006:SER:OG	2.41	0.53
1:B:740:ARG:NH2	1:B:818:VAL:O	2.40	0.53
1:B:734:LYS:O	1:B:738:LEU:CD1	2.57	0.53
1:A:659:GLU:OE1	1:A:998:TYR:OH	2.26	0.53
1:C:547:ARG:NH1	1:C:951:LEU:O	2.42	0.53
1:C:759:TYR:O	1:C:762:ILE:HG22	2.08	0.53
1:D:542:LEU:HD21	1:D:1027:GLU:CA	2.37	0.53
1:B:679:ILE:HD13	1:B:700:LEU:CD2	2.39	0.52
1:C:672:ASN:O	1:C:675:ILE:HG22	2.10	0.52
1:C:807:LYS:NZ	1:C:825:GLU:OE2	2.36	0.52
1:D:650:THR:HG23	1:D:652:SER:H	1.75	0.52
1:B:931:LEU:HD11	1:B:948:LEU:HD22	1.91	0.52
1:D:812:PHE:CE2	1:D:826:LEU:HD22	2.44	0.52
1:D:998:LEU:HD21	1:D:1002:TYR:HE2	1.75	0.52
1:B:630:LEU:HD12	1:C:634:ASN:OD1	2.09	0.52
1:C:749:PHE:CE1	1:C:882:ILE:HG23	2.45	0.52
1:D:559:HIS:ND1	1:D:609:LEU:HD11	2.25	0.51
1:A:686:GLU:OE1	1:A:688:ARG:NH1	2.43	0.51
1:C:675:ILE:HG23	1:C:676:LEU:HD22	1.92	0.51
1:D:750:ALA:O	1:D:941:PHE:HB2	2.11	0.51
1:D:789:GLN:HG2	1:D:839:GLN:HE21	1.74	0.51
1:C:764:ARG:NE	1:C:768:LEU:HD21	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:THR:OG1	1:A:978:LYS:HB2	2.11	0.51
1:C:835:LEU:HD21	1:C:999:ILE:CG1	2.41	0.51
1:A:672:ASN:O	1:A:675:ILE:HG22	2.10	0.51
1:A:961:LEU:HD11	1:A:1013:MET:HE2	1.92	0.51
1:B:770:ASN:O	1:B:773:LYS:HG2	2.11	0.51
1:B:589:LEU:HD22	2:B:2001:GOL:H2	1.93	0.51
1:C:823:ILE:HD13	1:C:871:LEU:HB3	1.93	0.51
1:B:838:ARG:HD2	1:B:993:LEU:HD12	1.92	0.51
1:B:718:LEU:HD21	1:B:898:LEU:HD13	1.93	0.50
1:D:771:TYR:CZ	1:D:775:ILE:HD11	2.46	0.50
1:A:987:ASP:O	1:A:991:VAL:HG23	2.11	0.50
1:D:770:ASN:O	1:D:773:LYS:HG2	2.12	0.50
1:D:545:ILE:O	1:D:1023:GLN:HA	2.11	0.50
1:A:656:GLN:HB3	1:A:954:LEU:HD12	1.93	0.50
1:A:874:PHE:CG	1:A:874:PHE:O	2.63	0.50
1:B:794:THR:O	1:B:795:SER:OG	2.25	0.50
1:C:762:ILE:HD12	1:C:871:LEU:HD13	1.94	0.50
1:D:762:ILE:HG23	1:D:815:ALA:HB1	1.93	0.50
1:A:892:LEU:HD12	1:A:896:LEU:HD12	1.92	0.50
1:B:714:ARG:HG2	1:B:717:LEU:HD12	1.93	0.50
1:C:945:ARG:HA	1:C:948:LEU:HD13	1.94	0.50
1:D:542:LEU:O	1:D:985:VAL:N	2.34	0.50
1:D:780:PHE:CE1	1:D:844:ILE:HD11	2.46	0.50
1:D:595:ALA:HB1	1:D:600:ALA:HB3	1.94	0.49
1:D:823:ILE:HD13	1:D:938:LEU:HB3	1.94	0.49
1:C:769:MET:SD	1:C:864:LEU:HD21	2.52	0.49
1:A:770:ASN:O	1:A:773:LYS:HG2	2.12	0.49
1:B:771:TYR:CE2	1:B:775:ILE:HD11	2.47	0.49
1:A:903:LEU:HD21	1:A:1020:LEU:CD1	2.41	0.49
1:D:718:LEU:HD21	1:D:965:LEU:HD13	1.94	0.49
1:A:605:LYS:O	1:A:609:LEU:HD13	2.12	0.49
1:D:839:GLN:O	1:D:842:GLU:HG2	2.12	0.49
1:B:888:LEU:HD21	1:B:936:GLU:HB2	1.94	0.49
1:D:575:GLU:N	1:D:575:GLU:OE1	2.46	0.49
1:B:659:GLU:CD	1:B:998:TYR:OH	2.52	0.48
1:C:558:LYS:O	1:C:559:HIS:CD2	2.66	0.48
1:A:834:ALA:O	1:A:838:ARG:HG3	2.13	0.48
1:A:985:THR:OG1	1:A:991:VAL:HG21	2.13	0.48
1:C:804:ARG:NH1	1:C:833:ASP:OD1	2.46	0.48
1:C:900:LYS:HD2	5:C:1111:ACT:H3	1.96	0.48
1:D:838:ARG:NH2	1:D:1058:VAL:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:LEU:HD23	1:A:898:LEU:HA	1.95	0.48
1:D:998:LEU:O	1:D:998:LEU:HD23	2.13	0.48
1:C:956:GLN:HG2	1:C:980:SER:HB3	1.95	0.48
1:A:745:ALA:O	1:A:746:PRO:C	2.52	0.48
1:B:615:LYS:HE3	1:B:795:SER:O	2.13	0.48
1:C:931:LEU:O	1:C:931:LEU:HD23	2.13	0.48
1:D:679:ILE:HD12	1:D:701:PHE:CE1	2.48	0.48
1:A:819:ASP:OD2	1:A:821:SER:HB3	2.14	0.48
1:B:931:LEU:HA	1:B:934:ILE:HD12	1.96	0.48
1:B:967:ALA:O	1:B:968:SER:OG	2.17	0.48
1:C:602:ASN:O	1:C:606:ILE:HD12	2.13	0.48
1:C:630:LEU:CD1	1:C:636:VAL:HG22	2.44	0.48
1:C:659:GLU:OE2	1:C:998:TYR:CZ	2.67	0.48
1:A:796:GLU:OE1	1:A:804:ARG:NH1	2.45	0.48
1:C:770:ASN:O	1:C:773:LYS:HG2	2.14	0.48
1:C:892:LEU:O	1:C:896:LEU:HB2	2.14	0.48
1:D:839:GLN:NE2	6:D:1301:HOH:O	2.38	0.48
1:B:836:HIS:HA	1:B:997:HIS:CD2	2.49	0.47
1:B:931:LEU:HD23	1:B:931:LEU:O	2.13	0.47
1:C:727:LEU:HD22	1:C:893:LEU:HD12	1.97	0.47
1:C:870:VAL:O	1:C:874:PHE:HD2	1.97	0.47
1:B:734:LYS:NZ	1:B:886:GLU:OE2	2.37	0.47
1:B:999:ILE:HG22	1:B:1000:SER:O	2.14	0.47
1:C:870:VAL:O	1:C:874:PHE:CD2	2.66	0.47
1:B:848:GLY:O	1:B:857:ARG:NH1	2.48	0.47
1:B:874:PHE:CG	1:B:874:PHE:O	2.67	0.47
1:A:848:GLY:O	1:A:857:ARG:NH1	2.47	0.47
1:D:683:SER:HB3	1:D:713:ILE:HD13	1.97	0.47
1:D:728:MET:O	1:D:732:LYS:HD3	2.14	0.47
1:B:797:ASP:HB2	1:B:798:PRO:CD	2.45	0.47
1:A:746:PRO:CB	1:A:747:PRO:CD	2.93	0.47
1:C:749:PHE:HE1	1:C:882:ILE:HG23	1.80	0.47
1:D:797:ASP:OD1	1:D:800:LEU:HD23	2.14	0.47
1:B:672:ASN:O	1:B:675:ILE:HG22	2.14	0.47
1:C:891:GLY:O	1:C:933:ILE:HD11	2.15	0.47
1:D:835:LEU:HD22	1:D:836:HIS:NE2	2.30	0.47
1:A:792:TRP:HB3	1:A:796:GLU:O	2.15	0.46
1:A:745:ALA:O	1:A:746:PRO:O	2.33	0.46
1:A:984:HIS:O	1:A:1002:ILE:HD11	2.14	0.46
1:C:849:SER:O	1:C:850:SER:OG	2.26	0.46
1:D:735:LEU:HD23	1:D:738:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:789:GLN:HG3	1:D:791:ARG:H	1.80	0.46
1:D:998:LEU:HD13	1:D:1018:LEU:HD11	1.96	0.46
1:D:547:ARG:O	1:D:1021:LEU:HD23	2.15	0.46
1:D:812:PHE:HE1	1:D:818:VAL:HG13	1.80	0.46
1:D:949:ILE:HG13	1:D:950:SER:H	1.80	0.46
1:C:931:LEU:HD12	1:C:951:LEU:HD11	1.97	0.46
1:D:789:GLN:CD	1:D:839:GLN:HG3	2.36	0.46
1:D:736:LYS:HB3	1:D:737:PRO:HD3	1.98	0.46
1:D:1024:ILE:HG22	1:D:1026:PHE:CE1	2.50	0.46
1:B:676:LEU:HA	1:B:679:ILE:HD11	1.98	0.46
1:B:896:LEU:HD23	1:B:896:LEU:O	2.16	0.46
1:C:685:SER:OG	1:C:715:LYS:HG2	2.16	0.46
1:A:614:GLU:HA	1:A:617:LEU:HD23	1.98	0.46
1:B:632:LYS:O	1:B:632:LYS:HG2	2.16	0.46
1:A:662:GLU:OE2	6:A:2101:HOH:O	2.21	0.46
1:B:679:ILE:HD12	1:B:701:PHE:CZ	2.52	0.45
1:B:764:ARG:HA	1:B:767:GLU:HG2	1.98	0.45
1:D:811:GLU:HB3	1:D:822:LYS:HD3	1.98	0.45
1:B:685:SER:OG	1:B:715:LYS:HG2	2.16	0.45
1:B:771:TYR:CZ	1:B:775:ILE:HD11	2.51	0.45
1:C:865:TYR:CE2	1:C:989:LEU:HD21	2.52	0.45
1:A:797:ASP:OD1	1:A:800:LEU:HD23	2.17	0.45
1:B:958:THR:OG1	1:B:978:LYS:HB2	2.17	0.45
1:A:830:MET:HE2	1:A:865:TYR:CD1	2.52	0.45
1:D:955:LEU:O	1:D:959:LEU:HD13	2.16	0.45
1:A:589:LEU:O	1:A:593:ARG:HD2	2.17	0.45
1:B:751:TRP:CH2	1:B:761:VAL:HG21	2.52	0.45
1:B:892:LEU:HD23	1:B:896:LEU:HD12	1.99	0.45
1:D:941:PHE:CG	1:D:941:PHE:O	2.69	0.45
1:C:854:ASP:N	1:C:854:ASP:OD1	2.50	0.45
1:D:656:GLN:HB3	1:D:1021:LEU:HD12	1.99	0.44
1:D:797:ASP:HB2	1:D:798:PRO:CD	2.46	0.44
1:B:797:ASP:OD1	1:B:800:LEU:HD23	2.17	0.44
1:D:547:ARG:NH2	1:D:991:GLU:OE1	2.50	0.44
1:C:910:LYS:HD2	1:C:1013:MET:SD	2.57	0.44
1:D:1046:MET:HB3	1:D:1074:LEU:HD21	2.00	0.44
1:A:961:LEU:HD11	1:A:1013:MET:HE3	2.00	0.44
1:A:981:PRO:HG2	1:A:1002:ILE:HD12	2.00	0.44
1:B:839:GLN:O	1:B:842:GLU:HG2	2.18	0.44
1:C:581:ASN:O	1:C:585:LEU:HD12	2.18	0.44
1:D:949:ILE:HG13	1:D:950:SER:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:680:LYS:O	1:D:985:VAL:HA	2.18	0.43
1:D:764:ARG:NH2	1:D:768:LEU:HD21	2.33	0.43
1:C:603:PRO:HB2	1:C:607:LYS:HE3	1.99	0.43
1:B:652:SER:OG	1:B:996:ARG:O	2.30	0.43
1:B:812:PHE:CD2	1:B:826:LEU:HD22	2.53	0.43
1:B:978:LYS:NZ	1:B:1006:SER:OG	2.51	0.43
1:A:805:TRP:NE1	1:A:833:ASP:OD2	2.46	0.43
1:C:545:ILE:O	1:C:956:GLN:HA	2.18	0.43
1:C:738:LEU:HD23	1:C:746:PRO:HG2	2.00	0.43
1:C:819:ASP:OD2	1:C:821:SER:HB3	2.18	0.43
1:C:965:THR:HG22	1:C:971:LYS:CD	2.49	0.43
1:D:739:LEU:HD11	1:D:942:ILE:CD1	2.49	0.43
1:D:995:TYR:CD1	1:D:1018:LEU:HD12	2.53	0.43
1:A:659:GLU:CD	1:A:998:TYR:OH	2.57	0.43
1:A:668:PHE:HB3	1:A:675:ILE:CG2	2.49	0.43
1:B:838:ARG:HD2	1:B:993:LEU:CD1	2.49	0.43
1:D:955:LEU:O	1:D:959:LEU:CD1	2.67	0.43
1:A:559:HIS:ND1	1:A:605:LYS:HE2	2.33	0.43
1:B:792:TRP:HB3	1:B:796:GLU:O	2.19	0.43
1:C:632:LYS:O	1:C:632:LYS:HG2	2.19	0.43
1:A:761:VAL:HG13	1:A:867:LEU:HD22	2.01	0.43
1:B:905:ASP:OD2	1:B:920:TYR:OH	2.34	0.43
1:C:630:LEU:HD13	1:C:636:VAL:HG22	2.01	0.43
1:C:734:LYS:O	1:C:738:LEU:CD1	2.67	0.43
1:D:549:ALA:HB2	1:D:1021:LEU:HD21	2.00	0.43
1:A:739:LEU:HD21	1:A:875:ILE:HD11	2.01	0.43
1:C:762:ILE:HD12	1:C:871:LEU:CD1	2.49	0.42
1:C:764:ARG:O	1:C:767:GLU:HG3	2.19	0.42
1:C:892:LEU:HB3	1:C:896:LEU:HD12	2.01	0.42
1:D:789:GLN:OE1	1:D:839:GLN:HG3	2.19	0.42
1:C:547:ARG:HG2	1:C:548:HIS:N	2.34	0.42
1:A:934:ILE:HG22	1:A:941:MET:CE	2.50	0.42
1:B:779:ASN:ND2	1:B:844:ILE:O	2.43	0.42
1:B:922:THR:OG1	1:B:926:HIS:HB2	2.19	0.42
1:C:604:ALA:HA	1:C:607:LYS:HD2	2.01	0.42
1:C:756:PRO:HB2	1:C:760:LEU:HD12	2.02	0.42
1:B:793:CYS:O	1:B:794:THR:OG1	2.32	0.42
1:A:791:ARG:HD2	1:A:995:ASP:OD1	2.20	0.42
1:B:545:ILE:O	1:B:956:GLN:HA	2.20	0.42
1:C:741:GLU:HG3	1:C:742:GLY:N	2.34	0.42
1:A:661:GLY:HA3	1:A:699:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:LEU:HD22	1:A:746:PRO:HG2	2.01	0.42
1:D:547:ARG:NH1	1:D:1018:LEU:O	2.53	0.42
1:D:629:VAL:HG21	1:D:638:LYS:HE3	2.02	0.42
1:A:680:LYS:HE2	1:A:918:VAL:HG22	2.02	0.42
1:A:779:ASN:ND2	1:A:844:ILE:O	2.43	0.42
1:A:788:MET:HB2	1:A:840:PHE:HD1	1.85	0.42
1:B:630:LEU:HD23	1:B:636:VAL:HA	2.01	0.42
1:D:772:HIS:CD2	1:D:928:LEU:HD13	2.55	0.42
1:A:934:ILE:HG22	1:A:941:MET:HE3	2.01	0.41
1:B:835:LEU:O	1:B:997:HIS:HB3	2.19	0.41
1:B:928:TYR:CE1	1:B:951:LEU:HD12	2.55	0.41
1:C:596:LEU:HD12	1:C:596:LEU:HA	1.91	0.41
1:C:750:ALA:O	1:C:874:PHE:HD1	2.01	0.41
1:D:589:LEU:HD11	1:D:614:GLU:HB2	2.01	0.41
1:D:1002:TYR:CD1	1:D:1008:MET:HG3	2.55	0.41
1:A:543:ALA:HB3	1:A:959:PHE:HB2	2.02	0.41
1:A:891:GLY:HA2	1:A:929:THR:HB	2.02	0.41
1:C:643:LEU:HD23	1:C:645:TRP:CE3	2.55	0.41
1:D:941:PHE:O	1:D:941:PHE:CD1	2.73	0.41
1:D:1069:ILE:HG23	1:D:1070:PRO:HD2	2.02	0.41
1:C:764:ARG:CZ	1:C:768:LEU:HD21	2.50	0.41
1:D:672:ASN:O	1:D:675:ILE:HG22	2.20	0.41
1:B:559:HIS:HD2	1:B:605:LYS:HE2	1.84	0.41
1:B:812:PHE:HE1	1:B:818:VAL:HG13	1.83	0.41
1:B:910:LYS:HG3	1:B:973:HIS:CE1	2.55	0.41
1:D:547:ARG:HG2	1:D:548:HIS:N	2.36	0.41
1:C:738:LEU:HD22	1:C:749:PHE:HE2	1.86	0.41
1:D:764:ARG:HA	1:D:767:GLU:HG2	2.03	0.41
1:C:664:MET:CE	1:C:696:TRP:HE1	2.34	0.41
1:C:714:ARG:NH2	1:C:717:LEU:HD11	2.35	0.41
1:C:791:ARG:O	1:C:791:ARG:HG3	2.20	0.41
1:A:736:LYS:HB3	1:A:740:ARG:HH12	1.85	0.41
1:C:588:VAL:HG12	1:C:592:LEU:CD1	2.51	0.41
1:D:668:PHE:HB3	1:D:675:ILE:CG2	2.51	0.41
1:D:542:LEU:N	1:D:984:CYS:HA	2.35	0.41
1:D:584:ASP:O	1:D:588:VAL:HG23	2.20	0.41
1:A:562:THR:HG22	1:A:638:LYS:CB	2.51	0.41
1:A:658:THR:HA	1:A:699:ALA:HB2	2.03	0.41
1:B:557:PHE:CE2	1:B:645:TRP:HH2	2.39	0.41
1:C:656:GLN:HB3	1:C:954:LEU:CD1	2.50	0.41
1:C:664:MET:HE3	1:C:696:TRP:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:736:LYS:N	1:C:737:PRO:HD2	2.36	0.41
1:D:558:LYS:HD2	1:D:640:GLN:OE1	2.20	0.41
1:A:675:ILE:HG23	1:A:676:LEU:HD22	2.03	0.41
1:B:634:ASN:ND2	1:C:630:LEU:HB3	2.36	0.41
1:D:749:PHE:CD1	1:D:945:LYS:HE3	2.56	0.41
1:D:812:PHE:CD2	1:D:826:LEU:HD22	2.56	0.41
1:A:747:PRO:HG2	1:A:749:PHE:CE1	2.56	0.40
1:B:846:ASP:OD1	1:B:846:ASP:O	2.38	0.40
1:C:717:LEU:HD21	1:C:901:GLN:HB2	2.03	0.40
1:A:764:ARG:O	1:A:768:LEU:HD23	2.22	0.40
1:B:927:ILE:HG22	1:B:951:LEU:HD13	2.04	0.40
1:C:976:ARG:HE	1:C:978:LYS:HZ3	1.69	0.40
1:B:811:GLU:HG2	1:B:822:LYS:HG3	2.03	0.40
1:D:585:LEU:HB2	1:D:617:LEU:CD1	2.51	0.40
1:A:557:PHE:HD1	1:A:558:LYS:N	2.19	0.40
1:A:605:LYS:O	1:A:609:LEU:CD1	2.70	0.40
1:C:797:ASP:OD1	1:C:800:LEU:HD23	2.22	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:B:990:ASP:O	1:D:919:GLN:NE2[3_556]	2.13	0.07

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	462/507 (91%)	446 (96%)	15 (3%)	1 (0%)	44	72
1	B	473/507 (93%)	462 (98%)	11 (2%)	0	100	100
1	C	480/507 (95%)	463 (96%)	16 (3%)	1 (0%)	44	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	456/507 (90%)	443 (97%)	13 (3%)	0	100	100
All	All	1871/2028 (92%)	1814 (97%)	55 (3%)	2 (0%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	746	PRO
1	C	741	GLU

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	429/459 (94%)	425 (99%)	4 (1%)	75	86
1	B	436/459 (95%)	435 (100%)	1 (0%)	92	96
1	C	438/459 (95%)	437 (100%)	1 (0%)	92	96
1	D	421/459 (92%)	419 (100%)	2 (0%)	86	91
All	All	1724/1836 (94%)	1716 (100%)	8 (0%)	86	91

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

Mol	Chain	Res	Type
1	A	551	ARG
1	A	557	PHE
1	A	874	PHE
1	A	998	TYR
1	B	814	ASN
1	C	672	ASN
1	D	791	ARG
1	D	941	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 38 ligands modelled in this entry, 6 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	GOL	A	2002	-	5,5,5	0.34	0	5,5,5	0.31	0
5	ACT	C	1106	-	3,3,3	1.11	0	3,3,3	1.23	0
2	GOL	B	2003	-	5,5,5	0.33	0	5,5,5	0.37	0
2	GOL	A	2007	-	5,5,5	0.33	0	5,5,5	0.34	0
2	GOL	A	2009	-	5,5,5	0.34	0	5,5,5	0.36	0
2	GOL	D	1202	-	5,5,5	0.34	0	5,5,5	0.40	0
5	ACT	C	1111	-	3,3,3	1.09	0	3,3,3	1.25	0
2	GOL	C	1103	-	5,5,5	0.34	0	5,5,5	0.30	0
2	GOL	A	2004	-	5,5,5	0.33	0	5,5,5	0.34	0
2	GOL	A	2010	-	5,5,5	0.35	0	5,5,5	0.35	0
2	GOL	C	1109	-	5,5,5	0.34	0	5,5,5	0.35	0
2	GOL	B	2006	-	5,5,5	0.34	0	5,5,5	0.35	0
4	LPC	B	2004	-	29,29,30	1.16	2 (6%)	34,36,37	0.65	1 (2%)
5	ACT	C	1110	-	3,3,3	1.07	0	3,3,3	1.24	0
5	ACT	D	1204	-	3,3,3	1.07	0	3,3,3	1.22	0
2	GOL	B	2001	-	5,5,5	0.33	0	5,5,5	0.36	0
2	GOL	A	2003	-	5,5,5	0.33	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	ACT	D	1205	-	3,3,3	1.09	0	3,3,3	1.21	0
2	GOL	B	2005	-	5,5,5	0.36	0	5,5,5	0.39	0
5	ACT	D	1203	-	3,3,3	1.10	0	3,3,3	1.20	0
5	ACT	C	1105	-	3,3,3	1.10	0	3,3,3	1.18	0
2	GOL	B	2002	-	5,5,5	0.34	0	5,5,5	0.36	0
2	GOL	A	2006	-	5,5,5	0.34	0	5,5,5	0.38	0
2	GOL	A	2001	-	5,5,5	0.34	0	5,5,5	0.34	0
2	GOL	A	2008	-	5,5,5	0.35	0	5,5,5	0.35	0
2	GOL	A	2005	-	5,5,5	0.33	0	5,5,5	0.35	0
5	ACT	C	1104	-	3,3,3	1.09	0	3,3,3	1.21	0
2	GOL	C	1108	-	5,5,5	0.33	0	5,5,5	0.29	0
2	GOL	C	1101	-	5,5,5	0.34	0	5,5,5	0.36	0
5	ACT	C	1102	-	3,3,3	1.10	0	3,3,3	1.19	0
2	GOL	D	1201	-	5,5,5	0.34	0	5,5,5	0.23	0
2	GOL	C	1107	-	5,5,5	0.35	0	5,5,5	0.33	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
2	GOL	A	2002	-	-	0/4/4/4	-
2	GOL	B	2003	-	-	2/4/4/4	-
2	GOL	A	2007	-	-	2/4/4/4	-
2	GOL	A	2009	-	-	0/4/4/4	-
2	GOL	D	1202	-	-	2/4/4/4	-
2	GOL	C	1103	-	-	4/4/4/4	-
2	GOL	A	2004	-	-	0/4/4/4	-
2	GOL	A	2010	-	-	0/4/4/4	-
2	GOL	C	1109	-	-	0/4/4/4	-
2	GOL	B	2006	-	-	0/4/4/4	-
4	LPC	B	2004	-	-	17/31/31/32	-
2	GOL	B	2001	-	-	1/4/4/4	-
2	GOL	A	2003	-	-	0/4/4/4	-
2	GOL	B	2005	-	-	2/4/4/4	-
2	GOL	B	2002	-	-	0/4/4/4	-
2	GOL	A	2006	-	-	0/4/4/4	-
2	GOL	A	2001	-	-	0/4/4/4	-
2	GOL	A	2008	-	-	0/4/4/4	-
2	GOL	A	2005	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	1108	-	-	<mark>2/4/4/4</mark>	-
2	GOL	C	1101	-	-	0/4/4/4	-
2	GOL	D	1201	-	-	<mark>2/4/4/4</mark>	-
2	GOL	C	1107	-	-	<mark>2/4/4/4</mark>	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2004	LPC	OQ2-CA	3.22	1.42	1.33
4	B	2004	LPC	P5-O4	2.06	1.67	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2004	LPC	OQ2-CA-CB	2.47	119.67	111.91

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2005	GOL	O1-C1-C2-C3
2	B	2003	GOL	C1-C2-C3-O3
2	C	1103	GOL	O1-C1-C2-O2
2	C	1103	GOL	O1-C1-C2-C3
2	C	1103	GOL	C1-C2-C3-O3
2	C	1108	GOL	C1-C2-C3-O3
2	D	1201	GOL	C1-C2-C3-O3
4	B	2004	LPC	C3-O4-P5-O5A
4	B	2004	LPC	C3-O4-P5-O5B
4	B	2004	LPC	C7-O6-P5-O4
4	B	2004	LPC	C7-O6-P5-O5A
4	B	2004	LPC	C7-O6-P5-O5B
4	B	2004	LPC	C7-C8-C9-OQ2
4	B	2004	LPC	O8-C8-C9-OQ2
4	B	2004	LPC	CB-CA-OQ2-C9
4	B	2004	LPC	OQ1-CA-OQ2-C9
2	A	2007	GOL	O1-C1-C2-O2
2	D	1201	GOL	O2-C2-C3-O3
4	B	2004	LPC	C3-O4-P5-O6
4	B	2004	LPC	CF-CG-CH-CI

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Mol	Chain	Res	Type	Atoms
2	A	2007	GOL	O1-C1-C2-C3
2	B	2005	GOL	O1-C1-C2-C3
2	C	1107	GOL	C1-C2-C3-O3
2	A	2005	GOL	O1-C1-C2-O2
2	B	2003	GOL	O2-C2-C3-O3
2	B	2005	GOL	O1-C1-C2-O2
2	C	1103	GOL	O2-C2-C3-O3
2	C	1108	GOL	O2-C2-C3-O3
4	B	2004	LPC	CC-CD-CE-CF
4	B	2004	LPC	CH-CI-CJ-CK
4	B	2004	LPC	CJ-CK-CL-CM
2	D	1202	GOL	O1-C1-C2-O2
2	C	1107	GOL	O2-C2-C3-O3
4	B	2004	LPC	CA-CB-CC-CD
4	B	2004	LPC	C8-C7-O6-P5
2	B	2001	GOL	O1-C1-C2-C3
2	D	1202	GOL	O1-C1-C2-C3
4	B	2004	LPC	OQ2-CA-CB-CC

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1111	ACT	2	0
2	B	2001	GOL	1	0
2	A	2001	GOL	1	0
2	A	2008	GOL	1	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 then 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.

Ligand LPC B 2004	
Bond lengths	Bond angles
Torsions	Rings
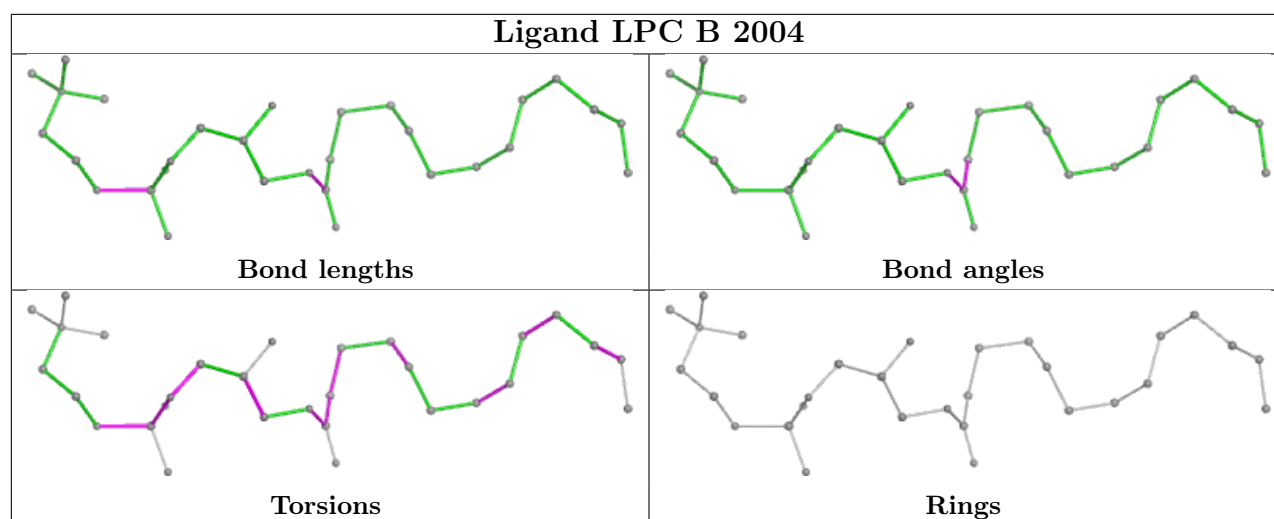
5.7 Other polymers ⓘ

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 ⓘ

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	470/507 (92%)	-0.25	3 (0%)	85	80	58, 110, 163, 227	0
1	B	479/507 (94%)	-0.23	1 (0%)	92	92	66, 113, 162, 194	0
1	C	484/507 (95%)	-0.14	6 (1%)	76	68	59, 112, 166, 201	0
1	D	462/507 (91%)	-0.17	1 (0%)	92	92	68, 120, 183, 224	0
All	All	1895/2028 (93%)	-0.20	11 (0%)	85	80	58, 114, 171, 227	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	557	PHE	4.6
1	A	851	GLY	3.7
1	C	874	PHE	3.2
1	C	937	SER	2.8
1	A	844	ILE	2.5
1	C	979	MET	2.3
1	C	703	ALA	2.3
1	A	749	PHE	2.2
1	C	609	LEU	2.2
1	C	831	LYS	2.2
1	D	1072	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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.
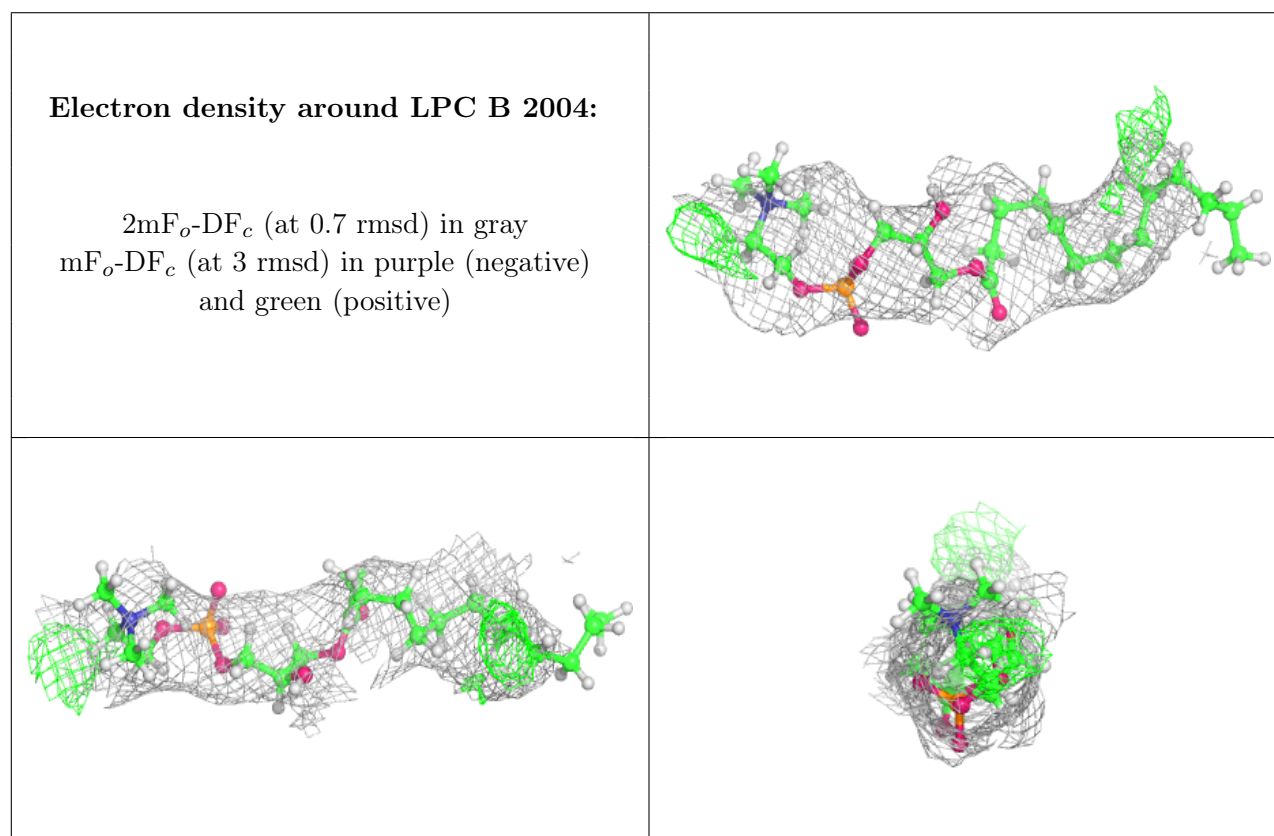
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
5	ACT	D	1205	4/4	0.26	0.14	99,119,122,130	0
2	GOL	C	1107	6/6	0.40	0.14	116,143,173,173	0
2	GOL	B	2006	6/6	0.41	0.12	98,134,161,161	0
5	ACT	D	1204	4/4	0.46	0.18	118,132,141,141	0
2	GOL	A	2008	6/6	0.50	0.13	107,129,149,155	0
5	ACT	C	1102	4/4	0.50	0.11	96,107,115,115	0
2	GOL	B	2001	6/6	0.55	0.14	89,115,137,144	0
5	ACT	D	1203	4/4	0.55	0.29	84,101,102,105	0
2	GOL	A	2003	6/6	0.58	0.09	120,145,166,166	0
2	GOL	A	2007	6/6	0.64	0.14	101,131,150,161	0
5	ACT	C	1111	4/4	0.65	0.13	83,103,135,135	0
4	LPC	B	2004	30/31	0.65	0.16	83,141,199,226	0
2	GOL	A	2009	6/6	0.67	0.09	86,135,160,172	0
5	ACT	C	1104	4/4	0.67	0.19	79,99,99,104	0
5	ACT	C	1105	4/4	0.78	0.15	73,87,95,97	0
2	GOL	C	1101	6/6	0.79	0.10	68,107,126,129	0
2	GOL	A	2004	6/6	0.80	0.10	79,125,153,153	0
2	GOL	A	2005	6/6	0.81	0.11	70,101,133,135	0
2	GOL	A	2010	6/6	0.82	0.11	87,125,152,166	0
5	ACT	C	1110	4/4	0.82	0.18	79,95,118,118	0
2	GOL	A	2001	6/6	0.82	0.08	93,128,153,153	0
2	GOL	D	1201	6/6	0.83	0.12	81,116,149,167	0
2	GOL	A	2006	6/6	0.84	0.08	102,122,136,136	0
2	GOL	A	2002	6/6	0.85	0.09	84,108,125,130	0
2	GOL	C	1108	6/6	0.85	0.12	79,116,126,139	0
5	ACT	C	1106	4/4	0.86	0.14	59,70,78,79	0
2	GOL	C	1109	6/6	0.86	0.08	76,109,142,142	0
2	GOL	B	2002	6/6	0.87	0.14	71,107,128,128	0
2	GOL	B	2003	6/6	0.87	0.09	49,96,117,117	0
2	GOL	B	2005	6/6	0.89	0.23	69,93,109,112	0
2	GOL	C	1103	6/6	0.90	0.15	100,120,133,142	0
2	GOL	D	1202	6/6	0.94	0.15	59,72,83,90	0
3	ZN	B	2007	1/1	0.98	0.10	134,134,134,134	0
3	ZN	A	2012	1/1	0.99	0.04	108,108,108,108	0
3	ZN	A	2011	1/1	0.99	0.02	58,58,58,58	0
3	ZN	B	2008	1/1	0.99	0.03	115,115,115,115	0
3	ZN	C	1112	1/1	0.99	0.09	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	ZN	D	1206	1/1	0.99	0.03	95,95,95,95	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 LPC B 2004:

$2mF_o$-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 ⓘ

There are no such residues in this entry.