Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:12 PM GMT

PDB ID	:	1EIN
Title	:	THE STRUCTURAL ORIGINS OF INTERFACIAL ACTIVATION IN THERMOMYCES (HUMICOLA) LANUGINOSA LIPASE
Authors	:	Brozozowski, A.M.; Savage, H.
Deposited on	:	2000-02-26
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

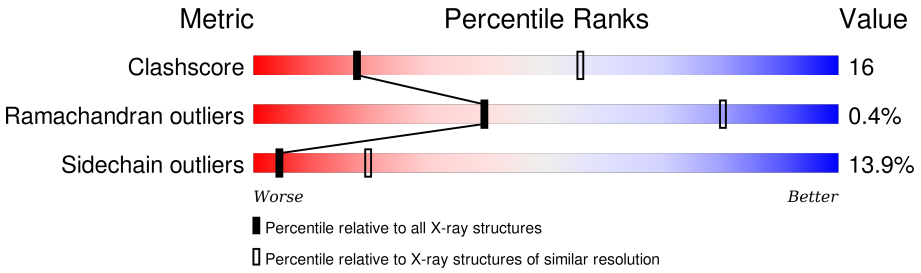
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	269	62% 30% 6% •
1	B	269	60% 33% 5% •
1	C	269	58% 34% 6% •

2 Entry composition

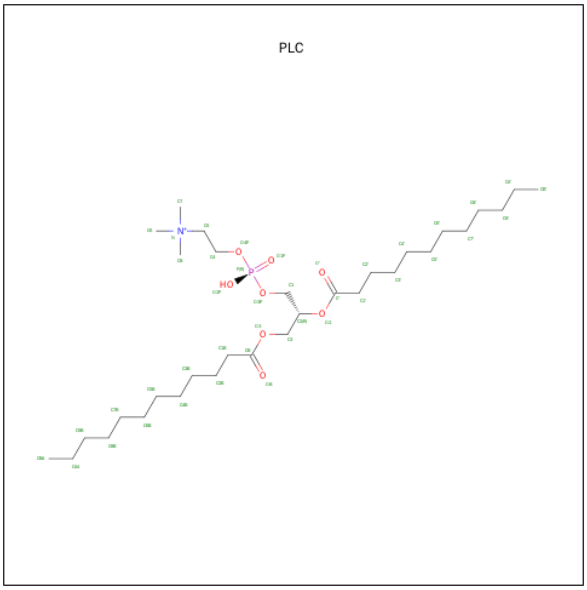
There are 3 unique types of molecules in this entry. The entry contains 6499 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LIPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2063	1301	356	400	6			
1	B	269	Total	C	N	O	S	0	0	0
			2063	1301	356	400	6			
1	C	269	Total	C	N	O	S	0	0	0
			2063	1301	356	400	6			

- Molecule 2 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			42	32	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			42	32	1	8	1		
2	C	1	Total	C	N	O	P	0	0
			42	32	1	8	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	68	Total O 68 68	0	0
3	B	57	Total O 57 57	0	0
3	C	59	Total O 59 59	0	0

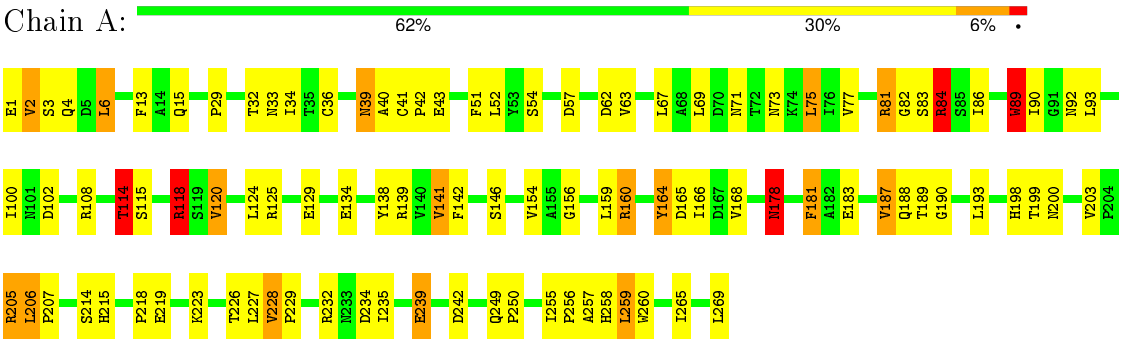
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

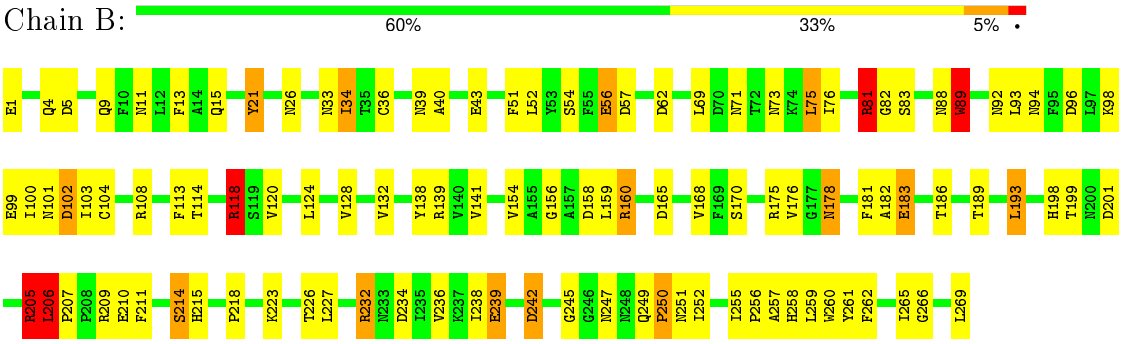
- Molecule 1: LIPASE

Chain A:



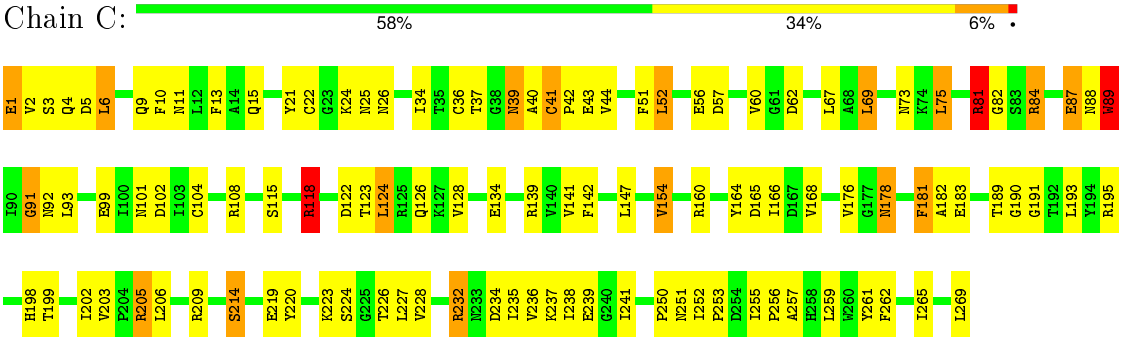
- Molecule 1: LIPASE

Chain B:



- Molecule 1: LIPASE

Chain C:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	135.95Å 135.95Å 149.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.40 – 3.00	Depositor
% Data completeness (in resolution range)	99.8 (27.40-3.00)	Depositor
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6499	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.43	0/2113	1.21	12/2878 (0.4%)
1	B	0.43	0/2113	1.30	18/2878 (0.6%)
1	C	0.42	0/2113	1.27	14/2878 (0.5%)
All	All	0.43	0/6339	1.26	44/8634 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	7
1	C	0	10
All	All	0	28

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	118	ARG	NE-CZ-NH1	11.11	125.85	120.30
1	C	81	ARG	CD-NE-CZ	10.95	138.93	123.60
1	B	160	ARG	NE-CZ-NH1	-10.88	114.86	120.30
1	C	205	ARG	NE-CZ-NH2	10.60	125.60	120.30
1	C	209	ARG	NE-CZ-NH2	-10.57	115.01	120.30
1	B	205	ARG	NE-CZ-NH2	10.44	125.52	120.30
1	A	81	ARG	CG-CD-NE	8.95	130.59	111.80
1	C	209	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	C	195	ARG	CD-NE-CZ	8.66	135.73	123.60
1	C	118	ARG	NE-CZ-NH1	8.20	124.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	118	ARG	NE-CZ-NH1	8.15	124.37	120.30
1	B	5	ASP	CB-CG-OD1	-7.70	111.37	118.30
1	A	118	ARG	CD-NE-CZ	7.70	134.38	123.60
1	B	81	ARG	CD-NE-CZ	7.68	134.35	123.60
1	B	158	ASP	CB-CG-OD1	7.57	125.11	118.30
1	A	160	ARG	NE-CZ-NH1	-7.43	116.59	120.30
1	C	195	ARG	NE-CZ-NH1	-7.41	116.59	120.30
1	B	118	ARG	CD-NE-CZ	7.36	133.90	123.60
1	B	205	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	B	118	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	89	TRP	CA-CB-CG	-6.97	100.47	113.70
1	C	5	ASP	CB-CG-OD1	-6.87	112.11	118.30
1	B	89	TRP	CA-CB-CG	-6.77	100.83	113.70
1	A	84	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	B	209	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	205	ARG	CD-NE-CZ	6.61	132.86	123.60
1	A	205	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	B	206	LEU	CA-CB-CG	6.50	130.24	115.30
1	C	89	TRP	CA-CB-CG	-6.43	101.48	113.70
1	A	242	ASP	CB-CG-OD1	-5.95	112.94	118.30
1	C	195	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	C	84	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	C	160	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	B	56	GLU	OE1-CD-OE2	5.56	129.97	123.30
1	B	242	ASP	CB-CG-OD1	-5.56	113.29	118.30
1	B	242	ASP	CB-CG-OD2	5.56	123.31	118.30
1	C	118	ARG	CD-NE-CZ	5.46	131.24	123.60
1	A	81	ARG	CA-CB-CG	5.37	125.22	113.40
1	B	102	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	91	GLY	O-C-N	-5.21	114.36	122.70
1	A	125	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	118	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	114	THR	CA-CB-CG2	-5.10	105.26	112.40
1	B	96	ASP	CB-CG-OD1	-5.01	113.79	118.30

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	GLU	Mainchain
1	A	134	GLU	Mainchain
1	A	141	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	A	164	TYR	Mainchain
1	A	178	ASN	Mainchain
1	A	214	SER	Mainchain
1	A	235	ILE	Mainchain
1	A	265	ILE	Mainchain
1	A	3	SER	Mainchain
1	A	41	CYS	Mainchain
1	A	92	ASN	Mainchain
1	B	113	PHE	Mainchain
1	B	165	ASP	Mainchain
1	B	21	TYR	Mainchain
1	B	250	PRO	Mainchain
1	B	33	ASN	Mainchain
1	B	76	ILE	Mainchain
1	B	94	ASN	Mainchain
1	C	134	GLU	Mainchain
1	C	203	VAL	Mainchain
1	C	262	PHE	Mainchain
1	C	3	SER	Mainchain
1	C	41	CYS	Mainchain
1	C	51	PHE	Mainchain
1	C	67	LEU	Mainchain
1	C	69	LEU	Mainchain
1	C	87	GLU	Mainchain
1	C	91	GLY	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2063	0	1956	50	0
1	B	2063	0	1956	62	0
1	C	2063	0	1956	64	0
2	A	42	0	64	15	0
2	B	42	0	64	12	0
2	C	42	0	64	16	0
3	A	68	0	0	1	0
3	B	57	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	59	0	0	0	0
All	All	6499	0	6060	197	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 16.

All (197) 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:15:GLN:HE22	1:B:43:GLU:H	1.09	0.97
1:A:15:GLN:HE22	1:A:43:GLU:H	1.18	0.91
2:A:601:PLC:H5'2	1:C:89:TRP:HZ3	1.39	0.87
1:B:81:ARG:HG2	1:B:81:ARG:HH21	1.39	0.87
1:C:36:CYS:HB3	1:C:40:ALA:HB3	1.56	0.86
1:C:118:ARG:HH11	1:C:118:ARG:HG3	1.43	0.84
2:C:801:PLC:H11	2:C:801:PLC:O'	1.77	0.83
1:B:36:CYS:HB3	1:B:40:ALA:HB3	1.65	0.79
2:B:701:PLC:HE'1	2:C:801:PLC:HT'1	1.66	0.78
1:A:178:ASN:ND2	1:A:181:PHE:H	1.82	0.76
1:A:118:ARG:HG3	1:A:118:ARG:HH11	1.52	0.75
1:A:15:GLN:HE22	1:A:43:GLU:N	1.84	0.73
1:B:118:ARG:HG3	1:B:118:ARG:HH11	1.54	0.72
1:A:73:ASN:HB2	1:A:75:LEU:HD22	1.70	0.72
2:A:601:PLC:H52	2:C:801:PLC:H72	1.72	0.71
1:B:261:TYR:HB2	1:B:265:ILE:HG21	1.74	0.70
1:C:202:ILE:HB	1:C:253:PRO:HB2	1.75	0.68
2:B:701:PLC:H81	2:C:801:PLC:O1P	1.93	0.68
1:B:15:GLN:HE22	1:B:43:GLU:N	1.89	0.67
1:A:218:PRO:HB3	1:A:239:GLU:HG3	1.77	0.67
1:A:100:ILE:HG21	1:A:114:THR:HG21	1.77	0.66
1:C:178:ASN:ND2	1:C:181:PHE:H	1.94	0.65
1:C:73:ASN:HB2	1:C:75:LEU:HD22	1.79	0.65
2:B:701:PLC:O'	2:B:701:PLC:H11	1.98	0.64
1:C:99:GLU:HA	1:C:108:ARG:HG2	1.81	0.63
1:B:252:ILE:HD12	1:B:252:ILE:H	1.63	0.63
1:A:36:CYS:HB3	1:A:40:ALA:HB3	1.81	0.63
1:A:226:THR:HG23	1:A:260:TRP:HB2	1.82	0.62
1:B:73:ASN:HB2	1:B:75:LEU:HD22	1.81	0.61
1:A:39:ASN:O	1:A:42:PRO:HD3	2.01	0.61
1:B:223:LYS:HG2	1:B:234:ASP:O	2.00	0.61
2:A:601:PLC:P	2:C:801:PLC:H61	2.40	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:GLN:HE22	1:C:43:GLU:H	1.49	0.60
1:A:100:ILE:CG2	1:A:114:THR:HG21	2.32	0.59
1:C:4:GLN:NE2	1:C:232:ARG:HD3	2.18	0.59
1:C:261:TYR:HB2	1:C:265:ILE:HG21	1.85	0.59
1:C:226:THR:O	1:C:227:LEU:HB2	2.03	0.58
1:B:176:VAL:HG12	3:B:738:HOH:O	2.03	0.58
1:C:81:ARG:HH21	1:C:81:ARG:HG2	1.69	0.58
1:C:223:LYS:HG2	1:C:234:ASP:O	2.04	0.57
2:C:801:PLC:O'	2:C:801:PLC:C1	2.46	0.57
1:C:10:PHE:HD2	1:C:235:ILE:HD13	1.69	0.57
1:C:21:TYR:OH	1:C:82:GLY:HA3	2.05	0.56
1:B:99:GLU:HA	1:B:108:ARG:HG2	1.87	0.56
1:A:156:GLY:O	1:A:160:ARG:HG3	2.05	0.56
1:C:124:LEU:O	1:C:128:VAL:HG23	2.05	0.56
1:C:183:GLU:HG3	1:C:241:ILE:HD12	1.88	0.56
1:A:81:ARG:HD2	1:A:82:GLY:O	2.05	0.56
1:A:34:ILE:HG13	1:A:51:PHE:CZ	2.41	0.56
1:A:146:SER:HB2	1:A:258:HIS:CE1	2.41	0.56
1:C:24:LYS:HE2	1:C:37:THR:HG23	1.87	0.56
1:B:4:GLN:HA	1:B:232:ARG:HD2	1.87	0.55
1:A:249:GLN:HB3	1:A:250:PRO:HD2	1.87	0.55
1:C:252:ILE:HD12	1:C:252:ILE:N	2.21	0.55
2:A:601:PLC:H51	2:C:801:PLC:H63	1.89	0.54
1:B:255:ILE:H	1:B:256:PRO:HD2	1.73	0.54
2:A:601:PLC:HT'1	2:C:801:PLC:HE'1	1.90	0.54
1:C:34:ILE:HG21	1:C:44:VAL:HG11	1.90	0.54
2:B:701:PLC:H61	2:C:801:PLC:P	2.48	0.53
1:B:108:ARG:H	1:B:178:ASN:ND2	2.06	0.53
1:B:255:ILE:N	1:B:256:PRO:HD2	2.24	0.53
1:A:203:VAL:HG22	2:A:601:PLC:H2	1.90	0.53
1:B:81:ARG:HG2	1:B:81:ARG:NH2	2.15	0.53
1:C:26:ASN:HB3	1:C:56:GLU:HB3	1.91	0.52
1:B:178:ASN:ND2	1:B:181:PHE:H	2.07	0.52
1:C:252:ILE:H	1:C:252:ILE:HD12	1.73	0.52
1:C:198:HIS:HD2	1:C:257:ALA:O	1.93	0.52
1:B:15:GLN:NE2	1:B:43:GLU:H	1.93	0.52
1:B:128:VAL:O	1:B:132:VAL:HG23	2.09	0.52
1:B:226:THR:O	1:B:227:LEU:HB2	2.10	0.51
2:B:701:PLC:C8	1:C:255:ILE:HG13	2.41	0.51
1:B:250:PRO:O	1:B:251:ASN:HB3	2.10	0.51
1:C:142:PHE:HB2	1:C:168:VAL:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:PLC:CA'	2:C:801:PLC:HE'1	2.41	0.51
1:C:198:HIS:HE1	1:C:224:SER:O	1.94	0.51
1:A:226:THR:O	1:A:227:LEU:HB2	2.11	0.51
1:C:13:PHE:CE2	1:C:141:VAL:HG11	2.46	0.51
1:A:73:ASN:CB	1:A:75:LEU:HD22	2.40	0.51
2:B:701:PLC:H71	2:C:801:PLC:O4P	2.11	0.51
1:C:164:TYR:HE2	1:C:166:ILE:HD11	1.76	0.50
1:B:26:ASN:HB3	1:B:56:GLU:HB3	1.92	0.50
1:C:236:VAL:HG12	1:C:238:ILE:HD12	1.92	0.50
2:B:701:PLC:CB'	2:C:801:PLC:HT'1	2.38	0.50
1:B:57:ASP:HA	1:B:62:ASP:OD1	2.11	0.49
1:A:255:ILE:N	1:A:256:PRO:HD2	2.28	0.49
1:C:118:ARG:NH1	1:C:118:ARG:HG3	2.15	0.49
1:B:4:GLN:NE2	1:B:232:ARG:HD3	2.27	0.49
1:C:57:ASP:HA	1:C:62:ASP:OD1	2.12	0.49
1:C:81:ARG:HG2	1:C:82:GLY:O	2.13	0.49
1:A:164:TYR:HE2	1:A:166:ILE:HD11	1.79	0.48
1:A:84:ARG:HD3	3:A:659:HOH:O	2.12	0.48
1:C:166:ILE:O	1:C:191:GLY:HA3	2.13	0.48
1:C:220:TYR:CE2	1:C:237:LYS:HG3	2.47	0.48
1:C:165:ASP:HA	1:C:190:GLY:O	2.14	0.48
1:B:21:TYR:OH	1:B:82:GLY:HA3	2.13	0.48
1:C:92:ASN:HB3	2:C:801:PLC:H3A1	1.94	0.48
1:C:39:ASN:O	1:C:42:PRO:HD3	2.14	0.48
2:A:601:PLC:O4P	2:C:801:PLC:H61	2.14	0.48
1:B:226:THR:HG23	1:B:260:TRP:HB2	1.96	0.48
1:A:2:VAL:HG13	1:A:6:LEU:HB3	1.95	0.48
1:C:101:ASN:HA	1:C:104:CYS:O	2.14	0.47
1:A:71:ASN:ND2	1:A:138:TYR:OH	2.44	0.47
1:B:156:GLY:O	1:B:160:ARG:HG3	2.14	0.47
1:A:57:ASP:HA	1:A:62:ASP:OD1	2.14	0.47
2:A:601:PLC:HE'1	2:B:701:PLC:HT'1	1.95	0.47
1:B:201:ASP:OD1	1:B:258:HIS:HB2	2.15	0.47
1:A:187:VAL:O	1:A:188:GLN:C	2.54	0.47
1:A:89:TRP:CZ3	1:A:93:LEU:HD11	2.49	0.47
1:B:92:ASN:HB3	2:B:701:PLC:H3A2	1.96	0.47
1:C:108:ARG:H	1:C:178:ASN:ND2	2.13	0.47
1:B:34:ILE:HD12	1:B:51:PHE:CE2	2.49	0.47
1:B:102:ASP:OD1	1:B:118:ARG:NH2	2.48	0.46
1:C:102:ASP:OD1	1:C:118:ARG:NH2	2.46	0.46
2:A:601:PLC:C1	2:A:601:PLC:O'	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:H	1:A:178:ASN:ND2	2.14	0.46
1:C:154:VAL:HG12	1:C:176:VAL:HG21	1.97	0.46
1:B:211:PHE:HB3	1:C:227:LEU:HD12	1.97	0.46
1:B:178:ASN:HD22	1:B:178:ASN:N	2.13	0.46
1:B:13:PHE:CZ	1:B:141:VAL:HG21	2.50	0.46
1:B:175:ARG:HG2	1:B:215:HIS:CD2	2.50	0.46
1:A:165:ASP:HA	1:A:190:GLY:O	2.15	0.46
1:C:102:ASP:OD2	1:C:102:ASP:N	2.48	0.46
1:A:146:SER:HB2	1:A:258:HIS:NE2	2.31	0.46
2:A:601:PLC:C'	2:A:601:PLC:O3P	2.63	0.46
2:B:701:PLC:H42	2:B:701:PLC:H73	1.47	0.46
1:A:29:PRO:HD2	1:A:32:THR:HG21	1.97	0.46
1:A:39:ASN:HD22	1:A:39:ASN:HA	1.48	0.45
1:C:73:ASN:CB	1:C:75:LEU:HD22	2.45	0.45
1:A:67:LEU:HD12	1:A:77:VAL:O	2.16	0.45
1:C:122:ASP:O	1:C:123:THR:C	2.54	0.45
1:C:250:PRO:O	1:C:251:ASN:HB3	2.16	0.45
2:B:701:PLC:H1'2	2:B:701:PLC:H4'2	1.82	0.45
1:C:232:ARG:HG3	1:C:232:ARG:NH2	2.32	0.45
1:B:9:GLN:OE1	1:B:139:ARG:NH1	2.49	0.45
1:B:261:TYR:O	1:B:262:PHE:HB2	2.17	0.45
1:C:87:GLU:O	1:C:88:ASN:C	2.54	0.45
1:B:89:TRP:HZ3	2:C:801:PLC:H4'1	1.82	0.45
1:A:4:GLN:NE2	1:A:232:ARG:HD3	2.31	0.45
1:C:182:ALA:HB2	1:C:214:SER:HB3	1.98	0.45
1:A:206:LEU:HA	1:A:207:PRO:C	2.36	0.45
1:B:249:GLN:HB3	1:B:250:PRO:HD2	1.99	0.44
1:B:21:TYR:CD2	1:B:266:GLY:HA2	2.52	0.44
1:C:75:LEU:HD12	1:C:139:ARG:HB3	1.99	0.44
1:B:198:HIS:HD2	1:B:257:ALA:O	1.99	0.44
1:C:22:CYS:HB2	1:C:25:ASN:ND2	2.33	0.44
2:C:801:PLC:H1'2	2:C:801:PLC:H4'2	1.55	0.44
1:B:101:ASN:HA	1:B:104:CYS:O	2.18	0.44
1:B:98:LYS:HE2	1:B:114:THR:HG21	1.99	0.44
1:A:84:ARG:O	2:A:601:PLC:H8'2	2.18	0.44
1:A:200:ASN:OD1	1:A:200:ASN:N	2.50	0.44
1:C:1:GLU:HB3	1:C:235:ILE:O	2.18	0.43
1:B:182:ALA:HB2	1:B:214:SER:HB3	2.00	0.43
1:A:15:GLN:NE2	1:A:43:GLU:HB2	2.34	0.43
1:A:102:ASP:OD1	1:A:118:ARG:NH2	2.51	0.43
1:C:92:ASN:ND2	1:C:147:LEU:HD13	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PHE:CZ	1:A:141:VAL:HG21	2.54	0.43
1:B:21:TYR:HA	1:B:81:ARG:HD3	1.99	0.43
1:A:198:HIS:HD2	1:A:257:ALA:O	2.01	0.43
2:A:601:PLC:H5'2	1:C:89:TRP:CZ3	2.32	0.43
1:B:218:PRO:HB3	1:B:239:GLU:HG3	2.01	0.43
2:B:701:PLC:H1A2	2:B:701:PLC:H32	1.63	0.43
1:A:223:LYS:NZ	1:A:234:ASP:HA	2.34	0.43
1:B:98:LYS:HG2	1:B:99:GLU:H	1.84	0.43
1:B:245:GLY:H	1:B:249:GLN:HG2	1.84	0.43
1:B:214:SER:OG	1:B:242:ASP:OD1	2.37	0.43
1:A:228:VAL:HG23	1:A:229:PRO:HD2	2.01	0.43
2:A:601:PLC:H41	2:A:601:PLC:H82	1.85	0.43
1:B:88:ASN:HA	1:B:88:ASN:HD22	1.65	0.43
1:C:255:ILE:HB	1:C:256:PRO:HD3	2.01	0.43
1:C:255:ILE:N	1:C:256:PRO:HD2	2.34	0.42
1:B:100:ILE:HB	1:B:103:ILE:HG13	2.00	0.42
1:A:255:ILE:H	1:A:256:PRO:HD2	1.85	0.42
1:C:52:LEU:HD22	1:C:69:LEU:HB2	2.02	0.42
1:C:10:PHE:CD2	1:C:235:ILE:HD13	2.52	0.42
1:B:206:LEU:HA	1:B:207:PRO:C	2.40	0.42
1:B:75:LEU:HD12	1:B:139:ARG:HB3	2.02	0.42
1:B:183:GLU:O	1:B:186:THR:HB	2.20	0.42
1:C:255:ILE:H	1:C:256:PRO:HD2	1.85	0.42
1:B:108:ARG:H	1:B:178:ASN:HD21	1.66	0.42
1:B:210:GLU:H	1:B:210:GLU:CD	2.23	0.42
1:C:232:ARG:HG3	1:C:232:ARG:HH21	1.83	0.42
1:C:6:LEU:HD23	1:C:6:LEU:HA	1.83	0.42
1:C:9:GLN:OE1	1:C:139:ARG:NH1	2.50	0.41
1:B:236:VAL:HG12	1:B:238:ILE:CD1	2.49	0.41
2:A:601:PLC:H1A1	2:A:601:PLC:H32	1.21	0.41
1:B:71:ASN:ND2	1:B:138:TYR:OH	2.53	0.41
1:A:142:PHE:O	1:A:168:VAL:HA	2.21	0.41
1:C:15:GLN:NE2	1:C:41:CYS:HA	2.36	0.41
1:B:93:LEU:HD23	1:B:93:LEU:HA	1.88	0.41
1:A:259:LEU:HD21	1:C:93:LEU:HD22	2.02	0.41
1:B:205:ARG:HG2	1:B:247:ASN:HD21	1.86	0.41
1:A:226:THR:HG23	1:A:260:TRP:CB	2.49	0.40
1:A:86:ILE:O	1:A:90:ILE:HG12	2.20	0.40
1:B:168:VAL:CG1	1:B:193:LEU:HD23	2.51	0.40
1:B:118:ARG:HG3	1:B:118:ARG:NH1	2.25	0.40
1:A:4:GLN:HA	1:A:232:ARG:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:VAL:HG11	1:A:120:VAL:HG11	2.03	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	267/269 (99%)	246 (92%)	20 (8%)	1 (0%)	39 80
1	B	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	39 80
1	C	267/269 (99%)	246 (92%)	20 (8%)	1 (0%)	39 80
All	All	801/807 (99%)	742 (93%)	56 (7%)	3 (0%)	39 80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	THR
1	C	199	THR
1	B	199	THR

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	218/220 (99%)	184 (84%)	34 (16%)	3 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	218/220 (99%)	190 (87%)	28 (13%)	5 23
1	C	218/220 (99%)	189 (87%)	29 (13%)	5 21
All	All	654/660 (99%)	563 (86%)	91 (14%)	4 19

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	2	VAL
1	A	6	LEU
1	A	33	ASN
1	A	39	ASN
1	A	52	LEU
1	A	54	SER
1	A	69	LEU
1	A	75	LEU
1	A	83	SER
1	A	84	ARG
1	A	89	TRP
1	A	114	THR
1	A	115	SER
1	A	118	ARG
1	A	120	VAL
1	A	124	LEU
1	A	139	ARG
1	A	154	VAL
1	A	159	LEU
1	A	178	ASN
1	A	181	PHE
1	A	183	GLU
1	A	187	VAL
1	A	189	THR
1	A	193	LEU
1	A	205	ARG
1	A	206	LEU
1	A	215	HIS
1	A	219	GLU
1	A	228	VAL
1	A	239	GLU
1	A	259	LEU
1	A	269	LEU

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Mol	Chain	Res	Type
1	B	1	GLU
1	B	11	ASN
1	B	34	ILE
1	B	39	ASN
1	B	52	LEU
1	B	54	SER
1	B	69	LEU
1	B	75	LEU
1	B	81	ARG
1	B	83	SER
1	B	89	TRP
1	B	118	ARG
1	B	120	VAL
1	B	124	LEU
1	B	154	VAL
1	B	159	LEU
1	B	170	SER
1	B	178	ASN
1	B	183	GLU
1	B	189	THR
1	B	193	LEU
1	B	205	ARG
1	B	206	LEU
1	B	214	SER
1	B	232	ARG
1	B	239	GLU
1	B	259	LEU
1	B	269	LEU
1	C	1	GLU
1	C	2	VAL
1	C	6	LEU
1	C	11	ASN
1	C	39	ASN
1	C	52	LEU
1	C	60	VAL
1	C	75	LEU
1	C	81	ARG
1	C	84	ARG
1	C	89	TRP
1	C	115	SER
1	C	118	ARG
1	C	124	LEU

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Mol	Chain	Res	Type
1	C	126	GLN
1	C	154	VAL
1	C	178	ASN
1	C	181	PHE
1	C	189	THR
1	C	193	LEU
1	C	205	ARG
1	C	206	LEU
1	C	214	SER
1	C	219	GLU
1	C	228	VAL
1	C	232	ARG
1	C	239	GLU
1	C	259	LEU
1	C	269	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	11	ASN
1	A	15	GLN
1	A	39	ASN
1	A	71	ASN
1	A	73	ASN
1	A	92	ASN
1	A	178	ASN
1	A	198	HIS
1	A	247	ASN
1	B	4	GLN
1	B	11	ASN
1	B	15	GLN
1	B	39	ASN
1	B	71	ASN
1	B	73	ASN
1	B	92	ASN
1	B	178	ASN
1	B	198	HIS
1	B	247	ASN
1	C	4	GLN
1	C	11	ASN
1	C	15	GLN

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Mol	Chain	Res	Type
1	C	39	ASN
1	C	71	ASN
1	C	73	ASN
1	C	92	ASN
1	C	178	ASN
1	C	198	HIS
1	C	247	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

3 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	PLC	A	601	-	41,41,41	0.74	0	45,49,49	1.13	6 (13%)
2	PLC	B	701	-	41,41,41	0.73	0	45,49,49	1.18	5 (11%)
2	PLC	C	801	-	41,41,41	0.70	0	45,49,49	1.02	5 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLC	A	601	-	-	0/45/45/45	0/0/0/0
2	PLC	B	701	-	-	0/45/45/45	0/0/0/0
2	PLC	C	801	-	-	0/45/45/45	0/0/0/0

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	PLC	C4-C5-N	-3.73	104.03	116.03
2	A	601	PLC	C2-O2-C'	-3.11	110.42	117.89
2	A	601	PLC	O2P-P-O4P	-2.64	95.15	108.46
2	C	801	PLC	C2B-C1B-CB	-2.41	104.14	113.59
2	C	801	PLC	C3-O3-CB	-2.34	110.29	116.85
2	A	601	PLC	C8-N-C7	-2.34	102.95	108.98
2	B	701	PLC	C8-N-C7	-2.23	103.24	108.98
2	C	801	PLC	C4-C5-N	-2.13	109.19	116.03
2	B	701	PLC	C2B-C1B-CB	-2.12	105.28	113.59
2	B	701	PLC	OB-CB-C1B	-2.03	115.59	123.72
2	C	801	PLC	O2P-P-O4P	-2.02	98.29	108.46
2	B	701	PLC	C7-N-C6	2.01	114.15	108.98
2	C	801	PLC	O3-CB-OB	2.05	128.79	123.49
2	A	601	PLC	O4P-P-O1P	2.11	117.79	109.62
2	A	601	PLC	O2-C2-C3	2.39	116.79	108.36
2	A	601	PLC	C7-N-C6	2.53	115.48	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PLC	15	0
2	B	701	PLC	12	0
2	C	801	PLC	16	0

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.