Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:43 PM GMT

PDB ID	:	1LPB
Title	:	THE 2.46 ANGSTROMS RESOLUTION STRUCTURE OF THE PANCREATIC LIPASE COLIPASE COMPLEX INHIBITED BY A C11 ALKYL PHOSPHONATE
Authors	:	Egloff, M.-P.; Van Tilbeurgh, H.; Cambillau, C.
Deposited on	:	1994-08-19
Resolution	:	2.46 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:

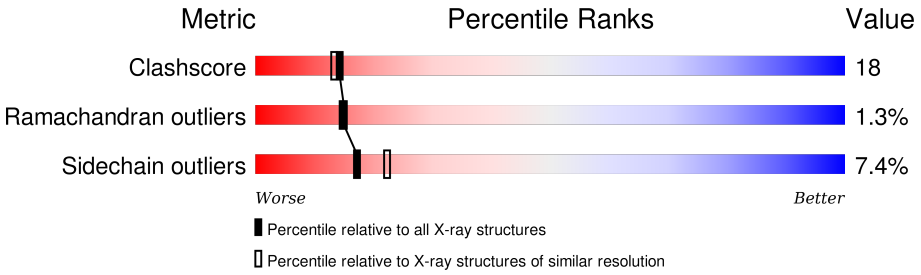
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.46 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	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)

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	95	51% 35% • 11%
2	B	449	67% 29% •

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
3	BOG	A	97	-	-	X	-
3	BOG	B	451[A]	X	-	-	-
3	BOG	B	452[A]	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6110 atoms, of which 1525 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.

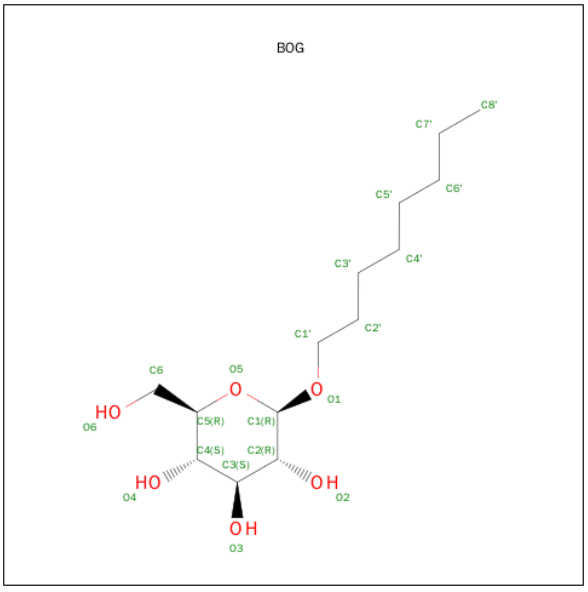
- Molecule 1 is a protein called COLIPASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	85	786	389	148	111	128	10	0	0	0

- Molecule 2 is a protein called LIPASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	449	4270	2212	779	600	661	18	0	0	0

- Molecule 3 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	B	1	24	14	4	6	4	0
3	A	1	Total	C	H	O	4	0
			24	14	4	6		

Continued on next page...

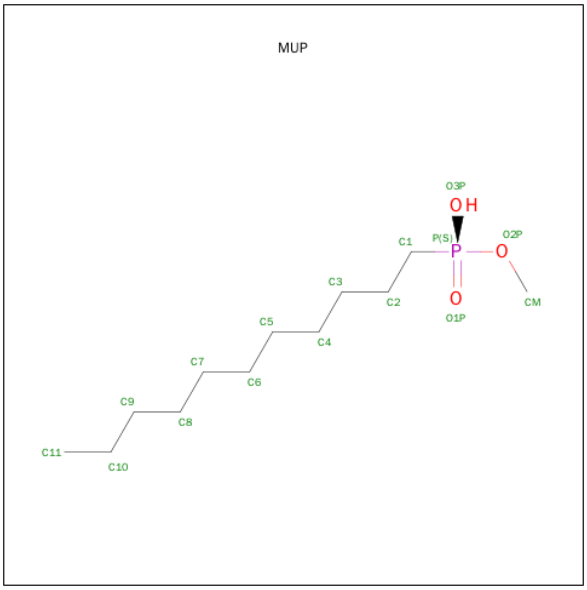
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 24 14 4 6	4	0
3	B	1	Total C H O 48 28 8 12	8	1
3	B	1	Total C H O 48 28 8 12	8	1

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0

- Molecule 5 is METHOXYUNDECYLPHOSPHINIC ACID (three-letter code: MUP) (formula: $C_{12}H_{27}O_3P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O P 30 24 4 2	0	1

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	44	Total H O 132 88 44	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	241	Total	H	O	0	0
			723	482	241		

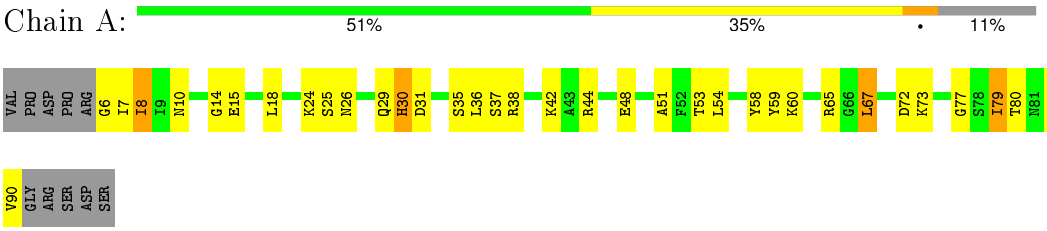
3 Residue-property plots (i)

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.

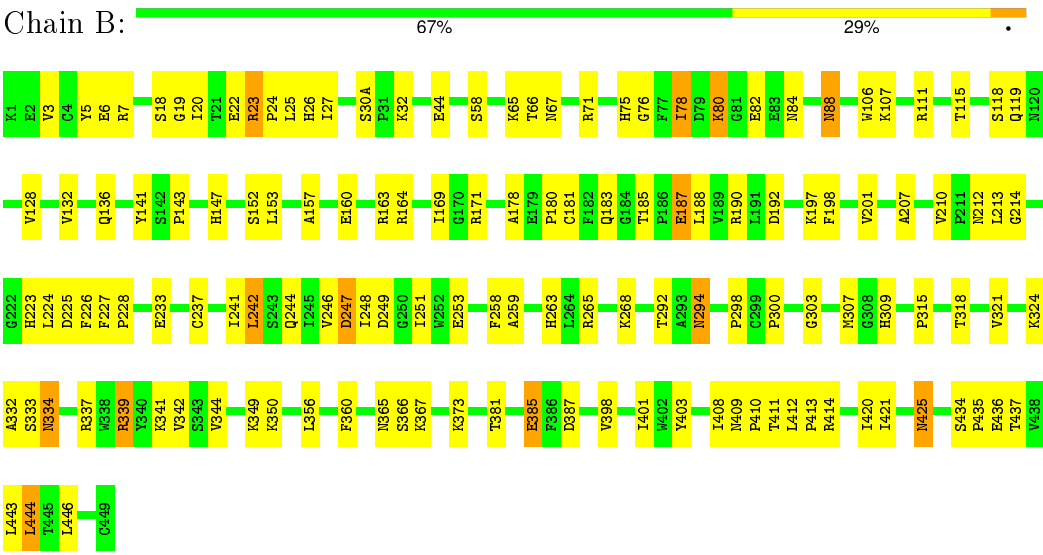
- Molecule 1: COLIPASE

Chain A:



- Molecule 2: LIPASE

Chain B:



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 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	133.70Å 133.70Å 93.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.46	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.46)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.183 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6110	wwPDB-VP
Average B, all atoms (Å^2)	24.0	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: CA, MUP, BOG

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	0.54	0/645	0.84	1/869 (0.1%)
2	B	0.58	0/3583	0.84	1/4864 (0.0%)
All	All	0.58	0/4228	0.84	2/5733 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	SER	N-CA-C	-5.76	95.46	111.00
2	B	334	ASN	N-CA-CB	5.55	120.59	110.60

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	638	148	610	35	0
2	B	3491	779	3351	118	0
3	A	40	8	56	14	0
3	B	100	20	140	23	0
4	B	1	0	0	0	0
5	B	30	0	52	3	0
6	A	44	88	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	241	482	0	12	0
All	All	4585	1525	4209	154	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 18.

All (154) 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)
2:B:333:SER:HB3	3:B:452[A]:BOG:H3'1	1.30	1.11
2:B:258:PHE:O	3:B:451[B]:BOG:H2	1.51	1.07
1:A:31:ASP:H	3:A:97:BOG:H6'2	1.28	0.98
2:B:307:MET:HE3	2:B:327:LEU:HD21	1.52	0.90
2:B:121:ILE:HD12	2:B:157:ALA:HB2	1.52	0.90
3:B:452[A]:BOG:O2	3:B:452[A]:BOG:H3'2	1.75	0.84
2:B:268:LYS:HE3	3:B:452[A]:BOG:H5	1.58	0.83
2:B:259:ALA:HA	3:B:451[B]:BOG:H2'2	1.58	0.83
2:B:147:HIS:CD2	2:B:171:ARG:HG3	2.14	0.82
1:A:35:SER:CB	3:A:97:BOG:H8'3	2.09	0.81
1:A:30:HIS:HA	3:A:97:BOG:H4'1	1.63	0.81
2:B:307:MET:CE	2:B:327:LEU:HD21	2.11	0.80
2:B:228:PRO:HD3	2:B:307:MET:HE2	1.64	0.80
2:B:349:LYS:HD3	2:B:413:PRO:HB3	1.66	0.77
1:A:58:TYR:HB3	1:A:60:LYS:O	1.85	0.75
2:B:333:SER:CB	3:B:452[A]:BOG:H3'1	2.15	0.75
2:B:244:GLN:HE21	3:B:451[B]:BOG:H62	1.55	0.71
2:B:25:LEU:HD12	2:B:115:THR:HG21	1.73	0.71
2:B:258:PHE:O	3:B:451[B]:BOG:C2	2.35	0.67
2:B:78:ILE:O	2:B:111:ARG:HD2	1.96	0.66
2:B:122:ARG:NH1	6:B:994:HOH:O	2.29	0.65
1:A:14:GLY:HA3	3:A:97:BOG:H4	1.78	0.65
1:A:44:ARG:NH2	2:B:367:LYS:HE3	2.12	0.64
2:B:119:GLN:O	2:B:122:ARG:HG2	1.98	0.64
2:B:228:PRO:HB3	2:B:307:MET:HE1	1.79	0.64
2:B:227:PHE:HE1	2:B:324:LYS:HG2	1.64	0.62
2:B:294:ASN:HD22	2:B:294:ASN:N	1.97	0.62
1:A:14:GLY:CA	3:A:97:BOG:H4	2.29	0.62
1:A:18:LEU:HD11	3:A:96:BOG:H2'2	1.83	0.61
2:B:27:ILE:HB	2:B:119:GLN:HG3	1.82	0.61
2:B:183:GLN:OE1	2:B:217:MET:HB2	2.00	0.61
2:B:160:GLU:OE2	2:B:164:ARG:HD2	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:GLU:OE1	3:B:452[A]:BOG:H61	2.01	0.60
2:B:366:SER:HB2	6:B:913:HOH:O	2.01	0.60
1:A:35:SER:OG	3:A:97:BOG:H8'3	2.01	0.59
2:B:333:SER:H	3:B:452[B]:BOG:H62	1.66	0.59
1:A:35:SER:HB2	3:A:97:BOG:H8'3	1.85	0.59
2:B:201:VAL:HG21	2:B:221:VAL:HG23	1.85	0.58
2:B:75:HIS:HD2	2:B:76:GLY:O	1.87	0.58
1:A:31:ASP:N	3:A:97:BOG:H6'2	2.10	0.57
2:B:233:GLU:HG3	6:B:949:HOH:O	2.04	0.57
2:B:20:ILE:HD11	2:B:23:ARG:HG3	1.85	0.57
2:B:425:ASN:N	2:B:425:ASN:HD22	2.01	0.57
2:B:84:ASN:O	2:B:88:ASN:HB2	2.05	0.57
1:A:30:HIS:HB3	1:A:37:SER:HB3	1.87	0.56
2:B:224:LEU:HD22	2:B:325:PHE:CE1	2.40	0.56
2:B:6:GLU:O	2:B:7:ARG:HB2	2.07	0.56
2:B:75:HIS:HE1	2:B:106:TRP:H	1.55	0.55
2:B:434:SER:HB2	2:B:446:LEU:HG	1.90	0.54
2:B:409:ASN:OD1	2:B:410:PRO:HD2	2.06	0.54
1:A:82:THR:O	1:A:82:THR:HG22	2.08	0.54
1:A:35:SER:O	3:A:96:BOG:H4	2.08	0.53
2:B:298:PRO:HB2	2:B:425:ASN:O	2.07	0.53
2:B:71:ARG:HA	2:B:147:HIS:O	2.08	0.53
2:B:292:THR:HA	6:B:1055:HOH:O	2.08	0.52
2:B:349:LYS:HG2	2:B:350:LYS:N	2.25	0.52
2:B:332:ALA:HA	3:B:452[A]:BOG:O3	2.10	0.52
2:B:242:LEU:O	2:B:246:VAL:HG23	2.10	0.52
1:A:36:LEU:HA	3:A:96:BOG:H2	1.91	0.52
1:A:51:ALA:O	1:A:53:THR:HG23	2.10	0.52
2:B:247:ASP:HB3	6:B:1013:HOH:O	2.11	0.51
1:A:67:LEU:HD13	2:B:443:LEU:HD21	1.92	0.51
2:B:22:GLU:HB2	2:B:185:THR:HG22	1.92	0.51
2:B:164:ARG:NH2	6:B:1063:HOH:O	2.43	0.51
1:A:72:ASP:HB2	6:A:136:HOH:O	2.11	0.51
2:B:440:GLU:OE2	2:B:441:GLU:HG3	2.11	0.51
1:A:73:LYS:HA	1:A:83:ASN:OD1	2.11	0.51
2:B:244:GLN:HE21	3:B:451[B]:BOG:C6	2.24	0.50
2:B:75:HIS:CE1	2:B:106:TRP:H	2.28	0.50
1:A:36:LEU:O	3:A:97:BOG:H4'2	2.10	0.50
1:A:38:ARG:NH1	2:B:246:VAL:O	2.45	0.50
2:B:220:VAL:HG22	2:B:225:ASP:CG	2.31	0.50
2:B:65:LYS:HB3	2:B:67:ASN:OD1	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:PHE:CE1	2:B:324:LYS:HG2	2.45	0.49
2:B:207:ALA:O	2:B:214:GLY:HA3	2.13	0.49
2:B:339:ARG:NH1	2:B:385:GLU:OE1	2.45	0.49
2:B:333:SER:HB2	3:B:452[A]:BOG:H1	1.95	0.49
2:B:265:ARG:HD3	6:B:1080:HOH:O	2.13	0.49
2:B:82:GLU:OE1	2:B:107:LYS:NZ	2.46	0.48
2:B:136:GLN:HA	2:B:141:TYR:O	2.13	0.48
2:B:263:HIS:NE2	5:B:901[B]:MUP:H12	2.28	0.48
2:B:143:PRO:O	2:B:169:ILE:HA	2.13	0.48
2:B:249:ASP:HB3	2:B:253:GLU:HG3	1.96	0.47
2:B:412:LEU:HD23	2:B:439:ARG:NH2	2.29	0.47
1:A:48:GLU:HB3	1:A:60:LYS:HD3	1.96	0.47
2:B:268:LYS:HE3	3:B:452[A]:BOG:C5	2.39	0.47
2:B:349:LYS:HE2	2:B:350:LYS:O	2.14	0.47
2:B:294:ASN:CG	2:B:385:GLU:HG3	2.35	0.47
2:B:411:THR:HG21	6:B:1038:HOH:O	2.15	0.47
2:B:180:PRO:O	2:B:181:CYS:HB2	2.15	0.46
1:A:26:ASN:HB2	1:A:42:LYS:HZ1	1.79	0.46
2:B:337:ARG:HB3	2:B:387:ASP:HB3	1.96	0.46
2:B:3:VAL:HG12	2:B:5:TYR:CE2	2.51	0.46
2:B:124:VAL:O	2:B:128:VAL:HG23	2.16	0.46
2:B:398:VAL:HG11	2:B:420:ILE:HG21	1.96	0.46
1:A:77:GLY:HA2	1:A:80:THR:HG22	1.96	0.46
2:B:408:ILE:HG13	2:B:408:ILE:O	2.15	0.46
1:A:30:HIS:HB3	1:A:37:SER:CB	2.46	0.46
1:A:6:GLY:O	1:A:8:ILE:HG22	2.16	0.45
1:A:30:HIS:O	1:A:59:TYR:HA	2.16	0.45
2:B:341:LYS:HE2	6:B:1092:HOH:O	2.16	0.45
2:B:344:VAL:O	2:B:381:THR:HA	2.16	0.45
2:B:339:ARG:NH2	6:B:1055:HOH:O	2.49	0.45
1:A:26:ASN:HB2	1:A:42:LYS:NZ	2.32	0.45
2:B:342:VAL:CG1	2:B:420:ILE:HG23	2.47	0.45
2:B:237:CYS:O	2:B:244:GLN:NE2	2.50	0.45
2:B:356:LEU:HB2	2:B:401:ILE:CG2	2.47	0.45
1:A:14:GLY:HA2	3:A:97:BOG:H2	1.98	0.45
2:B:249:ASP:OD1	3:B:452[B]:BOG:H1	2.17	0.45
2:B:210:VAL:O	2:B:210:VAL:HG23	2.17	0.45
2:B:294:ASN:N	2:B:294:ASN:ND2	2.65	0.44
2:B:187:GLU:HB3	2:B:192:ASP:OD1	2.17	0.44
2:B:251:ILE:HD12	2:B:251:ILE:N	2.32	0.44
3:B:452[B]:BOG:H1'2	3:B:452[B]:BOG:O2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:TYR:HA	2:B:440:GLU:HB2	1.98	0.44
2:B:223:HIS:HD2	2:B:321:VAL:HG12	1.82	0.44
2:B:332:ALA:HA	3:B:452[B]:BOG:O6	2.16	0.44
2:B:78:ILE:HG22	2:B:78:ILE:O	2.17	0.44
2:B:198:PHE:HA	2:B:223:HIS:CE1	2.53	0.43
1:A:38:ARG:NH1	6:A:119:HOH:O	2.50	0.43
2:B:163:ARG:HD2	2:B:188:LEU:HD12	2.00	0.43
2:B:268:LYS:HE2	3:B:452[A]:BOG:O4	2.19	0.43
2:B:356:LEU:N	2:B:356:LEU:HD12	2.33	0.43
2:B:30(A):SER:HB3	2:B:32:LYS:HG2	2.01	0.43
1:A:10:ASN:O	1:A:24:LYS:HE3	2.19	0.43
2:B:268:LYS:CE	3:B:452[A]:BOG:H5	2.39	0.43
2:B:342:VAL:HA	2:B:421:ILE:O	2.18	0.42
2:B:444:LEU:HD13	2:B:446:LEU:HD11	2.02	0.42
1:A:79:ILE:HD13	1:A:80:THR:N	2.35	0.42
1:A:44:ARG:HH22	2:B:367:LYS:HE3	1.84	0.42
2:B:360:PHE:CD2	2:B:365:ASN:HB3	2.55	0.42
2:B:223:HIS:CE1	2:B:318:THR:HG22	2.55	0.41
2:B:18:SER:OG	2:B:26:HIS:HA	2.20	0.41
2:B:198:PHE:HA	2:B:223:HIS:ND1	2.35	0.41
2:B:412:LEU:HD23	2:B:439:ARG:HH21	1.85	0.41
3:B:452[A]:BOG:O2	3:B:452[A]:BOG:C3'	2.56	0.41
2:B:171:ARG:NH2	2:B:309:HIS:O	2.53	0.41
2:B:178:ALA:CB	5:B:901[A]:MUP:H22	2.51	0.41
2:B:412:LEU:N	2:B:413:PRO:HD3	2.36	0.41
2:B:19:GLY:O	2:B:20:ILE:HG23	2.21	0.41
2:B:258:PHE:O	3:B:451[B]:BOG:C1	2.68	0.41
3:B:450:BOG:H5'1	3:B:450:BOG:H8'3	1.68	0.41
3:B:451[A]:BOG:H6'2	5:B:901[A]:MUP:H113	2.03	0.41
1:A:31:ASP:HB2	3:A:97:BOG:H6'2	2.03	0.41
2:B:226:PHE:CG	2:B:307:MET:HG3	2.55	0.41
2:B:300:PRO:HG2	2:B:303:GLY:O	2.21	0.41
2:B:80:LYS:HE3	6:B:1058:HOH:O	2.21	0.41
1:A:29:GLN:NE2	1:A:59:TYR:O	2.54	0.41
2:B:44:GLU:HG2	6:B:1030:HOH:O	2.21	0.41
2:B:118:SER:O	2:B:121:ILE:HB	2.21	0.40
2:B:425:ASN:H	2:B:425:ASN:HD22	1.70	0.40
2:B:414:ARG:HB3	2:B:437:THR:HB	2.03	0.40
2:B:121:ILE:HA	2:B:121:ILE:HD13	1.71	0.40
2:B:212:ASN:O	2:B:213:LEU:HB2	2.21	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	83/95 (87%)	78 (94%)	3 (4%)	2 (2%)	7 4
2	B	447/449 (100%)	417 (93%)	25 (6%)	5 (1%)	17 19
All	All	530/544 (97%)	495 (93%)	28 (5%)	7 (1%)	15 15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	78	ILE
1	A	8	ILE
2	B	248	ILE
2	B	334	ASN
1	A	7	ILE
2	B	435	PRO
2	B	24	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	74/83 (89%)	66 (89%)	8 (11%)	8 8
2	B	383/383 (100%)	357 (93%)	26 (7%)	20 26
All	All	457/466 (98%)	423 (93%)	34 (7%)	17 22

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	30	HIS
1	A	54	LEU
1	A	65	ARG
1	A	67	LEU
1	A	79	ILE
1	A	89	ASN
1	A	90	VAL
2	B	23	ARG
2	B	58	SER
2	B	66	THR
2	B	80	LYS
2	B	88	ASN
2	B	121	ILE
2	B	122	ARG
2	B	132	VAL
2	B	152	SER
2	B	153	LEU
2	B	187	GLU
2	B	190	ARG
2	B	197	LYS
2	B	220	VAL
2	B	241	ILE
2	B	242	LEU
2	B	247	ASP
2	B	294	ASN
2	B	315	PRO
2	B	339	ARG
2	B	373	LYS
2	B	385	GLU
2	B	425	ASN
2	B	436	GLU
2	B	440	GLU
2	B	444	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	35	ASN
2	B	75	HIS
2	B	88	ASN
2	B	151	HIS
2	B	244	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	289	ASN
2	B	294	ASN
2	B	319	ASN
2	B	425	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

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	$\#\|Z\| > 2$
3	BOG	A	96	-	20,20,20	0.84	1 (5%)	25,25,25	1.33	3 (12%)
3	BOG	A	97	-	20,20,20	0.85	1 (5%)	25,25,25	1.91	6 (24%)
3	BOG	B	450	-	20,20,20	0.70	0	25,25,25	1.55	6 (24%)
3	BOG	B	451[A]	-	20,20,20	0.91	1 (5%)	25,25,25	1.81	7 (28%)
3	BOG	B	451[B]	-	20,20,20	1.35	3 (15%)	25,25,25	3.16	7 (28%)
3	BOG	B	452[A]	-	20,20,20	1.04	1 (5%)	25,25,25	2.45	9 (36%)
3	BOG	B	452[B]	-	20,20,20	0.59	0	25,25,25	1.74	3 (12%)
5	MUP	B	901[A]	2	11,14,15	0.63	0	10,14,17	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MUP	B	901[B]	2	11,14,15	0.33	0	10,14,17	1.25	1 (10%)

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	BOG	A	96	-	-	0/11/31/31	0/1/1/1
3	BOG	A	97	-	-	0/11/31/31	0/1/1/1
3	BOG	B	450	-	-	0/11/31/31	0/1/1/1
3	BOG	B	451[A]	-	1/1/5/5	0/11/31/31	0/1/1/1
3	BOG	B	451[B]	-	-	0/11/31/31	0/1/1/1
3	BOG	B	452[A]	-	-	0/11/31/31	0/1/1/1
3	BOG	B	452[B]	-	-	1/11/31/31	0/1/1/1
5	MUP	B	901[A]	2	-	0/9/13/15	0/0/0/0
5	MUP	B	901[B]	2	-	0/9/13/15	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	451[A]	BOG	C1-C2	2.26	1.59	1.52
3	A	96	BOG	C4-C5	2.30	1.58	1.53
3	B	451[B]	BOG	C1-C2	2.47	1.59	1.52
3	B	452[A]	BOG	O1-C1	2.50	1.44	1.40
3	A	97	BOG	C4-C5	2.60	1.58	1.53
3	B	451[B]	BOG	O1-C1	3.24	1.46	1.40
3	B	451[B]	BOG	C4-C5	3.38	1.60	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	451[B]	BOG	O4-C4-C3	-5.94	96.97	110.34
3	B	451[A]	BOG	C6-C5-C4	-4.56	101.77	113.02
3	B	452[A]	BOG	C4-C3-C2	-4.54	102.32	110.79
3	A	97	BOG	C4-C3-C2	-4.26	102.84	110.79
3	B	452[A]	BOG	C1-C2-C3	-3.81	102.47	109.97
3	A	97	BOG	C1-C2-C3	-3.52	103.04	109.97
3	B	452[A]	BOG	O4-C4-C3	-3.34	102.83	110.34
3	A	96	BOG	C1-C2-C3	-3.15	103.76	109.97
3	B	450	BOG	C6-C5-C4	-3.01	105.58	113.02
3	A	96	BOG	O4-C4-C3	-2.90	103.82	110.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	451[A]	BOG	O3-C3-C4	-2.60	104.48	110.34
3	B	450	BOG	C1-C2-C3	-2.33	105.38	109.97
3	B	451[A]	BOG	O2-C2-C1	-2.25	105.09	110.02
3	A	96	BOG	C4-C3-C2	-2.10	106.87	110.79
3	B	451[B]	BOG	O4-C4-C5	-2.07	103.76	109.24
3	B	450	BOG	O4-C4-C5	-2.06	103.78	109.24
3	A	97	BOG	O4-C4-C5	2.01	114.56	109.24
3	B	451[A]	BOG	C1-O5-C5	2.02	117.67	113.75
3	A	97	BOG	O3-C3-C4	2.11	115.09	110.34
3	B	452[B]	BOG	O3-C3-C2	2.13	115.12	110.34
3	B	452[A]	BOG	O4-C4-C5	2.18	115.00	109.24
3	A	97	BOG	O2-C2-C3	2.30	115.51	110.34
3	B	452[A]	BOG	C1-O5-C5	2.39	118.38	113.75
3	B	450	BOG	C1'-O1-C1	2.42	118.17	113.94
3	B	452[A]	BOG	O3-C3-C2	2.49	115.94	110.34
3	B	452[B]	BOG	O1-C1-C2	2.49	111.18	108.04
3	B	451[A]	BOG	O5-C1-C2	2.55	115.51	110.28
3	B	451[B]	BOG	O2-C2-C1	2.59	115.69	110.02
3	B	450	BOG	O1-C1-C2	2.71	111.46	108.04
3	B	451[B]	BOG	O5-C1-O1	2.82	116.83	110.05
3	B	451[A]	BOG	C1'-O1-C1	3.32	119.75	113.94
5	B	901[B]	MUP	P-C1-C2	3.59	121.85	112.36
3	B	450	BOG	C3-C4-C5	3.61	116.50	110.20
3	B	452[A]	BOG	O2-C2-C1	3.70	118.13	110.02
3	B	451[A]	BOG	O1-C1-C2	3.98	113.06	108.04
3	B	452[A]	BOG	O1-C1-C2	4.31	113.48	108.04
3	A	97	BOG	C1'-O1-C1	5.55	123.64	113.94
3	B	451[B]	BOG	C3-C4-C5	5.84	120.37	110.20
3	B	452[A]	BOG	C1'-O1-C1	5.97	124.37	113.94
3	B	452[B]	BOG	C1'-O1-C1	7.18	126.50	113.94
3	B	451[B]	BOG	C1'-O1-C1	8.44	128.69	113.94
3	B	451[B]	BOG	O1-C1-C2	8.78	119.13	108.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	451[A]	BOG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	452[B]	BOG	C1'-O1-C1-O5

There are no ring outliers.

9 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	96	BOG	3	0
3	A	97	BOG	11	0
3	B	450	BOG	1	0
3	B	451[A]	BOG	1	0
3	B	451[B]	BOG	6	0
3	B	452[A]	BOG	11	0
3	B	452[B]	BOG	4	0
5	B	901[A]	MUP	2	0
5	B	901[B]	MUP	1	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.