Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 05:36 PM EST

PDB ID	:	2ZZX
Title	:	Crystal Structure of a Periplasmic Substrate Binding Protein in Complex with Lactate
Authors	:	Akiyama, N.; Takeda, K.; Miki, K.
Deposited on	:	2009-02-27
Resolution	:	1.75 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

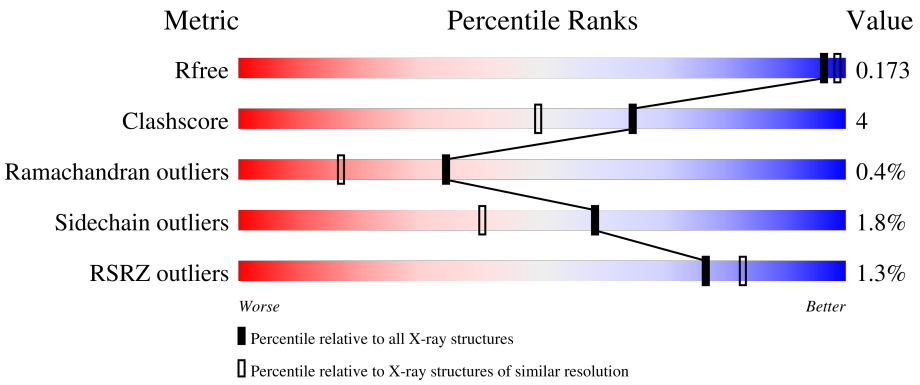
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	361	2%, 81%, 10%, 9%
1	B	361	2%, 79%, 12%, •, 9%
1	C	361	82%, 8%, •, 10%
1	D	361	%, 80%, 11%, 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
2	LAC	A	401	X	-	-	-
2	LAC	B	402	X	-	-	-
2	LAC	C	403	X	-	-	-
2	LAC	D	404	X	-	-	-

2 Entry composition (i)

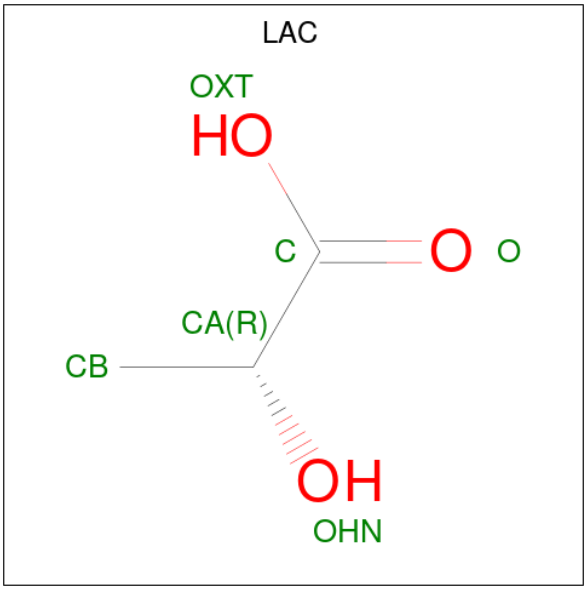
There are 6 unique types of molecules in this entry. The entry contains 11513 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ABC transporter, solute-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	2654	1729	456	461	8	0	0	0
1	B	328	2615	1705	443	459	8	0	0	0
1	C	326	2630	1712	452	458	8	0	1	0
1	D	329	2646	1723	454	461	8	0	1	0

- Molecule 2 is LACTIC ACID (three-letter code: LAC) (formula: $C_3H_6O_3$).



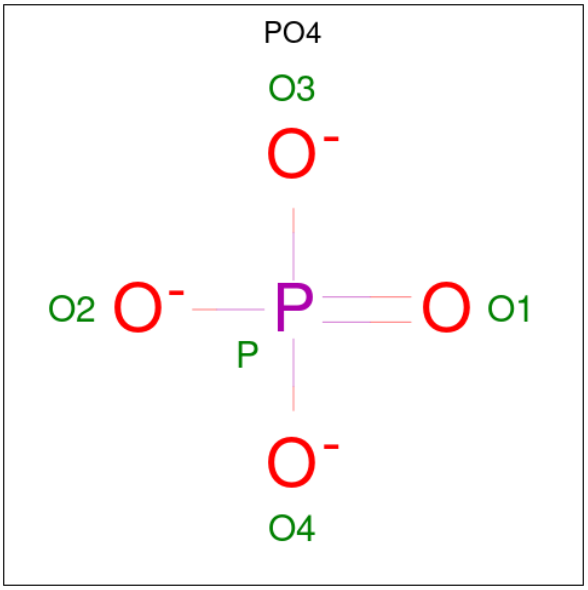
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
2	B	1	6	3	3	0	0

Continued on next page...

Continued from previous page...

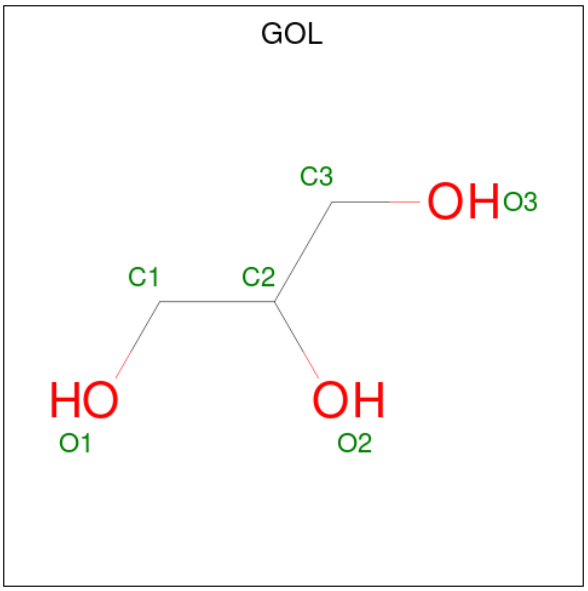
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	C	1	6	3	3	0	0
			Total	C	O		
2	D	1	6	3	3	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	A	1	5	4	1	0	0
			Total	O	P		
3	B	1	5	4	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	D	1	6	3	3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	C	1	1	1	0	0

- Molecule 6 is water.

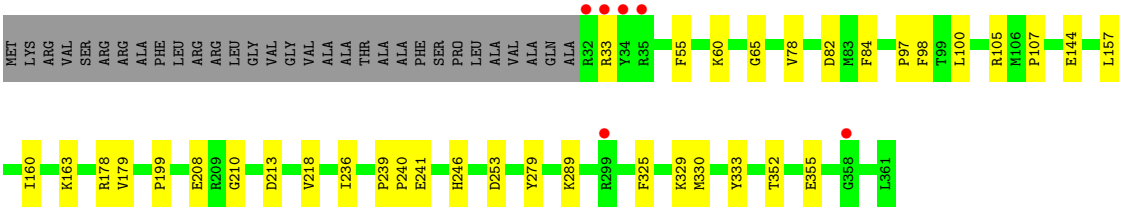
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	245	245	245	0	0
			Total	O		
6	B	207	207	207	0	0
			Total	O		
6	C	259	259	259	0	0
			Total	O		
6	D	210	210	210	0	0

3 Residue-property plots (i)

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.

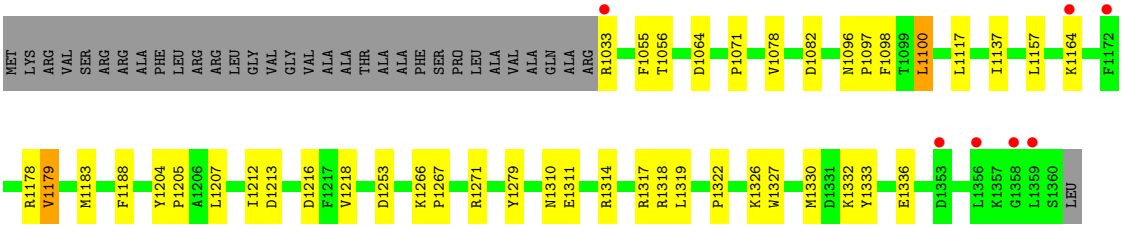
• Molecule 1: ABC transporter, solute-binding protein

Chain A:



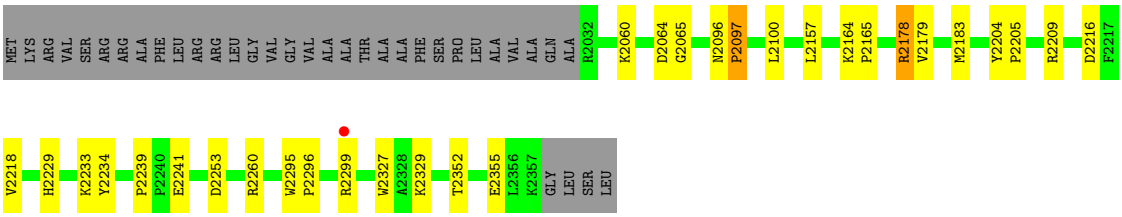
• Molecule 1: ABC transporter, solute-binding protein

Chain B:



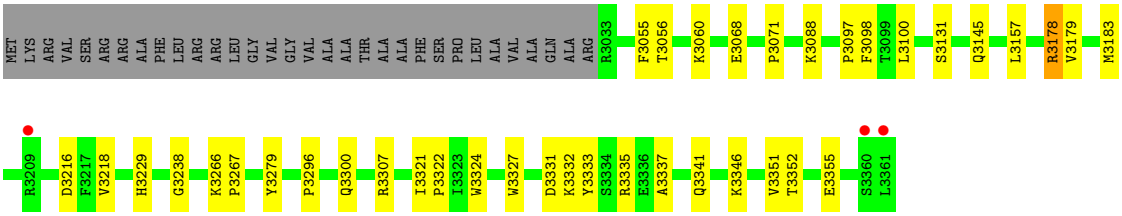
• Molecule 1: ABC transporter, solute-binding protein

Chain C:



• Molecule 1: ABC transporter, solute-binding protein

Chain D:


MET
LYS
ARG
VAL
SER
ARG
ARG
ALA
PHE
LEU
ARG
ARG
LEU
GLY
VAL
GLY
VAL
ALA
ALA
THR
ALA
ALA
PHE
SER
PRO
LEU
ALA
VAL
ALA
GLN
ALA
ARG
R3033
F3055
T3056
K3060
E3068
P3071
K3088
P3097
F3098
T3099
L3100
S3131
Q3145
L3157
R3178
V3179
M3183
R3209
D3216
F3217
V3218
H3229
G3238
K3266
P3267
Y3279
P3296
Q3300
R3307
I3321
P3322
I3323
W3324
W3327
D3331
K3332
Y3333
S3334
R3335
E3336
A3337
Q3341
K3346
V3351
T3352
E3355
S3360
L3361

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.79Å 103.50Å 90.76Å 90.00° 101.86° 90.00°	Depositor
Resolution (Å)	45.29 – 1.75 45.29 – 1.75	Depositor EDS
% Data completeness (in resolution range)	90.1 (45.29-1.75) 89.9 (45.29-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.78 (at 1.75Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.177 , 0.207 0.175 , 0.173	Depositor DCC
R_{free} test set	6591 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	18.1	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11513	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, PO4, LAC

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	0.46	0/2733	0.66	1/3710 (0.0%)
1	B	0.43	0/2694	0.64	1/3663 (0.0%)
1	C	0.47	0/2709	0.68	0/3679
1	D	0.42	0/2726	0.63	1/3703 (0.0%)
All	All	0.45	0/10862	0.65	3/14755 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	3098	PHE	N-CA-C	-5.82	95.30	111.00
1	A	98	PHE	N-CA-C	-5.70	95.60	111.00
1	B	1098	PHE	N-CA-C	-5.28	96.74	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2654	0	2624	22	0
1	B	2615	0	2556	29	0
1	C	2630	0	2587	20	0
1	D	2646	0	2597	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	6	0	0	0	0
2	B	6	0	0	1	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	6	0	8	1	0
4	D	6	0	8	0	0
5	C	1	0	0	0	0
6	A	245	0	0	2	0
6	B	207	0	0	1	1
6	C	259	0	0	2	0
6	D	210	0	0	0	0
All	All	11513	0	10380	85	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 4.

All (85) 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:1204:TYR:HB3	1:B:1205:PRO:HD3	1.65	0.76
1:A:84:PHE:CE2	1:A:105:ARG:HD2	2.29	0.67
1:A:107:PRO:HG3	1:A:330:MET:HE2	1.78	0.66
1:B:1117:LEU:HD12	1:B:1317:ARG:HA	1.76	0.66
1:D:3352:THR:OG1	1:D:3355:GLU:HG3	1.97	0.64
1:D:3346:LYS:HG2	1:D:3351:VAL:HG23	1.80	0.63
1:D:3331:ASP:O	1:D:3335:ARG:HG3	1.99	0.62
1:D:3321:ILE:HB	1:D:3322:PRO:HD3	1.83	0.59
1:B:1310:ASN:O	1:B:1314:ARG:HG3	2.01	0.59
1:B:1327:TRP:O	1:B:1330:MET:HG3	2.03	0.58
1:B:1137:ILE:HD13	1:B:1336:GLU:HG2	1.84	0.58
1:C:2204:TYR:HB3	1:C:2205:PRO:HD3	1.86	0.57
1:C:2164:LYS:HE2	6:C:4248:HOH:O	2.04	0.57
1:B:1271:ARG:HH22	1:C:2064:ASP:CG	2.08	0.56
1:B:1178:ARG:HD3	1:B:1178:ARG:C	2.28	0.54
1:C:2165:PRO:HG3	1:C:2234:TYR:CZ	2.42	0.54
1:B:1137:ILE:CD1	1:B:1336:GLU:HG2	2.37	0.54
1:B:1179:VAL:HG23	6:B:4884:HOH:O	2.08	0.54
1:D:3229:HIS:H	1:D:3229:HIS:CD2	2.26	0.54
1:C:2178:ARG:HD3	1:C:2178:ARG:C	2.28	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:THR:OG1	1:A:355:GLU:HG3	2.09	0.53
1:B:1157:LEU:HD12	1:B:1157:LEU:C	2.30	0.52
1:B:1056:THR:HG21	1:B:1071:PRO:HB3	1.92	0.52
1:D:3332:LYS:HE3	1:D:3333:TYR:CE2	2.45	0.52
1:A:208:GLU:OE2	1:C:2329:LYS:HE2	2.10	0.52
1:D:3178:ARG:HD3	1:D:3178:ARG:C	2.29	0.51
1:B:1207:LEU:HD23	1:B:1212:ILE:HG13	1.93	0.51
1:D:3157:LEU:C	1:D:3157:LEU:HD12	2.31	0.51
1:B:1311:GLU:HA	1:B:1314:ARG:NH1	2.26	0.50
1:D:3088:LYS:HE2	1:D:3145:GLN:O	2.11	0.50
1:B:1332:LYS:HE3	1:B:1333:TYR:CE2	2.47	0.50
1:B:1271:ARG:NH2	1:C:2064:ASP:OD2	2.46	0.49
1:C:2296:PRO:HA	1:C:2299:ARG:HD2	1.95	0.49
1:C:2239:PRO:HB2	1:C:2241:GLU:OE1	2.13	0.48
1:A:199:PRO:HB2	4:A:601:GOL:H31	1.96	0.48
1:C:2229:HIS:H	1:C:2229:HIS:CD2	2.31	0.48
1:D:3296:PRO:O	1:D:3300:GLN:HG3	2.12	0.48
1:A:325:PHE:O	1:A:329:LYS:HG3	2.13	0.47
1:B:1078:VAL:HG22	1:B:1082:ASP:HB2	1.95	0.47
1:A:239:PRO:HB2	1:A:241:GLU:OE1	2.15	0.47
1:D:3266:LYS:HB3	1:D:3267:PRO:HD3	1.96	0.47
1:A:246:HIS:CE1	6:A:4192:HOH:O	2.67	0.46
1:B:1117:LEU:HD12	1:B:1317:ARG:CA	2.46	0.46
1:A:240:PRO:HG2	1:A:241:GLU:OE2	2.16	0.46
1:B:1271:ARG:NH2	1:C:2064:ASP:CG	2.70	0.46
1:A:163:LYS:HE2	1:A:213:ASP:HA	1.98	0.45
1:B:1100:LEU:HD11	2:B:402:LAC:CB	2.46	0.45
1:A:78:VAL:HG22	1:A:82:ASP:HB2	1.99	0.45
1:B:1326:LYS:HE2	1:B:1326:LYS:HB3	1.80	0.45
1:C:2295:TRP:HB2	1:C:2296:PRO:HD3	1.99	0.44
1:A:163:LYS:NZ	1:A:210:GLY:HA2	2.33	0.44
1:A:33:ARG:NH1	1:A:65:GLY:O	2.50	0.44
1:A:84:PHE:HB3	6:A:4550:HOH:O	2.16	0.44
1:B:1314:ARG:O	1:B:1318:ARG:HG3	2.17	0.44
1:A:60:LYS:HG3	1:A:65:GLY:HA2	2.00	0.43
1:B:1319:LEU:O	1:B:1322:PRO:HD2	2.18	0.43
1:A:253:ASP:OD1	1:A:253:ASP:C	2.57	0.43
1:B:1164:LYS:HE3	1:B:1213:ASP:HB3	2.01	0.43
1:A:178:ARG:C	1:A:178:ARG:HD3	2.38	0.43
1:C:2352:THR:O	1:C:2355:GLU:HB3	2.19	0.43
1:A:144:GLU:OE2	1:A:333:TYR:OH	2.29	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1266:LYS:HB3	1:B:1267:PRO:HD3	2.01	0.42
1:A:289:LYS:HD2	1:D:3131:SER:O	2.19	0.42
1:A:157:LEU:C	1:A:157:LEU:HD12	2.40	0.42
1:B:1055:PHE:HB2	1:B:1279:TYR:CE1	2.55	0.42
1:C:2096:ASN:HA	1:C:2253:ASP:O	2.20	0.42
1:C:2233:LYS:O	1:C:2233:LYS:HG2	2.20	0.42
1:D:3055:PHE:HB2	1:D:3279:TYR:CE1	2.55	0.42
1:C:2205:PRO:O	1:C:2209:ARG:HG2	2.21	0.41
1:B:1179:VAL:HG11	1:B:1188:PHE:CD2	2.55	0.41
1:B:1327:TRP:HA	1:B:1330:MET:HG3	2.02	0.41
1:D:3060:LYS:HE3	1:D:3068:GLU:OE2	2.21	0.41
1:D:3183:MET:HG3	1:D:3327:TRP:CD1	2.55	0.41
1:D:3337:ALA:O	1:D:3341:GLN:HG3	2.20	0.41
1:B:1096:ASN:HA	1:B:1253:ASP:O	2.20	0.41
1:C:2183:MET:HG3	1:C:2327:TRP:CG	2.55	0.41
1:D:3321:ILE:HD13	1:D:3324:TRP:CH2	2.56	0.41
1:A:55:PHE:HB2	1:A:279:TYR:CE1	2.56	0.41
1:D:3056:THR:HG21	1:D:3071:PRO:HB3	2.03	0.41
1:D:3238:GLY:O	1:D:3307:ARG:HD2	2.21	0.41
1:C:2260:ARG:HD3	6:C:4866:HOH:O	2.22	0.40
1:C:2157:LEU:C	1:C:2157:LEU:HD12	2.41	0.40
1:C:2060:LYS:HG3	1:C:2065:GLY:HA2	2.04	0.40
1:A:160:ILE:HB	1:A:236:ILE:HB	2.03	0.40
1:B:1183:MET:HG3	1:B:1327:TRP:CD1	2.56	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)
6:B:4583:HOH:O	6:B:4583:HOH:O[2_555]	2.05	0.15

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	328/361 (91%)	320 (98%)	7 (2%)	1 (0%)	41	22
1	B	326/361 (90%)	317 (97%)	8 (2%)	1 (0%)	41	22
1	C	325/361 (90%)	316 (97%)	7 (2%)	2 (1%)	25	10
1	D	328/361 (91%)	320 (98%)	7 (2%)	1 (0%)	41	22
All	All	1307/1444 (90%)	1273 (97%)	29 (2%)	5 (0%)	34	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1218	VAL
1	A	218	VAL
1	D	3218	VAL
1	C	2097	PRO
1	C	2218	VAL

5.3.2 Protein sidechains (i)

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	269/291 (92%)	266 (99%)	3 (1%)	73	60
1	B	263/291 (90%)	257 (98%)	6 (2%)	50	28
1	C	266/291 (91%)	261 (98%)	5 (2%)	57	37
1	D	267/291 (92%)	262 (98%)	5 (2%)	57	37
All	All	1065/1164 (92%)	1046 (98%)	19 (2%)	59	40

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	PRO
1	A	100	LEU
1	A	179	VAL
1	B	1033	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1064	ASP
1	B	1097	PRO
1	B	1100	LEU
1	B	1179	VAL
1	B	1216	ASP
1	C	2097	PRO
1	C	2100	LEU
1	C	2178	ARG
1	C	2179	VAL
1	C	2216	ASP
1	D	3097	PRO
1	D	3100	LEU
1	D	3178	ARG
1	D	3179	VAL
1	D	3216	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	ASN
1	B	1229	HIS
1	B	1300	GLN
1	C	2229	HIS
1	C	2310	ASN
1	D	3229	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	PO4	A	501	-	4,4,4	2.68	1 (25%)	6,6,6	0.82	0
2	LAC	D	404	-	5,5,5	1.13	1 (20%)	4,6,6	1.43	1 (25%)
4	GOL	A	601	-	5,5,5	0.27	0	5,5,5	0.21	0
2	LAC	A	401	-	5,5,5	1.04	0	4,6,6	1.44	0
3	PO4	B	502	-	4,4,4	2.59	1 (25%)	6,6,6	0.88	0
4	GOL	D	602	-	5,5,5	0.28	0	5,5,5	0.27	0
2	LAC	B	402	-	5,5,5	1.12	1 (20%)	4,6,6	1.51	1 (25%)
2	LAC	C	403	5	5,5,5	1.07	0	4,6,6	1.35	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	LAC	D	404	-	1/1/2/2	1/4/4/4	-
4	GOL	A	601	-	-	4/4/4/4	-
2	LAC	A	401	-	1/1/2/2	1/4/4/4	-
4	GOL	D	602	-	-	0/4/4/4	-
2	LAC	B	402	-	1/1/2/2	0/4/4/4	-
2	LAC	C	403	5	1/1/2/2	1/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	PO4	P-O1	5.09	1.62	1.50
3	B	502	PO4	P-O1	4.97	1.62	1.50
2	B	402	LAC	CB-CA	-2.16	1.40	1.50
2	D	404	LAC	CB-CA	-2.09	1.40	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	402	LAC	CB-CA-C	2.20	115.61	110.63
2	D	404	LAC	CB-CA-C	2.02	115.21	110.63

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	401	LAC	CA
2	B	402	LAC	CA
2	C	403	LAC	CA
2	D	404	LAC	CA

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	GOL	O1-C1-C2-C3
4	A	601	GOL	C1-C2-C3-O3
4	A	601	GOL	O1-C1-C2-O2
4	A	601	GOL	O2-C2-C3-O3
2	D	404	LAC	OXT-C-CA-OHN
2	A	401	LAC	OXT-C-CA-OHN
2	C	403	LAC	OXT-C-CA-OHN

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	GOL	1	0
2	B	402	LAC	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	330/361 (91%)	-0.23	6 (1%)	68	76	10, 19, 36, 53	0
1	B	328/361 (90%)	-0.05	7 (2%)	63	71	12, 25, 40, 53	0
1	C	326/361 (90%)	-0.30	1 (0%)	94	95	10, 18, 33, 58	0
1	D	329/361 (91%)	-0.22	3 (0%)	84	89	11, 24, 38, 56	0
All	All	1313/1444 (90%)	-0.20	17 (1%)	77	83	10, 21, 38, 58	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3361	LEU	5.1
1	B	1172	PHE	3.1
1	B	1164	LYS	2.8
1	C	2299	ARG	2.7
1	B	1358	GLY	2.7
1	A	32	ARG	2.6
1	B	1353	ASP	2.5
1	A	33	ARG	2.5
1	B	1356	LEU	2.5
1	A	35	ARG	2.4
1	A	299	ARG	2.3
1	B	1033	ARG	2.3
1	A	34	TYR	2.3
1	D	3360	SER	2.2
1	A	358	GLY	2.2
1	D	3209	ARG	2.1
1	B	1359	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LAC	B	402	6/6	0.85	0.16	40,43,44,47	0
2	LAC	A	401	6/6	0.90	0.17	32,33,35,38	0
4	GOL	D	602	6/6	0.90	0.10	43,48,49,50	0
4	GOL	A	601	6/6	0.94	0.15	29,40,42,44	0
2	LAC	C	403	6/6	0.94	0.10	21,24,25,28	0
3	PO4	B	502	5/5	0.95	0.19	42,44,44,47	0
3	PO4	A	501	5/5	0.96	0.12	25,37,38,39	0
2	LAC	D	404	6/6	0.96	0.07	27,28,29,32	0
5	CA	C	701	1/1	0.99	0.07	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.