Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 04:40 am BST

PDB ID	:	6M7Z
Title	:	A divergent kinase lacking the glycine-rich loop regulates membrane ultrastructure of the Toxoplasma parasitophorous vacuole
Authors	:	Beraki, T.; Borek, D.M.; Reese, M.L.
Deposited on	:	2018-08-21
Resolution	:	2.50 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 following versions of software and data (see references (1)) were used in the production of this report:

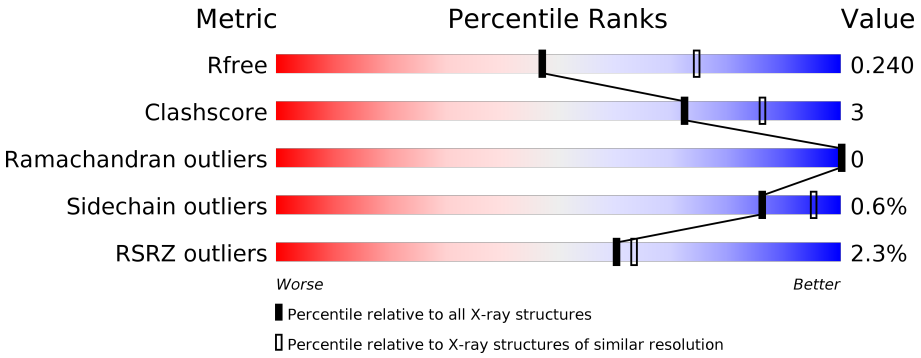
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	319	76% 7% 18%
1	B	319	74% 7% 19%
1	C	319	77% 5% 18%
1	D	319	73% 6% 20%
1	E	319	3% 76% 8% 16%
1	F	319	3% 75% 6% 19%

2 Entry composition

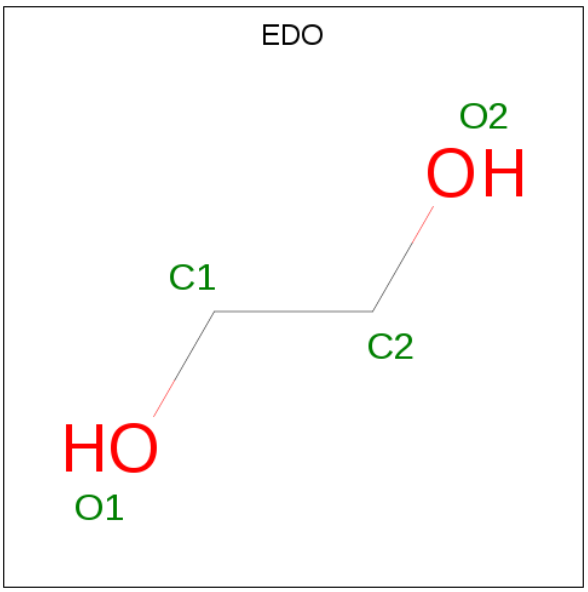
There are 4 unique types of molecules in this entry. The entry contains 12870 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bradyzoite pseudokinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2081	1333	360	382	6			
1	B	258	Total	C	N	O	S	0	0	0
			2043	1313	345	379	6			
1	C	262	Total	C	N	O	S	0	0	0
			2079	1334	356	383	6			
1	D	255	Total	C	N	O	S	0	1	0
			2023	1297	347	374	5			
1	E	269	Total	C	N	O	S	0	1	0
			2141	1370	373	392	6			
1	F	259	Total	C	N	O	S	0	0	0
			2055	1317	351	381	6			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Cl 1 1	0	0
3	E	2	Total Cl 2 2	0	0

- Molecule 4 is water.

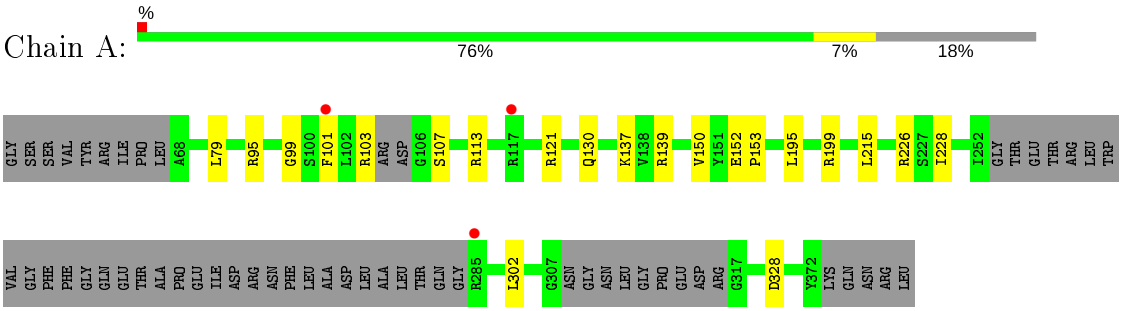
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	46	Total O 46 46	0	0
4	B	51	Total O 51 51	0	0
4	C	93	Total O 93 93	0	0
4	D	67	Total O 67 67	0	0
4	E	82	Total O 82 82	0	0
4	F	42	Total O 42 42	0	0

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 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.

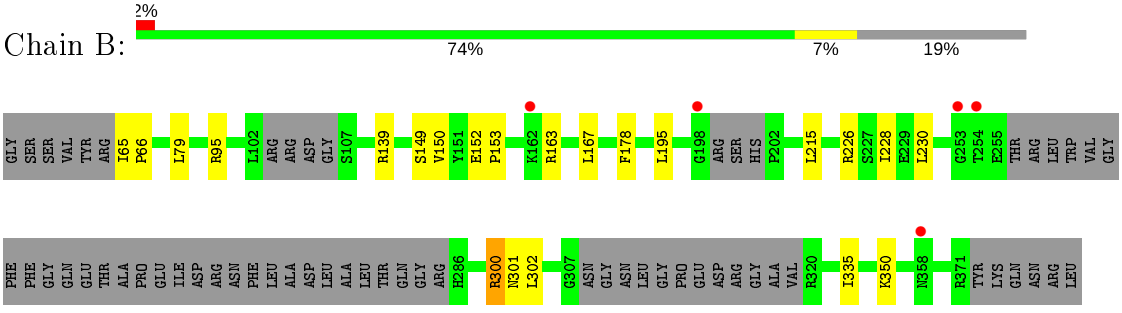
- Molecule 1: Bradyzoite pseudokinase 1

Chain A:



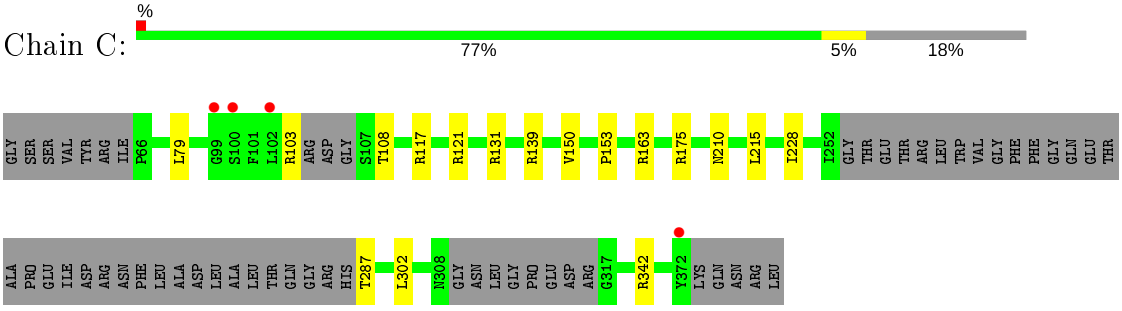
- Molecule 1: Bradyzoite pseudokinase 1

Chain B:



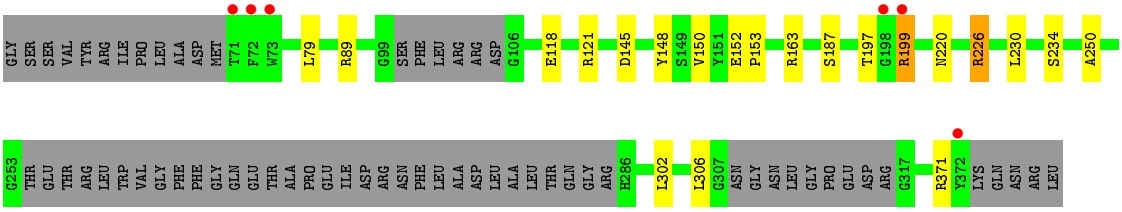
- Molecule 1: Bradyzoite pseudokinase 1

Chain C:

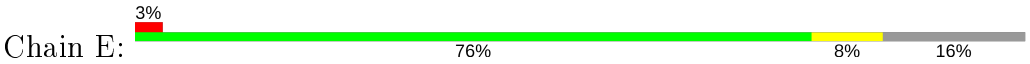


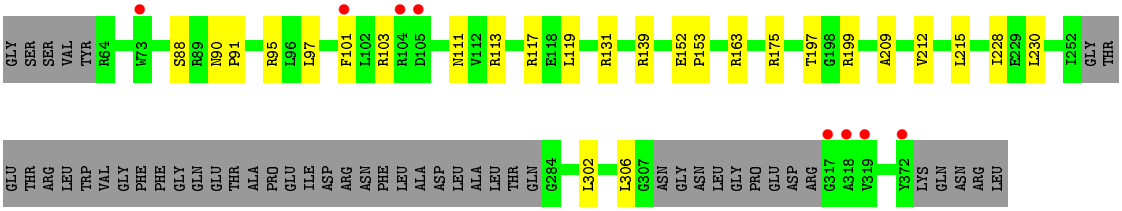
- Molecule 1: Bradyzoite pseudokinase 1

Chain D:

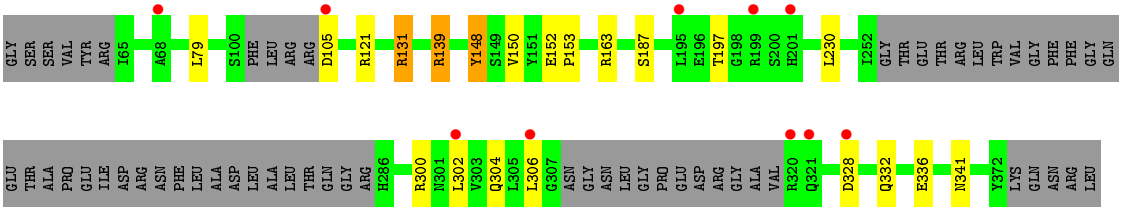


- Molecule 1: Bradyzoite pseudokinase 1





- Molecule 1: Bradyzoite pseudokinase 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	171.47Å 123.07Å 86.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.70 – 2.50 47.71 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.9 (47.70-2.50) 91.0 (47.71-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.63 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.197 , 0.239 0.200 , 0.240	Depositor DCC
R_{free} test set	2987 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12870	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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

5.1 Standard geometry

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

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	0.47	0/2122	0.63	0/2871
1	B	0.47	0/2082	0.61	0/2818
1	C	0.52	0/2120	0.64	0/2870
1	D	0.52	1/2066 (0.0%)	0.64	0/2797
1	E	0.51	0/2187	0.66	0/2960
1	F	0.46	0/2096	0.61	0/2839
All	All	0.49	1/12673 (0.0%)	0.63	0/17155

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	4
1	B	0	3
1	C	0	1
1	D	0	4
1	E	0	3
1	F	0	4
All	All	0	19

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	118	GLU	CD-OE2	5.25	1.31	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ARG	Sidechain
1	A	199	ARG	Sidechain
1	A	226	ARG	Sidechain
1	A	95	ARG	Sidechain
1	B	163	ARG	Sidechain
1	B	226	ARG	Sidechain
1	B	300	ARG	Sidechain
1	C	121	ARG	Sidechain
1	D	163	ARG	Sidechain
1	D	199	ARG	Sidechain
1	D	226	ARG	Sidechain
1	D	89	ARG	Sidechain
1	E	117	ARG	Sidechain
1	E	163	ARG	Sidechain
1	E	199	ARG	Sidechain
1	F	121	ARG	Sidechain
1	F	131	ARG	Sidechain
1	F	139	ARG	Sidechain
1	F	163	ARG	Sidechain

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	2081	0	2124	14	0
1	B	2043	0	2089	19	0
1	C	2079	0	2126	10	0
1	D	2023	0	2064	13	0
1	E	2141	0	2192	22	0
1	F	2055	0	2094	17	0
2	A	8	0	12	2	0
2	B	16	0	24	3	0
2	C	24	0	36	3	0
2	E	8	0	12	2	0
2	F	8	0	12	0	0
3	C	1	0	0	0	0
3	E	2	0	0	0	0
4	A	46	0	0	2	0
4	B	51	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	93	0	0	2	0
4	D	67	0	0	3	0
4	E	82	0	0	2	0
4	F	42	0	0	2	0
All	All	12870	0	12785	86	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 3.

All (86) 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:E:139:ARG:NH1	2:E:402:EDO:O1	1.97	0.97
1:D:199:ARG:HB3	1:E:197:THR:O	1.66	0.95
1:C:139:ARG:NH1	2:C:404:EDO:O1	2.04	0.91
1:B:350:LYS:NZ	4:B:501:HOH:O	2.02	0.90
1:B:178:PHE:HE2	1:E:97:LEU:HD12	1.35	0.90
1:E:113:ARG:O	1:F:304:GLN:NE2	2.15	0.77
1:A:139:ARG:NH1	2:A:402:EDO:O2	2.20	0.75
1:E:95:ARG:NH1	1:E:111:ASN:O	2.25	0.70
1:B:178:PHE:CE2	1:E:97:LEU:HD12	2.25	0.66
1:E:175:ARG:NH2	4:E:502:HOH:O	2.29	0.66
1:A:328:ASP:OD2	1:C:131:ARG:HD2	1.99	0.62
1:F:187:SER:HB2	4:F:501:HOH:O	1.99	0.62
1:A:195:LEU:CD1	1:A:302:LEU:CD1	2.79	0.60
1:F:300:ARG:NH2	1:F:332:GLN:HG2	2.18	0.58
1:B:139:ARG:HD2	2:B:404:EDO:H21	1.85	0.58
1:C:175:ARG:HD2	4:C:563:HOH:O	2.04	0.57
1:A:195:LEU:CD1	1:A:302:LEU:HD13	2.35	0.57
1:D:234:SER:OG	4:D:401:HOH:O	2.17	0.57
1:D:199:ARG:CB	1:E:197:THR:O	2.48	0.56
1:B:139:ARG:NH1	2:B:404:EDO:O2	2.38	0.56
1:B:230:LEU:HD12	1:B:301:ASN:OD1	2.06	0.55
1:E:88:SER:HB3	1:E:119:LEU:HD13	1.88	0.55
1:E:131:ARG:HD3	1:F:328:ASP:OD2	2.07	0.54
1:B:195:LEU:CD1	1:B:302:LEU:CD1	2.86	0.53
1:A:195:LEU:HD13	1:A:302:LEU:CD1	2.39	0.53
1:B:95:ARG:HH11	1:B:95:ARG:HG3	1.73	0.53
1:A:137:LYS:HD3	4:A:513:HOH:O	2.09	0.53
1:D:187:SER:HB2	4:D:401:HOH:O	2.08	0.52
1:B:167:LEU:HB2	2:B:401:EDO:H12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:ARG:HH11	2:E:402:EDO:C1	2.23	0.51
1:F:336:GLU:HG2	1:F:341:ASN:CB	2.40	0.51
1:A:139:ARG:HH11	2:A:402:EDO:C2	2.23	0.50
1:D:220:ASN:ND2	4:D:402:HOH:O	2.29	0.50
1:B:195:LEU:CD1	1:B:302:LEU:HD13	2.40	0.50
1:B:65:ILE:N	1:B:66:PRO:CD	2.75	0.50
1:E:175:ARG:HD2	4:E:533:HOH:O	2.11	0.50
1:E:90:ASN:N	1:E:91:PRO:HD2	2.27	0.49
1:E:113:ARG:HB3	1:F:304:GLN:OE1	2.12	0.49
1:C:210:ASN:ND2	4:C:501:HOH:O	2.18	0.48
1:F:336:GLU:HG2	1:F:341:ASN:HB2	1.95	0.48
1:B:195:LEU:HD13	1:B:302:LEU:CD1	2.43	0.48
1:A:99:GLY:HA3	1:A:101:PHE:CE1	2.49	0.47
1:E:209:ALA:HA	1:E:212:VAL:HG22	1.97	0.47
1:F:139:ARG:NH1	1:F:148:TYR:CE2	2.83	0.47
1:F:300:ARG:HH21	1:F:332:GLN:HG2	1.80	0.47
1:F:187:SER:HB3	4:F:512:HOH:O	2.14	0.46
1:A:215:LEU:HD13	1:A:228:ILE:HD11	1.97	0.46
1:D:79:LEU:HD13	1:D:150:VAL:CG1	2.46	0.45
1:B:79:LEU:HD13	1:B:150:VAL:CG1	2.47	0.45
1:A:130:GLN:NE2	4:A:506:HOH:O	2.49	0.45
1:F:197:THR:O	1:F:197:THR:HG22	2.17	0.45
1:A:113:ARG:HD2	1:B:301:ASN:HD21	1.82	0.45
1:C:215:LEU:HD13	1:C:228:ILE:HD11	1.98	0.45
1:F:302:LEU:CD2	1:F:306:LEU:HD12	2.46	0.44
1:C:103:ARG:HB2	1:C:108:THR:OG1	2.18	0.44
1:C:79:LEU:HD13	1:C:150:VAL:CG1	2.49	0.43
1:F:152:GLU:HB3	1:F:153:PRO:HD3	2.00	0.43
1:E:101:PHE:O	1:E:103:ARG:HG3	2.18	0.43
1:E:90:ASN:N	1:E:91:PRO:CD	2.82	0.43
1:C:153:PRO:HD3	2:C:404:EDO:H11	2.00	0.42
1:E:302:LEU:C	1:E:302:LEU:HD23	2.40	0.42
1:C:342:ARG:HH22	2:C:401:EDO:H12	1.84	0.42
1:F:79:LEU:HD13	1:F:150:VAL:CG1	2.50	0.42
1:A:79:LEU:HD13	1:A:150:VAL:CG1	2.50	0.42
1:D:152:GLU:HB3	1:D:153:PRO:HD3	2.02	0.42
1:D:302:LEU:C	1:D:302:LEU:HD23	2.40	0.42
1:B:152:GLU:HB3	1:B:153:PRO:HD3	2.02	0.42
1:A:103:ARG:NH1	1:A:107:SER:O	2.53	0.41
1:D:226:ARG:HD2	1:D:250:ALA:HB3	2.02	0.41
1:B:95:ARG:HH11	1:B:95:ARG:CG	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:GLU:HB3	1:E:153:PRO:HD3	2.02	0.41
1:D:230:LEU:HD23	1:D:230:LEU:HA	1.96	0.41
1:D:197:THR:HG22	1:D:197:THR:O	2.21	0.41
1:F:230:LEU:HD23	1:F:230:LEU:HA	1.94	0.41
1:C:302:LEU:HD23	1:C:302:LEU:C	2.41	0.41
1:E:215:LEU:HD13	1:E:228:ILE:HD11	2.02	0.41
1:F:302:LEU:HD21	1:F:306:LEU:HD12	2.02	0.41
1:E:302:LEU:CD2	1:E:306:LEU:HD12	2.51	0.40
1:F:302:LEU:HD23	1:F:302:LEU:C	2.41	0.40
1:B:215:LEU:HD13	1:B:228:ILE:HD11	2.02	0.40
1:A:152:GLU:HB3	1:A:153:PRO:HD3	2.02	0.40
1:B:300:ARG:HD2	1:B:335:ILE:HD13	2.03	0.40
1:D:145:ASP:HB3	1:D:148:TYR:HD2	1.86	0.40
1:E:230:LEU:HA	1:E:230:LEU:HD23	1.97	0.40
1:B:149:SER:HB2	4:B:522:HOH:O	2.22	0.40
1:D:302:LEU:CD2	1:D:306:LEU:HD12	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/319 (80%)	251 (99%)	3 (1%)	0	100	100
1	B	248/319 (78%)	245 (99%)	3 (1%)	0	100	100
1	C	254/319 (80%)	249 (98%)	5 (2%)	0	100	100
1	D	248/319 (78%)	245 (99%)	3 (1%)	0	100	100
1	E	264/319 (83%)	258 (98%)	6 (2%)	0	100	100
1	F	251/319 (79%)	248 (99%)	3 (1%)	0	100	100
All	All	1519/1914 (79%)	1496 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	231/278 (83%)	231 (100%)	0	100 100
1	B	229/278 (82%)	229 (100%)	0	100 100
1	C	232/278 (84%)	229 (99%)	3 (1%)	69 87
1	D	225/278 (81%)	223 (99%)	2 (1%)	78 92
1	E	238/278 (86%)	238 (100%)	0	100 100
1	F	230/278 (83%)	227 (99%)	3 (1%)	69 87
All	All	1385/1668 (83%)	1377 (99%)	8 (1%)	86 95

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

Mol	Chain	Res	Type
1	C	117	ARG
1	C	163	ARG
1	C	287	THR
1	D	121	ARG
1	D	371	ARG
1	F	105	ASP
1	F	131	ARG
1	F	148	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	ASN
1	C	301	ASN
1	D	341	ASN
1	F	341	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 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	EDO	C	404	-	3,3,3	0.60	0	2,2,2	0.10	0
2	EDO	A	401	-	3,3,3	0.39	0	2,2,2	0.42	0
2	EDO	B	404	-	3,3,3	0.57	0	2,2,2	0.11	0
2	EDO	E	401	-	3,3,3	0.51	0	2,2,2	0.37	0
2	EDO	B	403	-	3,3,3	0.59	0	2,2,2	0.06	0
2	EDO	C	401	-	3,3,3	0.52	0	2,2,2	0.23	0
2	EDO	B	402	-	3,3,3	0.55	0	2,2,2	0.09	0
2	EDO	C	405	-	3,3,3	0.34	0	2,2,2	0.45	0
2	EDO	A	402	-	3,3,3	0.55	0	2,2,2	0.33	0
2	EDO	F	402	-	3,3,3	0.58	0	2,2,2	0.11	0
2	EDO	C	402	-	3,3,3	0.44	0	2,2,2	0.45	0
2	EDO	E	402	-	3,3,3	0.64	0	2,2,2	0.14	0
2	EDO	C	403	-	3,3,3	0.50	0	2,2,2	0.25	0
2	EDO	C	406	-	3,3,3	0.54	0	2,2,2	0.11	0
2	EDO	B	401	-	3,3,3	0.50	0	2,2,2	0.20	0
2	EDO	F	401	-	3,3,3	0.55	0	2,2,2	0.18	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	EDO	C	404	-	-	1/1/1/1	-
2	EDO	A	401	-	-	1/1/1/1	-
2	EDO	B	404	-	-	1/1/1/1	-
2	EDO	E	401	-	-	1/1/1/1	-
2	EDO	B	403	-	-	0/1/1/1	-
2	EDO	C	401	-	-	0/1/1/1	-
2	EDO	B	402	-	-	0/1/1/1	-
2	EDO	C	405	-	-	1/1/1/1	-
2	EDO	A	402	-	-	0/1/1/1	-
2	EDO	F	402	-	-	1/1/1/1	-
2	EDO	C	402	-	-	1/1/1/1	-
2	EDO	E	402	-	-	1/1/1/1	-
2	EDO	C	403	-	-	0/1/1/1	-
2	EDO	C	406	-	-	1/1/1/1	-
2	EDO	B	401	-	-	1/1/1/1	-
2	EDO	F	401	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	404	EDO	O1-C1-C2-O2
2	A	401	EDO	O1-C1-C2-O2
2	E	401	EDO	O1-C1-C2-O2
2	C	405	EDO	O1-C1-C2-O2
2	C	406	EDO	O1-C1-C2-O2
2	C	402	EDO	O1-C1-C2-O2
2	B	404	EDO	O1-C1-C2-O2
2	F	402	EDO	O1-C1-C2-O2
2	E	402	EDO	O1-C1-C2-O2
2	B	401	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	404	EDO	2	0
2	B	404	EDO	2	0
2	C	401	EDO	1	0
2	A	402	EDO	2	0
2	E	402	EDO	2	0
2	B	401	EDO	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

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, 95^{th} 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	262/319 (82%)	-0.12	3 (1%)	80	82	24, 46, 90, 110	0
1	B	258/319 (80%)	-0.07	5 (1%)	66	69	23, 41, 86, 109	0
1	C	262/319 (82%)	-0.18	4 (1%)	73	75	21, 30, 73, 138	1 (0%)
1	D	255/319 (79%)	-0.14	6 (2%)	59	62	21, 33, 81, 120	1 (0%)
1	E	269/319 (84%)	-0.12	8 (2%)	50	53	21, 34, 80, 127	0
1	F	259/319 (81%)	0.06	10 (3%)	39	42	25, 48, 95, 109	1 (0%)
All	All	1565/1914 (81%)	-0.09	36 (2%)	60	63	21, 39, 86, 138	3 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	100	SER	5.5
1	D	72	PHE	4.4
1	C	102	LEU	4.3
1	D	372	TYR	4.2
1	E	372	TYR	3.9
1	E	105	ASP	3.7
1	D	73	TRP	3.6
1	B	253	GLY	3.6
1	B	358	ASN	3.4
1	C	99	GLY	3.3
1	D	199	ARG	3.2
1	F	302	LEU	3.2
1	B	198	GLY	3.2
1	B	254	THR	3.1
1	F	105	ASP	3.1
1	E	317	GLY	3.0
1	E	101	PHE	2.9
1	F	321	GLN	2.8
1	F	328	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	285	ARG	2.6
1	F	306	LEU	2.6
1	C	372	TYR	2.5
1	F	195	LEU	2.5
1	E	104	ARG	2.5
1	E	318	ALA	2.5
1	D	198	GLY	2.4
1	E	73	TRP	2.4
1	A	117	ARG	2.4
1	D	71	THR	2.3
1	B	162	LYS	2.3
1	E	319	VAL	2.2
1	F	320	ARG	2.2
1	F	68	ALA	2.2
1	F	199	ARG	2.2
1	A	101	PHE	2.1
1	F	201	HIS	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 carbohydrates 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, 95^{th} 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	EDO	C	403	4/4	0.76	0.27	54,59,68,76	0
2	EDO	C	401	4/4	0.80	0.15	56,57,61,69	0
2	EDO	B	403	4/4	0.81	0.34	41,53,64,65	0
3	CL	E	404	1/1	0.82	0.10	62,62,62,62	0
2	EDO	C	406	4/4	0.83	0.22	43,45,51,62	0
2	EDO	F	402	4/4	0.87	0.39	53,58,59,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	B	404	4/4	0.91	0.30	42,49,54,55	0
2	EDO	B	401	4/4	0.92	0.22	34,41,50,52	0
2	EDO	C	402	4/4	0.93	0.18	31,38,45,48	0
2	EDO	C	405	4/4	0.94	0.17	32,32,36,36	0
3	CL	E	403	1/1	0.94	0.12	49,49,49,49	0
2	EDO	C	404	4/4	0.95	0.21	24,39,51,55	0
2	EDO	A	401	4/4	0.96	0.14	32,43,49,51	0
2	EDO	A	402	4/4	0.97	0.16	29,42,43,47	0
2	EDO	B	402	4/4	0.97	0.11	36,39,40,41	0
2	EDO	E	401	4/4	0.97	0.13	27,28,30,33	0
2	EDO	F	401	4/4	0.97	0.09	38,39,46,48	0
3	CL	C	407	1/1	0.98	0.10	59,59,59,59	0
2	EDO	E	402	4/4	0.98	0.20	28,32,58,60	0

6.5 Other polymers

There are no such residues in this entry.