W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:38 PM GMT

|		
PDB ID	:	1PZG
Title	:	T.gondii LDH1 complexed with APAD and sulfate at 1.6 Angstroms
Authors	:	Kavanagh, K.L.; Elling, R.A.; Wilson, D.K.
Deposited on	:	2003-07-10
Resolution	:	1.60 Å(reported)

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 1.60 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.197
Clashscore		4
Ramachandran outliers		0.3%
Sidechain outliers		0.6%
RSRZ outliers		7.6%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
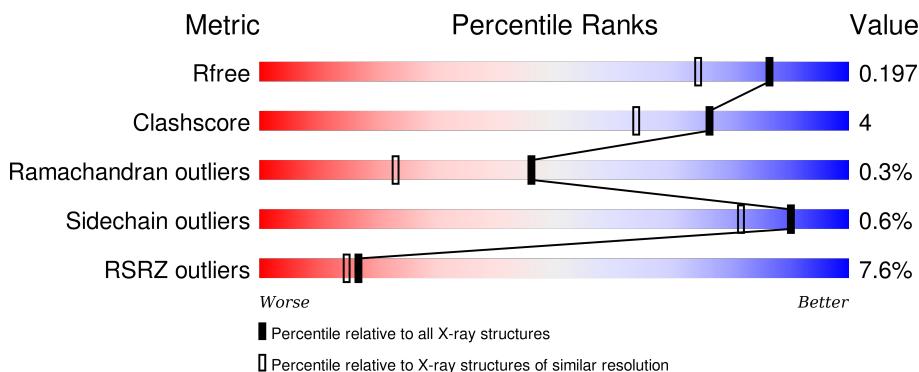
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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.

Mol	Chain	Length	Quality of chain
1	A	331	5% / 93% / 6% ·
1	B	331	5% / 89% / 10% ·
1	C	331	10% / 86% / 11% ··
1	D	331	10% / 87% / 11% ·
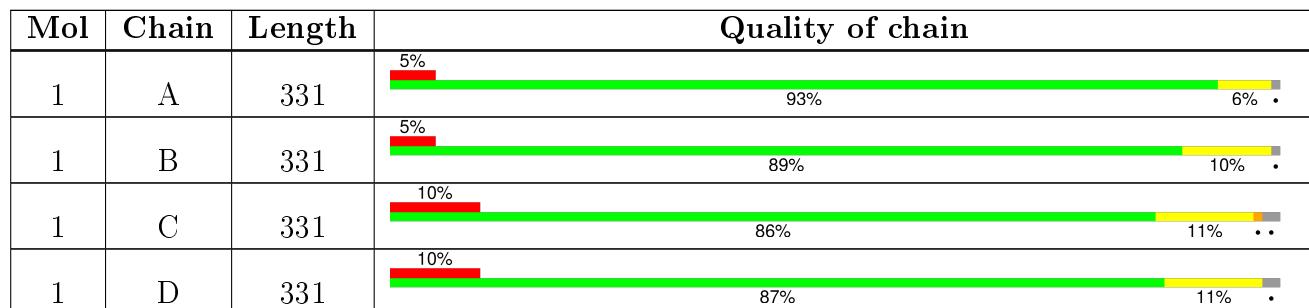
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10639 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 lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total 2478	C 1568	N 418	O 468	S 24	0	0	0
1	B	328	Total 2478	C 1568	N 418	O 468	S 24	0	0	0
1	C	325	Total 2459	C 1555	N 415	O 465	S 24	0	0	0
1	D	326	Total 2466	C 1560	N 416	O 466	S 24	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	CME	CYS	MODIFIED RESIDUE	UNP P90613
A	334	PRO	-	CLONING ARTIFACT	UNP P90613
A	335	GLY	-	CLONING ARTIFACT	UNP P90613
B	150	CME	CYS	MODIFIED RESIDUE	UNP P90613
B	334	PRO	-	CLONING ARTIFACT	UNP P90613
B	335	GLY	-	CLONING ARTIFACT	UNP P90613
C	150	CME	CYS	MODIFIED RESIDUE	UNP P90613
C	334	PRO	-	CLONING ARTIFACT	UNP P90613
C	335	GLY	-	CLONING ARTIFACT	UNP P90613
D	150	CME	CYS	MODIFIED RESIDUE	UNP P90613
D	334	PRO	-	CLONING ARTIFACT	UNP P90613
D	335	GLY	-	CLONING ARTIFACT	UNP P90613

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
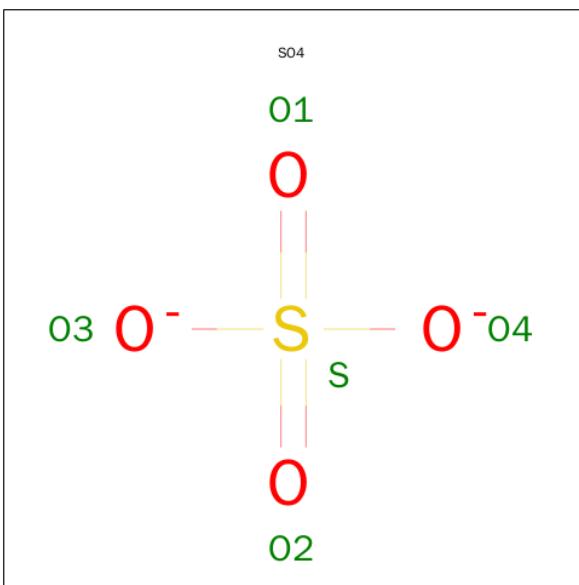
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

• Molecule 3 is 3-ACETYLPYRIDINE ADENINE DINUCLEOTIDE (three-letter code: A3D) (formula: $C_{22}H_{28}N_6O_{14}P_2$).
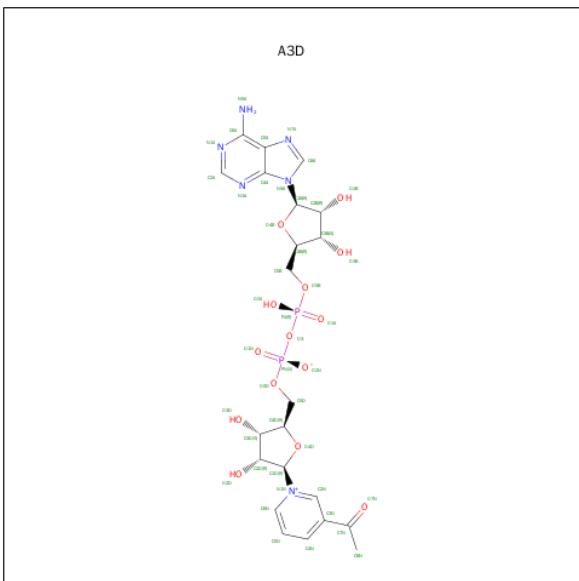
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	22	6	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	22	6	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	22	6	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	22	6	14	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	160	Total	O	0	0
			160	160		
4	B	149	Total	O	0	0
			149	149		
4	C	121	Total	O	0	0
			121	121		
4	D	132	Total	O	0	0
			132	132		

3 Residue-property plots ⓘ

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.

- Molecule 1: lactate dehydrogenase
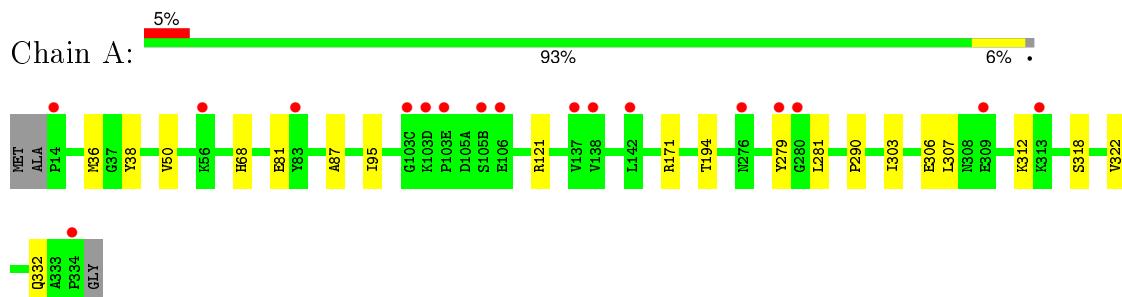
- Molecule 1: lactate dehydrogenase
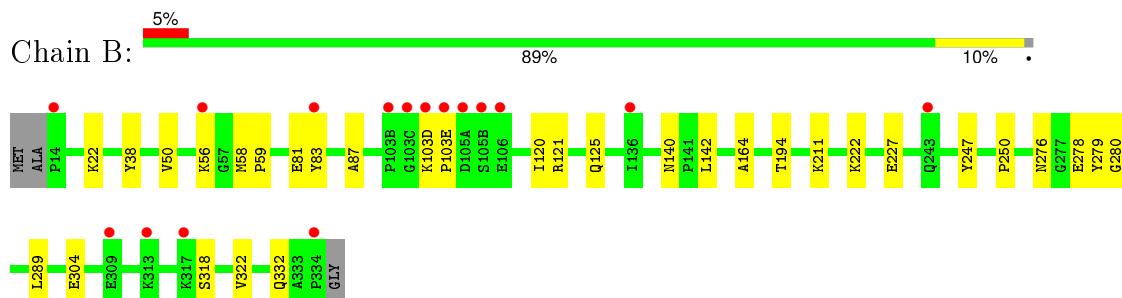
- Molecule 1: lactate dehydrogenase
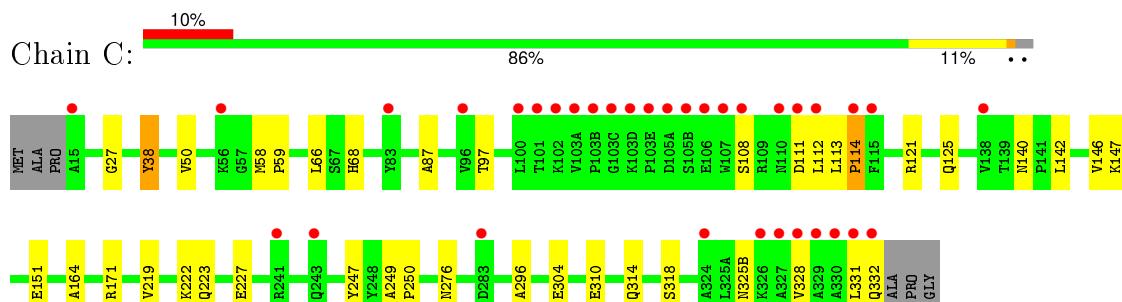
- Molecule 1: lactate dehydrogenase
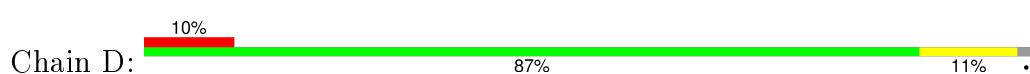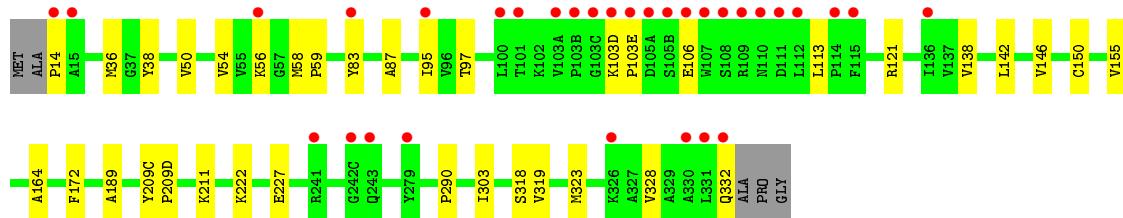
4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.94Å 124.98Å 86.39Å 90.00° 105.94° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 28.95 – 1.60	Depositor EDS
% Data completeness (in resolution range)	91.8 (30.00-1.60) 91.8 (28.95-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 1.60Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.176 , 0.198 0.175 , 0.197	Depositor DCC
R_{free} test set	8417 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 45.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 167151 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10639	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CME, SO4, A3D

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	0/2506	0.68	0/3389
1	B	0.46	0/2506	0.68	0/3389
1	C	0.46	0/2485	0.67	1/3359 (0.0%)
1	D	0.43	0/2493	0.67	0/3370
All	All	0.45	0/9990	0.68	1/13507 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	27	GLY	N-CA-C	-5.02	100.55	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	38	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	38	TYR	Sidechain
1	C	38	TYR	Sidechain
1	D	38	TYR	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	2478	0	2533	12	0
1	B	2478	0	2533	21	0
1	C	2459	0	2513	26	0
1	D	2466	0	2521	22	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	44	0	27	0	0
3	B	44	0	27	0	0
3	C	44	0	27	1	0
3	D	44	0	27	2	0
4	A	160	0	0	1	0
4	B	149	0	0	0	0
4	C	121	0	0	0	0
4	D	132	0	0	0	0
All	All	10639	0	10208	76	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 4.

All (76) 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:C:112:LEU:C	1:C:114:PRO:HD2	1.82	0.99
1:C:113:LEU:N	1:C:114:PRO:HD2	1.87	0.90
1:C:113:LEU:HD11	1:C:328:VAL:HG12	1.60	0.83
1:C:113:LEU:HD11	1:C:328:VAL:CG1	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ARG:O	1:C:125:GLN:HG3	1.92	0.69
1:D:113:LEU:HD11	1:D:328:VAL:CG2	2.25	0.66
1:D:103(D):LYS:HE3	1:D:106:GLU:HB3	1.78	0.65
1:C:296:ALA:HB1	1:D:14:PRO:HB2	1.80	0.63
1:B:56:LYS:HE3	1:B:83:TYR:HD2	1.67	0.59
1:D:113:LEU:HD11	1:D:328:VAL:HG22	1.84	0.58
1:D:121:ARG:NH1	1:D:332:GLN:HB2	2.19	0.57
1:B:211:LYS:HE2	1:C:304:GLU:O	2.05	0.56
1:C:50:VAL:HG11	1:C:87:ALA:HA	1.87	0.56
1:C:113:LEU:N	1:C:114:PRO:CD	2.66	0.56
1:B:194:THR:HG21	1:B:322:VAL:HB	1.88	0.56
1:C:310:GLU:HG3	1:C:314:GLN:HE21	1.71	0.55
1:D:142:LEU:O	1:D:146:VAL:HG23	2.07	0.54
1:A:50:VAL:HG11	1:A:87:ALA:HA	1.90	0.53
1:B:22:LYS:HE3	1:B:50:VAL:HG21	1.90	0.53
1:D:290:PRO:HB2	1:D:303:ILE:HB	1.91	0.52
1:C:219:VAL:HG23	1:C:223:GLN:CD	2.30	0.51
1:A:194:THR:HG21	1:A:322:VAL:HB	1.93	0.51
1:B:222:LYS:O	1:B:227:GLU:HG3	2.10	0.51
1:A:121:ARG:NH1	1:A:332:GLN:HG2	2.25	0.51
1:B:50:VAL:HG13	1:B:81:GLU:HG2	1.93	0.51
1:B:56:LYS:HG3	1:B:83:TYR:CD2	2.46	0.51
1:B:121:ARG:NH1	1:B:332:GLN:HG3	2.25	0.51
1:C:310:GLU:HG3	1:C:314:GLN:NE2	2.26	0.50
1:A:290:PRO:HB2	1:A:303:ILE:HB	1.92	0.50
1:A:307:LEU:O	1:A:312:LYS:HE3	2.12	0.50
1:D:319:VAL:O	1:D:323:MET:HG3	2.11	0.50
1:B:22:LYS:HE3	1:B:50:VAL:CG2	2.42	0.50
1:C:147:LYS:O	1:C:151:GLU:HG3	2.12	0.50
1:D:50:VAL:HG11	1:D:87:ALA:HA	1.95	0.49
1:D:56:LYS:HA	1:D:83:TYR:CE2	2.49	0.48
1:C:108:SER:HB3	1:C:111:ASP:OD2	2.14	0.47
1:D:58:MET:HB3	1:D:59:PRO:HD3	1.97	0.47
1:B:279:TYR:CZ	1:B:304:GLU:HA	2.50	0.46
1:C:142:LEU:O	1:C:146:VAL:HG23	2.15	0.46
1:B:103(D):LYS:HA	1:B:103(E):PRO:HD3	1.86	0.45
1:C:140:ASN:HA	1:C:142:LEU:N	2.31	0.45
1:C:331:LEU:O	1:C:332:GLN:HB2	2.16	0.45
1:B:279:TYR:CE2	1:B:304:GLU:HA	2.52	0.45
1:D:222:LYS:O	1:D:227:GLU:HG3	2.17	0.44
1:D:150:CME:HE2	1:D:155:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:TYR:HB2	1:A:281:LEU:HG	1.99	0.44
1:B:278:GLU:C	1:B:280:GLY:H	2.21	0.44
1:B:278:GLU:C	1:B:280:GLY:N	2.71	0.44
1:C:222:LYS:O	1:C:227:GLU:HG3	2.18	0.44
1:D:36:MET:SD	1:D:95:ILE:HG21	2.58	0.44
1:B:279:TYR:CE2	1:B:289:LEU:HD22	2.53	0.43
1:B:121:ARG:O	1:B:125:GLN:HG3	2.17	0.43
1:C:97:THR:HB	3:C:605:A3D:H51N	1.99	0.43
1:D:103(D):LYS:HE3	1:D:106:GLU:CB	2.47	0.43
1:D:97:THR:HB	3:D:607:A3D:H51N	2.00	0.42
1:B:50:VAL:HG11	1:B:87:ALA:HA	2.00	0.42
1:D:172:PHE:CD2	1:D:189:ALA:HB1	2.54	0.42
1:A:306:GLU:HG3	1:D:211:LYS:HD3	2.00	0.42
1:D:97:THR:HG22	1:D:138:VAL:HB	2.02	0.42
1:B:58:MET:HB3	1:B:59:PRO:HD3	2.02	0.42
1:D:54:VAL:HG13	3:D:607:A3D:N1A	2.35	0.42
1:C:38:TYR:HA	1:C:66:LEU:HD22	2.01	0.42
1:A:171:ARG:HG2	1:C:68:HIS:CE1	2.55	0.41
1:D:209(C):TYR:HA	1:D:209(D):PRO:HD3	1.93	0.41
1:A:36:MET:SD	1:A:95:ILE:HG21	2.60	0.41
1:A:50:VAL:HG13	1:A:81:GLU:HG2	2.02	0.41
1:A:332:GLN:NE2	4:A:677:HOH:O	2.52	0.41
1:B:247:TYR:C	1:B:250:PRO:HD2	2.41	0.41
1:C:249:ALA:N	1:C:250:PRO:CD	2.83	0.41
1:A:68:HIS:CE1	1:C:171:ARG:HG2	2.56	0.41
1:C:325(B):ASN:O	1:C:328:VAL:HG22	2.20	0.41
1:C:58:MET:HB3	1:C:59:PRO:HD3	2.02	0.41
1:B:140:ASN:HA	1:B:142:LEU:N	2.36	0.40
1:B:120:ILE:HD13	1:B:120:ILE:HA	1.94	0.40
1:C:247:TYR:C	1:C:250:PRO:HD2	2.41	0.40
1:D:103(D):LYS:HA	1:D:103(E):PRO:HD3	1.98	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	325/331 (98%)	320 (98%)	5 (2%)	0	100	100
1	B	325/331 (98%)	319 (98%)	5 (2%)	1 (0%)	46	23
1	C	322/331 (97%)	314 (98%)	6 (2%)	2 (1%)	30	9
1	D	323/331 (98%)	318 (98%)	4 (1%)	1 (0%)	46	23
All	All	1295/1324 (98%)	1271 (98%)	20 (2%)	4 (0%)	46	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	114	PRO
1	B	164	ALA
1	D	164	ALA
1	C	164	ALA

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	269/270 (100%)	268 (100%)	1 (0%)	93	88
1	B	269/270 (100%)	267 (99%)	2 (1%)	88	78
1	C	267/270 (99%)	265 (99%)	2 (1%)	88	78
1	D	268/270 (99%)	267 (100%)	1 (0%)	93	88
All	All	1073/1080 (99%)	1067 (99%)	6 (1%)	90	82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	SER
1	B	276	ASN
1	B	318	SER
1	C	276	ASN

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Mol	Chain	Res	Type
1	C	318	SER
1	D	318	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	332	GLN
1	B	276	ASN
1	C	276	ASN
1	C	314	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
1	CME	A	150	1	8,9,10	1.19	1 (12%)	6,9,11	1.44	1 (16%)
1	CME	B	150	1	8,9,10	1.16	1 (12%)	6,9,11	1.36	1 (16%)
1	CME	C	150	1	8,9,10	1.16	1 (12%)	6,9,11	1.51	2 (33%)
1	CME	D	150	1	8,9,10	1.23	1 (12%)	6,9,11	1.29	1 (16%)

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
1	CME	A	150	1	-	0/5/8/10	0/0/0/0
1	CME	B	150	1	-	0/5/8/10	0/0/0/0
1	CME	C	150	1	-	0/5/8/10	0/0/0/0
1	CME	D	150	1	-	0/5/8/10	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	CME	OH-CZ	-3.16	1.25	1.42
1	D	150	CME	OH-CZ	-3.16	1.25	1.42
1	B	150	CME	OH-CZ	-3.06	1.25	1.42
1	C	150	CME	OH-CZ	-3.03	1.25	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	150	CME	OH-CZ-CE	2.00	119.59	110.83
1	C	150	CME	OH-CZ-CE	2.10	120.04	110.83
1	C	150	CME	CZ-CE-SD	2.17	118.46	113.16
1	B	150	CME	OH-CZ-CE	2.21	120.53	110.83
1	D	150	CME	OH-CZ-CE	2.26	120.73	110.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	150	CME	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	$\#|Z| > 2$
3	A3D	A	601	-	38,48,48	1.66	8 (21%)	47,73,73	1.80	7 (14%)
2	SO4	A	602	-	4,4,4	0.41	0	6,6,6	0.84	0
3	A3D	B	603	-	38,48,48	1.81	9 (23%)	47,73,73	1.77	6 (12%)
2	SO4	B	604	-	4,4,4	0.48	0	6,6,6	0.58	0
3	A3D	C	605	-	38,48,48	1.81	10 (26%)	47,73,73	1.77	6 (12%)
2	SO4	C	606	-	4,4,4	0.35	0	6,6,6	0.50	0
3	A3D	D	607	-	38,48,48	1.77	10 (26%)	47,73,73	1.76	7 (14%)
2	SO4	D	608	-	4,4,4	0.35	0	6,6,6	0.25	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
3	A3D	A	601	-	-	0/22/62/62	0/5/5/5
2	SO4	A	602	-	-	0/0/0/0	0/0/0/0
3	A3D	B	603	-	-	0/22/62/62	0/5/5/5
2	SO4	B	604	-	-	0/0/0/0	0/0/0/0
3	A3D	C	605	-	-	0/22/62/62	0/5/5/5
2	SO4	C	606	-	-	0/0/0/0	0/0/0/0
3	A3D	D	607	-	-	0/22/62/62	0/5/5/5
2	SO4	D	608	-	-	0/0/0/0	0/0/0/0

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	607	A3D	PA-O1A	-2.89	1.40	1.51
3	B	603	A3D	PA-O1A	-2.42	1.42	1.51
3	A	601	A3D	PA-O1A	-2.22	1.43	1.51
3	C	605	A3D	PA-O1A	-2.21	1.43	1.51
3	D	607	A3D	C3D-C4D	2.01	1.58	1.53
3	D	607	A3D	C6N-C5N	2.03	1.43	1.38
3	C	605	A3D	C6N-C5N	2.08	1.43	1.38
3	B	603	A3D	C5N-C4N	2.11	1.43	1.38
3	C	605	A3D	C3B-C4B	2.14	1.58	1.53
3	C	605	A3D	O4B-C4B	2.28	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	A3D	C4A-N3A	2.28	1.39	1.35
3	D	607	A3D	O4D-C1D	2.31	1.44	1.41
3	D	607	A3D	C3B-C4B	2.32	1.59	1.53
3	B	603	A3D	C3B-C4B	2.34	1.59	1.53
3	A	601	A3D	C3B-C4B	2.39	1.59	1.53
3	B	603	A3D	C4A-N3A	2.52	1.39	1.35
3	D	607	A3D	C4A-N3A	2.61	1.39	1.35
3	C	605	A3D	C4A-N3A	2.72	1.39	1.35
3	A	601	A3D	O4D-C1D	2.89	1.44	1.41
3	A	601	A3D	C6N-N1N	2.99	1.43	1.35
3	D	607	A3D	C6N-N1N	3.00	1.43	1.35
3	B	603	A3D	C6N-N1N	3.22	1.44	1.35
3	C	605	A3D	C6N-N1N	3.23	1.44	1.35
3	B	603	A3D	O4D-C1D	3.48	1.45	1.41
3	A	601	A3D	C2A-N1A	3.77	1.41	1.33
3	C	605	A3D	C2A-N3A	3.79	1.38	1.32
3	C	605	A3D	C2A-N1A	3.81	1.41	1.33
3	A	601	A3D	C2A-N3A	3.98	1.39	1.32
3	B	603	A3D	C2A-N1A	4.04	1.41	1.33
3	D	607	A3D	C2A-N1A	4.17	1.41	1.33
3	A	601	A3D	C4N-C3N	4.20	1.46	1.39
3	C	605	A3D	O4D-C1D	4.25	1.46	1.41
3	D	607	A3D	C2A-N3A	4.30	1.39	1.32
3	B	603	A3D	C2A-N3A	4.49	1.40	1.32
3	B	603	A3D	C4N-C3N	4.65	1.47	1.39
3	D	607	A3D	C4N-C3N	4.67	1.47	1.39
3	C	605	A3D	C4N-C3N	4.74	1.47	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	A3D	N3A-C2A-N1A	-8.49	122.40	128.89
3	A	601	A3D	N3A-C2A-N1A	-8.46	122.42	128.89
3	D	607	A3D	N3A-C2A-N1A	-8.33	122.52	128.89
3	C	605	A3D	N3A-C2A-N1A	-8.08	122.71	128.89
3	C	605	A3D	C1B-N9A-C4A	-4.22	120.57	126.94
3	A	601	A3D	C1B-N9A-C4A	-3.84	121.15	126.94
3	B	603	A3D	O5B-C5B-C4B	-3.51	96.17	109.12
3	D	607	A3D	C1B-N9A-C4A	-3.50	121.66	126.94
3	D	607	A3D	O5B-C5B-C4B	-3.49	96.24	109.12
3	A	601	A3D	O5B-C5B-C4B	-3.46	96.37	109.12
3	C	605	A3D	O5B-C5B-C4B	-3.26	97.09	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	A3D	C1B-N9A-C4A	-3.25	122.03	126.94
3	C	605	A3D	O4D-C1D-N1N	-2.32	105.58	108.13
3	D	607	A3D	O4D-C1D-N1N	-2.09	105.83	108.13
3	A	601	A3D	C5N-C6N-N1N	-2.08	116.87	120.47
3	B	603	A3D	C5N-C6N-N1N	-2.04	116.94	120.47
3	D	607	A3D	C5N-C6N-N1N	-2.03	116.96	120.47
3	A	601	A3D	O4D-C1D-N1N	-2.03	105.90	108.13
3	B	603	A3D	O4B-C1B-N9A	2.46	113.24	108.10
3	B	603	A3D	C2N-C3N-C4N	2.55	121.13	118.29
3	D	607	A3D	C2N-C3N-C4N	2.56	121.14	118.29
3	A	601	A3D	C2N-C3N-C4N	2.65	121.24	118.29
3	D	607	A3D	O4B-C1B-N9A	2.71	113.78	108.10
3	C	605	A3D	C2N-C3N-C4N	2.78	121.38	118.29
3	A	601	A3D	O4B-C1B-N9A	2.85	114.07	108.10
3	C	605	A3D	O4B-C1B-N9A	2.91	114.19	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	605	A3D	1	0
3	D	607	A3D	2	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(Å²)	Q<0.9
1	A	327/331 (98%)	0.01	17 (5%)	31	28	12, 17, 34, 47	0
1	B	327/331 (98%)	0.08	16 (4%)	33	30	13, 19, 36, 52	0
1	C	324/331 (97%)	0.43	34 (10%)	8	7	12, 20, 48, 61	0
1	D	325/331 (98%)	0.30	32 (9%)	10	8	13, 20, 43, 59	0
All	All	1303/1324 (98%)	0.20	99 (7%)	17	15	12, 19, 39, 61	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	103(E)	PRO	9.9
1	C	115	PHE	9.6
1	C	103(C)	GLY	7.9
1	C	105(B)	SER	7.8
1	C	103(B)	PRO	7.4
1	D	103(A)	VAL	6.6
1	C	107	TRP	6.5
1	B	83	TYR	6.2
1	D	103(B)	PRO	6.0
1	C	331	LEU	6.0
1	D	103(E)	PRO	5.9
1	C	330	ALA	5.7
1	D	115	PHE	5.5
1	C	108	SER	5.4
1	C	106	GLU	5.3
1	D	103(C)	GLY	5.2
1	C	105(A)	ASP	5.1
1	C	332	GLN	5.1
1	C	103(D)	LYS	5.1
1	B	105(B)	SER	4.9
1	C	112	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	56	LYS	4.9
1	A	103(C)	GLY	4.7
1	D	331	LEU	4.6
1	D	103(D)	LYS	4.6
1	D	56	LYS	4.6
1	C	15	ALA	4.5
1	C	100	LEU	4.5
1	A	83	TYR	4.4
1	C	101	THR	4.4
1	D	83	TYR	4.3
1	D	330	ALA	4.3
1	C	56	LYS	4.2
1	C	103(A)	VAL	4.2
1	D	332	GLN	4.1
1	C	328	VAL	4.1
1	C	110	ASN	4.0
1	B	103(B)	PRO	4.0
1	B	103(C)	GLY	4.0
1	B	103(E)	PRO	3.9
1	A	280	GLY	3.8
1	B	309	GLU	3.8
1	D	243	GLN	3.8
1	D	108	SER	3.7
1	A	14	PRO	3.7
1	D	100	LEU	3.7
1	D	107	TRP	3.7
1	C	329	ALA	3.7
1	D	105(B)	SER	3.6
1	D	241	ARG	3.7
1	D	105(A)	ASP	3.6
1	D	14	PRO	3.5
1	C	326	LYS	3.5
1	C	114	PRO	3.4
1	B	103(D)	LYS	3.4
1	C	327	ALA	3.4
1	D	106	GLU	3.4
1	C	111	ASP	3.2
1	B	14	PRO	3.2
1	A	106	GLU	3.2
1	D	101	THR	3.2
1	D	112	LEU	3.1
1	A	105(B)	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	56	LYS	3.0
1	B	334	PRO	2.9
1	C	83	TYR	2.9
1	A	103(E)	PRO	2.9
1	B	106	GLU	2.9
1	D	326	LYS	2.9
1	A	309	GLU	2.7
1	D	114	PRO	2.7
1	D	110	ASN	2.6
1	A	334	PRO	2.6
1	C	243	GLN	2.6
1	A	276	ASN	2.5
1	A	279	TYR	2.5
1	B	243	GLN	2.5
1	A	103(D)	LYS	2.5
1	D	15	ALA	2.5
1	D	111	ASP	2.4
1	C	241	ARG	2.3
1	D	242(C)	GLY	2.3
1	A	313	LYS	2.3
1	C	96	VAL	2.3
1	B	317	LYS	2.3
1	A	142	LEU	2.2
1	A	137	VAL	2.2
1	C	138	VAL	2.2
1	B	105(A)	ASP	2.1
1	D	95	ILE	2.1
1	A	138	VAL	2.1
1	D	136	ILE	2.1
1	C	102	LYS	2.0
1	D	109	ARG	2.0
1	B	136	ILE	2.0
1	C	283	ASP	2.0
1	C	324	ALA	2.0
1	D	279	TYR	2.0
1	B	313	LYS	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å^2)	Q<0.9
1	CME	D	150	10/11	0.96	0.08	-	19,25,34,34	0
1	CME	C	150	10/11	0.93	0.11	-	22,25,38,39	0
1	CME	B	150	10/11	0.95	0.08	-	19,22,34,35	0
1	CME	A	150	10/11	0.95	0.08	-	15,18,31,31	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	602	5/5	0.95	0.09	-0.00	22,22,25,28	0
2	SO4	C	606	5/5	0.95	0.08	-0.35	23,25,28,30	0
3	A3D	B	603	44/44	0.95	0.09	-0.36	16,18,29,32	0
2	SO4	B	604	5/5	0.96	0.09	-0.37	23,24,27,29	0
3	A3D	A	601	44/44	0.96	0.09	-0.38	14,17,29,33	0
3	A3D	D	607	44/44	0.95	0.08	-0.52	19,22,32,35	0
3	A3D	C	605	44/44	0.95	0.08	-0.65	19,24,31,33	0
2	SO4	D	608	5/5	0.98	0.05	-1.08	24,26,27,29	0

6.5 Other polymers (i)

There are no such residues in this entry.