



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:50 PM BST

PDB ID : 4D9K
Title : Crystal structure of Escherichia coli Diaminopropionate ammonia lyase in apo form
Authors : Bisht, S.; Rajaram, V.; Bharath, S.R.; Murthy, M.R.N.
Deposited on : 2012-01-11
Resolution : 2.19 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

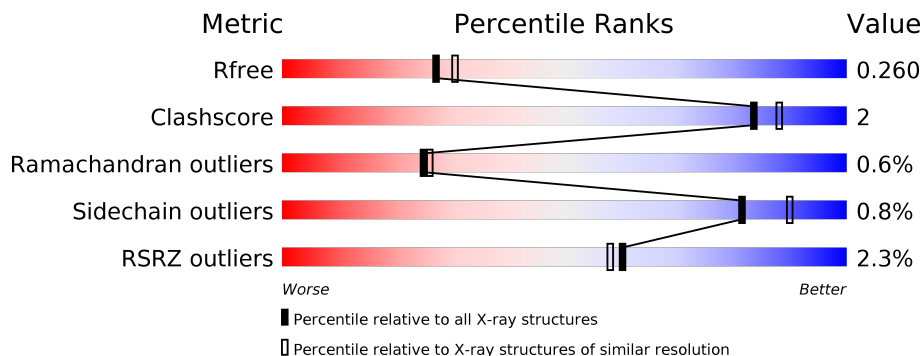
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 $\leq 5\%$. 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	398	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4% 86% 6% 8%</p>
1	B	398	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">% 82% 8% 10%</p>
1	C	398	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2% 86% 5% 9%</p>
1	D	398	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2% 85% 6% 8%</p>

2 Entry composition [i](#)

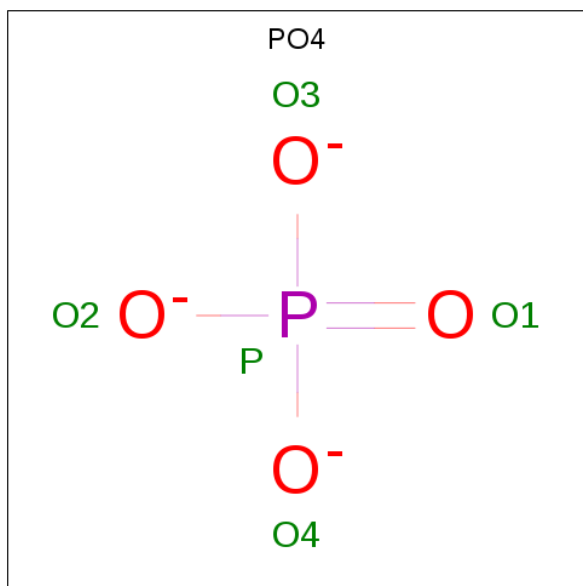
There are 4 unique types of molecules in this entry. The entry contains 11560 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Diaminopropionate ammonia-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	366	Total 2786	C 1767	N 477	O 525	S 17	0	0	0
1	D	367	Total 2793	C 1773	N 478	O 525	S 17	0	0	0
1	B	357	Total 2713	C 1719	N 464	O 513	S 17	0	0	0
1	C	363	Total 2730	C 1727	N 469	O 517	S 17	0	1	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	Total 5	O 4	P 1	0	0
2	D	1	Total 5	O 4	P 1	0	0

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

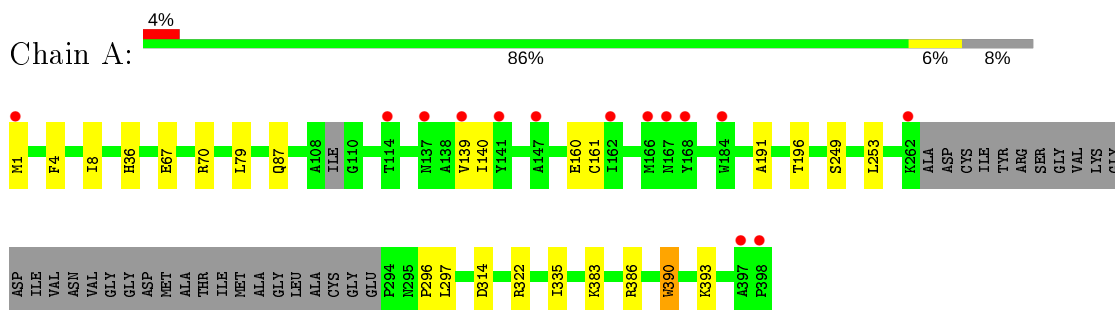
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	166	Total O 166 166	0	0
4	D	97	Total O 97 97	0	0
4	B	153	Total O 153 153	0	0
4	C	87	Total O 87 87	0	0

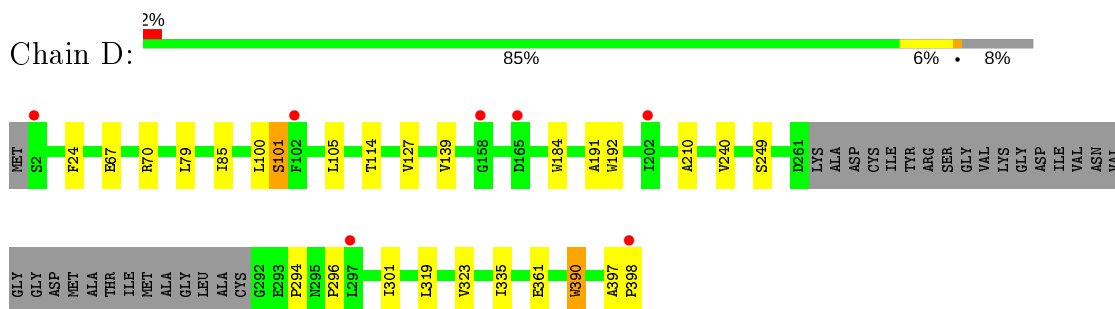
3 Residue-property plots [i](#)

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.

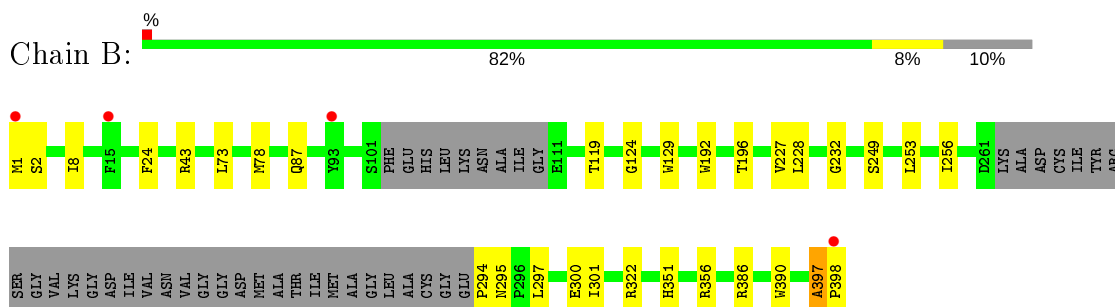
- Molecule 1: Diaminopropionate ammonia-lyase



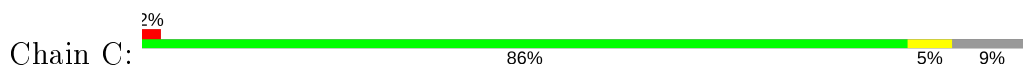
- Molecule 1: Diaminopropionate ammonia-lyase

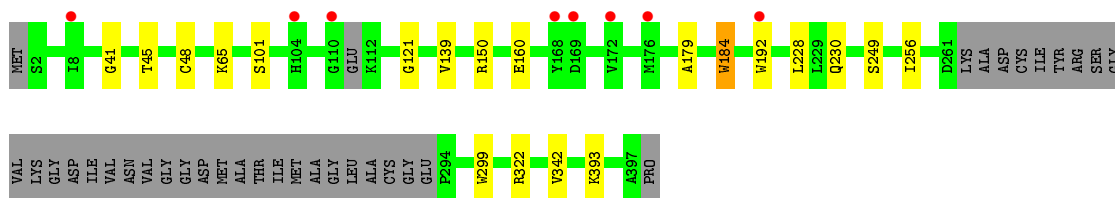


- Molecule 1: Diaminopropionate ammonia-lyase



- Molecule 1: Diaminopropionate ammonia-lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.78Å 94.14Å 94.69Å 90.00° 110.01° 90.00°	Depositor
Resolution (Å)	40.65 – 2.19 40.65 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.0 (40.65-2.19) 98.1 (40.65-2.19)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.213 , 0.261 0.212 , 0.260	Depositor DCC
R_{free} test set	3590 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtrriage
Anisotropy	0.415	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11560	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.4131e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: CME, PO4, SO4

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	1/2833 (0.0%)	0.51	0/3847
1	B	0.47	1/2758 (0.0%)	0.51	0/3748
1	C	0.46	3/2768 (0.1%)	0.48	0/3765
1	D	0.46	2/2841 (0.1%)	0.50	0/3859
All	All	0.47	7/11200 (0.1%)	0.50	0/15219

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	390	TRP	CD2-CE2	5.24	1.47	1.41
1	D	192	TRP	CD2-CE2	5.13	1.47	1.41
1	B	192	TRP	CD2-CE2	5.07	1.47	1.41
1	D	390	TRP	CD2-CE2	5.06	1.47	1.41
1	C	192	TRP	CD2-CE2	5.04	1.47	1.41
1	C	299	TRP	CD2-CE2	5.04	1.47	1.41
1	C	184	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

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	2786	0	2714	13	0
1	B	2713	0	2635	19	0
1	C	2730	0	2604	10	0
1	D	2793	0	2723	14	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	10	0	0	0	0
3	C	5	0	0	0	0
4	A	166	0	0	1	0
4	B	153	0	0	0	0
4	C	87	0	0	0	0
4	D	97	0	0	1	0
All	All	11560	0	10676	52	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 2.

All (52) 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:A:383:LYS:HG3	1:B:1:MET:HA	1.64	0.78
1:B:398:PRO:HB3	1:C:41:GLY:HA2	1.67	0.76
1:B:397:ALA:HB1	1:B:398:PRO:CD	2.19	0.73
1:D:67:GLU:OE1	1:D:70:ARG:HD2	1.94	0.67
1:A:8:ILE:HG22	1:A:8:ILE:O	1.95	0.65
1:C:139:VAL:HG12	1:C:160:GLU:HB2	1.80	0.63
1:D:100:LEU:O	1:D:101:SER:HB3	2.00	0.61
1:D:397:ALA:HB3	1:D:398:PRO:HD3	1.80	0.61
1:A:67:GLU:OE1	1:A:70:ARG:HD2	2.01	0.60
1:B:24:PHE:CD2	1:B:301:ILE:HD11	2.35	0.60
1:C:121:GLY:HA3	1:C:150:ARG:HD3	1.84	0.60
1:D:390:TRP:O	1:C:322:ARG:HD2	2.04	0.56
1:B:351:HIS:HD2	1:B:356:ARG:HH21	1.54	0.56
1:A:390:TRP:O	1:B:322:ARG:HD2	2.05	0.56
1:A:196:THR:HG23	1:A:297:LEU:HD11	1.89	0.54
1:D:100:LEU:O	1:D:101:SER:CB	2.56	0.53
1:D:335:ILE:HD11	4:D:597:HOH:O	2.07	0.53
1:B:73:LEU:HD11	1:B:129:TRP:CD1	2.44	0.52
1:D:70:ARG:HD3	1:D:79:LEU:HG	1.93	0.50
1:B:232:GLY:HA3	2:B:401:PO4:O1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:VAL:HG12	1:A:160:GLU:HB2	1.94	0.49
1:A:335:ILE:HD11	4:A:762:HOH:O	2.13	0.48
1:B:397:ALA:CB	1:B:398:PRO:CD	2.91	0.48
1:B:397:ALA:HB1	1:B:398:PRO:HD2	1.95	0.48
1:D:210:ALA:HB2	1:D:240:VAL:HG13	1.96	0.48
1:D:319:LEU:O	1:D:323:VAL:HG23	2.14	0.47
1:C:230:GLN:HG3	1:C:342:VAL:HG12	1.97	0.47
1:A:322:ARG:NH2	1:A:393:LYS:O	2.48	0.47
1:C:48[A]:CME:HE3	1:C:48[A]:CME:HA	1.97	0.46
1:A:191:ALA:HB3	1:A:296:PRO:HD2	1.98	0.45
1:D:24:PHE:CD2	1:D:301:ILE:HD11	2.52	0.45
1:B:196:THR:HG23	1:B:297:LEU:HD11	1.98	0.44
1:B:73:LEU:HD22	1:B:78:MET:HB3	2.00	0.44
1:D:114:THR:HB	1:D:184:TRP:CD1	2.52	0.44
1:A:386:ARG:O	1:A:390:TRP:HB2	2.18	0.43
1:B:8:ILE:O	1:B:8:ILE:HG22	2.18	0.43
1:D:85:ILE:HD11	1:D:127:VAL:HG13	2.01	0.43
1:B:397:ALA:HB1	1:B:398:PRO:HD3	1.97	0.43
1:C:179:ALA:HA	1:C:184:TRP:HB2	2.01	0.42
1:A:1:MET:HG3	1:A:4:PHE:HB3	2.01	0.42
1:B:227:VAL:HG12	1:B:253:LEU:HD11	2.02	0.42
1:C:45:THR:OG1	1:C:65:LYS:HE3	2.20	0.42
1:B:119:THR:HG21	1:B:124:GLY:HA3	2.02	0.42
1:C:322:ARG:NH2	1:C:393:LYS:O	2.53	0.42
1:D:139:VAL:HG21	1:D:184:TRP:CZ3	2.55	0.41
1:B:294:PRO:HB2	1:B:295:ASN:H	1.66	0.41
1:B:386:ARG:O	1:B:390:TRP:HB2	2.20	0.41
1:B:228:LEU:HG	1:B:256:ILE:HB	2.03	0.41
1:A:140:ILE:O	1:A:161:CYS:HA	2.21	0.41
1:D:191:ALA:HB3	1:D:296:PRO:HD2	2.03	0.41
1:C:228:LEU:HG	1:C:256:ILE:HB	2.02	0.41
1:A:36:HIS:NE2	1:A:79:LEU:HA	2.35	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	359/398 (90%)	346 (96%)	12 (3%)	1 (0%)	41	46
1	B	350/398 (88%)	337 (96%)	11 (3%)	2 (1%)	25	26
1	C	356/398 (89%)	342 (96%)	12 (3%)	2 (1%)	25	26
1	D	362/398 (91%)	345 (95%)	14 (4%)	3 (1%)	19	19
All	All	1427/1592 (90%)	1370 (96%)	49 (3%)	8 (1%)	25	26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	101	SER
1	B	397	ALA
1	C	101	SER
1	D	294	PRO
1	A	249	SER
1	B	249	SER
1	D	249	SER
1	C	249	SER

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	286/318 (90%)	283 (99%)	3 (1%)	76	86
1	B	278/318 (87%)	274 (99%)	4 (1%)	67	80
1	C	270/318 (85%)	270 (100%)	0	100	100
1	D	286/318 (90%)	284 (99%)	2 (1%)	84	91
All	All	1120/1272 (88%)	1111 (99%)	9 (1%)	81	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	253	LEU
1	A	314	ASP
1	D	105	LEU
1	D	361	GLU
1	B	2	SER
1	B	43	ARG
1	B	87	GLN
1	B	300	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	133	GLN
1	A	330	ASN
1	A	355	GLN
1	D	37	GLN
1	D	137	ASN
1	D	252	ASN
1	D	394	HIS
1	B	87	GLN
1	B	330	ASN
1	B	351	HIS
1	C	330	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

5 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	B	48	1	8,9,10	0.79	0	5,9,11	0.70	0
1	CME	C	48[B]	-	8,9,10	0.77	0	5,9,11	0.69	0
1	CME	C	48[A]	-	8,9,10	0.80	0	5,9,11	0.83	0
1	CME	A	48	1	8,9,10	0.87	0	5,9,11	1.10	0
1	CME	D	48	1	8,9,10	0.81	0	5,9,11	0.74	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
1	CME	B	48	1	-	2/5/8/10	-
1	CME	C	48[B]	-	-	1/5/8/10	-
1	CME	C	48[A]	-	-	3/5/8/10	-
1	CME	A	48	1	-	1/5/8/10	-
1	CME	D	48	1	-	2/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	48[B]	CME	SD-CE-CZ-OH
1	C	48[A]	CME	N-CA-CB-SG
1	A	48	CME	SD-CE-CZ-OH
1	D	48	CME	SD-CE-CZ-OH
1	C	48[A]	CME	SD-CE-CZ-OH
1	C	48[A]	CME	CE-SD-SG-CB
1	B	48	CME	CE-SD-SG-CB
1	B	48	CME	CA-CB-SG-SD
1	D	48	CME	CZ-CE-SD-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	48[A]	CME	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	SO4	A	502	-	4,4,4	0.33	0	6,6,6	0.07	0
2	PO4	C	401	-	4,4,4	0.97	0	6,6,6	0.42	0
2	PO4	A	501	-	4,4,4	1.08	0	6,6,6	0.59	0
2	PO4	B	401	-	4,4,4	1.00	0	6,6,6	0.70	0
2	PO4	D	401	-	4,4,4	0.98	0	6,6,6	0.40	0
3	SO4	C	402	-	4,4,4	0.34	0	6,6,6	0.06	0
3	SO4	A	503	-	4,4,4	0.35	0	6,6,6	0.16	0

There are no bond length outliers.

There are no bond angle outliers.

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
2	B	401	PO4	1	0

5.7 Other polymers [i](#)

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, 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	365/398 (91%)	0.28	14 (3%) 40 38	23, 36, 72, 88	0
1	B	356/398 (89%)	0.11	4 (1%) 80 79	22, 37, 56, 83	0
1	C	362/398 (90%)	0.26	8 (2%) 62 59	29, 50, 87, 109	0
1	D	366/398 (91%)	0.20	7 (1%) 66 65	31, 45, 67, 83	0
All	All	1449/1592 (91%)	0.21	33 (2%) 60 58	22, 41, 71, 109	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	6.3
1	A	1	MET	5.6
1	C	176	MET	4.8
1	A	184	TRP	4.4
1	A	168	TYR	4.1
1	B	398	PRO	4.1
1	C	104	HIS	3.7
1	D	2	SER	3.6
1	B	15	PHE	3.6
1	D	165	ASP	3.4
1	A	162	ILE	3.3
1	D	102	PHE	3.1
1	C	110	GLY	3.1
1	A	166	MET	3.1
1	A	137	ASN	3.0
1	A	262	LYS	3.0
1	C	169	ASP	3.0
1	A	139	VAL	3.0
1	C	172	VAL	2.8
1	A	167	ASN	2.8
1	A	141	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	192	TRP	2.5
1	A	398	PRO	2.5
1	B	93	TYR	2.5
1	A	114	THR	2.4
1	A	397	ALA	2.4
1	C	8	ILE	2.2
1	D	398	PRO	2.2
1	D	202	ILE	2.2
1	C	168	TYR	2.2
1	D	297	LEU	2.1
1	A	147	ALA	2.0
1	D	158	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CME	C	48[B]	10/11	0.80	0.19	34,36,40,40	7
1	CME	C	48[A]	10/11	0.80	0.19	34,36,37,38	7
1	CME	D	48	10/11	0.86	0.12	37,41,50,50	0
1	CME	A	48	10/11	0.89	0.15	29,33,45,45	0
1	CME	B	48	10/11	0.89	0.14	32,35,46,48	0

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
3	SO4	C	402	5/5	0.90	0.22	82,83,84,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	B	401	5/5	0.95	0.14	38,42,43,44	0
2	PO4	D	401	5/5	0.95	0.12	59,62,62,63	0
2	PO4	C	401	5/5	0.95	0.15	63,64,66,66	0
3	SO4	A	503	5/5	0.95	0.16	47,48,48,49	0
2	PO4	A	501	5/5	0.97	0.14	46,47,49,50	0
3	SO4	A	502	5/5	0.98	0.17	53,53,54,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.