



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:57 pm BST

PDB ID : 6QAP
Title : Structure of the human aldehyde dehydrogenase 9A1 in C2 space group
Authors : Morera, S.; Vigouroux, A.
Deposited on : 2018-12-19
Resolution : 2.30 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 : 2.11
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

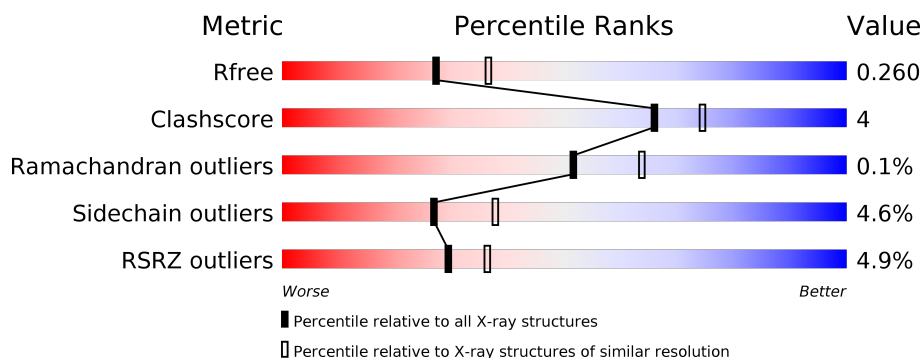
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	508	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>7%</div> </div> </div>
1	B	508	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>7%</div> </div> </div>
1	C	508	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>7%</div> </div> </div>
1	D	508	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>7%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	505	-	-	X	-
2	EDO	D	507	-	-	X	-
3	PEG	B	504	-	-	X	-
3	PEG	C	506	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14878 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 4-trimethylaminobutyraldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3600	2279	615	678	28			
1	B	470	Total	C	N	O	S	0	0	0
			3600	2279	615	678	28			
1	C	471	Total	C	N	O	S	0	0	0
			3604	2281	616	679	28			
1	D	471	Total	C	N	O	S	0	2	0
			3620	2291	622	679	28			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP P49189
A	-12	GLY	-	expression tag	UNP P49189
A	-11	SER	-	expression tag	UNP P49189
A	-10	SER	-	expression tag	UNP P49189
A	-9	HIS	-	expression tag	UNP P49189
A	-8	HIS	-	expression tag	UNP P49189
A	-7	HIS	-	expression tag	UNP P49189
A	-6	HIS	-	expression tag	UNP P49189
A	-5	HIS	-	expression tag	UNP P49189
A	-4	HIS	-	expression tag	UNP P49189
A	-3	SER	-	expression tag	UNP P49189
A	-2	GLN	-	expression tag	UNP P49189
A	-1	ASP	-	expression tag	UNP P49189
A	0	PRO	-	expression tag	UNP P49189
B	-13	MET	-	initiating methionine	UNP P49189
B	-12	GLY	-	expression tag	UNP P49189
B	-11	SER	-	expression tag	UNP P49189
B	-10	SER	-	expression tag	UNP P49189
B	-9	HIS	-	expression tag	UNP P49189
B	-8	HIS	-	expression tag	UNP P49189
B	-7	HIS	-	expression tag	UNP P49189

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP P49189
B	-5	HIS	-	expression tag	UNP P49189
B	-4	HIS	-	expression tag	UNP P49189
B	-3	SER	-	expression tag	UNP P49189
B	-2	GLN	-	expression tag	UNP P49189
B	-1	ASP	-	expression tag	UNP P49189
B	0	PRO	-	expression tag	UNP P49189
C	-13	MET	-	initiating methionine	UNP P49189
C	-12	GLY	-	expression tag	UNP P49189
C	-11	SER	-	expression tag	UNP P49189
C	-10	SER	-	expression tag	UNP P49189
C	-9	HIS	-	expression tag	UNP P49189
C	-8	HIS	-	expression tag	UNP P49189
C	-7	HIS	-	expression tag	UNP P49189
C	-6	HIS	-	expression tag	UNP P49189
C	-5	HIS	-	expression tag	UNP P49189
C	-4	HIS	-	expression tag	UNP P49189
C	-3	SER	-	expression tag	UNP P49189
C	-2	GLN	-	expression tag	UNP P49189
C	-1	ASP	-	expression tag	UNP P49189
C	0	PRO	-	expression tag	UNP P49189
D	-13	MET	-	initiating methionine	UNP P49189
D	-12	GLY	-	expression tag	UNP P49189
D	-11	SER	-	expression tag	UNP P49189
D	-10	SER	-	expression tag	UNP P49189
D	-9	HIS	-	expression tag	UNP P49189
D	-8	HIS	-	expression tag	UNP P49189
D	-7	HIS	-	expression tag	UNP P49189
D	-6	HIS	-	expression tag	UNP P49189
D	-5	HIS	-	expression tag	UNP P49189
D	-4	HIS	-	expression tag	UNP P49189
D	-3	SER	-	expression tag	UNP P49189
D	-2	GLN	-	expression tag	UNP P49189
D	-1	ASP	-	expression tag	UNP P49189
D	0	PRO	-	expression tag	UNP P49189

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	5	Total	Na	0	0
			5	5		
4	C	3	Total	Na	0	0
			3	3		

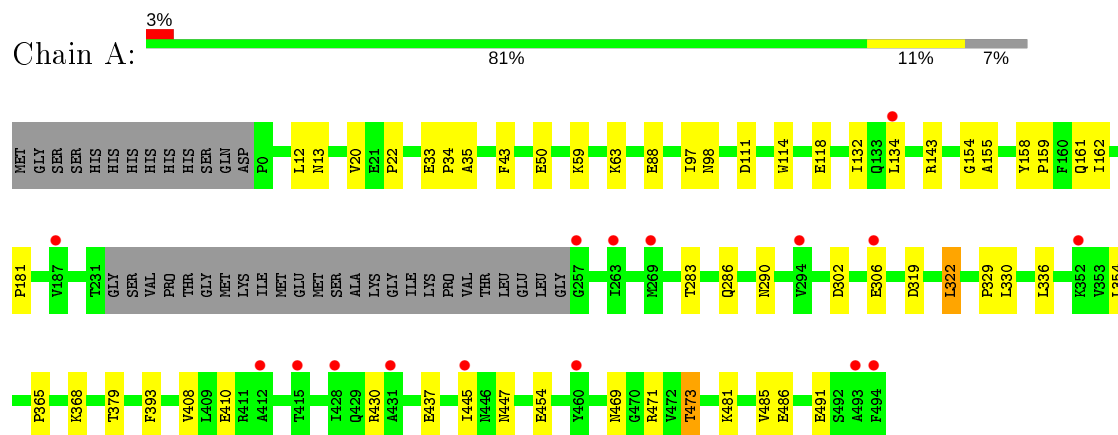
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	94	Total 94	O 94	0	0
5	B	85	Total 85	O 85	0	0
5	C	96	Total 96	O 96	0	0
5	D	83	Total 83	O 83	0	0

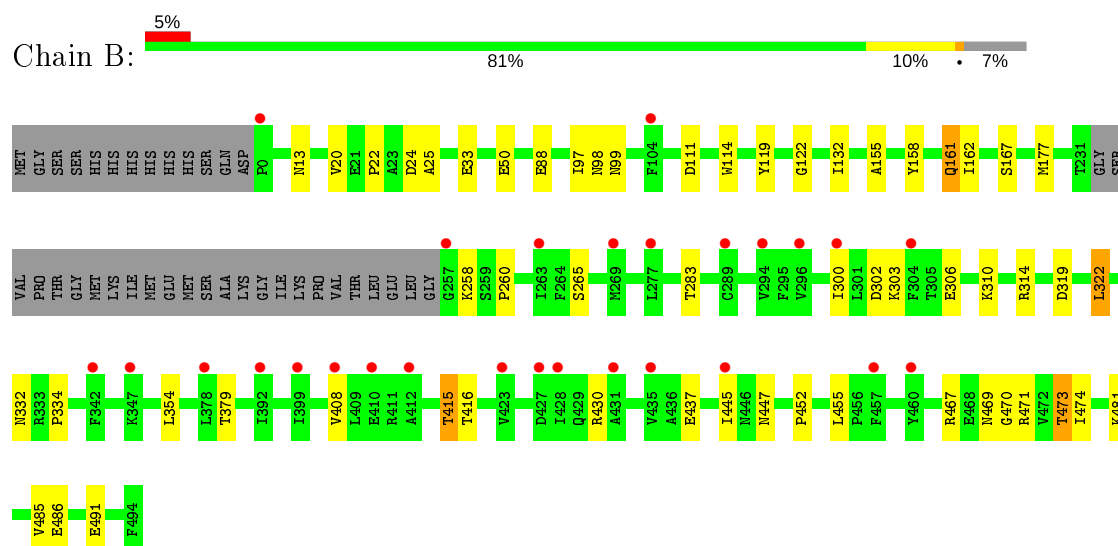
3 Residue-property plots [i](#)

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.

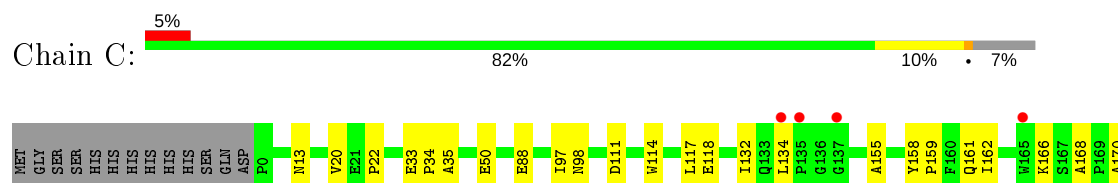
- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase



- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase



- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.29Å 160.03Å 84.60Å 90.00° 91.09° 90.00°	Depositor
Resolution (Å)	47.74 – 2.30 47.74 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.74-2.30) 99.7 (47.74-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.220 , 0.251 0.228 , 0.260	Depositor DCC
R_{free} test set	4843 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l 0.006 for -k,-h,-l 0.289 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14878	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.51	0/3672	0.71	0/4966
1	B	0.51	0/3672	0.69	0/4966
1	C	0.51	0/3676	0.70	0/4971
1	D	0.50	0/3698	0.69	0/4999
All	All	0.51	0/14718	0.70	0/19902

There are no bond length outliers.

There are no bond angle outliers.

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	3600	0	3574	31	0
1	B	3600	0	3574	31	0
1	C	3604	0	3577	30	0
1	D	3620	0	3603	33	0
2	A	20	0	30	8	0
2	B	12	0	18	3	0
2	C	4	0	6	0	0
2	D	24	0	35	12	0
3	B	7	0	10	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	21	0	30	6	0
4	C	3	0	0	0	0
4	D	5	0	0	0	0
5	A	94	0	0	0	0
5	B	85	0	0	2	0
5	C	96	0	0	1	0
5	D	83	0	0	0	0
All	All	14878	0	14457	117	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 (117) 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:159:PRO:HA	2:A:505:EDO:H22	1.45	0.99
1:B:332:ASN:HB3	1:B:334:PRO:HD2	1.52	0.90
1:C:469:ASN:O	1:C:473:THR:HG23	1.72	0.87
1:B:24:ASP:HB2	3:B:504:PEG:H21	1.56	0.85
1:A:469:ASN:O	1:A:473:THR:HG23	1.78	0.83
1:D:144:ARG:HG3	2:D:511:EDO:H22	1.60	0.82
1:B:25:ALA:H	3:B:504:PEG:H41	1.44	0.80
1:B:122:GLY:HA2	3:C:506:PEG:H21	1.64	0.79
1:B:469:ASN:O	1:B:473:THR:HG23	1.84	0.76
1:D:43:PHE:HB2	2:D:508:EDO:H11	1.66	0.75
1:D:203:PRO:HA	2:D:507:EDO:H11	1.70	0.74
1:C:155:ALA:HB3	1:C:162:ILE:HD13	1.70	0.72
1:D:201:VAL:CG2	2:D:507:EDO:H21	2.19	0.71
1:A:159:PRO:CA	2:A:505:EDO:H22	2.19	0.70
1:D:201:VAL:HG23	2:D:507:EDO:H21	1.72	0.70
1:C:118:GLU:O	3:C:506:PEG:H12	1.92	0.68
2:B:502:EDO:H22	1:C:467:ARG:HH11	1.61	0.65
1:D:155:ALA:HB3	1:D:162:ILE:HD13	1.77	0.64
1:A:43:PHE:HB2	2:A:503:EDO:H11	1.80	0.63
1:C:118:GLU:OE1	3:C:506:PEG:H41	2.00	0.62
1:B:155:ALA:HB3	1:B:162:ILE:HD13	1.82	0.61
1:C:265:SER:HA	1:C:300:ILE:HG12	1.83	0.61
1:B:265:SER:HA	1:B:300:ILE:HG12	1.83	0.59
1:D:144:ARG:HG3	2:D:511:EDO:C2	2.31	0.59
1:D:265:SER:HA	1:D:300:ILE:HG12	1.86	0.57
1:A:486:GLU:HB2	1:B:447:ASN:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:610:HOH:O	3:C:506:PEG:H22	2.05	0.56
1:A:155:ALA:HB3	1:A:162:ILE:HD13	1.87	0.55
1:C:486:GLU:HB2	1:D:447:ASN:HB2	1.87	0.55
1:A:12:LEU:HB2	2:A:503:EDO:H21	1.89	0.55
1:A:181:PRO:HA	2:A:505:EDO:H11	1.89	0.55
1:A:447:ASN:HB2	1:B:486:GLU:HB2	1.88	0.54
1:A:319:ASP:HB3	1:A:322:LEU:HD22	1.88	0.53
1:A:471:ARG:HD2	5:B:601:HOH:O	2.08	0.53
1:B:354:LEU:HD11	1:B:379:THR:HB	1.91	0.53
1:A:365:PRO:O	1:A:368:LYS:HB2	2.09	0.53
1:D:258:LYS:HE2	1:D:292:THR:OG1	2.09	0.52
1:C:34:PRO:HB2	1:C:329:PRO:HG2	1.92	0.52
1:A:13:ASN:HB2	1:A:20:VAL:O	2.10	0.52
1:B:13:ASN:HB2	1:B:20:VAL:O	2.11	0.51
1:D:13:ASN:HB2	1:D:20:VAL:O	2.11	0.51
1:B:319:ASP:HB3	1:B:322:LEU:HD22	1.92	0.51
1:D:354:LEU:HD11	1:D:379:THR:HB	1.91	0.51
1:C:159:PRO:HG2	5:C:611:HOH:O	2.10	0.51
1:C:13:ASN:HB2	1:C:20:VAL:O	2.11	0.51
1:D:201:VAL:HG23	2:D:507:EDO:C2	2.40	0.51
1:C:447:ASN:HB2	1:D:486:GLU:HB2	1.93	0.51
1:C:287:VAL:HG12	1:C:289:CYS:H	1.77	0.50
1:C:35:ALA:HA	1:C:329:PRO:HG3	1.93	0.50
1:C:354:LEU:HD11	1:C:379:THR:HB	1.92	0.50
1:B:260:PRO:HD3	1:B:415:THR:HG21	1.94	0.50
1:B:24:ASP:HB2	3:B:504:PEG:H32	1.94	0.50
1:C:162:ILE:O	1:C:166:LYS:HG3	2.12	0.50
1:D:33:GLU:HA	1:D:97:ILE:O	2.12	0.49
1:A:330:LEU:HD23	1:A:336:LEU:HA	1.93	0.49
1:B:167:SER:HB3	1:B:177:MET:HE2	1.95	0.49
1:C:485:VAL:HG22	1:D:445:ILE:HD12	1.95	0.49
1:A:34:PRO:HB2	1:A:329:PRO:HG2	1.95	0.48
1:B:452:PRO:HD2	1:B:455:LEU:HD22	1.96	0.48
1:A:469:ASN:O	1:A:473:THR:CG2	2.56	0.48
1:A:33:GLU:HA	1:A:97:ILE:O	2.13	0.48
1:B:22:PRO:HB3	1:B:50:GLU:HG2	1.96	0.48
1:B:33:GLU:HA	1:B:97:ILE:O	2.13	0.48
1:B:469:ASN:O	1:B:473:THR:CG2	2.61	0.48
1:D:111:ASP:HA	1:D:114:TRP:NE1	2.30	0.47
1:A:35:ALA:HA	1:A:329:PRO:HG3	1.95	0.47
1:D:129:GLY:HA2	2:D:511:EDO:H21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:VAL:HG22	1:B:445:ILE:HD12	1.97	0.47
1:C:183:PRO:HD2	3:C:507:PEG:H21	1.95	0.47
1:A:154:GLY:HA3	2:A:505:EDO:H11	1.96	0.47
1:A:111:ASP:HA	1:A:114:TRP:NE1	2.30	0.46
1:C:111:ASP:HA	1:C:114:TRP:NE1	2.30	0.46
1:C:452:PRO:HB2	1:C:455:LEU:HD13	1.96	0.46
1:B:161:GLN:HE22	1:B:452:PRO:HG2	1.80	0.46
1:C:33:GLU:HA	1:C:97:ILE:O	2.15	0.46
1:B:471:ARG:HH11	2:B:502:EDO:H12	1.81	0.46
1:A:22:PRO:HB3	1:A:50:GLU:HG2	1.99	0.45
1:B:111:ASP:HA	1:B:114:TRP:NE1	2.30	0.45
1:D:162:ILE:O	1:D:166:LYS:HG3	2.16	0.45
1:C:445:ILE:HD12	1:D:485:VAL:HG22	1.97	0.45
1:A:155:ALA:HB3	1:A:162:ILE:CD1	2.46	0.45
1:D:202:PRO:O	2:D:507:EDO:H22	2.16	0.45
1:D:203:PRO:HA	2:D:507:EDO:C1	2.43	0.45
1:D:22:PRO:HB3	1:D:50:GLU:HG2	1.99	0.45
1:C:22:PRO:HB3	1:C:50:GLU:HG2	1.99	0.45
1:D:34:PRO:HB2	1:D:329:PRO:HG2	1.98	0.45
1:C:300:ILE:HA	1:C:303:LYS:HE2	2.00	0.44
1:A:158:TYR:HB3	1:A:161:GLN:HB3	2.00	0.44
1:C:158:TYR:HB2	1:C:162:ILE:HD12	1.99	0.44
1:A:155:ALA:O	2:A:505:EDO:H12	2.18	0.44
1:B:24:ASP:CB	3:B:504:PEG:H32	2.48	0.44
1:C:303:LYS:HG2	1:C:303:LYS:H	1.59	0.43
1:A:486:GLU:CB	1:B:447:ASN:HB2	2.48	0.43
1:B:470:GLY:O	1:B:474:ILE:HG12	2.18	0.43
1:D:281:PHE:HB3	1:D:327:MET:HE1	2.01	0.43
1:A:118:GLU:HB3	2:A:504:EDO:H22	2.00	0.43
1:D:35:ALA:HA	1:D:329:PRO:HG3	1.99	0.43
1:C:170:ALA:O	1:C:175:ASN:HB2	2.19	0.42
1:D:409:LEU:O	1:D:413:ASN:HB2	2.18	0.42
1:B:119:TYR:HA	2:B:501:EDO:C2	2.49	0.42
1:A:354:LEU:HD11	1:A:379:THR:HB	2.02	0.42
1:B:122:GLY:HA2	3:C:506:PEG:C2	2.43	0.42
1:B:158:TYR:HB2	1:B:162:ILE:HD12	2.01	0.42
1:D:197:SER:OG	2:D:507:EDO:H12	2.20	0.42
1:C:117:LEU:HD12	1:C:168:ALA:HB2	2.01	0.42
1:D:470:GLY:O	1:D:474:ILE:HG12	2.20	0.42
1:A:286:GLN:O	1:A:393:PHE:HD1	2.02	0.41
1:A:445:ILE:HD12	1:B:485:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:TYR:HA	2:D:506:EDO:C1	2.51	0.41
1:C:469:ASN:O	1:C:473:THR:CG2	2.58	0.41
1:C:470:GLY:O	1:C:474:ILE:HG12	2.21	0.41
1:B:310:LYS:HE2	1:B:314:ARG:HH22	1.84	0.41
1:D:167:SER:HB3	1:D:177:MET:HE1	2.02	0.41
1:C:310:LYS:HE2	1:C:314:ARG:HH22	1.85	0.41
1:D:310:LYS:HE2	1:D:314:ARG:HH22	1.86	0.41
1:A:59:LYS:HG2	1:A:63:LYS:HE3	2.03	0.40
1:D:59:LYS:HG2	1:D:63:LYS:HE3	2.04	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	466/508 (92%)	454 (97%)	11 (2%)	1 (0%)	47	58
1	B	466/508 (92%)	455 (98%)	11 (2%)	0	100	100
1	C	467/508 (92%)	454 (97%)	13 (3%)	0	100	100
1	D	469/508 (92%)	458 (98%)	11 (2%)	0	100	100
All	All	1868/2032 (92%)	1821 (98%)	46 (2%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	ASN

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	384/416 (92%)	367 (96%)	17 (4%)	28	39
1	B	384/416 (92%)	364 (95%)	20 (5%)	23	32
1	C	384/416 (92%)	369 (96%)	15 (4%)	32	46
1	D	386/416 (93%)	368 (95%)	18 (5%)	26	37
All	All	1538/1664 (92%)	1468 (95%)	70 (5%)	27	38

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	GLU
1	A	98	ASN
1	A	132	ILE
1	A	134	LEU
1	A	143	ARG
1	A	283	THR
1	A	302	ASP
1	A	306	GLU
1	A	322	LEU
1	A	408	VAL
1	A	410	GLU
1	A	430	ARG
1	A	437	GLU
1	A	454	GLU
1	A	473	THR
1	A	481	LYS
1	A	491	GLU
1	B	88	GLU
1	B	98	ASN
1	B	99	ASN
1	B	132	ILE
1	B	161	GLN
1	B	258	LYS
1	B	283	THR
1	B	302	ASP
1	B	303	LYS
1	B	306	GLU
1	B	322	LEU

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Mol	Chain	Res	Type
1	B	408	VAL
1	B	415	THR
1	B	416	THR
1	B	430	ARG
1	B	437	GLU
1	B	467	ARG
1	B	473	THR
1	B	481	LYS
1	B	491	GLU
1	C	88	GLU
1	C	98	ASN
1	C	132	ILE
1	C	134	LEU
1	C	161	GLN
1	C	283	THR
1	C	303	LYS
1	C	408	VAL
1	C	430	ARG
1	C	437	GLU
1	C	454	GLU
1	C	467	ARG
1	C	473	THR
1	C	481	LYS
1	C	491	GLU
1	D	88	GLU
1	D	98	ASN
1	D	99	ASN
1	D	132	ILE
1	D	161	GLN
1	D	258	LYS
1	D	283	THR
1	D	287	VAL
1	D	302	ASP
1	D	303	LYS
1	D	306	GLU
1	D	363	GLU
1	D	408	VAL
1	D	430	ARG
1	D	437	GLU
1	D	475	GLU
1	D	481	LYS
1	D	491	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	447	ASN
1	C	447	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](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 8 are monoatomic - leaving 19 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	PEG	C	506	-	6,6,6	0.22	0	5,5,5	0.31	0
2	EDO	A	503	-	3,3,3	0.68	0	2,2,2	0.45	0
2	EDO	B	501	-	3,3,3	1.41	1 (33%)	2,2,2	0.41	0
3	PEG	C	505	-	6,6,6	0.23	0	5,5,5	0.14	0
3	PEG	B	504	-	6,6,6	0.24	0	5,5,5	0.29	0
2	EDO	D	511	-	3,3,3	0.69	0	2,2,2	0.20	0
2	EDO	B	502	-	3,3,3	0.60	0	2,2,2	0.21	0
3	PEG	C	507	-	6,6,6	0.25	0	5,5,5	0.17	0
2	EDO	A	502	-	3,3,3	0.72	0	2,2,2	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	505	-	3,3,3	0.56	0	2,2,2	0.33	0
2	EDO	D	509	-	3,3,3	0.71	0	2,2,2	0.16	0
2	EDO	A	501	-	3,3,3	0.81	0	2,2,2	0.15	0
2	EDO	D	510	-	3,3,3	0.55	0	2,2,2	0.38	0
2	EDO	D	508	-	3,3,3	0.63	0	2,2,2	0.54	0
2	EDO	C	504	-	3,3,3	0.71	0	2,2,2	0.06	0
2	EDO	B	503	-	3,3,3	0.71	0	2,2,2	0.16	0
2	EDO	A	504	-	3,3,3	0.69	0	2,2,2	0.12	0
2	EDO	D	506	-	3,3,3	1.22	0	2,2,2	0.27	0
2	EDO	D	507	4	3,3,3	0.46	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
3	PEG	C	506	-	-	2/4/4/4	-
2	EDO	A	503	-	-	0/1/1/1	-
2	EDO	B	501	-	-	1/1/1/1	-
3	PEG	C	505	-	-	2/4/4/4	-
3	PEG	B	504	-	-	1/4/4/4	-
2	EDO	D	511	-	-	0/1/1/1	-
2	EDO	B	502	-	-	1/1/1/1	-
3	PEG	C	507	-	-	2/4/4/4	-
2	EDO	A	502	-	-	0/1/1/1	-
2	EDO	A	505	-	-	0/1/1/1	-
2	EDO	D	509	-	-	0/1/1/1	-
2	EDO	A	501	-	-	0/1/1/1	-
2	EDO	D	510	-	-	0/1/1/1	-
2	EDO	D	508	-	-	1/1/1/1	-
2	EDO	C	504	-	-	0/1/1/1	-
2	EDO	B	503	-	-	0/1/1/1	-
2	EDO	A	504	-	-	1/1/1/1	-
2	EDO	D	506	-	-	1/1/1/1	-
2	EDO	D	507	4	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	EDO	C2-C1	2.13	1.63	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	508	EDO	O1-C1-C2-O2
3	B	504	PEG	C1-C2-O2-C3
3	C	507	PEG	C1-C2-O2-C3
3	C	507	PEG	C4-C3-O2-C2
3	C	505	PEG	C4-C3-O2-C2
2	D	506	EDO	O1-C1-C2-O2
3	C	505	PEG	C1-C2-O2-C3
3	C	506	PEG	O2-C3-C4-O4
2	A	504	EDO	O1-C1-C2-O2
2	B	501	EDO	O1-C1-C2-O2
2	B	502	EDO	O1-C1-C2-O2
3	C	506	PEG	C1-C2-O2-C3

There are no ring outliers.

12 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	506	PEG	5	0
2	A	503	EDO	2	0
2	B	501	EDO	1	0
3	B	504	PEG	4	0
2	D	511	EDO	3	0
2	B	502	EDO	2	0
3	C	507	PEG	1	0
2	A	505	EDO	5	0
2	D	508	EDO	1	0
2	A	504	EDO	1	0
2	D	506	EDO	1	0
2	D	507	EDO	7	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 ⓘ

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	470/508 (92%)	0.35	16 (3%) 45 52	32, 58, 95, 114	0
1	B	470/508 (92%)	0.41	27 (5%) 23 30	33, 61, 109, 134	0
1	C	471/508 (92%)	0.40	27 (5%) 23 30	34, 56, 102, 119	0
1	D	471/508 (92%)	0.35	23 (4%) 29 36	34, 55, 99, 116	0
All	All	1882/2032 (92%)	0.38	93 (4%) 29 36	32, 57, 101, 134	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	428	ILE	9.6
1	D	428	ILE	7.4
1	A	428	ILE	7.2
1	C	137	GLY	7.0
1	C	134	LEU	4.8
1	C	264	PHE	4.3
1	D	431	ALA	4.2
1	C	423	VAL	4.2
1	C	428	ILE	4.1
1	D	137	GLY	3.9
1	B	342	PHE	3.4
1	B	423	VAL	3.4
1	A	134	LEU	3.4
1	A	431	ALA	3.4
1	B	392	ILE	3.3
1	B	431	ALA	3.3
1	B	460	TYR	3.2
1	C	165	TRP	3.2
1	B	263	ILE	3.1
1	D	426	ARG	3.1
1	D	134	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	457	PHE	3.1
1	A	257	GLY	3.0
1	D	264	PHE	3.0
1	D	462	LYS	3.0
1	A	352	LYS	3.0
1	A	494	PHE	2.9
1	B	304	PHE	2.9
1	C	257	GLY	2.9
1	C	445	ILE	2.8
1	C	135	PRO	2.8
1	D	135	PRO	2.8
1	B	412	ALA	2.8
1	B	294	VAL	2.8
1	B	410	GLU	2.8
1	C	387	CYS	2.8
1	D	300	ILE	2.8
1	A	415	THR	2.7
1	B	300	ILE	2.7
1	C	402	PHE	2.7
1	D	460	TYR	2.6
1	A	445	ILE	2.6
1	C	462	LYS	2.6
1	D	423	VAL	2.6
1	D	415	THR	2.6
1	A	460	TYR	2.6
1	C	393	PHE	2.5
1	D	187	VAL	2.5
1	B	399	ILE	2.5
1	B	257	GLY	2.5
1	B	347	LYS	2.5
1	C	261	LEU	2.5
1	A	269	MET	2.4
1	A	412	ALA	2.4
1	A	187	VAL	2.4
1	D	455	LEU	2.3
1	C	427	ASP	2.3
1	C	415	THR	2.3
1	A	294	VAL	2.3
1	C	347	LYS	2.3
1	A	493	ALA	2.3
1	D	458	GLY	2.3
1	B	289	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	304	PHE	2.2
1	B	445	ILE	2.2
1	D	257	GLY	2.2
1	C	426	ARG	2.2
1	C	289	CYS	2.2
1	B	427	ASP	2.2
1	C	262	ILE	2.2
1	B	0	PRO	2.2
1	D	424	PHE	2.2
1	D	289	CYS	2.2
1	A	263	ILE	2.2
1	C	314	ARG	2.1
1	D	399	ILE	2.1
1	D	310	LYS	2.1
1	B	296	VAL	2.1
1	B	408	VAL	2.1
1	B	435	VAL	2.1
1	B	378	LEU	2.1
1	C	300	ILE	2.1
1	C	187	VAL	2.1
1	D	450	VAL	2.1
1	B	457	PHE	2.1
1	C	460	TYR	2.1
1	D	304	PHE	2.1
1	B	104	PHE	2.0
1	C	352	LYS	2.0
1	B	277	LEU	2.0
1	B	269	MET	2.0
1	A	306	GLU	2.0
1	D	354	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

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, 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	EDO	A	502	4/4	0.70	0.20	59,61,62,63	0
2	EDO	D	506	4/4	0.72	0.18	46,46,46,48	0
4	NA	C	501	1/1	0.73	0.16	74,74,74,74	0
3	PEG	B	504	7/7	0.74	0.27	63,66,70,71	0
2	EDO	B	503	4/4	0.74	0.15	64,66,66,66	0
2	EDO	B	502	4/4	0.77	0.12	76,76,76,76	0
2	EDO	C	504	4/4	0.78	0.15	74,75,76,77	0
2	EDO	B	501	4/4	0.79	0.18	41,44,50,50	0
2	EDO	D	509	4/4	0.80	0.16	69,70,72,72	0
3	PEG	C	507	7/7	0.81	0.18	54,64,71,72	0
4	NA	D	501	1/1	0.83	0.12	47,47,47,47	0
3	PEG	C	505	7/7	0.84	0.12	72,74,75,76	0
2	EDO	A	504	4/4	0.86	0.27	55,57,59,60	0
2	EDO	A	501	4/4	0.87	0.16	55,56,57,59	0
3	PEG	C	506	7/7	0.88	0.42	52,55,60,63	0
2	EDO	D	510	4/4	0.88	0.12	68,70,70,72	0
4	NA	D	502	1/1	0.88	0.16	65,65,65,65	0
4	NA	D	505	1/1	0.91	0.24	72,72,72,72	0
2	EDO	A	505	4/4	0.91	0.21	41,44,46,47	0
4	NA	C	502	1/1	0.91	0.21	71,71,71,71	0
2	EDO	A	503	4/4	0.92	0.23	39,50,55,57	0
2	EDO	D	507	4/4	0.92	0.36	48,51,51,53	0
2	EDO	D	508	4/4	0.93	0.31	50,56,59,62	0
4	NA	C	503	1/1	0.94	0.15	60,60,60,60	0
2	EDO	D	511	4/4	0.94	0.14	44,45,46,46	0
4	NA	D	504	1/1	0.96	0.17	56,56,56,56	0
4	NA	D	503	1/1	0.97	0.17	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.