



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2018 – 02:21 PM EDT

PDB ID : 6B4R
Title : The crystal structure of the aldehyde dehydrogenase KauB from *Pseudomonas aeruginosa*
Authors : Gonzalez-Segura, L.; Cardona-Cardona, Y.; Carrillo-Campos, J.; Munoz-Clares, R.A.
Deposited on : 2017-09-27
Resolution : 2.55 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031172
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

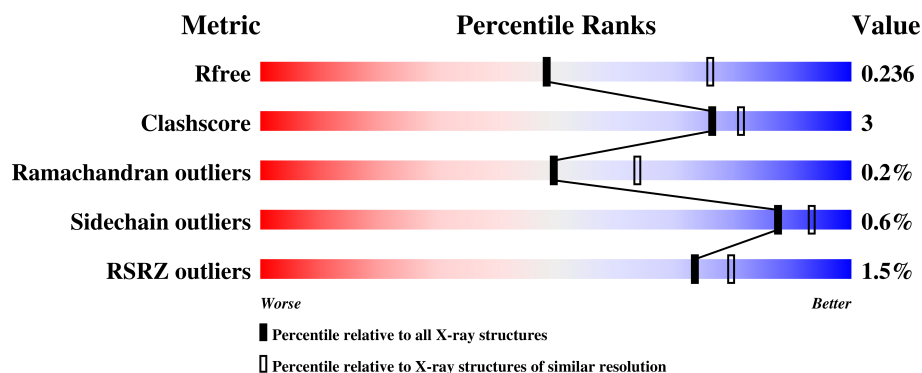
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	111664	1053 (2.56-2.52)
Clashscore	122126	1098 (2.56-2.52)
Ramachandran outliers	120053	1088 (2.56-2.52)
Sidechain outliers	120020	1088 (2.56-2.52)
RSRZ outliers	108989	1043 (2.56-2.52)

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 $\leq 5\%$. 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	497	<div> <div>91%</div> <div>9%</div> </div>
1	C	497	<div> <div>2%</div> <div>90%</div> <div>10%</div> </div>
2	B	497	<div> <div>92%</div> <div>8%</div> </div>
2	D	497	<div> <div>4%</div> <div>90%</div> <div>9%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CSD	C	302	-	-	X	-
5	TOE	C	503	-	-	X	-
6	GOL	B	503	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 15533 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.

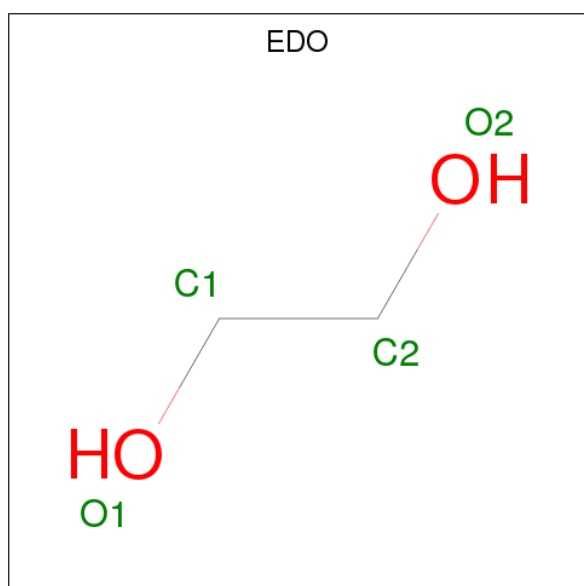
- Molecule 1 is a protein called KauB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	1	0
			3752	2380	640	718	14			
1	C	495	Total	C	N	O	S	0	1	0
			3737	2371	638	715	13			

- Molecule 2 is a protein called KauB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	495	Total	C	N	O	S	0	1	0
			3735	2371	638	713	13			
2	D	495	Total	C	N	O	S	0	1	0
			3735	2371	638	713	13			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

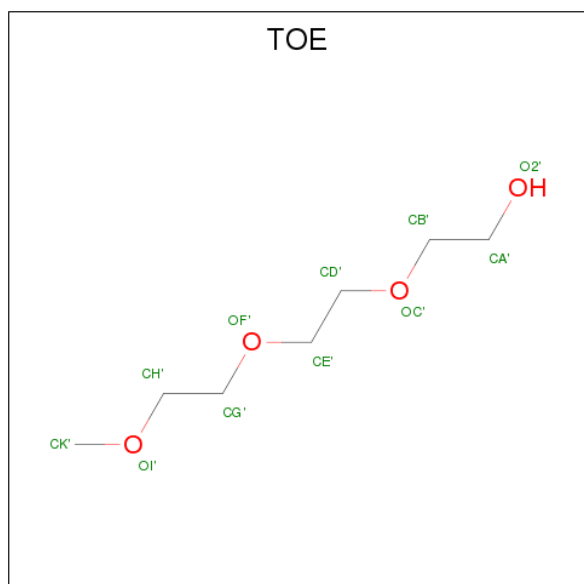


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 5 is 2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXYL (three-letter code: TOE) (formula: C₇H₁₆O₄).



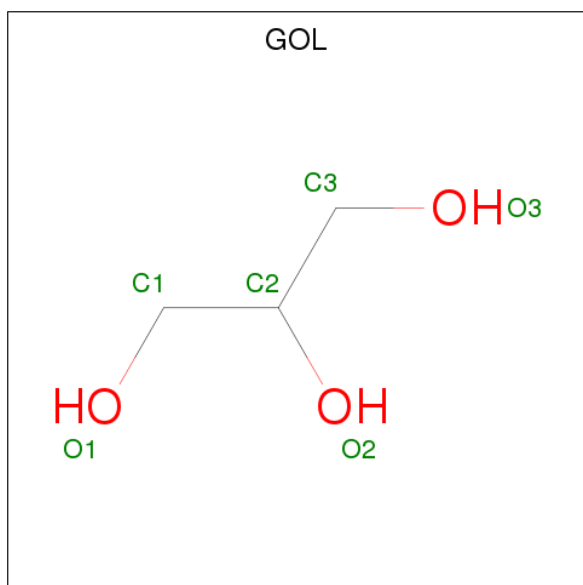
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	7	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			11	7	4		
5	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

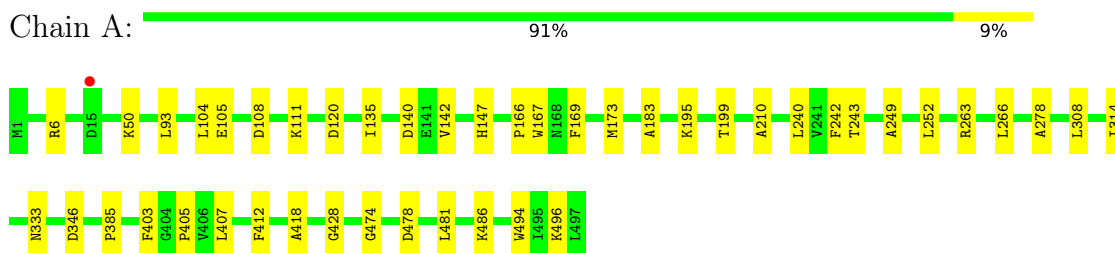
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	170	Total	O	0	0
			170	170		
7	B	146	Total	O	0	0
			146	146		
7	C	123	Total	O	0	0
			123	123		
7	D	77	Total	O	0	0
			77	77		

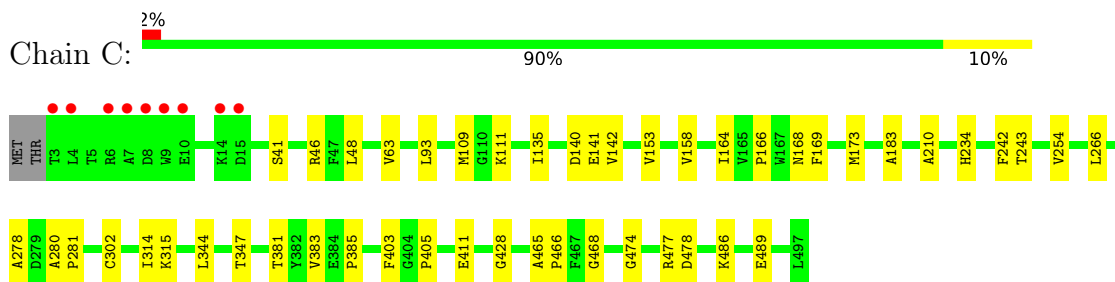
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

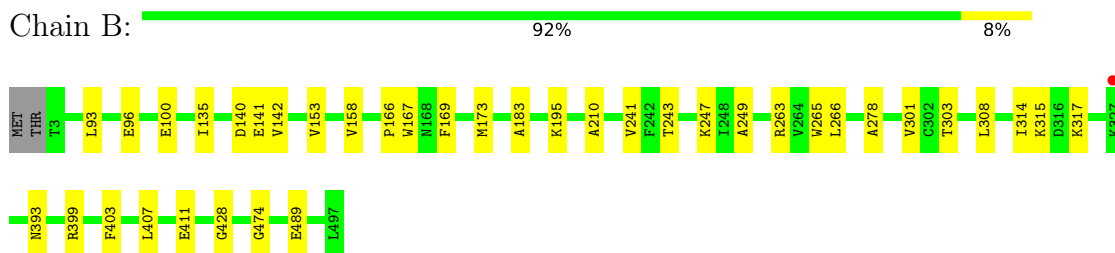
- Molecule 1: KauB



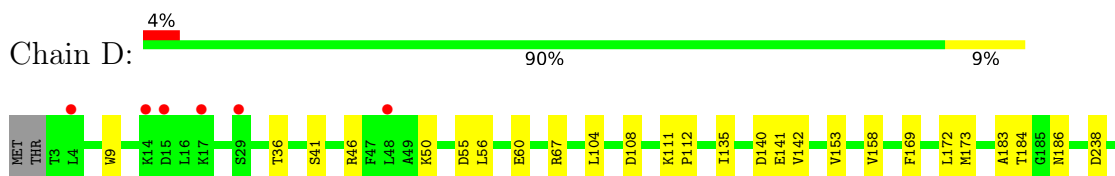
- Molecule 1: KauB

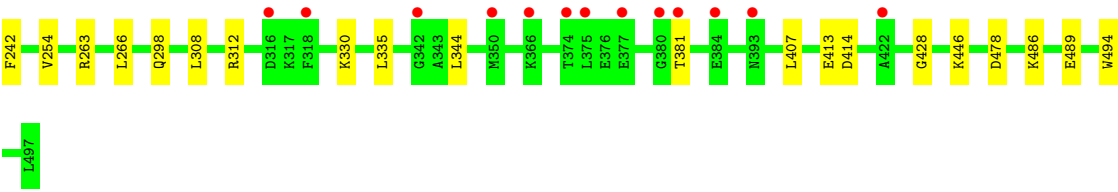


- Molecule 2: KauB



- Molecule 2: KauB





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.64Å 93.81Å 128.86Å 90.00° 92.28° 90.00°	Depositor
Resolution (Å)	46.12 – 2.55 46.91 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.12-2.55) 99.4 (46.91-2.55)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.178 , 0.234 0.180 , 0.236	Depositor DCC
R_{free} test set	3486 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15533	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: GOL, K, TOE, EDO, CSD

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	0.21	0/3818	0.39	0/5186
1	C	0.21	0/3803	0.38	0/5166
2	B	0.21	0/3809	0.38	0/5174
2	D	0.21	0/3809	0.37	0/5174
All	All	0.21	0/15239	0.38	0/20700

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	3752	0	3760	26	0
1	C	3737	0	3741	33	0
2	B	3735	0	3741	23	0
2	D	3735	0	3741	25	0
3	A	8	0	12	2	0
3	B	4	0	6	2	0
3	C	4	0	6	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	11	0	16	0	0
5	B	11	0	16	0	0
5	C	10	0	13	8	0
6	B	6	0	8	0	0
7	A	170	0	0	1	1
7	B	146	0	0	1	0
7	C	123	0	0	0	0
7	D	77	0	0	0	0
All	All	15533	0	15060	98	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (98) 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:302:CSD:CB	5:C:503:TOE:H3	1.88	1.04
1:C:302:CSD:HB3	5:C:503:TOE:H3	1.33	1.03
1:C:302:CSD:SG	5:C:503:TOE:H3	2.02	0.99
1:C:302:CSD:HB3	5:C:503:TOE:CA'	2.01	0.89
1:C:302:CSD:SG	5:C:503:TOE:CA'	2.80	0.70
2:D:312:ARG:HH12	2:D:413:GLU:HG3	1.58	0.68
2:D:36:THR:HG21	2:D:50:LYS:HB3	1.80	0.64
1:A:142:VAL:HB	1:C:140:ASP:HB2	1.80	0.64
2:B:249:ALA:HB1	2:B:266:LEU:HD13	1.83	0.60
1:C:254:VAL:HG13	2:D:254:VAL:HG13	1.82	0.60
2:B:166:PRO:HD3	2:B:243:THR:HB	1.83	0.59
2:D:158:VAL:HG12	2:D:489:GLU:HG2	1.83	0.58
1:A:385:PRO:HA	1:A:405:PRO:HB2	1.86	0.58
1:C:242:PHE:HB3	1:C:266:LEU:HD23	1.86	0.57
1:C:302:CSD:CB	5:C:503:TOE:CA'	2.71	0.57
1:A:263:ARG:NH2	2:B:474:GLY:O	2.38	0.57
1:C:474:GLY:O	2:D:263:ARG:NH2	2.37	0.57
1:A:105:GLU:HG2	1:A:199:THR:HG21	1.88	0.56
1:A:140:ASP:HB2	1:C:142:VAL:HB	1.88	0.55
2:D:111:LYS:HD2	2:D:112:PRO:HD2	1.88	0.55
1:A:166:PRO:HD3	1:A:243:THR:HB	1.88	0.55
1:A:249:ALA:HB1	1:A:266:LEU:HD13	1.87	0.55
2:B:158:VAL:HG12	2:B:489:GLU:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:184:THR:OG1	2:D:186:ASN:ND2	2.40	0.54
1:C:158:VAL:HG12	1:C:489:GLU:HG2	1.89	0.54
2:B:140:ASP:HB2	2:D:142:VAL:HB	1.90	0.54
1:A:481:LEU:HD12	3:A:502:EDO:H22	1.88	0.53
2:B:315:LYS:HD2	2:B:411:GLU:HB3	1.89	0.53
2:B:169:PHE:HB2	2:B:173:MET:HG2	1.90	0.52
1:A:167:TRP:CD1	1:A:195:LYS:HD2	2.45	0.52
1:A:50:LYS:NZ	7:A:606:HOH:O	2.44	0.51
2:D:135:ILE:HG12	2:D:183:ALA:HB1	1.93	0.51
1:C:278:ALA:HA	1:C:314:ILE:HD13	1.93	0.51
2:B:100:GLU:H	3:B:501:EDO:H11	1.76	0.50
2:B:393:ASN:O	2:B:399:ARG:NH2	2.41	0.50
1:A:308:LEU:HB2	1:A:407:LEU:HD11	1.92	0.50
2:B:135:ILE:HG12	2:B:183:ALA:HB1	1.94	0.50
1:C:478:ASP:OD1	1:C:486:LYS:NZ	2.42	0.50
2:D:9:TRP:HB3	2:D:335:LEU:HD12	1.94	0.50
1:A:481:LEU:HB2	3:A:502:EDO:H22	1.93	0.50
1:C:135:ILE:HG12	1:C:183:ALA:HB1	1.93	0.50
2:B:317:LYS:NZ	7:B:602:HOH:O	2.45	0.49
2:D:242:PHE:HB3	2:D:266:LEU:HD23	1.94	0.49
2:B:141:GLU:HB2	2:B:153:VAL:HB	1.95	0.49
2:D:344:LEU:HB2	2:D:381:THR:HG22	1.95	0.49
1:A:240:LEU:HD11	1:A:252:LEU:HD13	1.95	0.49
1:C:468:GLY:HA3	1:C:477:ARG:HD3	1.95	0.48
2:D:308:LEU:HB2	2:D:407:LEU:HD11	1.95	0.48
2:B:241:VAL:HG12	2:B:265:TRP:HB2	1.94	0.48
1:A:104:LEU:O	1:A:108:ASP:HB2	2.13	0.48
2:B:301:VAL:HG12	2:B:303:THR:H	1.78	0.48
1:A:278:ALA:HA	1:A:314:ILE:HD13	1.94	0.48
1:A:169:PHE:HB2	1:A:173:MET:HG2	1.95	0.48
1:C:344:LEU:HD11	1:C:383:VAL:HG12	1.96	0.48
1:C:169:PHE:HB2	1:C:173:MET:HG2	1.96	0.47
1:C:41:SER:HB3	1:C:46:ARG:HG2	1.95	0.47
2:D:141:GLU:HB2	2:D:153:VAL:HB	1.97	0.47
1:A:147:HIS:O	2:D:446:LYS:NZ	2.46	0.46
1:C:302:CSD:OD1	5:C:503:TOE:CA'	2.63	0.46
2:B:142:VAL:HB	2:D:140:ASP:HB2	1.97	0.46
1:C:41:SER:HB2	1:C:48:LEU:HD21	1.96	0.46
2:D:478:ASP:OD1	2:D:486:LYS:NZ	2.43	0.46
1:C:164:ILE:HB	1:C:242:PHE:HD1	1.81	0.46
1:C:166:PRO:HD3	1:C:243:THR:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:ASN:ND2	5:C:503:TOE:O2'	2.49	0.45
1:A:474:GLY:O	2:B:263:ARG:NH2	2.48	0.45
1:A:478:ASP:OD1	1:A:486:LYS:NZ	2.48	0.45
1:A:242:PHE:HB3	1:A:266:LEU:HD23	1.99	0.45
1:C:385:PRO:HA	1:C:405:PRO:HB2	1.98	0.45
2:D:55:ASP:CG	2:D:56:LEU:H	2.20	0.45
2:D:312:ARG:NH1	2:D:413:GLU:HG3	2.29	0.44
2:B:278:ALA:HA	2:B:314:ILE:HD13	1.99	0.44
1:A:195:LYS:NZ	1:A:346:ASP:OD1	2.36	0.44
1:A:135:ILE:HG12	1:A:183:ALA:HB1	1.98	0.44
2:D:41:SER:HB3	2:D:46:ARG:HG2	1.99	0.44
1:C:93:LEU:HD12	1:C:210:ALA:HB2	2.00	0.44
2:B:314:ILE:HA	2:B:317:LYS:HE2	1.99	0.43
2:B:167:TRP:CD1	2:B:195:LYS:HD2	2.53	0.43
1:A:6:ARG:HD2	1:A:333:ASN:HD22	1.83	0.43
2:B:308:LEU:HB2	2:B:407:LEU:HD11	1.99	0.43
2:D:414:ASP:N	2:D:414:ASP:OD1	2.52	0.42
1:A:111:LYS:NZ	1:A:120:ASP:OD1	2.52	0.42
2:D:169:PHE:HB2	2:D:173:MET:HG2	2.02	0.42
2:D:104:LEU:O	2:D:108:ASP:HB2	2.20	0.41
1:C:141:GLU:HB2	1:C:153:VAL:HB	2.01	0.41
2:B:93:LEU:HD12	2:B:210:ALA:HB2	2.03	0.41
2:B:247:LYS:HB3	2:B:247:LYS:HE2	1.85	0.41
2:D:169:PHE:HB3	2:D:172:LEU:HB3	2.02	0.41
1:A:93:LEU:HD12	1:A:210:ALA:HB2	2.03	0.41
1:C:63:VAL:HG11	1:C:234:HIS:CE1	2.55	0.41
1:C:465:ALA:HA	1:C:466:PRO:HD2	1.95	0.41
2:D:67:ARG:NH2	2:D:238:ASP:OD2	2.49	0.41
1:A:412:PHE:CD2	1:A:418:ALA:HB2	2.55	0.41
1:C:347:THR:HA	1:C:381:THR:HG21	2.01	0.41
2:B:96:GLU:O	3:B:501:EDO:H22	2.21	0.41
1:C:315:LYS:HG3	1:C:411:GLU:HG2	2.02	0.41
1:C:109:MET:SD	1:C:111:LYS:HE3	2.61	0.40
1:C:280:ALA:HA	1:C:281:PRO:HD3	1.97	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:601:HOH:O	7:A:601:HOH:O[2_756]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	495/497 (100%)	474 (96%)	20 (4%)	1 (0%)	49	64
1	C	493/497 (99%)	473 (96%)	19 (4%)	1 (0%)	49	64
2	B	494/497 (99%)	475 (96%)	18 (4%)	1 (0%)	49	64
2	D	494/497 (99%)	474 (96%)	19 (4%)	1 (0%)	49	64
All	All	1976/1988 (99%)	1896 (96%)	76 (4%)	4 (0%)	49	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	428	GLY
1	A	428	GLY
2	B	428	GLY
1	C	428	GLY

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	385/384 (100%)	382 (99%)	3 (1%)	83	90
1	C	383/384 (100%)	382 (100%)	1 (0%)	93	97
2	B	384/385 (100%)	383 (100%)	1 (0%)	93	97
2	D	384/385 (100%)	380 (99%)	4 (1%)	78	86
All	All	1536/1538 (100%)	1527 (99%)	9 (1%)	87	93

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

Mol	Chain	Res	Type
1	A	403	PHE
1	A	494	TRP
1	A	496	LYS
2	B	403	PHE
1	C	403	PHE
2	D	60	GLU
2	D	298	GLN
2	D	330	LYS
2	D	494	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	CSD	A	302	1	4,7,8	1.24	0	2,8,10	0.31	0
1	CSD	C	302	1	4,7,8	1.34	1 (25%)	2,8,10	0.26	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	CSD	A	302	1	-	0/2/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	C	302	1	-	0/2/6/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	302	CSD	CA-C	2.28	1.53	1.50

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 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	302	CSD	7	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	501	-	3,3,3	0.47	0	2,2,2	0.40	0
3	EDO	A	502	-	3,3,3	0.48	0	2,2,2	0.30	0
5	TOE	A	504	-	10,10,10	0.45	0	9,9,9	0.29	0
3	EDO	B	501	-	3,3,3	0.48	0	2,2,2	0.32	0
6	GOL	B	503	-	5,5,5	0.37	0	5,5,5	0.20	0
5	TOE	B	504	-	10,10,10	0.44	0	9,9,9	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	C	501	-	3,3,3	0.48	0	2,2,2	0.29	0
5	TOE	C	503	-	9,9,10	0.50	0	8,8,9	0.57	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	EDO	A	501	-	-	0/1/1/1	0/0/0/0
3	EDO	A	502	-	-	0/1/1/1	0/0/0/0
5	TOE	A	504	-	-	0/8/8/8	0/0/0/0
3	EDO	B	501	-	-	0/1/1/1	0/0/0/0
6	GOL	B	503	-	-	0/4/4/4	0/0/0/0
5	TOE	B	504	-	-	0/8/8/8	0/0/0/0
3	EDO	C	501	-	-	0/1/1/1	0/0/0/0
5	TOE	C	503	-	-	0/7/7/8	0/0/0/0

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.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	EDO	2	0
3	B	501	EDO	2	0
5	C	503	TOE	8	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	496/497 (99%)	-0.33	1 (0%) 94 97	17, 29, 41, 57	0
1	C	494/497 (99%)	0.01	9 (1%) 68 75	22, 37, 53, 75	0
2	B	495/497 (99%)	-0.21	1 (0%) 94 97	19, 30, 49, 60	0
2	D	495/497 (99%)	0.25	19 (3%) 40 47	19, 45, 68, 84	0
All	All	1980/1988 (99%)	-0.07	30 (1%) 73 79	17, 34, 58, 84	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	48	LEU	3.8
1	C	3	THR	3.4
1	C	4	LEU	3.2
2	D	350	MET	3.1
2	D	375	LEU	3.0
2	D	381	THR	2.9
2	D	422	ALA	2.7
1	C	9	TRP	2.7
1	C	7	ALA	2.7
1	A	15	ASP	2.6
2	D	380	GLY	2.6
1	C	14	LYS	2.5
2	D	377	GLU	2.5
2	D	393	ASN	2.4
1	C	15	ASP	2.4
2	D	374	THR	2.4
2	D	318	PHE	2.3
2	D	14	LYS	2.2
2	D	342	GLY	2.2
2	D	366	LYS	2.2
1	C	10	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	8	ASP	2.1
2	D	15	ASP	2.1
2	D	29	SER	2.1
2	B	327	LYS	2.1
1	C	6	ARG	2.1
2	D	384	GLU	2.1
2	D	17	LYS	2.0
2	D	4	LEU	2.0
2	D	316	ASP	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	CSD	C	302	8/9	0.90	0.19	45,50,65,66	0
1	CSD	A	302	8/9	0.91	0.16	27,33,50,63	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. 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
6	GOL	B	503	6/6	0.67	0.43	32,40,49,51	0
5	TOE	B	504	11/11	0.78	0.25	51,55,61,69	0
5	TOE	C	503	10/11	0.80	0.23	49,54,63,67	0
4	K	D	501	1/1	0.83	0.09	58,58,58,58	0
5	TOE	A	504	11/11	0.85	0.22	44,51,58,59	0
3	EDO	A	501	4/4	0.87	0.31	38,41,46,50	0
3	EDO	B	501	4/4	0.88	0.23	34,42,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	A	502	4/4	0.88	0.23	26,33,35,41	0
3	EDO	C	501	4/4	0.90	0.21	38,41,44,44	0
4	K	C	502	1/1	0.93	0.06	48,48,48,48	0
4	K	A	503	1/1	0.98	0.14	32,32,32,32	0
4	K	B	502	1/1	0.99	0.06	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.