



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:23 PM UTC

PDB ID : 3FPC / pdb\_00003fpc  
Title : Chimera of alcohol dehydrogenase by exchange of the cofactor binding domain res 153-294 of *T. brockii* ADH by *E. histolytica* ADH  
Authors : Felix, F.; Goihberg, E.; Shimon, L.; Burstein, Y.  
Deposited on : 2009-01-05  
Resolution : 1.40 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

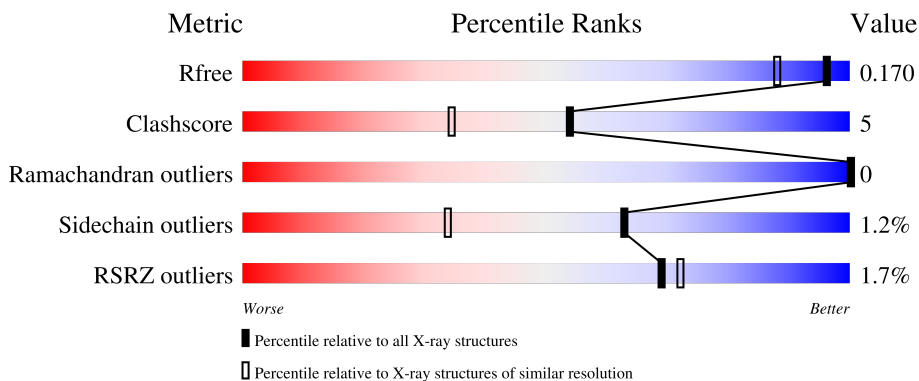
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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))
$R_{free}$	180053	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	352	 92% 7%
1	B	352	 93% 7%
1	C	352	 92% 8%
1	D	352	 92% 7%

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
5	EDO	C	360	-	-	X	-
5	EDO	D	358	-	-	X	-
7	IMD	C	355	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13056 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.

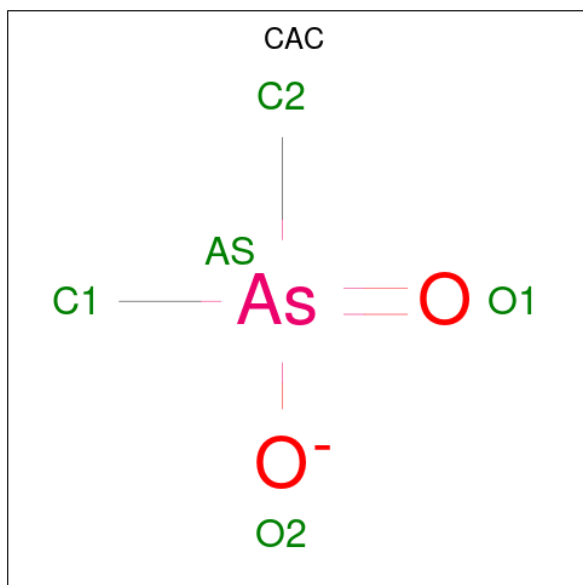
- Molecule 1 is a protein called NADP-dependent alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	352	Total 2728	C 1746	N 473	O 489	S 20	0	10	0
1	B	352	Total 2746	C 1759	N 477	O 490	S 20	0	12	0
1	C	352	Total 2751	C 1756	N 480	O 495	S 20	0	11	0
1	D	352	Total 2734	C 1748	N 475	O 491	S 20	0	10	0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

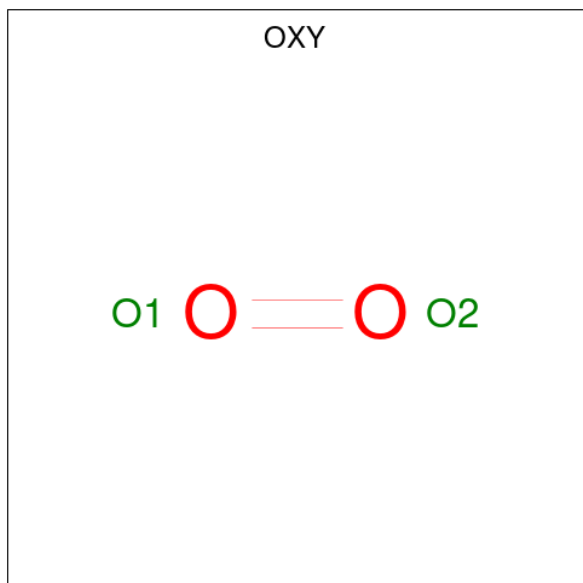
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0

- Molecule 3 is CACODYLATE ION (CCD ID: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>).



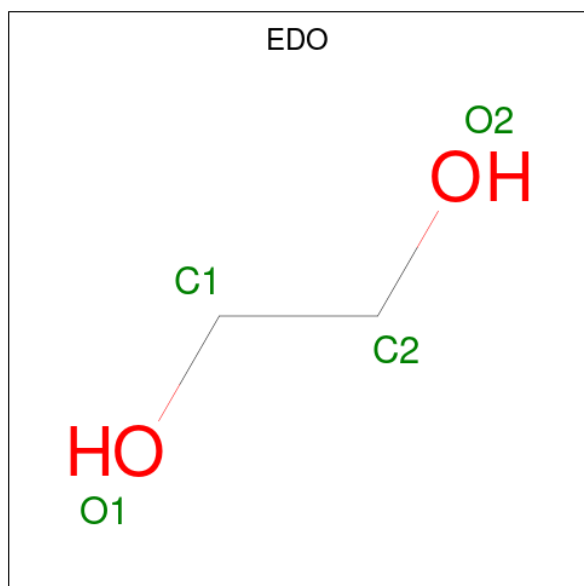
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	As	C	O		
3	A	1	5	1	2	2	0	0
3	B	1	5	1	2	2	0	0
3	C	1	5	1	2	2	0	0
3	D	1	5	1	2	2	0	0

- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O<sub>2</sub>).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



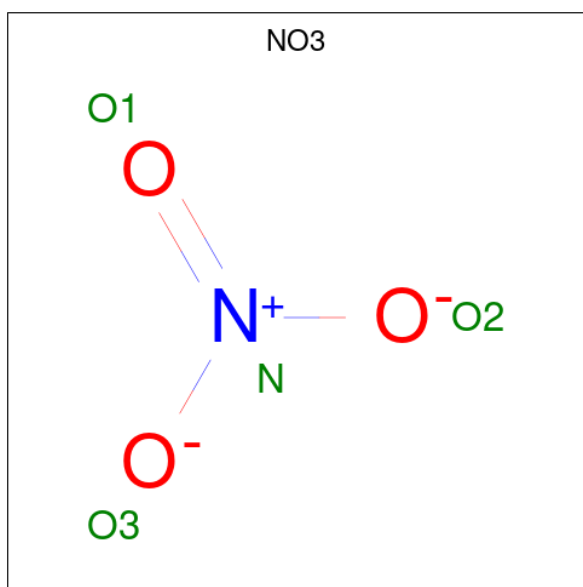
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 8 4 4	0	1
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 8 4 4	0	1
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

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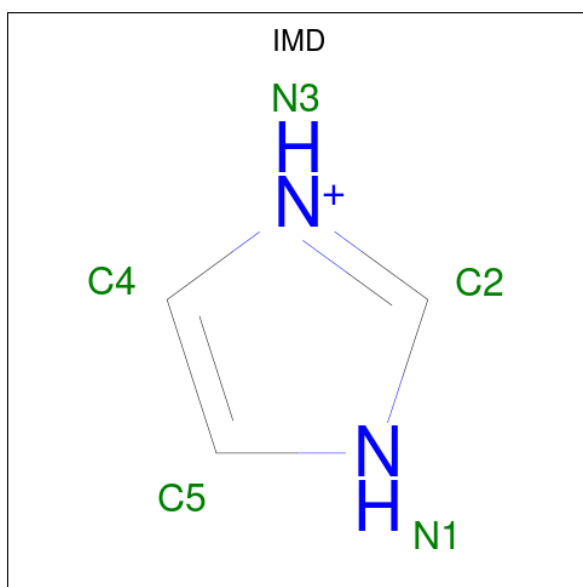
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	1
			8	4	4		

- Molecule 6 is NITRATE ION (CCD ID: NO3) (formula:  $\text{NO}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	N	O	0	0
			4	1	3		
6	D	1	Total	N	O	0	0
			4	1	3		

- Molecule 7 is IMIDAZOLE (CCD ID: IMD) (formula:  $\text{C}_3\text{H}_5\text{N}_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C N 5 3 2	0	0

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Na 1 1	0	0
8	D	1	Total Na 1 1	0	0

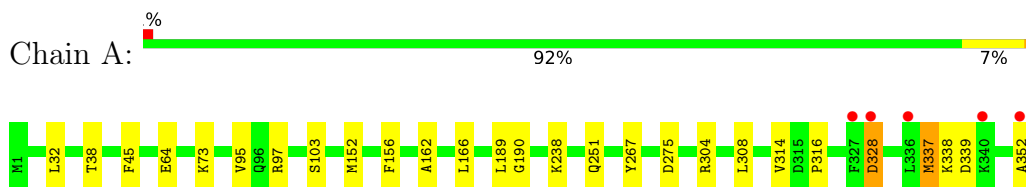
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	477	Total O 477 477	0	0
9	B	520	Total O 520 520	0	0
9	C	510	Total O 510 510	0	0
9	D	481	Total O 481 481	0	0

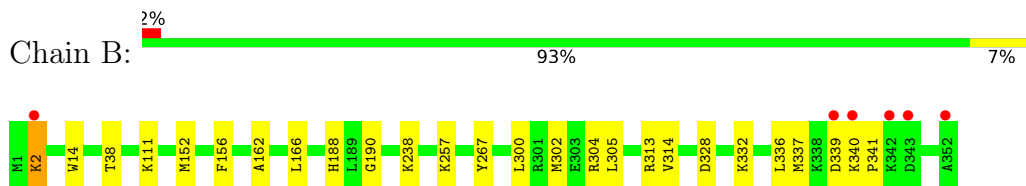
### 3 Residue-property plots [i](#)

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.

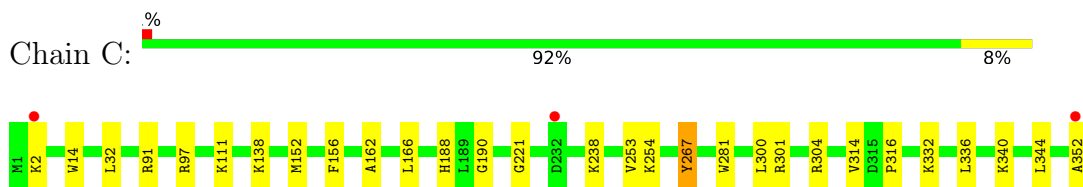
- Molecule 1: NADP-dependent alcohol dehydrogenase



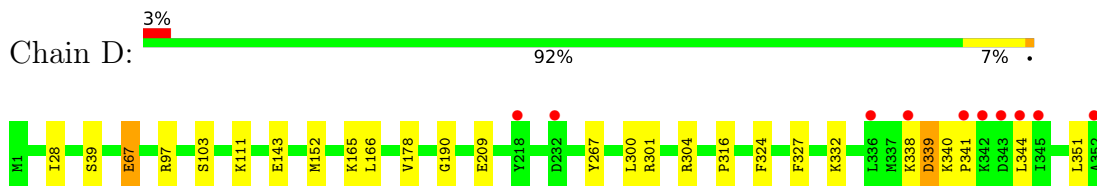
- Molecule 1: NADP-dependent alcohol dehydrogenase



- Molecule 1: NADP-dependent alcohol dehydrogenase



- Molecule 1: NADP-dependent alcohol dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.74Å 82.43Å 118.25Å 90.00° 99.89° 90.00°	Depositor
Resolution (Å)	48.77 – 1.40 48.77 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.77-1.40) 99.1 (48.77-1.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 1.40Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.116 , 0.155 0.139 , 0.170	Depositor DCC
$R_{free}$ test set	14820 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.6	Xtrriage
Anisotropy	0.045	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13056	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, IMD, NO3, EDO, CAC, ZN, OXY

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	0.80	0/2817	0.81	0/3803
1	B	0.78	0/2841	0.83	0/3836
1	C	0.79	1/2828 (0.0%)	0.83	0/3818
1	D	0.76	0/2822	0.82	0/3810
All	All	0.78	1/11308 (0.0%)	0.82	0/15267

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	221	GLY	C-O	-5.39	1.18	1.23

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	2728	0	2765	18	0
1	B	2746	0	2793	20	0
1	C	2751	0	2767	32	0
1	D	2734	0	2769	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	2	0	0	0	0
5	B	20	0	30	2	0
5	C	24	0	36	7	0
5	D	24	0	36	13	0
6	B	4	0	0	0	0
6	D	4	0	0	0	0
7	C	5	0	5	5	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	477	0	0	7	0
9	B	520	0	0	9	0
9	C	510	0	0	15	0
9	D	481	0	0	12	0
All	All	13056	0	11201	108	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 5.

All (108) 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:138:LYS:HB2	9:C:2044:HOH:O	1.39	1.17
1:A:275[B]:ASP:OD2	9:A:465:HOH:O	1.68	1.12
1:B:111[A]:LYS:NZ	9:B:2021:HOH:O	1.97	0.94
7:C:355:IMD:C5	9:C:590:HOH:O	2.16	0.92
1:C:138:LYS:CB	9:C:2044:HOH:O	2.08	0.85
7:C:355:IMD:H5	9:C:590:HOH:O	1.74	0.85
1:C:253:VAL:HG12	9:C:1956:HOH:O	1.76	0.84
1:D:301:ARG:HA	5:D:358:EDO:H22	1.64	0.79
1:B:305:LEU:HD21	9:B:1621:HOH:O	1.82	0.78
1:D:166[A]:LEU:HD23	1:D:190:GLY:HA3	1.68	0.74
7:C:355:IMD:N1	9:C:590:HOH:O	2.21	0.71
1:C:111:LYS:NZ	9:C:2023:HOH:O	2.23	0.70
1:B:302:MET:HE3	9:B:1887:HOH:O	1.91	0.69
1:C:188[A]:HIS:CE1	1:C:314:VAL:HG22	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:MET:CE	9:B:1887:HOH:O	2.40	0.68
1:C:301:ARG:HH11	5:C:360:EDO:C2	2.06	0.68
1:D:39:SER:OG	5:D:360[A]:EDO:H11	1.94	0.66
1:C:2:LYS:HG2	1:C:14:TRP:CE3	2.30	0.66
1:C:301:ARG:HD3	5:C:360:EDO:H21	1.76	0.66
1:D:67:GLU:OE1	9:D:1872:HOH:O	2.13	0.65
1:C:156[B]:PHE:HZ	1:C:314:VAL:HG21	1.62	0.64
1:A:166[A]:LEU:HD23	1:A:190:GLY:HA3	1.81	0.62
1:B:304[C]:ARG:HD3	9:B:2061:HOH:O	1.97	0.62
1:D:28:ILE:HB	1:D:67:GLU:CG	2.29	0.62
1:B:332:LYS:O	1:B:336:LEU:HD13	1.99	0.62
1:D:165:LYS:O	9:D:1890:HOH:O	2.15	0.60
1:C:166[A]:LEU:HD23	1:C:190:GLY:HA3	1.83	0.60
1:D:111:LYS:NZ	9:D:2016:HOH:O	2.27	0.60
1:C:188[A]:HIS:CE1	1:C:314:VAL:CG2	2.85	0.59
1:D:28:ILE:HB	1:D:67:GLU:HG2	1.83	0.59
1:D:301:ARG:HH11	5:D:358:EDO:H12	1.69	0.58
1:D:165:LYS:C	9:D:1890:HOH:O	2.47	0.58
7:C:355:IMD:H5	9:C:1495:HOH:O	2.02	0.58
1:A:251:GLN:NE2	9:A:385:HOH:O	2.36	0.57
1:C:2:LYS:NZ	9:C:815:HOH:O	2.29	0.57
1:C:254:LYS:HG3	9:C:1956:HOH:O	2.03	0.57
1:A:64:GLU:HG3	9:A:1989:HOH:O	2.05	0.57
5:C:360:EDO:C1	9:C:2058:HOH:O	2.54	0.56
1:B:166[A]:LEU:HD23	1:B:190:GLY:HA3	1.87	0.55
1:D:340:LYS:HD2	1:D:344:LEU:HD23	1.88	0.55
1:B:257:LYS:HZ1	5:B:359[A]:EDO:H22	1.72	0.54
1:C:32:LEU:CD2	1:C:352:ALA:HB3	2.38	0.54
1:D:301:ARG:HH11	5:D:358:EDO:C1	2.21	0.53
1:C:32:LEU:HD22	1:C:352:ALA:HB3	1.91	0.53
1:C:352:ALA:HB1	9:C:937:HOH:O	2.07	0.53
1:D:304[C]:ARG:HD2	5:D:358:EDO:C2	2.39	0.52
1:A:103[B]:SER:OG	9:A:449:HOH:O	2.03	0.52
1:A:73:LYS:NZ	9:A:1950:HOH:O	2.42	0.52
1:B:339:ASP:O	1:B:341:PRO:HD3	2.09	0.52
1:D:301:ARG:HD3	5:D:358:EDO:C2	2.41	0.51
1:A:38[B]:THR:HG23	1:A:337:MET:HE3	1.91	0.51
1:B:328:ASP:HB2	9:B:741:HOH:O	2.10	0.51
5:B:355:EDO:H22	9:B:1180:HOH:O	2.10	0.51
1:A:32:LEU:HD22	1:A:352:ALA:HB3	1.93	0.51
1:A:97:ARG:HG2	1:B:300:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:LEU:HD21	1:D:97:ARG:HG2	1.93	0.50
1:D:324:PHE:CE1	1:D:332:LYS:HD2	2.47	0.50
1:B:188[B]:HIS:NE2	1:B:314:VAL:HG22	2.27	0.49
1:C:97:ARG:HG2	1:D:300:LEU:HD21	1.94	0.49
1:A:328:ASP:OD2	1:A:328:ASP:N	2.45	0.48
1:C:91:ARG:HD3	7:C:355:IMD:C5	2.44	0.48
1:D:304[A]:ARG:NE	9:D:506:HOH:O	2.46	0.48
1:B:304[C]:ARG:CD	9:B:2061:HOH:O	2.59	0.48
1:D:209:GLU:HB2	9:D:1941:HOH:O	2.14	0.47
1:A:189:LEU:HD13	9:A:1373:HOH:O	2.14	0.47
1:A:304[A]:ARG:NH1	9:D:1890:HOH:O	2.47	0.47
1:B:2:LYS:HG2	1:B:14:TRP:CE3	2.49	0.47
1:C:156[B]:PHE:CZ	1:C:314:VAL:HG21	2.47	0.47
5:D:358:EDO:H21	9:D:918:HOH:O	2.15	0.47
1:C:340:LYS:HD3	1:C:344:LEU:HD23	1.96	0.46
1:B:38[B]:THR:HG23	1:B:337:MET:HE3	1.97	0.46
1:D:28:ILE:CG1	1:D:67:GLU:HG3	2.45	0.46
1:D:28:ILE:HB	1:D:67:GLU:HG3	1.98	0.46
1:A:45:PHE:CZ	1:A:338:LYS:HE2	2.51	0.46
1:C:2:LYS:HG2	1:C:14:TRP:HE3	1.77	0.46
1:C:253:VAL:CG1	9:C:1956:HOH:O	2.50	0.46
1:C:301:ARG:HH11	5:C:360:EDO:H21	1.81	0.45
1:A:95:VAL:HG11	9:A:1972:HOH:O	2.15	0.45
1:A:162:ALA:O	1:A:238:LYS:HD2	2.17	0.45
1:D:339:ASP:O	1:D:341:PRO:HD3	2.16	0.45
1:B:152[A]:MET:HG2	1:B:156[A]:PHE:CE2	2.51	0.45
1:D:304[C]:ARG:CD	5:D:358:EDO:O1	2.65	0.44
1:D:178:VAL:HG21	5:D:360[A]:EDO:H21	1.99	0.43
1:B:336:LEU:CD1	9:B:671:HOH:O	2.66	0.43
1:D:152[A]:MET:HE1	1:D:316:PRO:HG3	1.99	0.43
1:A:308:LEU:HD11	1:D:166[B]:LEU:HG	1.99	0.43
1:B:162:ALA:O	1:B:238:LYS:HD2	2.18	0.43
5:D:358:EDO:C1	9:D:1116:HOH:O	2.66	0.43
1:C:267:TYR:H	5:C:357[A]:EDO:C1	2.32	0.42
1:D:327:PHE:HB2	1:D:351:LEU:HD12	2.01	0.42
1:B:188[B]:HIS:CE1	1:B:313:ARG:HB3	2.55	0.42
5:D:358:EDO:H11	9:D:1116:HOH:O	2.19	0.42
5:D:360[A]:EDO:H22	9:D:1209:HOH:O	2.18	0.42
1:C:336:LEU:CD1	9:C:1044:HOH:O	2.68	0.42
1:B:337:MET:O	1:B:340:LYS:HD3	2.20	0.42
1:C:152[A]:MET:HE1	1:C:316:PRO:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ALA:O	1:C:238:LYS:HD2	2.19	0.41
1:C:304[B]:ARG:NE	5:C:360:EDO:H12	2.35	0.41
1:D:332:LYS:NZ	9:D:1903:HOH:O	2.52	0.41
1:A:152[A]:MET:HE1	1:A:316:PRO:HG3	2.03	0.41
1:C:2:LYS:HE3	1:C:14:TRP:CE3	2.54	0.41
1:D:301:ARG:CA	5:D:358:EDO:H22	2.45	0.41
1:D:28:ILE:HG12	1:D:67:GLU:HG3	2.02	0.41
5:C:357[B]:EDO:C2	9:C:626:HOH:O	2.69	0.40
1:C:152[A]:MET:HE3	1:C:152[A]:MET:HB2	1.87	0.40
1:C:332:LYS:O	1:C:336:LEU:HD13	2.20	0.40
1:A:156[B]:PHE:HZ	1:A:314:VAL:HG21	1.87	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	360/352 (102%)	342 (95%)	18 (5%)	0	100	100
1	B	363/352 (103%)	343 (94%)	20 (6%)	0	100	100
1	C	361/352 (103%)	343 (95%)	18 (5%)	0	100	100
1	D	361/352 (103%)	346 (96%)	15 (4%)	0	100	100
All	All	1445/1408 (103%)	1374 (95%)	71 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	291/281 (104%)	287 (99%)	4 (1%)	59	28
1	B	294/281 (105%)	292 (99%)	2 (1%)	76	52
1	C	292/281 (104%)	290 (99%)	2 (1%)	76	52
1	D	292/281 (104%)	287 (98%)	5 (2%)	53	21
All	All	1169/1124 (104%)	1156 (99%)	13 (1%)	63	37

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	TYR
1	A	328	ASP
1	A	337	MET
1	A	339	ASP
1	B	2	LYS
1	B	267	TYR
1	C	267	TYR
1	C	281	TRP
1	D	67	GLU
1	D	143	GLU
1	D	267	TYR
1	D	338	LYS
1	D	339	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
1	B	53	HIS
1	B	226	GLN
1	D	53	HIS
1	D	220	ASN
1	D	329	ASN

### 5.3.3 RNA

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 6 are monoatomic - leaving 25 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
5	EDO	B	359[B]	-	3,3,3	0.51	0	2,2,2	0.04	0
5	EDO	D	358	-	3,3,3	0.56	0	2,2,2	0.26	0
3	CAC	B	354	2	2,4,4	1.72	1 (50%)	4,6,6	1.25	0
3	CAC	C	354	2	2,4,4	1.13	0	4,6,6	2.58	2 (50%)
5	EDO	C	357[A]	-	3,3,3	0.51	0	2,2,2	0.32	0
5	EDO	C	358	-	3,3,3	0.37	0	2,2,2	0.27	0
6	NO3	D	359	-	1,3,3	3.10	1 (100%)	0,3,3	-	-
5	EDO	B	355	-	3,3,3	0.50	0	2,2,2	0.63	0
5	EDO	D	360[B]	-	3,3,3	0.39	0	2,2,2	0.49	0
5	EDO	C	357[B]	-	3,3,3	0.62	0	2,2,2	0.53	0
5	EDO	B	358	-	3,3,3	0.52	0	2,2,2	0.25	0
5	EDO	C	360	-	3,3,3	0.57	0	2,2,2	0.32	0
7	IMD	C	355	-	5,5,5	0.69	0	5,5,5	0.72	0
5	EDO	D	356	-	3,3,3	0.35	0	2,2,2	0.47	0
3	CAC	D	354	2	2,4,4	1.45	1 (50%)	4,6,6	1.79	1 (25%)
5	EDO	C	356	-	3,3,3	0.42	0	2,2,2	0.48	0
4	OXY	A	355	-	1,1,1	0.01	0	-	-	-
5	EDO	B	356	-	3,3,3	0.26	0	2,2,2	0.39	0
5	EDO	C	359	-	3,3,3	0.53	0	2,2,2	0.62	0
5	EDO	B	359[A]	-	3,3,3	0.49	0	2,2,2	0.47	0
6	NO3	B	357	-	1,3,3	2.96	1 (100%)	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CAC	A	354	2	2,4,4	1.43	0	4,6,6	1.59	1 (25%)
5	EDO	D	355	-	3,3,3	0.66	0	2,2,2	0.54	0
5	EDO	D	360[A]	-	3,3,3	0.62	0	2,2,2	0.12	0
5	EDO	D	357	-	3,3,3	0.42	0	2,2,2	0.71	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
5	EDO	C	359	-	-	1/1/1/1	-
5	EDO	B	359[B]	-	-	1/1/1/1	-
5	EDO	D	356	-	-	0/1/1/1	-
5	EDO	C	357[B]	-	-	1/1/1/1	-
5	EDO	D	358	-	-	1/1/1/1	-
5	EDO	B	359[A]	-	-	1/1/1/1	-
5	EDO	C	356	-	-	0/1/1/1	-
5	EDO	C	357[A]	-	-	0/1/1/1	-
5	EDO	C	358	-	-	1/1/1/1	-
5	EDO	B	358	-	-	0/1/1/1	-
5	EDO	B	355	-	-	1/1/1/1	-
5	EDO	D	360[B]	-	-	0/1/1/1	-
5	EDO	D	355	-	-	0/1/1/1	-
5	EDO	B	356	-	-	0/1/1/1	-
5	EDO	D	360[A]	-	-	0/1/1/1	-
5	EDO	C	360	-	-	0/1/1/1	-
7	IMD	C	355	-	-	-	0/1/1/1
5	EDO	D	357	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	359	NO3	O1-N	3.10	1.39	1.24
6	B	357	NO3	O1-N	2.96	1.38	1.24
3	B	354	CAC	AS-C1	2.06	1.95	1.90
3	D	354	CAC	AS-C2	2.05	1.95	1.90

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	354	CAC	O2-AS-C2	3.80	115.06	105.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	354	CAC	O1-AS-C1	-2.66	108.19	111.50
3	D	354	CAC	O2-AS-C2	2.62	112.18	105.84
3	A	354	CAC	O2-AS-C2	2.43	111.72	105.84

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	359	EDO	O1-C1-C2-O2
5	D	358	EDO	O1-C1-C2-O2
5	C	357[B]	EDO	O1-C1-C2-O2
5	B	355	EDO	O1-C1-C2-O2
5	B	359[B]	EDO	O1-C1-C2-O2
5	B	359[A]	EDO	O1-C1-C2-O2
5	C	358	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	358	EDO	10	0
5	C	357[A]	EDO	1	0
5	B	355	EDO	1	0
5	C	357[B]	EDO	1	0
5	C	360	EDO	5	0
7	C	355	IMD	5	0
5	B	359[A]	EDO	1	0
5	D	360[A]	EDO	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	352/352 (100%)	-0.28	5 (1%) 73 76	4, 9, 23, 39	10 (2%)
1	B	352/352 (100%)	-0.40	6 (1%) 69 72	4, 9, 22, 43	12 (3%)
1	C	352/352 (100%)	-0.42	3 (0%) 81 84	4, 8, 20, 36	11 (3%)
1	D	352/352 (100%)	-0.23	10 (2%) 55 57	3, 10, 23, 44	10 (2%)
All	All	1408/1408 (100%)	-0.33	24 (1%) 69 72	3, 9, 22, 44	43 (3%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	352	ALA	8.6
1	A	352	ALA	6.5
1	B	352	ALA	4.1
1	D	352	ALA	4.0
1	D	232	ASP	3.4
1	C	232	ASP	3.3
1	B	340	LYS	3.2
1	A	327	PHE	2.9
1	A	340	LYS	2.8
1	D	345	ILE	2.7
1	B	342	LYS	2.5
1	B	2	LYS	2.5
1	D	343	ASP	2.4
1	D	336	LEU	2.4
1	B	339	ASP	2.3
1	B	343	ASP	2.3
1	A	336	LEU	2.3
1	A	328	ASP	2.2
1	D	342	LYS	2.2
1	D	344	LEU	2.1
1	C	2	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	338	LYS	2.1
1	D	218	TYR	2.1
1	D	341	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	EDO	D	360[A]	4/4	0.71	0.21	19,20,22,22	4
5	EDO	D	360[B]	4/4	0.71	0.21	15,19,20,21	4
5	EDO	C	357[A]	4/4	0.82	0.19	14,22,26,29	4
5	EDO	C	357[B]	4/4	0.82	0.19	10,13,14,14	4
5	EDO	C	358	4/4	0.84	0.15	33,36,38,38	0
5	EDO	B	359[B]	4/4	0.86	0.11	15,19,21,23	4
4	OXY	A	355	2/2	0.86	0.18	27,27,27,30	0
5	EDO	B	359[A]	4/4	0.86	0.11	20,20,21,23	4
6	NO3	B	357	4/4	0.86	0.14	24,26,31,34	0
6	NO3	D	359	4/4	0.87	0.14	23,24,29,33	0
7	IMD	C	355	5/5	0.87	0.14	17,24,27,28	0
5	EDO	D	358	4/4	0.88	0.12	21,26,32,32	0
5	EDO	B	356	4/4	0.89	0.13	20,27,30,30	0
5	EDO	C	356	4/4	0.90	0.10	22,23,28,31	0
5	EDO	C	360	4/4	0.91	0.10	20,26,28,29	0
5	EDO	D	356	4/4	0.91	0.11	25,26,28,29	0
5	EDO	D	357	4/4	0.91	0.11	20,21,25,27	0
5	EDO	C	359	4/4	0.92	0.13	15,23,30,34	0
5	EDO	B	355	4/4	0.94	0.13	15,18,24,24	0
5	EDO	D	355	4/4	0.94	0.10	14,18,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	B	358	4/4	0.95	0.08	18,20,21,22	0
8	NA	C	361	1/1	0.98	0.21	28,28,28,28	0
8	NA	D	361	1/1	0.99	0.18	24,24,24,24	0
3	CAC	D	354	5/5	1.00	0.03	8,11,12,13	0
2	ZN	A	353	1/1	1.00	0.01	7,7,7,7	0
2	ZN	B	353	1/1	1.00	0.01	8,8,8,8	0
2	ZN	C	353	1/1	1.00	0.01	6,6,6,6	0
2	ZN	D	353	1/1	1.00	0.01	7,7,7,7	0
3	CAC	A	354	5/5	1.00	0.03	8,10,12,13	0
3	CAC	B	354	5/5	1.00	0.03	8,10,12,12	0
3	CAC	C	354	5/5	1.00	0.03	6,9,10,14	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.