



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2023 – 07:24 AM EDT

PDB ID : 2OUI  
Title : D275P mutant of alcohol dehydrogenase from protozoa *Entamoeba histolytica*  
Authors : Frolow, F.; Shimon, L.; Burstein, Y.; Goihberg, E.; Peretz, M.; Dym, O.  
Deposited on : 2007-02-11  
Resolution : 1.77 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

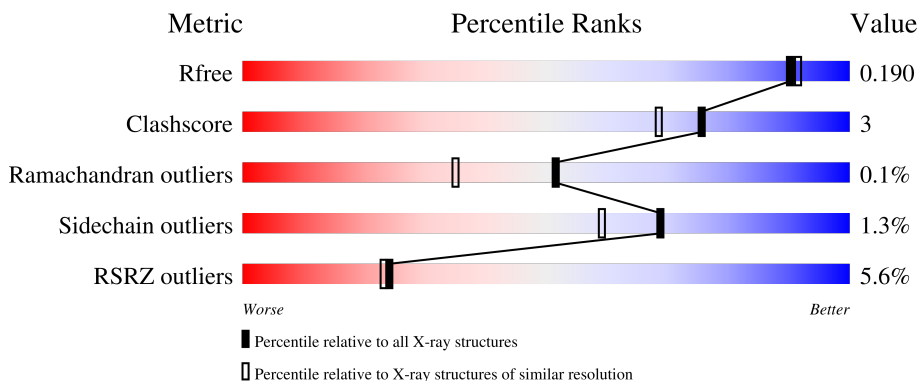
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

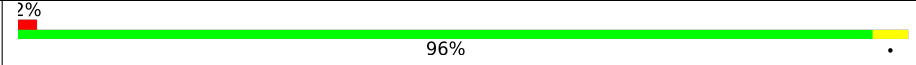
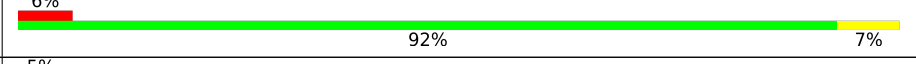
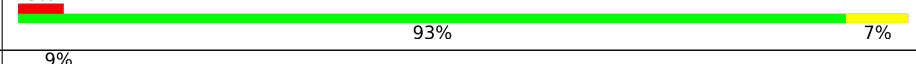
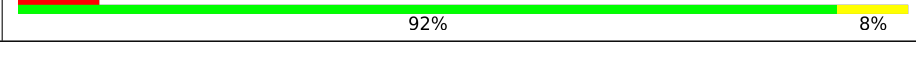
The reported resolution of this entry is 1.77 Å.

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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	360	 2% 96%
1	B	360	 6% 92% 7%
1	C	360	 5% 93% 7%
1	D	360	 9% 92% 8%

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	A	2007	-	-	X	-
8	CL	D	7001	-	-	-	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 12226 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	360	2728	1730	477	503	18	0	5	0
1	B	360	2763	1754	484	506	19	0	10	0
1	C	360	2761	1752	484	507	18	0	9	0
1	D	360	2743	1740	479	506	18	0	7	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	PRO	ASP	engineered mutation	UNP P35630
B	275	PRO	ASP	engineered mutation	UNP P35630
C	275	PRO	ASP	engineered mutation	UNP P35630
D	275	PRO	ASP	engineered mutation	UNP P35630

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

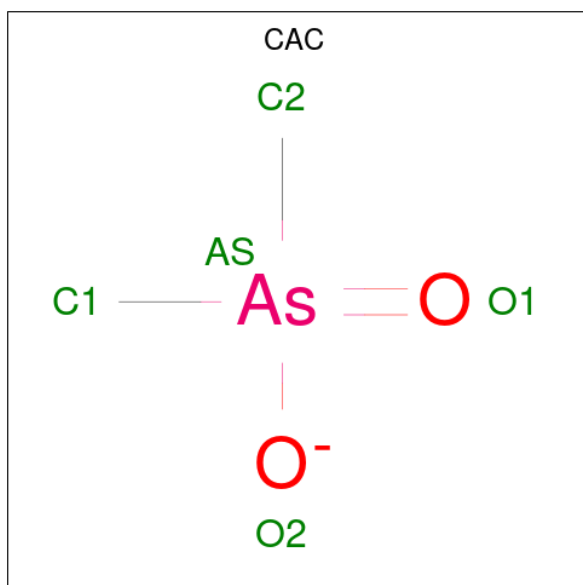
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



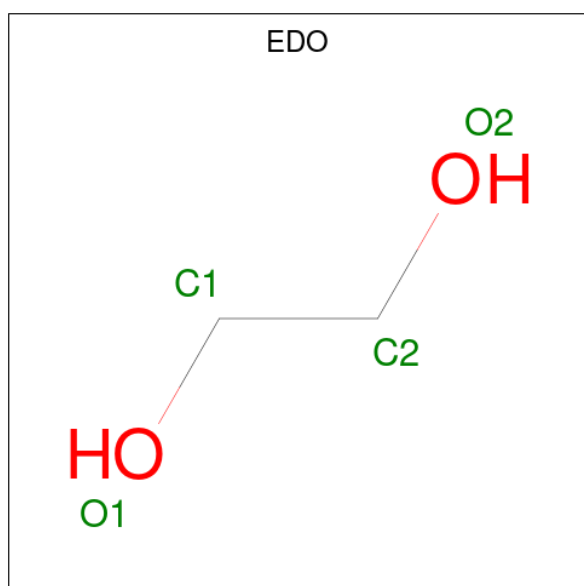
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		
3	B	1	Total	N	O	0	0
			4	1	3		
3	D	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is CACODYLATE ION (three-letter code: CAC) (formula:  $C_2H_6AsO_2$ ).



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

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



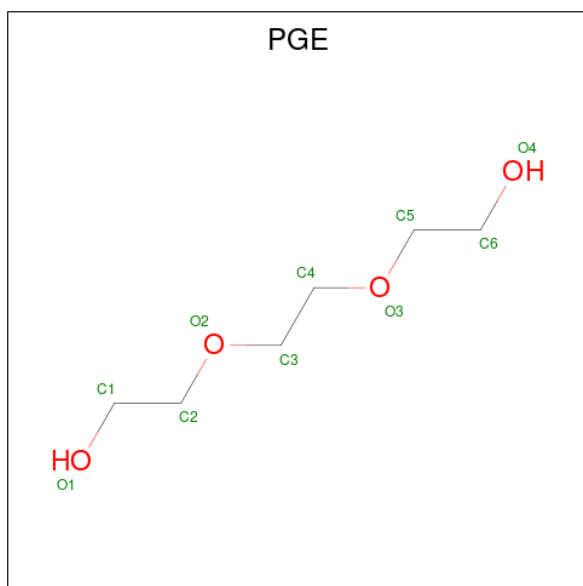
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	C	1	4	2	2	0	0

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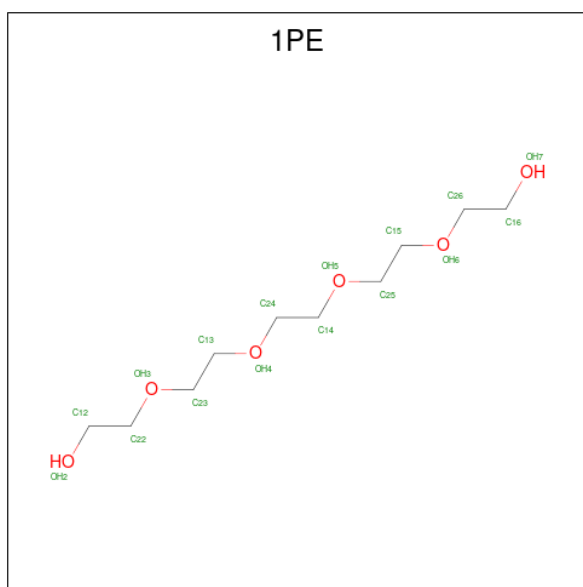
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).

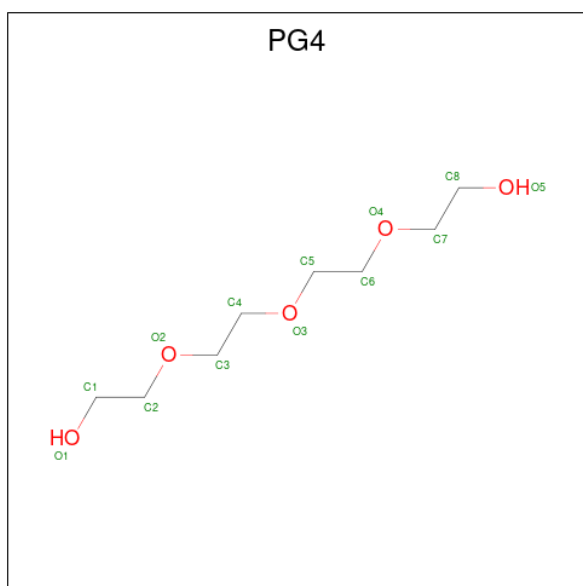


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 16 10 6	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Cl 1 1	0	0

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	276	Total	O	0	2
			278	278		
10	B	270	Total	O	0	3
			273	273		
10	C	276	Total	O	0	3
			279	279		
10	D	253	Total	O	0	2
			255	255		

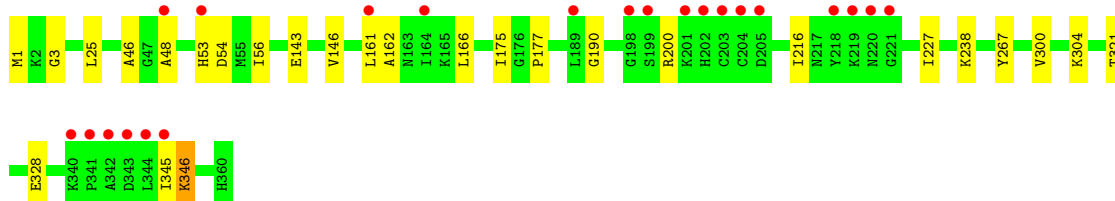
### 3 Residue-property plots [i](#)

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.

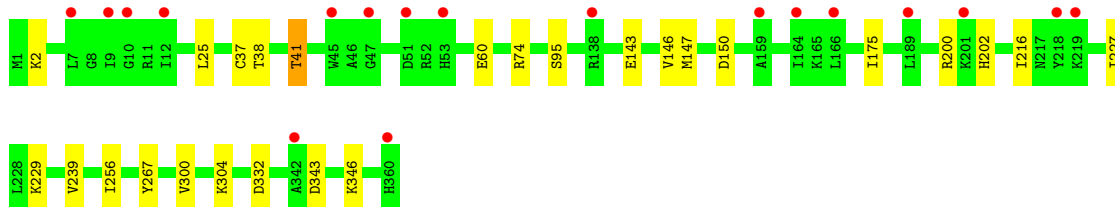
- Molecule 1: NADP-dependent alcohol dehydrogenase



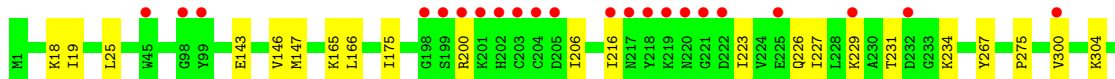
- Molecule 1: NADP-dependent alcohol dehydrogenase

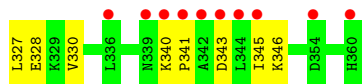


- Molecule 1: NADP-dependent alcohol dehydrogenase



- Molecule 1: NADP-dependent alcohol dehydrogenase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.92Å 144.10Å 80.07Å 90.00° 121.44° 90.00°	Depositor
Resolution (Å)	50.00 – 1.77 49.58 – 1.77	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-1.77) 99.9 (49.58-1.77)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 1.77Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.148 , 0.178 0.171 , 0.190	Depositor DCC
$R_{free}$ test set	6881 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.3	Xtrriage
Anisotropy	0.196	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.018 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12226	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: ZN, CAC, 1PE, EDO, CL, PGE, PG4, NO3

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	0.57	0/2797	0.68	0/3779
1	B	0.59	0/2842	0.70	0/3838
1	C	0.59	0/2840	0.67	0/3836
1	D	0.56	0/2811	0.66	0/3795
All	All	0.58	0/11290	0.68	0/15248

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	2728	0	2776	11	0
1	B	2763	0	2821	20	0
1	C	2761	0	2817	16	0
1	D	2743	0	2801	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	0	0
3	D	4	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
5	A	16	0	24	5	0
5	B	12	0	18	0	0
5	C	4	0	6	0	0
5	D	4	0	6	0	0
6	A	10	0	14	0	0
6	B	20	0	28	2	0
6	C	10	0	14	1	0
7	C	16	0	22	2	0
8	D	1	0	0	0	0
9	D	13	0	18	1	0
10	A	278	0	0	6	0
10	B	273	0	0	6	0
10	C	279	0	0	2	0
10	D	255	0	0	1	0
All	All	12226	0	11365	70	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 3.

All (70) 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:53[A]:HIS:CD2	10:A:5148[A]:HOH:O	2.22	0.92
1:D:226:GLN:HA	1:D:229:LYS:HD2	1.68	0.76
5:A:2007:EDO:H22	1:D:166:LEU:H	1.48	0.76
1:A:231:THR:O	1:A:234:LYS:HG2	1.91	0.70
5:A:2007:EDO:C2	1:D:166:LEU:H	2.05	0.69
1:C:41:THR:HG21	10:C:5180:HOH:O	1.93	0.66
1:D:216:ILE:HG13	1:D:227:ILE:HD11	1.80	0.64
1:B:328[A]:GLU:H	1:B:328[A]:GLU:CD	2.06	0.59
1:B:300:VAL:O	1:B:304:LYS:HG2	2.03	0.58
1:D:328[A]:GLU:H	1:D:328[A]:GLU:CD	2.07	0.57
5:A:2007:EDO:H11	1:D:165:LYS:HD2	1.86	0.57
1:C:38:THR:O	1:C:41:THR:HB	2.05	0.56
1:C:300:VAL:O	1:C:304:LYS:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:VAL:O	1:A:304:LYS:HG2	2.09	0.53
1:B:200:ARG:NH1	10:B:5197:HOH:O	2.42	0.53
1:C:37:CYS:HB2	1:C:60:GLU:OE2	2.08	0.53
1:C:143[B]:GLU:O	1:C:146:VAL:HG12	2.08	0.53
1:B:321:THR:HG21	1:B:345:ILE:H	1.74	0.53
1:A:53[A]:HIS:HD2	10:A:5148[A]:HOH:O	1.77	0.52
1:D:143:GLU:O	1:D:146:VAL:HG12	2.09	0.52
5:A:2008:EDO:H11	10:A:5078:HOH:O	2.10	0.52
1:D:146:VAL:HG13	1:D:147:MET:CE	2.39	0.52
1:C:150:ASP:OD1	4:C:1001:CAC:C1	2.57	0.51
5:A:2007:EDO:H22	1:D:166:LEU:N	2.23	0.50
1:B:3:GLY:HA3	1:B:56[B]:ILE:HD12	1.94	0.50
1:B:216:ILE:HG13	1:B:227:ILE:HD11	1.94	0.50
1:D:231:THR:O	1:D:234:LYS:HG2	2.12	0.49
1:B:54:ASP:N	10:B:5144:HOH:O	2.15	0.49
1:B:321:THR:HG21	1:B:345:ILE:N	2.27	0.49
1:B:46:ALA:HB3	10:B:5256:HOH:O	2.12	0.49
1:B:162:ALA:O	1:B:238:LYS:HD2	2.14	0.48
1:C:216:ILE:HG13	1:C:227[A]:ILE:HD11	1.96	0.48
1:A:166:LEU:HD23	1:A:190:GLY:HA3	1.97	0.47
1:B:143:GLU:O	1:B:146:VAL:HG12	2.14	0.47
1:C:2:LYS:HD3	7:C:4001:1PE:H231	1.96	0.47
1:D:300:VAL:O	1:D:304:LYS:HG2	2.15	0.46
1:D:223:ILE:O	1:D:227:ILE:HG12	2.15	0.46
1:D:216:ILE:HG13	1:D:227:ILE:CD1	2.44	0.46
1:C:202[A]:HIS:HD2	1:C:343:ASP:HA	1.81	0.45
1:D:206:ILE:HD12	1:D:345:ILE:HD11	1.98	0.44
1:D:25:LEU:HD22	10:D:7163:HOH:O	2.18	0.44
1:D:146:VAL:HG13	1:D:147:MET:HE3	1.99	0.44
1:A:323:ARG:NH1	10:A:5197:HOH:O	2.33	0.44
1:B:177:PRO:HG3	1:B:346:LYS:HG2	2.00	0.43
1:C:74:ARG:NH1	10:C:5155:HOH:O	2.42	0.43
1:B:25:LEU:HD22	10:B:5011:HOH:O	2.19	0.43
1:A:340:LYS:HE3	1:A:340:LYS:HB2	1.83	0.42
1:A:25:LEU:HD11	1:C:25:LEU:HD11	2.00	0.42
1:D:327:LEU:O	1:D:330:VAL:HG22	2.20	0.42
1:D:200:ARG:NH2	1:D:341:PRO:O	2.53	0.42
1:B:216:ILE:HG13	1:B:227:ILE:CD1	2.50	0.41
1:D:146:VAL:HG13	1:D:147:MET:HE2	2.01	0.41
1:C:95:SER:O	6:C:5002:PGE:H32	2.21	0.41
1:D:18[B]:LYS:HG2	1:D:19:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ALA:HB2	10:B:5256:HOH:O	2.20	0.41
1:B:166:LEU:HD23	1:B:190:GLY:HA3	2.02	0.41
1:C:2:LYS:HD3	7:C:4001:1PE:H222	2.03	0.41
1:A:352:HIS:HE1	10:A:5200:HOH:O	2.03	0.41
1:B:328[A]:GLU:HG3	6:B:5003:PGE:C4	2.51	0.41
1:C:146:VAL:HG13	1:C:147:MET:CE	2.50	0.41
1:C:239:VAL:HG23	1:C:256:ILE:HD12	2.03	0.41
1:D:328[A]:GLU:HG3	9:D:6001:PG4:O2	2.22	0.40
1:B:53[A]:HIS:HB3	10:B:5144:HOH:O	2.21	0.40
1:B:161:LEU:HD23	6:B:5004:PGE:H12	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	363/360 (101%)	351 (97%)	12 (3%)	0	100	100
1	B	368/360 (102%)	355 (96%)	13 (4%)	0	100	100
1	C	368/360 (102%)	355 (96%)	13 (4%)	0	100	100
1	D	365/360 (101%)	350 (96%)	14 (4%)	1 (0%)	41	25
All	All	1464/1440 (102%)	1411 (96%)	52 (4%)	1 (0%)	51	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	340	LYS



### 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	291/286 (102%)	289 (99%)	2 (1%)	84	79
1	B	296/286 (104%)	293 (99%)	3 (1%)	76	68
1	C	296/286 (104%)	290 (98%)	6 (2%)	55	40
1	D	293/286 (102%)	289 (99%)	4 (1%)	67	56
All	All	1176/1144 (103%)	1161 (99%)	15 (1%)	69	59

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	TYR
1	A	328	GLU
1	B	1	MET
1	B	267	TYR
1	B	346	LYS
1	C	41	THR
1	C	200	ARG
1	C	229	LYS
1	C	267	TYR
1	C	332	ASP
1	C	346	LYS
1	D	267	TYR
1	D	275	PRO
1	D	343	ASP
1	D	346	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	247	HIS
1	A	251	GLN
1	A	352	HIS

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Mol	Chain	Res	Type
1	B	187	ASN
1	B	251	GLN
1	C	187	ASN
1	C	226	GLN
1	C	251	GLN
1	C	360	HIS
1	D	187	ASN
1	D	188	HIS
1	D	226	GLN
1	D	251	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 5 are monoatomic - leaving 23 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	2006	-	3,3,3	0.60	0	2,2,2	0.13	0
7	1PE	C	4001	-	15,15,15	0.47	0	14,14,14	0.30	0
4	CAC	D	1001	2	0,4,4	-	-	0,6,6	-	-
4	CAC	B	1001	2	0,4,4	-	-	0,6,6	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	2003	-	3,3,3	0.48	0	2,2,2	0.40	0
6	PGE	A	5001	-	9,9,9	0.42	0	8,8,8	0.40	0
4	CAC	C	1001	2	0,4,4	-	-	0,6,6	-	-
3	NO3	A	3003	-	1,3,3	3.66	1 (100%)	0,3,3	-	-
5	EDO	B	2005	-	3,3,3	0.45	0	2,2,2	0.40	0
3	NO3	B	3002	-	1,3,3	3.51	1 (100%)	0,3,3	-	-
5	EDO	A	2001	-	3,3,3	0.54	0	2,2,2	0.25	0
5	EDO	C	2002	-	3,3,3	0.53	0	2,2,2	0.15	0
4	CAC	A	1001	2	0,4,4	-	-	0,6,6	-	-
3	NO3	D	3004	-	1,3,3	3.88	1 (100%)	0,3,3	-	-
6	PGE	C	5002	-	9,9,9	0.49	0	8,8,8	0.18	0
5	EDO	A	2007	-	3,3,3	0.38	0	2,2,2	0.72	0
3	NO3	A	3001	-	1,3,3	3.66	1 (100%)	0,3,3	-	-
6	PGE	B	5003	-	9,9,9	0.46	0	8,8,8	0.30	0
5	EDO	A	2008	-	3,3,3	0.49	0	2,2,2	0.38	0
5	EDO	D	2009	-	3,3,3	0.53	0	2,2,2	0.24	0
5	EDO	B	2004	-	3,3,3	0.64	0	2,2,2	0.33	0
6	PGE	B	5004	-	9,9,9	0.55	0	8,8,8	0.34	0
9	PG4	D	6001	-	12,12,12	0.47	0	11,11,11	0.30	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	B	2006	-	-	0/1/1/1	-
7	1PE	C	4001	-	-	5/13/13/13	-
6	PGE	C	5002	-	-	4/7/7/7	-
5	EDO	B	2004	-	-	0/1/1/1	-
5	EDO	B	2005	-	-	1/1/1/1	-
5	EDO	A	2007	-	-	1/1/1/1	-
5	EDO	A	2003	-	-	1/1/1/1	-
6	PGE	B	5004	-	-	5/7/7/7	-
6	PGE	B	5003	-	-	5/7/7/7	-
6	PGE	A	5001	-	-	2/7/7/7	-
5	EDO	A	2001	-	-	1/1/1/1	-
5	EDO	A	2008	-	-	1/1/1/1	-
5	EDO	C	2002	-	-	0/1/1/1	-
5	EDO	D	2009	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PG4	D	6001	-	-	4/10/10/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3004	NO3	O1-N	3.88	1.42	1.24
3	A	3001	NO3	O1-N	3.66	1.40	1.24
3	A	3003	NO3	O1-N	3.66	1.40	1.24
3	B	3002	NO3	O1-N	3.51	1.40	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	4001	1PE	OH4-C13-C23-OH3
6	A	5001	PGE	O3-C5-C6-O4
6	A	5001	PGE	O2-C3-C4-O3
6	B	5003	PGE	O2-C3-C4-O3
6	B	5003	PGE	O3-C5-C6-O4
6	B	5004	PGE	O3-C5-C6-O4
6	B	5004	PGE	O1-C1-C2-O2
6	C	5002	PGE	O1-C1-C2-O2
7	C	4001	1PE	OH2-C12-C22-OH3
9	D	6001	PG4	O1-C1-C2-O2
5	B	2005	EDO	O1-C1-C2-O2
5	D	2009	EDO	O1-C1-C2-O2
6	B	5004	PGE	O2-C3-C4-O3
9	D	6001	PG4	O2-C3-C4-O3
6	C	5002	PGE	O2-C3-C4-O3
9	D	6001	PG4	O3-C5-C6-O4
6	B	5003	PGE	O1-C1-C2-O2
9	D	6001	PG4	C5-C6-O4-C7
6	B	5003	PGE	C1-C2-O2-C3
6	B	5004	PGE	C6-C5-O3-C4
6	B	5003	PGE	C3-C4-O3-C5
6	B	5004	PGE	C3-C4-O3-C5
7	C	4001	1PE	C15-C25-OH5-C14
5	A	2008	EDO	O1-C1-C2-O2
6	C	5002	PGE	C4-C3-O2-C2
7	C	4001	1PE	C24-C14-OH5-C25

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Mol	Chain	Res	Type	Atoms
7	C	4001	1PE	C23-C13-OH4-C24
5	A	2001	EDO	O1-C1-C2-O2
5	A	2003	EDO	O1-C1-C2-O2
5	A	2007	EDO	O1-C1-C2-O2
6	C	5002	PGE	C6-C5-O3-C4

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	4001	1PE	2	0
4	C	1001	CAC	1	0
6	C	5002	PGE	1	0
5	A	2007	EDO	4	0
6	B	5003	PGE	1	0
5	A	2008	EDO	1	0
6	B	5004	PGE	1	0
9	D	6001	PG4	1	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	360/360 (100%)	0.00	9 (2%) 57 56	19, 25, 37, 48	0
1	B	360/360 (100%)	0.16	22 (6%) 21 20	17, 24, 44, 73	0
1	C	360/360 (100%)	0.16	18 (5%) 28 27	19, 24, 36, 53	0
1	D	360/360 (100%)	0.29	32 (8%) 9 9	19, 24, 43, 64	0
All	All	1440/1440 (100%)	0.15	81 (5%) 24 23	17, 24, 40, 73	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	218	TYR	7.6
1	D	344	LEU	6.8
1	D	343	ASP	6.2
1	B	218	TYR	6.1
1	B	202[A]	HIS	5.9
1	B	343	ASP	5.5
1	D	341	PRO	5.4
1	D	199	SER	5.4
1	D	203	CYS	5.3
1	B	345	ILE	5.3
1	D	342	ALA	5.2
1	B	342	ALA	4.9
1	D	201	LYS	4.3
1	B	341	PRO	4.2
1	D	345	ILE	4.1
1	C	218	TYR	4.1
1	D	202	HIS	4.1
1	C	9	ILE	4.1
1	B	203	CYS	3.9
1	D	200	ARG	3.9
1	D	198	GLY	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	221	GLY	3.7
1	D	340	LYS	3.7
1	D	219	LYS	3.6
1	B	344	LEU	3.6
1	B	204	CYS	3.5
1	B	219	LYS	3.5
1	D	220	ASN	3.5
1	C	53[A]	HIS	3.4
1	B	201	LYS	3.4
1	C	164	ILE	3.3
1	B	53[A]	HIS	3.3
1	D	205	ASP	3.0
1	D	45	TRP	3.0
1	A	53[A]	HIS	2.9
1	B	48	ALA	2.9
1	C	159	ALA	2.9
1	C	189	LEU	2.8
1	D	354	ASP	2.8
1	A	358	THR	2.8
1	B	221	GLY	2.8
1	D	204	CYS	2.7
1	D	217	ASN	2.7
1	C	342	ALA	2.6
1	C	47	GLY	2.6
1	D	225	GLU	2.6
1	B	340	LYS	2.6
1	B	199	SER	2.6
1	C	45	TRP	2.6
1	D	98	GLY	2.5
1	D	339	ASN	2.5
1	C	201	LYS	2.5
1	A	343	ASP	2.5
1	A	218	TYR	2.5
1	C	166	LEU	2.4
1	C	51	ASP	2.4
1	A	161	LEU	2.4
1	D	360	HIS	2.4
1	B	161	LEU	2.3
1	A	164	ILE	2.3
1	A	341	PRO	2.3
1	C	7	LEU	2.3
1	C	138	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	342	ALA	2.2
1	B	189	LEU	2.2
1	D	99	TYR	2.2
1	D	232	ASP	2.2
1	D	222	ASP	2.2
1	C	10	GLY	2.2
1	D	229	LYS	2.2
1	B	220	ASN	2.2
1	A	354	ASP	2.2
1	C	360	HIS	2.2
1	C	12	ILE	2.2
1	C	219	LYS	2.1
1	B	205	ASP	2.1
1	B	164	ILE	2.1
1	B	198	GLY	2.1
1	D	216	ILE	2.0
1	D	300	VAL	2.0
1	D	336	LEU	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 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, 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
8	CL	D	7001	1/1	0.31	0.81	158,158,158,158	0
5	EDO	D	2009	4/4	0.74	0.36	54,55,57,57	0
3	NO3	D	3004	4/4	0.78	0.16	32,41,44,45	0
6	PGE	C	5002	10/10	0.83	0.25	46,52,57,57	0
5	EDO	A	2008	4/4	0.85	0.18	40,43,47,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NO3	A	3003	4/4	0.86	0.17	48,51,52,54	0
6	PGE	B	5004	10/10	0.86	0.20	22,56,60,61	0
5	EDO	A	2001	4/4	0.88	0.12	30,31,33,37	0
5	EDO	B	2006	4/4	0.88	0.14	33,35,36,36	0
9	PG4	D	6001	13/13	0.88	0.16	44,52,70,72	0
6	PGE	B	5003	10/10	0.90	0.15	46,55,64,67	0
5	EDO	B	2004	4/4	0.91	0.12	23,33,38,38	0
5	EDO	A	2007	4/4	0.91	0.23	29,41,44,47	0
7	1PE	C	4001	16/16	0.93	0.14	38,47,74,74	0
6	PGE	A	5001	10/10	0.93	0.17	41,51,58,61	0
5	EDO	B	2005	4/4	0.93	0.28	45,46,50,59	0
3	NO3	B	3002	4/4	0.94	0.20	35,35,37,37	0
5	EDO	A	2003	4/4	0.95	0.21	30,31,32,35	0
5	EDO	C	2002	4/4	0.95	0.09	33,38,41,43	0
3	NO3	A	3001	4/4	0.97	0.15	23,31,32,37	0
4	CAC	C	1001	5/5	0.99	0.07	16,19,24,29	0
4	CAC	D	1001	5/5	0.99	0.05	21,22,25,26	0
2	ZN	A	361	1/1	0.99	0.03	19,19,19,19	0
4	CAC	A	1001	5/5	1.00	0.04	19,25,26,28	0
4	CAC	B	1001	5/5	1.00	0.04	19,20,24,29	0
2	ZN	C	361	1/1	1.00	0.01	18,18,18,18	0
2	ZN	D	361	1/1	1.00	0.02	19,19,19,19	0
2	ZN	B	361	1/1	1.00	0.02	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.