



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:19 PM GMT

PDB ID : 4XDZ  
Title : Holo structure of ketol-acid reductoisomerase from Ignisphaera aggregans  
Authors : Cahn, J.K.B.; Brinkmann-Chen, S.; Arnold, F.H.  
Deposited on : 2014-12-20  
Resolution : 1.15 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

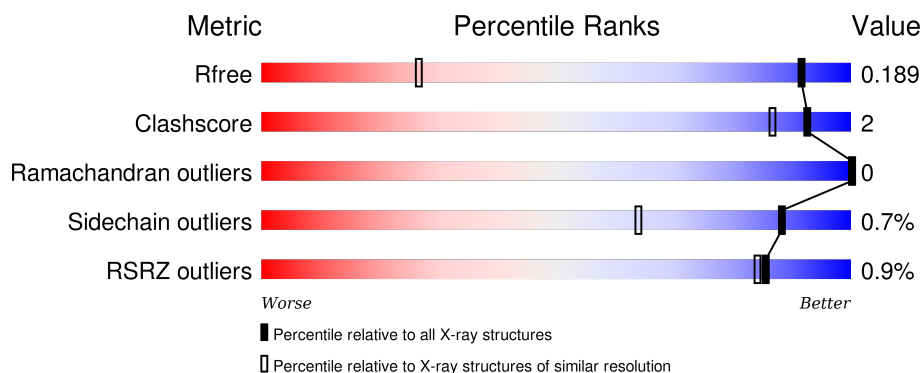
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.15 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))
$R_{free}$	91344	1495 (1.20-1.08)
Clashscore	102246	1593 (1.20-1.08)
Ramachandran outliers	100387	1521 (1.20-1.08)
Sidechain outliers	100360	1518 (1.20-1.08)
RSRZ outliers	91569	1498 (1.20-1.08)

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  $\geq 3$ , 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	343	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 9%, green 86%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>86%</span> <span>9% .</span> </div> </div>
1	B	343	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 9%, green 87%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>87%</span> <span>9% .</span> </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
5	EPE	A	405	-	-	-	X
5	EPE	B	405	-	-	-	X
6	GOL	A	407	-	-	-	X
6	GOL	A	408	-	-	-	X
6	GOL	B	406	-	-	-	X
6	GOL	B	407	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6039 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.

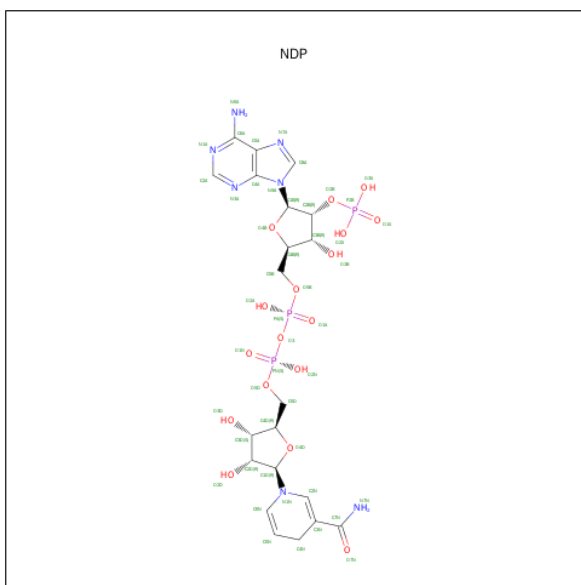
- Molecule 1 is a protein called Ketol-acid reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	11	0
			2634	1701	433	485	15			
1	B	329	Total	C	N	O	S	0	9	0
			2631	1693	436	487	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	336	LEU	-	expression tag	UNP E0SRA9
A	337	GLU	-	expression tag	UNP E0SRA9
A	338	HIS	-	expression tag	UNP E0SRA9
A	339	HIS	-	expression tag	UNP E0SRA9
A	340	HIS	-	expression tag	UNP E0SRA9
A	341	HIS	-	expression tag	UNP E0SRA9
A	342	HIS	-	expression tag	UNP E0SRA9
A	343	HIS	-	expression tag	UNP E0SRA9
B	336	LEU	-	expression tag	UNP E0SRA9
B	337	GLU	-	expression tag	UNP E0SRA9
B	338	HIS	-	expression tag	UNP E0SRA9
B	339	HIS	-	expression tag	UNP E0SRA9
B	340	HIS	-	expression tag	UNP E0SRA9
B	341	HIS	-	expression tag	UNP E0SRA9
B	342	HIS	-	expression tag	UNP E0SRA9
B	343	HIS	-	expression tag	UNP E0SRA9

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).

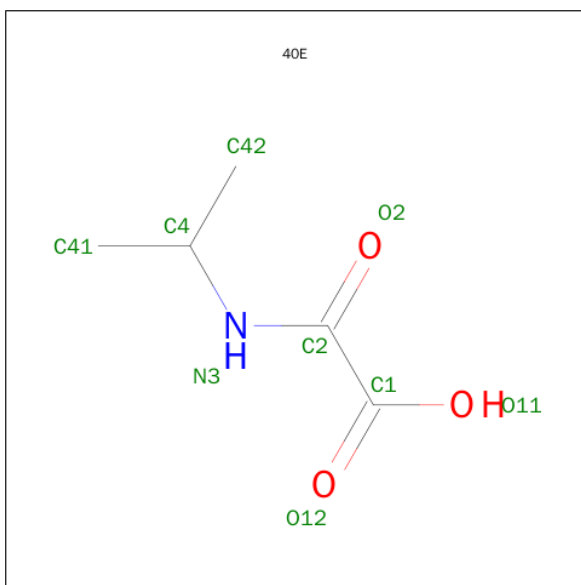


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

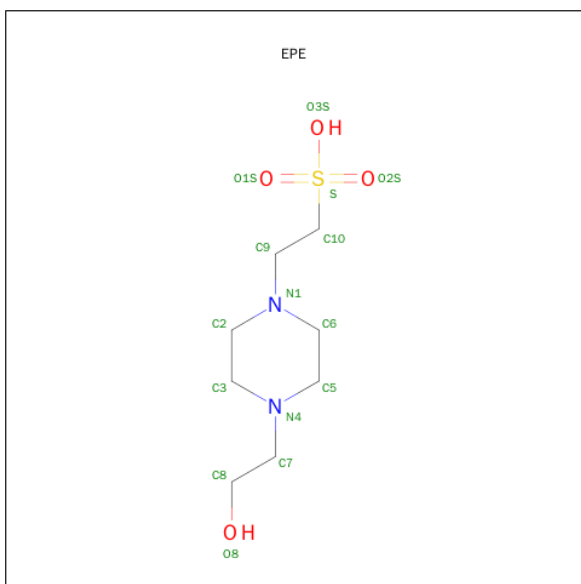
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0
3	A	2	Total Mg 2 2	0	0

- Molecule 4 is oxo(propan-2-ylamino)acetic acid (three-letter code: 40E) (formula:  $\text{C}_5\text{H}_9\text{NO}_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	5	1	3		
4	B	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



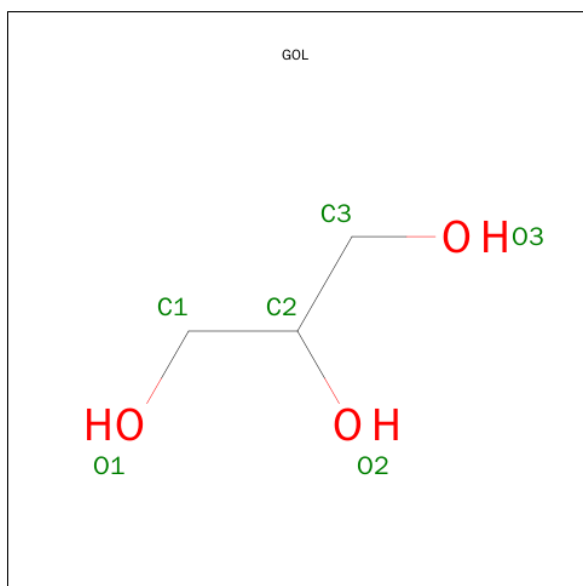
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	291	Total	O	0	0
			291	291		
7	B	304	Total	O	0	1
			305	305		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.58Å 90.75Å 69.53Å 90.00° 100.25° 90.00°	Depositor
Resolution (Å)	68.42 – 1.15 39.01 – 1.15	Depositor EDS
% Data completeness (in resolution range)	94.9 (68.42-1.15) 94.9 (39.01-1.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 1.15Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.157 , 0.190 0.156 , 0.189	Depositor DCC
$R_{free}$ test set	11211 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	9.3	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 224304 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	6039	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.48 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.5164e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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, 40E, EPE, MG, NDP

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	1.27	9/2706 (0.3%)	1.31	21/3639 (0.6%)
1	B	1.26	13/2700 (0.5%)	1.31	22/3633 (0.6%)
All	All	1.27	22/5406 (0.4%)	1.31	43/7272 (0.6%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	37	ARG	CZ-NH1	12.33	1.49	1.33
1	A	8	GLU	CD-OE2	11.99	1.38	1.25
1	B	53	SER	CB-OG	-11.75	1.26	1.42
1	A	53	SER	CB-OG	-11.54	1.27	1.42
1	B	8	GLU	CD-OE1	9.71	1.36	1.25
1	A	280	GLU	CG-CD	8.38	1.64	1.51
1	B	8	GLU	CD-OE2	8.32	1.34	1.25
1	A	281	ARG	CZ-NH2	7.27	1.42	1.33
1	B	205	GLU	CD-OE1	7.00	1.33	1.25
1	B	280	GLU	CD-OE1	6.70	1.33	1.25
1	B	187	GLU	CD-OE1	-6.41	1.18	1.25
1	A	280	GLU	CD-OE1	6.33	1.32	1.25
1	B	294	GLU	CD-OE2	-6.00	1.19	1.25
1	A	305	GLU	CD-OE1	5.62	1.31	1.25
1	B	305	GLU	CD-OE1	5.50	1.31	1.25
1	A	291	TRP	CG-CD1	-5.29	1.29	1.36
1	B	280	GLU	CG-CD	5.27	1.59	1.51
1	B	142	GLU	CD-OE2	-5.20	1.20	1.25
1	A	109	GLY	CA-C	5.13	1.60	1.51
1	B	37	ARG	NE-CZ	5.12	1.39	1.33
1	B	25	TYR	CE2-CZ	-5.11	1.31	1.38
1	A	8	GLU	CG-CD	5.04	1.59	1.51

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ARG	NE-CZ-NH1	-16.25	112.17	120.30
1	B	37	ARG	NE-CZ-NH2	-14.56	113.02	120.30
1	A	324[A]	MET	CG-SD-CE	12.90	120.84	100.20
1	A	324[B]	MET	CG-SD-CE	12.90	120.84	100.20
1	B	37	ARG	NE-CZ-NH1	10.43	125.52	120.30
1	A	30	ARG	NE-CZ-NH2	7.73	124.16	120.30
1	B	138	ARG	NE-CZ-NH2	7.64	124.12	120.30
1	B	100	LYS	CD-CE-NZ	-7.39	94.70	111.70
1	B	55	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	A	83	ASP	CB-CG-OD1	-7.27	111.76	118.30
1	B	30	ARG	NE-CZ-NH2	7.09	123.85	120.30
1	B	59	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	A	281	ARG	NH1-CZ-NH2	6.91	127.00	119.40
1	B	289[A]	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	B	289[B]	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	60	ASP	CB-CG-OD1	6.76	124.38	118.30
1	B	273	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	280	GLU	OE1-CD-OE2	-6.51	115.48	123.30
1	B	60	ASP	CB-CG-OD1	6.51	124.16	118.30
1	B	327	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	B	53	SER	CB-CA-C	6.43	122.31	110.10
1	A	268	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	303	PHE	CB-CG-CD1	-6.32	116.37	120.80
1	B	30	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	A	55	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	280	GLU	CA-CB-CG	6.06	126.73	113.40
1	B	319	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	B	289[A]	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	289[B]	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	25	TYR	CB-CG-CD1	-5.92	117.45	121.00
1	A	53	SER	CB-CA-C	5.86	121.23	110.10
1	A	5	TYR	CB-CG-CD2	5.81	124.48	121.00
1	A	274	LYS	CD-CE-NZ	5.67	124.74	111.70
1	B	143	MET	CG-SD-CE	5.56	109.09	100.20
1	A	59	ASP	CB-CG-OD2	-5.53	113.33	118.30
1	A	8	GLU	CG-CD-OE1	-5.28	107.75	118.30
1	B	322	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	257	TYR	CD1-CE1-CZ	-5.23	115.09	119.80
1	A	99	LYS	CB-CA-C	-5.22	99.96	110.40
1	B	241	GLU	OE1-CD-OE2	5.21	129.54	123.30
1	A	280	GLU	CG-CD-OE1	5.18	128.66	118.30
1	B	103	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	295	TYR	CB-CG-CD2	-5.05	117.97	121.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2634	0	2730	17	0
1	B	2631	0	2714	7	0
2	A	48	0	26	0	0
2	B	48	0	26	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	9	0	7	0	0
4	B	9	0	7	0	0
5	A	15	0	18	0	0
5	B	15	0	18	0	0
6	A	18	0	24	0	0
6	B	12	0	16	0	0
7	A	291	0	0	8	1
7	B	305	0	0	3	1
All	All	6039	0	5586	22	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 2.

All (22) 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:B:277:ILE:HD12	7:B:578:HOH:O	1.37	1.19
1:A:16[B]:LYS:O	7:A:501:HOH:O	1.72	1.06
1:B:16[A]:LYS:O	7:B:804:HOH:O	1.83	0.96
1:A:6[B]:LYS:NZ	7:A:683:HOH:O	2.08	0.87
1:B:277:ILE:CD1	7:B:578:HOH:O	2.10	0.81
1:A:118[B]:GLU:CA	1:A:119:PRO:N	2.45	0.78
1:A:16[B]:LYS:CE	7:A:529:HOH:O	2.41	0.69
1:A:16[A]:LYS:O	7:A:756:HOH:O	2.18	0.56
1:A:203:ILE:CD1	1:B:203:ILE:HD13	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324[A]:MET:CE	7:A:777:HOH:O	2.57	0.52
1:A:117:ILE:C	1:A:118[B]:GLU:CA	2.79	0.51
1:B:12:LEU:HB2	1:B:16[B]:LYS:HE3	1.94	0.49
1:B:13:GLU:HA	1:B:16[B]:LYS:HD2	1.95	0.48
1:A:16[B]:LYS:HE2	7:A:529:HOH:O	2.10	0.48
1:A:16[B]:LYS:HE3	7:A:529:HOH:O	2.12	0.47
1:A:13:GLU:CD	1:A:16[B]:LYS:HD2	2.35	0.47
1:A:118[B]:GLU:CA	1:A:119:PRO:CD	2.95	0.45
1:A:324[A]:MET:HE2	7:A:777:HOH:O	2.18	0.44
1:A:47:LEU:O	1:A:66:TYR:HA	2.18	0.43
1:A:203:ILE:HD13	1:B:203:ILE:CD1	2.49	0.43
1:A:13:GLU:OE2	1:A:16[B]:LYS:HD2	2.19	0.42
1:A:65[A]:MET:HE1	1:A:73:ILE:HD11	2.01	0.41

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:575:HOH:O	7:B:551:HOH:O[1_655]	2.14	0.06

## 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	338/343 (98%)	326 (96%)	12 (4%)	0	100	100
1	B	337/343 (98%)	330 (98%)	7 (2%)	0	100	100
All	All	675/686 (98%)	656 (97%)	19 (3%)	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	283/288 (98%)	282 (100%)	1 (0%)	93	78
1	B	283/288 (98%)	278 (98%)	5 (2%)	66	26
All	All	566/576 (98%)	560 (99%)	6 (1%)	88	47

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	B	16[A]	LYS
1	B	16[B]	LYS
1	B	17[A]	ASN
1	B	17[B]	ASN
1	B	49	ARG

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

### 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 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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$
2	NDP	A	401	-	42,52,52	1.35	4 (9%)	55,80,80	1.39	4 (7%)
4	40E	A	404	3	5,8,8	1.60	1 (20%)	6,10,10	3.36	2 (33%)
5	EPE	A	405	-	14,15,15	1.72	3 (21%)	18,20,20	3.39	7 (38%)
6	GOL	A	406	-	5,5,5	0.25	0	5,5,5	0.84	0
6	GOL	A	407	-	5,5,5	0.90	0	5,5,5	1.27	1 (20%)
6	GOL	A	408	-	5,5,5	1.40	1 (20%)	5,5,5	0.99	0
2	NDP	B	401	-	42,52,52	1.50	7 (16%)	55,80,80	1.54	6 (10%)
4	40E	B	404	3	5,8,8	1.49	1 (20%)	6,10,10	3.42	3 (50%)
5	EPE	B	405	-	14,15,15	1.85	2 (14%)	18,20,20	3.80	9 (50%)
6	GOL	B	406	-	5,5,5	0.73	0	5,5,5	1.00	0
6	GOL	B	407	-	5,5,5	0.62	0	5,5,5	1.08	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
2	NDP	A	401	-	-	0/30/77/77	0/5/5/5
4	40E	A	404	3	-	1/4/8/8	0/0/0/0
5	EPE	A	405	-	-	0/9/19/19	0/1/1/1
6	GOL	A	406	-	-	0/4/4/4	0/0/0/0
6	GOL	A	407	-	-	0/4/4/4	0/0/0/0
6	GOL	A	408	-	-	0/4/4/4	0/0/0/0
2	NDP	B	401	-	-	0/30/77/77	0/5/5/5
4	40E	B	404	3	-	1/4/8/8	0/0/0/0
5	EPE	B	405	-	-	0/9/19/19	0/1/1/1
6	GOL	B	406	-	-	0/4/4/4	0/0/0/0
6	GOL	B	407	-	-	0/4/4/4	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NDP	C4N-C5N	-3.91	1.40	1.49
2	A	401	NDP	C4A-N3A	-3.28	1.30	1.35
5	A	405	EPE	C6-N1	-2.97	1.38	1.46
2	A	401	NDP	C4N-C5N	-2.87	1.42	1.49
2	B	401	NDP	C5A-N7A	-2.79	1.29	1.39
2	B	401	NDP	C4A-N3A	-2.56	1.31	1.35
4	B	404	40E	C2-N3	-2.54	1.28	1.34
4	A	404	40E	C2-N3	-2.47	1.28	1.34
2	B	401	NDP	P2B-O3X	-2.03	1.47	1.54
2	B	401	NDP	PA-O2A	-2.00	1.46	1.54
2	A	401	NDP	C5A-C4A	2.03	1.45	1.40
5	A	405	EPE	O3S-S	2.49	1.52	1.46
6	A	408	GOL	O1-C1	2.63	1.53	1.42
2	B	401	NDP	C5A-C4A	3.00	1.47	1.40
2	A	401	NDP	C2A-N3A	3.52	1.38	1.32
2	B	401	NDP	C2A-N3A	4.05	1.39	1.32
5	B	405	EPE	C7-N4	4.37	1.57	1.47
5	B	405	EPE	O1S-S	4.52	1.59	1.45
5	A	405	EPE	O2S-S	4.57	1.59	1.45

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	405	EPE	O2S-S-C10	-10.38	98.05	106.91
5	B	405	EPE	O1S-S-C10	-9.02	99.21	106.91
2	B	401	NDP	N3A-C2A-N1A	-7.37	123.25	128.89
2	A	401	NDP	N3A-C2A-N1A	-6.38	124.01	128.89
2	B	401	NDP	O3-PA-O5B	-3.19	94.46	102.94
2	A	401	NDP	O2B-P2B-O1X	-2.80	100.13	107.11
2	A	401	NDP	O3-PA-O5B	-2.35	96.69	102.94
6	A	407	GOL	C3-C2-C1	-2.21	102.45	111.12
4	B	404	40E	O2-C2-N3	-2.14	118.57	122.44
2	B	401	NDP	PN-O3-PA	-2.05	126.98	132.73
2	B	401	NDP	O2A-PA-O1A	2.03	123.52	112.53
5	B	405	EPE	C3-C2-N1	2.10	114.38	110.63
5	A	405	EPE	O1S-S-C10	2.24	108.81	106.91
2	B	401	NDP	O3X-P2B-O1X	2.45	118.47	110.58
2	B	401	NDP	C2A-N1A-C6A	2.69	123.58	118.77
2	A	401	NDP	O3X-P2B-O2X	2.86	118.28	107.38
5	A	405	EPE	C6-C5-N4	3.06	116.10	110.63
5	A	405	EPE	C6-N1-C2	3.15	115.72	108.90
4	A	404	40E	C1-C2-N3	3.71	120.48	115.69
5	A	405	EPE	C3-C2-N1	3.97	117.74	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	40E	C1-C2-N3	4.00	120.85	115.69
5	B	405	EPE	C5-C6-N1	4.09	117.96	110.63
5	B	405	EPE	C2-C3-N4	4.22	118.19	110.63
5	A	405	EPE	C5-N4-C3	4.25	118.11	108.90
5	B	405	EPE	C6-C5-N4	4.25	118.24	110.63
5	B	405	EPE	C7-N4-C3	4.75	123.45	111.27
5	B	405	EPE	C9-N1-C2	4.84	123.69	111.27
5	A	405	EPE	C7-N4-C5	5.28	124.81	111.27
5	B	405	EPE	C5-N4-C3	5.36	120.52	108.90
5	B	405	EPE	C6-N1-C2	5.85	121.57	108.90
4	B	404	40E	C4-N3-C2	6.76	132.25	122.72
4	A	404	40E	C4-N3-C2	7.05	132.66	122.72

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	40E	C1-C2-N3-C4
4	B	404	40E	C1-C2-N3-C4

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	328/343 (95%)	-0.37	2 (0%) 90 88	7, 10, 21, 68	0
1	B	329/343 (95%)	-0.33	4 (1%) 81 79	6, 11, 21, 45	0
All	All	657/686 (95%)	-0.35	6 (0%) 85 84	6, 10, 21, 68	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	GLY	8.1
1	B	328	GLY	4.9
1	B	330	LYS	3.1
1	A	329	MET	2.9
1	B	329	MET	2.8
1	B	271	VAL	2.4

### 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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	A	408	6/6	0.90	0.11	14.53	19,22,25,42	0
5	EPE	A	405	15/15	0.97	0.13	9.92	14,19,40,62	0
5	EPE	B	405	15/15	0.97	0.14	7.55	18,21,44,65	0
6	GOL	A	407	6/6	0.94	0.11	6.03	18,22,23,23	0
6	GOL	B	407	6/6	0.95	0.12	3.84	21,23,28,35	0
6	GOL	B	406	6/6	0.97	0.07	3.41	13,18,21,33	0
6	GOL	A	406	6/6	0.98	0.08	1.12	14,19,22,34	0
2	NDP	B	401	48/48	0.99	0.06	0.02	5,8,15,17	0
4	40E	B	404	9/9	0.99	0.06	-0.07	7,7,10,10	0
2	NDP	A	401	48/48	0.99	0.06	-0.10	5,8,13,15	0
4	40E	A	404	9/9	0.99	0.06	-0.52	7,8,11,12	0
3	MG	A	403	1/1	1.00	0.02	-3.93	8,8,8,8	0
3	MG	B	402	1/1	1.00	0.02	-4.21	8,8,8,8	0
3	MG	B	403	1/1	1.00	0.03	-	6,6,6,6	0
3	MG	A	402	1/1	1.00	0.04	-	6,6,6,6	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.