



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 10:17 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

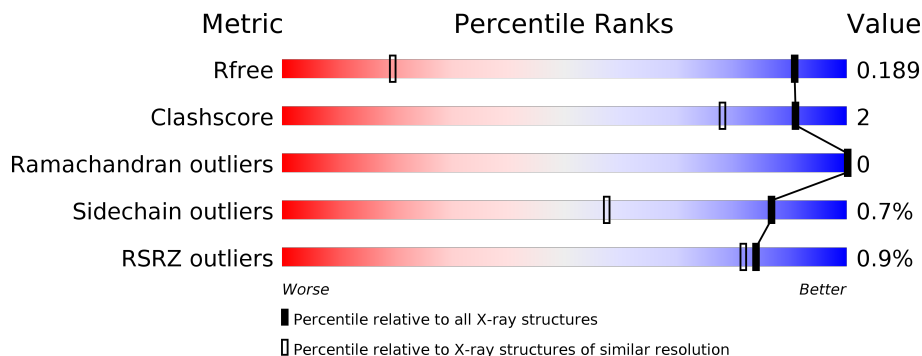
1 Overall quality at a glance

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}	100719	1078 (1.18-1.10)
Clashscore	112137	1123 (1.18-1.10)
Ramachandran outliers	110173	1074 (1.18-1.10)
Sidechain outliers	110143	1071 (1.18-1.10)
RSRZ outliers	101464	1082 (1.18-1.10)

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	343	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 10px; right: 0;">86%</div> <div style="position: absolute; top: 10px; right: 10px;">9%</div> <div style="position: absolute; top: 10px; right: 5px;">•</div> </div> </div>
1	B	343	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 10px; right: 0;">87%</div> <div style="position: absolute; top: 10px; right: 10px;">9%</div> <div style="position: absolute; top: 10px; right: 5px;">•</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit 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.

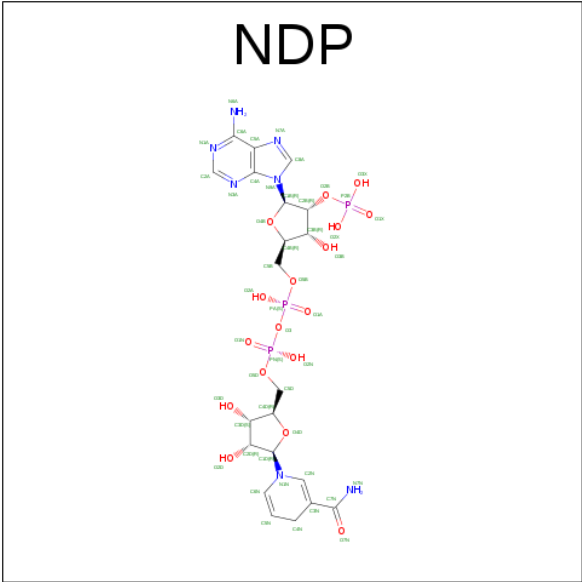
- Molecule 1 is a protein called Ketol-acid reductoisomerase.

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: C₂₁H₃₀N₇O₁₇P₃).

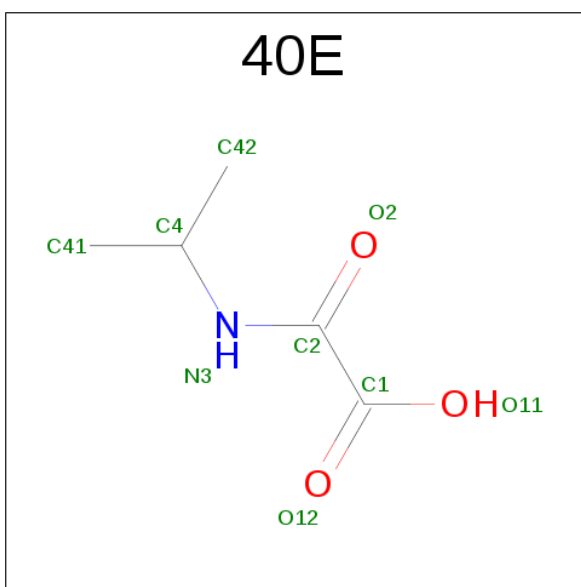


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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

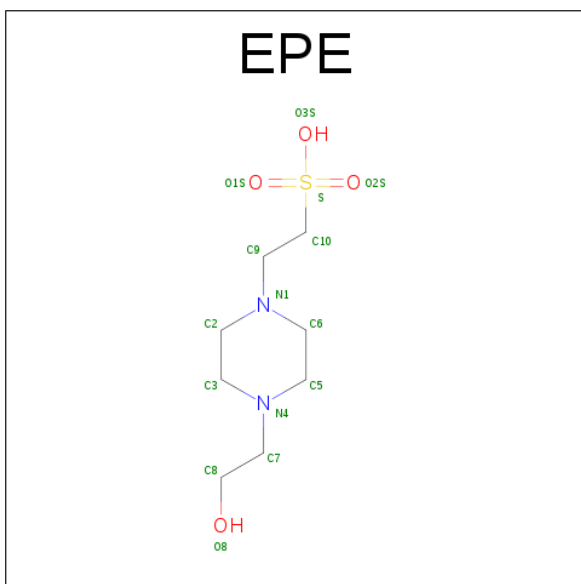
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is oxo(propan-2-ylamino)acetic acid (three-letter code: 40E) (formula: C₅H₉NO₃).



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: C₈H₁₈N₂O₄S).



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		

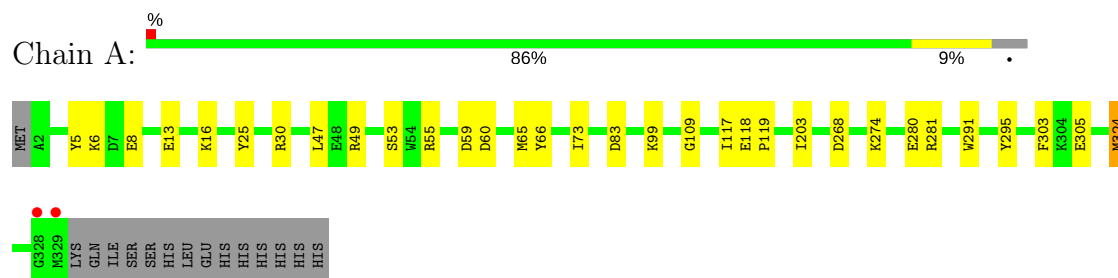
- Molecule 7 is water.

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

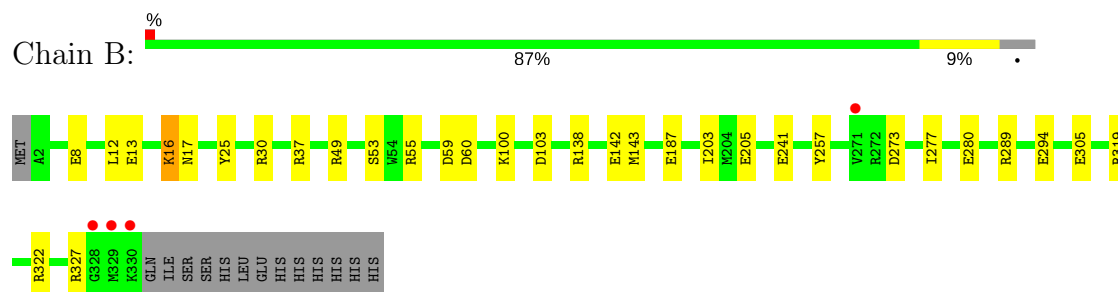
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ketol-acid reductoisomerase



- Molecule 1: Ketol-acid reductoisomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	9.3	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	6039	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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, 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%)

The worst 5 of 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

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
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

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	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.

The worst 5 of 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

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

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	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

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	77
1	B	283/288 (98%)	278 (98%)	5 (2%)	64	22
All	All	566/576 (98%)	560 (99%)	6 (1%)	87	40

5 of 6 residues with a non-rotameric sidechain are listed below:

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

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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	43,52,52	1.36	4 (9%)	49,80,80	1.28	3 (6%)
4	40E	A	404	3	5,8,8	1.61	1 (20%)	6,10,10	3.02	1 (16%)
5	EPE	A	405	-	15,15,15	2.12	3 (20%)	18,20,20	3.30	7 (38%)
6	GOL	A	406	-	5,5,5	0.26	0	5,5,5	0.80	0
6	GOL	A	407	-	5,5,5	0.92	0	5,5,5	1.26	1 (20%)
6	GOL	A	408	-	5,5,5	1.43	1 (20%)	5,5,5	0.97	0
2	NDP	B	401	-	43,52,52	1.51	6 (13%)	49,80,80	1.45	6 (12%)
4	40E	B	404	3	5,8,8	1.51	1 (20%)	6,10,10	3.06	3 (50%)
5	EPE	B	405	-	15,15,15	2.19	3 (20%)	18,20,20	3.67	8 (44%)
6	GOL	B	406	-	5,5,5	0.75	0	5,5,5	0.94	0
6	GOL	B	407	-	5,5,5	0.63	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

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	405	EPE	C10-S	-5.11	1.69	1.77
5	B	405	EPE	C10-S	-4.62	1.70	1.77
2	B	401	NDP	C4N-C5N	-3.89	1.40	1.49
2	A	401	NDP	C4A-N3A	-3.31	1.30	1.35
5	A	405	EPE	C6-N1	-2.99	1.38	1.47

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	405	EPE	O2S-S-C10	-10.18	98.05	106.79
5	B	405	EPE	O1S-S-C10	-8.83	99.21	106.79
2	B	401	NDP	N3A-C2A-N1A	-6.44	123.25	128.86
2	A	401	NDP	N3A-C2A-N1A	-5.57	124.01	128.86
2	A	401	NDP	O2B-P2B-O1X	-2.33	100.13	109.26

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, 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	328/343 (95%)	-0.36	2 (0%) 89 87	7, 10, 21, 68	0
1	B	329/343 (95%)	-0.32	4 (1%) 79 76	6, 11, 21, 45	0
All	All	657/686 (95%)	-0.34	6 (0%) 84 82	6, 10, 21, 68	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	GLY	8.2
1	B	328	GLY	4.9
1	B	330	LYS	3.2
1	A	329	MET	3.0
1	B	329	MET	2.9

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, 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	LLDF	B-factors(\AA^2)	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.