



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 11:24 AM EDT

PDB ID : 5EXF
Title : Thermostable aldehyde dehydrogenase from *Pyrobaculum* sp.1860 complexed with NADP+
Authors : Petrova, T.; Bezsudnova, E.Y.; Boyko, K.M.; Nikolaeva, A.Y.; Rakitina, T.V.; Popov, V.O.
Deposited on : 2015-11-23
Resolution : 2.19 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

<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>.

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	:	2.37.1
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)	:	2.37.1

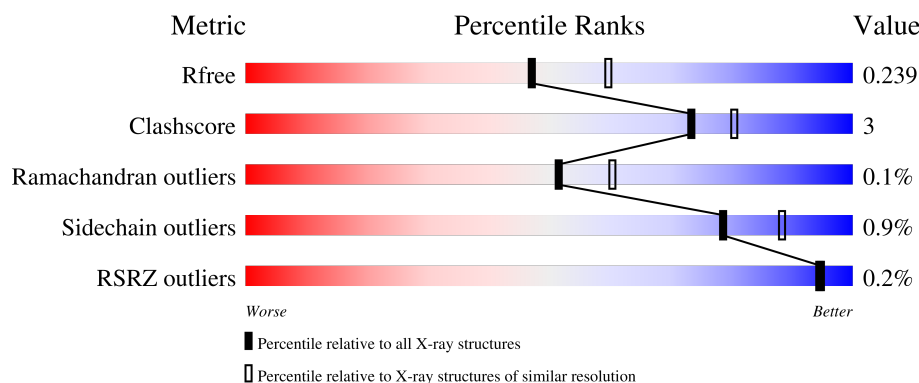
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 ≥ 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	491	<div><div style="width: 93%;"></div>93%<div style="width: 6%;"></div>6%</div>
1	B	491	<div><div style="width: 89%;"></div>89%<div style="width: 9%;"></div>9%<div style="width: 2%;"></div>2%</div>
1	C	491	<div><div style="width: 91%;"></div>91%<div style="width: 9%;"></div>9%</div>
1	D	491	<div><div style="width: 89%;"></div>89%<div style="width: 9%;"></div>9%<div style="width: 2%;"></div>2%</div>
1	E	491	<div><div style="width: 91%;"></div>91%<div style="width: 8%;"></div>8%<div style="width: 1%;"></div>1%</div>

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Mol	Chain	Length	Quality of chain
1	F	491	 92% 7% .
1	G	491	 88% 11% .
1	H	491	 91% 8% .

2 Entry composition

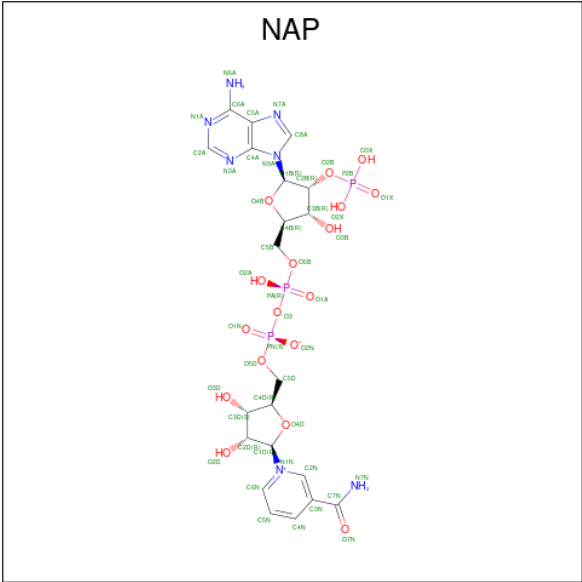
There are 4 unique types of molecules in this entry. The entry contains 33881 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	5	1
			3822	2438	664	708	12			
1	B	483	Total	C	N	O	S	0	6	0
			3772	2407	654	700	11			
1	C	490	Total	C	N	O	S	0	9	1
			3838	2448	669	709	12			
1	D	483	Total	C	N	O	S	0	8	0
			3797	2422	663	701	11			
1	E	483	Total	C	N	O	S	0	5	0
			3764	2402	657	694	11			
1	F	488	Total	C	N	O	S	0	6	0
			3817	2435	664	706	12			
1	G	484	Total	C	N	O	S	0	5	0
			3784	2416	654	703	11			
1	H	487	Total	C	N	O	S	0	6	1
			3788	2418	656	702	12			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

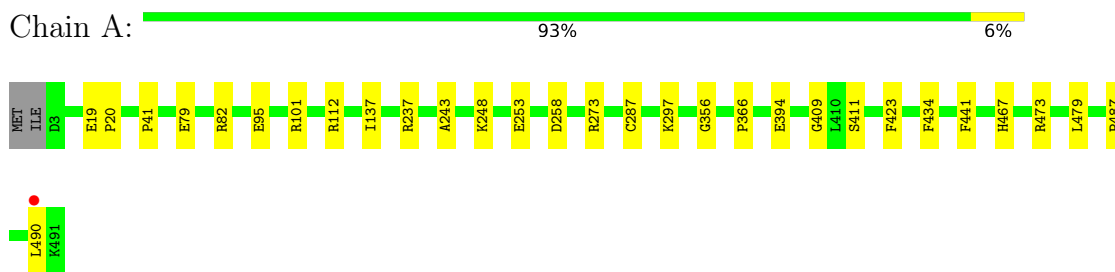
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	452	Total	O	0	0
			452	452		
4	B	391	Total	O	0	0
			391	391		
4	C	420	Total	O	0	0
			420	420		
4	D	342	Total	O	0	0
			342	342		
4	E	327	Total	O	0	0
			327	327		
4	F	393	Total	O	0	0
			393	393		
4	G	357	Total	O	0	0
			357	357		
4	H	427	Total	O	0	0
			427	427		

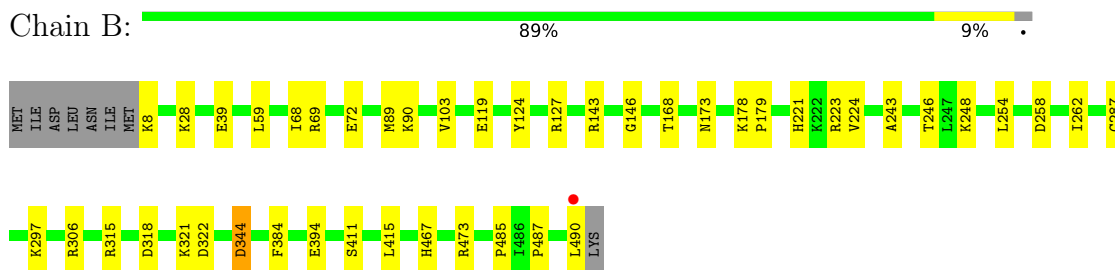
3 Residue-property plots

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.

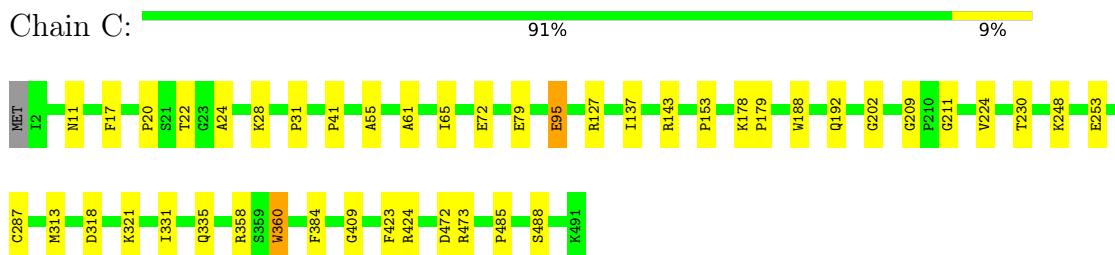
- Molecule 1: Aldehyde dehydrogenase



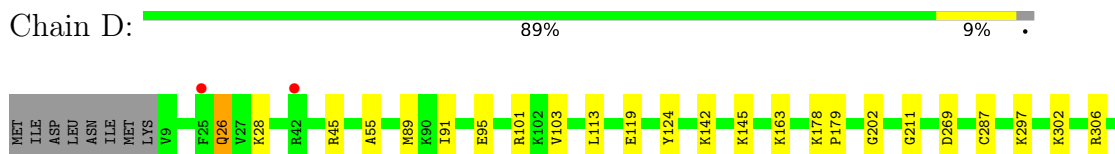
- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase





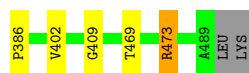
- Molecule 1: Aldehyde dehydrogenase

Chain E: 91% 8%



- Molecule 1: Aldehyde dehydrogenase

Chain F: 92% 7%



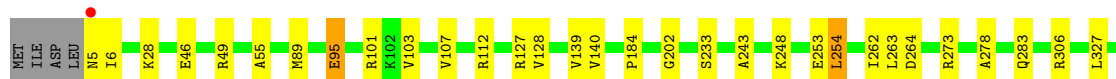
- Molecule 1: Aldehyde dehydrogenase

Chain G: 88% 11%



- Molecule 1: Aldehyde dehydrogenase

Chain H: 91% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	185.59Å 208.72Å 164.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.97 – 2.19 92.80 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.1 (90.97-2.19) 97.2 (92.80-2.19)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.206 , 0.245 0.198 , 0.239	Depositor DCC
R_{free} test set	15785 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33881	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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 46.39 % 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 1.1530e-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, NAP

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	0.43	0/3919	0.55	0/5313
1	B	0.45	2/3872 (0.1%)	0.55	0/5253
1	C	0.44	0/3944	0.54	0/5349
1	D	0.44	2/3900 (0.1%)	0.53	0/5287
1	E	0.38	0/3861	0.51	0/5238
1	F	0.42	0/3917	0.55	2/5309 (0.0%)
1	G	0.38	0/3879	0.51	0/5260
1	H	0.45	0/3889	0.54	0/5276
All	All	0.43	4/31181 (0.0%)	0.54	2/42285 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	D	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	344[A]	ASP	N-CA	6.31	1.58	1.46
1	D	344[B]	ASP	N-CA	6.31	1.58	1.46
1	B	344[A]	ASP	N-CA	5.96	1.58	1.46
1	B	344[B]	ASP	N-CA	5.96	1.58	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	473	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	F	473	ARG	NE-CZ-NH2	-5.27	117.67	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	344[A]	ASP	Mainchain
1	B	344[B]	ASP	Mainchain
1	D	344[A]	ASP	Mainchain
1	D	344[B]	ASP	Mainchain

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	3822	0	3826	23	0
1	B	3772	0	3763	33	0
1	C	3838	0	3829	32	0
1	D	3797	0	3799	30	0
1	E	3764	0	3753	21	0
1	F	3817	0	3816	23	0
1	G	3784	0	3777	31	0
1	H	3788	0	3763	25	0
2	A	48	0	13	2	0
2	B	48	0	13	3	0
2	C	48	0	13	3	0
2	D	48	0	13	2	0
2	E	48	0	13	2	0
2	F	48	0	13	4	0
2	G	48	0	13	2	0
2	H	48	0	13	3	0
3	A	6	0	8	1	0
4	A	452	0	0	3	0
4	B	391	0	0	3	0
4	C	420	0	0	5	0
4	D	342	0	0	5	0
4	E	327	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	393	0	0	4	0
4	G	357	0	0	0	1
4	H	427	0	0	2	0
All	All	33881	0	30438	201	1

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

The worst 5 of 201 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:H:233:SER:HA	1:H:254:LEU:HG	1.64	0.78
1:G:69:ARG:NH1	1:G:72[A]:GLU:OE2	2.17	0.77
1:C:358[B]:ARG:NH1	4:C:602:HOH:O	2.19	0.76
1:A:467[B]:HIS:NE2	4:A:601:HOH:O	2.20	0.75
1:A:467[B]:HIS:CE1	4:A:601:HOH:O	2.42	0.71

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)
4:E:871:HOH:O	4:G:912:HOH:O[4_455]	2.15	0.05

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	492/491 (100%)	474 (96%)	17 (4%)	1 (0%)	47	55
1	B	487/491 (99%)	473 (97%)	14 (3%)	0	100	100
1	C	497/491 (101%)	481 (97%)	15 (3%)	1 (0%)	47	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	489/491 (100%)	472 (96%)	17 (4%)	0	100	100
1	E	486/491 (99%)	470 (97%)	16 (3%)	0	100	100
1	F	492/491 (100%)	476 (97%)	15 (3%)	1 (0%)	47	55
1	G	487/491 (99%)	470 (96%)	16 (3%)	1 (0%)	47	55
1	H	491/491 (100%)	474 (96%)	17 (4%)	0	100	100
All	All	3921/3928 (100%)	3790 (97%)	127 (3%)	4 (0%)	51	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	409	GLY
1	C	409	GLY
1	G	153	PRO
1	F	409	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/408 (100%)	403 (99%)	3 (1%)	84	91
1	B	399/408 (98%)	398 (100%)	1 (0%)	92	97
1	C	405/408 (99%)	402 (99%)	3 (1%)	84	91
1	D	402/408 (98%)	400 (100%)	2 (0%)	88	94
1	E	396/408 (97%)	391 (99%)	5 (1%)	69	81
1	F	403/408 (99%)	398 (99%)	5 (1%)	71	83
1	G	400/408 (98%)	394 (98%)	6 (2%)	65	78
1	H	398/408 (98%)	393 (99%)	5 (1%)	69	81
All	All	3209/3264 (98%)	3179 (99%)	30 (1%)	78	88

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	4	LEU
1	H	306	ARG
1	F	306	ARG
1	H	473	ARG
1	G	473	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	26	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](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	A	502	-	5,5,5	0.34	0	5,5,5	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	502	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	GOL	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 [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	489/491 (99%)	-0.47	1 (0%) 95 94	8, 16, 32, 58	1 (0%)
1	B	483/491 (98%)	-0.47	1 (0%) 95 94	10, 18, 36, 50	1 (0%)
1	C	490/491 (99%)	-0.47	0 100 100	9, 18, 33, 51	1 (0%)
1	D	483/491 (98%)	-0.42	2 (0%) 92 91	9, 21, 41, 61	1 (0%)
1	E	483/491 (98%)	-0.46	1 (0%) 95 94	11, 24, 42, 55	1 (0%)
1	F	488/491 (99%)	-0.46	1 (0%) 95 94	11, 20, 35, 55	1 (0%)
1	G	484/491 (98%)	-0.47	2 (0%) 92 91	11, 23, 37, 46	1 (0%)
1	H	487/491 (99%)	-0.51	1 (0%) 95 94	10, 19, 34, 57	1 (0%)
All	All	3887/3928 (98%)	-0.46	9 (0%) 95 94	8, 20, 37, 61	8 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	490	LEU	3.5
1	B	490	LEU	2.9
1	H	5	ASN	2.8
1	G	490	LEU	2.2
1	D	25	PHE	2.2

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAP	D	500[A]	48/48	0.96	0.11	10,22,30,33	17
3	GOL	A	502	6/6	0.96	0.12	34,36,38,40	0
2	NAP	E	500[A]	48/48	0.97	0.09	13,25,30,35	17
2	NAP	F	500[A]	48/48	0.97	0.11	11,21,27,32	18
2	NAP	G	500[A]	48/48	0.97	0.12	12,23,28,32	17
2	NAP	H	500[A]	48/48	0.97	0.12	11,19,27,30	18
2	NAP	A	501[A]	48/48	0.97	0.12	11,17,22,28	17
2	NAP	B	500[A]	48/48	0.98	0.10	11,18,23,26	17
2	NAP	C	500[A]	48/48	0.98	0.12	11,20,24,27	17

6.5 Other polymers [i](#)

There are no such residues in this entry.