Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 04:49 pm GMT

PDB ID	:	6HCN
Title	:	Adenovirus Type 5 Fiber Knob protein at 1.49A resolution
Authors	:	Rizkallah, P.J.; Parker, A.L.; Baker, A.T.
Deposited on	:	2018-08-15
Resolution	:	1.49 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

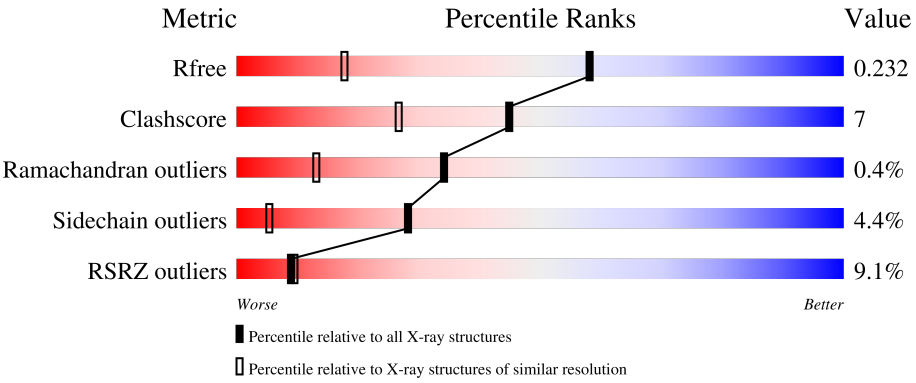
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.49 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 <=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	186	7% 88% 11%
1	C	186	8% 86% 12%
2	B	188	13% 89% 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
3	EDO	A	602	-	-	X	-
3	EDO	A	603	-	-	X	-
3	EDO	A	604	-	-	X	-
3	EDO	C	602	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4825 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.

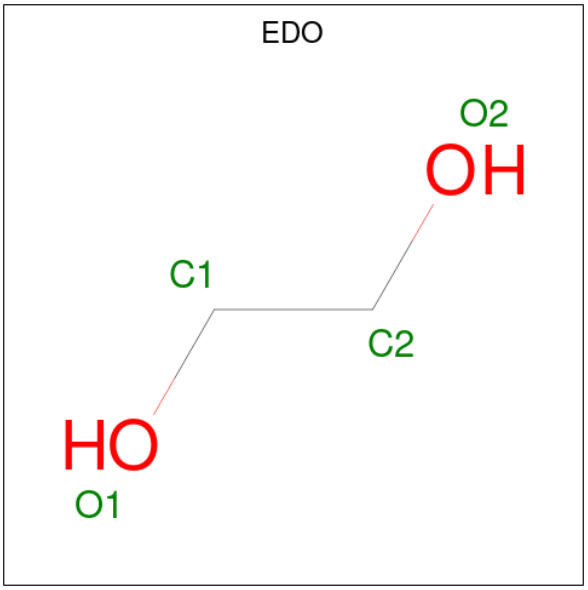
- Molecule 1 is a protein called Fiber protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	5	0
			1470	929	242	294	5			
1	C	186	Total	C	N	O	S	0	1	0
			1439	912	236	286	5			

- Molecule 2 is a protein called Fiber protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	188	Total	C	N	O	S	0	5	0
			1486	939	245	297	5			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is water.

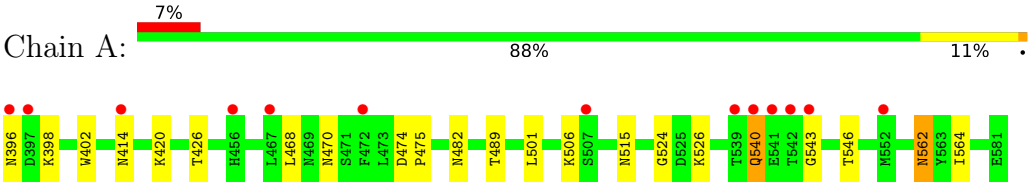
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	161	Total O 161 161	0	0
5	B	101	Total O 101 101	0	0
5	C	147	Total O 147 147	0	0

3 Residue-property plots (i)

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

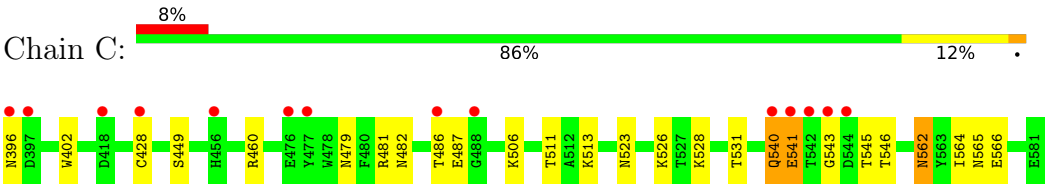
• Molecule 1: Fiber protein

Chain A:



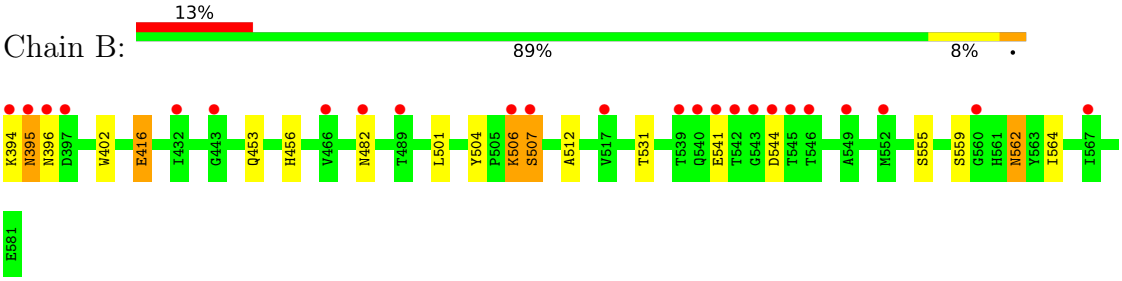
• Molecule 1: Fiber protein

Chain C:



• Molecule 2: Fiber protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.16Å 102.44Å 77.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.56 – 1.49 61.56 – 1.49	Depositor EDS
% Data completeness (in resolution range)	99.8 (61.56-1.49) 99.8 (61.56-1.49)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 1.49Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.211 , 0.233 0.217 , 0.232	Depositor DCC
R_{free} test set	6391 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.755	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4825	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EDO

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	0.64	0/1504	0.79	0/2052
1	C	0.59	0/1473	0.73	0/2010
2	B	0.63	0/1520	0.82	1/2071 (0.0%)
All	All	0.62	0/4497	0.78	1/6133 (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	A	0	1
1	C	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	504	TYR	CB-CG-CD1	6.20	124.72	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	543	GLY	Peptide
1	C	481	ARG	Sidechain
1	C	543	GLY	Peptide

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	1470	0	1427	22	0
1	C	1439	0	1402	19	0
2	B	1486	0	1446	17	0
3	A	16	0	24	15	0
3	C	4	0	6	6	0
4	C	1	0	0	0	0
5	A	161	0	0	3	0
5	B	101	0	0	1	0
5	C	147	0	0	1	0
All	All	4825	0	4305	57	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 7.

All (57) 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)
2:B:506[A]:LYS:HD2	2:B:506[A]:LYS:H	1.02	1.07
2:B:506[A]:LYS:HD2	2:B:506[A]:LYS:N	1.74	1.01
2:B:506[A]:LYS:H	2:B:506[A]:LYS:CD	1.62	0.97
1:C:511:THR:HG22	3:C:602:EDO:H11	1.65	0.76
2:B:506[B]:LYS:HD2	2:B:507:SER:N	2.03	0.74
1:C:511:THR:CG2	3:C:602:EDO:H11	2.18	0.73
2:B:453:GLN:HE21	2:B:559:SER:HA	1.54	0.72
1:A:501:LEU:HD22	3:A:601:EDO:H12	1.70	0.71
1:A:489:THR:HG22	5:A:743:HOH:O	1.94	0.66
1:A:470:ASN:HD22	3:A:604:EDO:H12	1.62	0.65
1:A:468:LEU:HD12	3:A:603:EDO:H21	1.79	0.65
1:A:546:THR:CG2	3:A:604:EDO:H22	2.26	0.64
1:A:562:ASN:HD22	1:A:562:ASN:C	2.05	0.60
1:A:546:THR:HG21	3:A:604:EDO:H22	1.85	0.59
1:A:414[B]:ASN:HD22	1:A:414[B]:ASN:C	2.04	0.59
2:B:453:GLN:NE2	2:B:559:SER:HA	2.18	0.58
1:C:511:THR:CG2	3:C:602:EDO:C1	2.83	0.56
2:B:562:ASN:C	2:B:562:ASN:HD22	2.09	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:GLY:O	1:C:540:GLN:OE1	2.24	0.55
1:C:562:ASN:C	1:C:562:ASN:HD22	2.10	0.55
1:C:528:LYS:NZ	1:C:566:GLU:OE2	2.28	0.55
1:A:515:ASN:OD1	1:A:540:GLN:HG2	2.07	0.55
1:A:470:ASN:HD22	3:A:604:EDO:C1	2.19	0.54
3:A:602:EDO:H21	1:C:513:LYS:NZ	2.23	0.54
2:B:416[A]:GLU:O	2:B:416[A]:GLU:OE2	2.26	0.53
1:A:526:LYS:HB2	1:C:531:THR:HG21	1.93	0.51
2:B:506[A]:LYS:HG2	5:B:695:HOH:O	2.11	0.50
2:B:456:HIS:CE1	2:B:555[B]:SER:HG	2.29	0.50
2:B:394:LYS:C	2:B:396:ASN:H	2.15	0.50
1:A:420:LYS:HB2	3:A:602:EDO:H12	1.94	0.49
2:B:501:LEU:HD22	2:B:506[A]:LYS:HG3	1.95	0.49
1:C:511:THR:HG23	3:C:602:EDO:H12	1.96	0.48
1:A:546:THR:HG23	3:A:604:EDO:H22	1.96	0.48
3:A:603:EDO:H22	3:A:604:EDO:H11	1.97	0.47
1:A:420:LYS:CB	3:A:602:EDO:H12	2.44	0.47
1:C:565:ASN:ND2	5:C:703:HOH:O	2.44	0.47
1:C:460:ARG:NE	1:C:546:THR:OG1	2.48	0.47
2:B:395:ASN:O	2:B:395:ASN:ND2	2.49	0.46
1:A:474[B]:ASP:OD1	1:A:475:PRO:HD2	2.16	0.45
3:A:603:EDO:H22	3:A:604:EDO:C1	2.46	0.45
1:A:414[B]:ASN:C	1:A:414[B]:ASN:ND2	2.69	0.44
1:A:474[B]:ASP:OD2	5:A:701:HOH:O	2.20	0.44
3:A:602:EDO:H11	3:C:602:EDO:H21	1.99	0.44
1:C:396:ASN:CG	1:C:487:GLU:OE2	2.55	0.44
1:A:526:LYS:CB	1:C:531:THR:HG21	2.47	0.44
1:C:511:THR:HG23	3:C:602:EDO:C1	2.49	0.43
2:B:562:ASN:HD22	2:B:564:ILE:H	1.67	0.42
1:A:562:ASN:HD22	1:A:564:ILE:H	1.67	0.42
2:B:531:THR:HG21	1:C:526:LYS:HB2	2.01	0.42
1:C:562:ASN:HD22	1:C:564:ILE:H	1.67	0.42
3:A:601:EDO:H21	5:A:822:HOH:O	2.20	0.42
1:A:426:THR:HG21	1:C:428:CYS:O	2.20	0.41
1:A:396:ASN:OD1	1:A:398:LYS:HD3	2.21	0.41
1:C:479:ASN:HB3	1:C:486:THR:HB	2.03	0.41
3:A:603:EDO:H22	3:A:604:EDO:H22	2.02	0.41
2:B:512:ALA:HB2	1:C:523:ASN:HA	2.03	0.41

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	189/186 (102%)	182 (96%)	7 (4%)	0	100 100
1	C	185/186 (100%)	175 (95%)	9 (5%)	1 (0%)	29 9
2	B	191/188 (102%)	183 (96%)	7 (4%)	1 (0%)	29 9
All	All	565/560 (101%)	540 (96%)	23 (4%)	2 (0%)	34 13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	541	GLU
1	C	541	GLU

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	165/160 (103%)	159 (96%)	6 (4%)	35 8
1	C	161/160 (101%)	153 (95%)	8 (5%)	24 4
2	B	167/162 (103%)	157 (94%)	10 (6%)	19 2
All	All	493/482 (102%)	469 (95%)	24 (5%)	28 4

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	402	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	482	ASN
1	A	506[A]	LYS
1	A	506[B]	LYS
1	A	540	GLN
1	A	562	ASN
2	B	395	ASN
2	B	402	TRP
2	B	416[A]	GLU
2	B	416[B]	GLU
2	B	482	ASN
2	B	506[A]	LYS
2	B	506[B]	LYS
2	B	507	SER
2	B	544	ASP
2	B	562	ASN
1	C	402	TRP
1	C	449	SER
1	C	482	ASN
1	C	506	LYS
1	C	540	GLN
1	C	541	GLU
1	C	545	THR
1	C	562	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	431	GLN
1	A	456	HIS
1	A	470	ASN
1	A	482	ASN
1	A	562	ASN
1	A	565	ASN
2	B	431	GLN
2	B	453	GLN
2	B	469	ASN
2	B	482	ASN
2	B	562	ASN
2	B	565	ASN
1	C	431	GLN
1	C	469	ASN
1	C	482	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	562	ASN
1	C	565	ASN

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 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\#\|Z\| > 2$
3	EDO	C	602	-	3,3,3	0.31	0	2,2,2	0.23	0
3	EDO	A	602	-	3,3,3	0.78	0	2,2,2	1.62	1 (50%)
3	EDO	A	603	-	3,3,3	0.46	0	2,2,2	0.20	0
3	EDO	A	604	-	3,3,3	0.58	0	2,2,2	0.65	0
3	EDO	A	601	-	3,3,3	0.42	0	2,2,2	0.33	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	EDO	C	602	-	-	0/1/1/1	-
3	EDO	A	602	-	-	1/1/1/1	-
3	EDO	A	603	-	-	0/1/1/1	-
3	EDO	A	604	-	-	0/1/1/1	-
3	EDO	A	601	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	EDO	O1-C1-C2	2.04	126.57	111.91

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	EDO	6	0
3	A	602	EDO	4	0
3	A	603	EDO	4	0
3	A	604	EDO	8	0
3	A	601	EDO	2	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^{th} 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	186/186 (100%)	0.99	13 (6%) 16 17	21, 29, 44, 68	0
1	C	186/186 (100%)	0.99	14 (7%) 14 14	23, 32, 48, 78	0
2	B	188/188 (100%)	1.11	24 (12%) 3 3	23, 32, 55, 80	0
All	All	560/560 (100%)	1.03	51 (9%) 9 9	21, 32, 50, 80	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	542	THR	19.2
1	C	542	THR	14.7
1	C	543	GLY	14.5
1	A	543	GLY	13.1
2	B	542	THR	12.9
2	B	544	ASP	10.4
1	A	396	ASN	9.8
1	A	541	GLU	8.5
2	B	395	ASN	6.7
2	B	543	GLY	6.6
2	B	396	ASN	6.4
1	C	396	ASN	6.3
1	C	541	GLU	5.9
1	A	397	ASP	5.3
2	B	545	THR	5.2
2	B	541	GLU	4.5
2	B	546	THR	4.4
1	C	488	GLY	4.2
1	A	507	SER	4.1
2	B	507	SER	3.7
1	A	540	GLN	3.6
2	B	443	GLY	3.3
2	B	482	ASN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	477	TYR	3.0
1	C	476	GLU	2.9
1	C	540	GLN	2.8
2	B	540	GLN	2.7
2	B	397	ASP	2.5
2	B	539	THR	2.5
2	B	552[A]	MET	2.5
1	A	472	PHE	2.5
1	C	428	CYS	2.5
1	A	467	LEU	2.4
2	B	432	ILE	2.4
2	B	560	GLY	2.4
1	A	456	HIS	2.3
1	A	539	THR	2.3
1	C	397	ASP	2.3
1	A	414[A]	ASN	2.3
2	B	567	ILE	2.3
2	B	489	THR	2.3
2	B	506[A]	LYS	2.3
1	C	418	ASP	2.2
2	B	394	LYS	2.1
1	C	544	ASP	2.1
1	A	552[A]	MET	2.1
1	C	456	HIS	2.1
2	B	466	VAL	2.1
1	C	486	THR	2.1
2	B	517	VAL	2.0
2	B	549	ALA	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^{th} 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
3	EDO	A	602	4/4	0.71	0.22	28,30,33,38	0
3	EDO	A	604	4/4	0.77	0.24	38,39,40,40	0
3	EDO	A	601	4/4	0.83	0.23	32,33,33,34	0
3	EDO	A	603	4/4	0.85	0.28	39,39,39,41	0
3	EDO	C	602	4/4	0.88	0.20	30,30,31,31	0
4	MG	C	601	1/1	0.98	0.14	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.