Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 05:40 AM EDT

PDB ID	:	6PQH
Title	:	Crystal structure of Asparagine-tRNA ligase from Elizabethkingia sp. CCUG 26117
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2019-07-09
Resolution	:	2.00 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 (i)) were used in the production of this report:

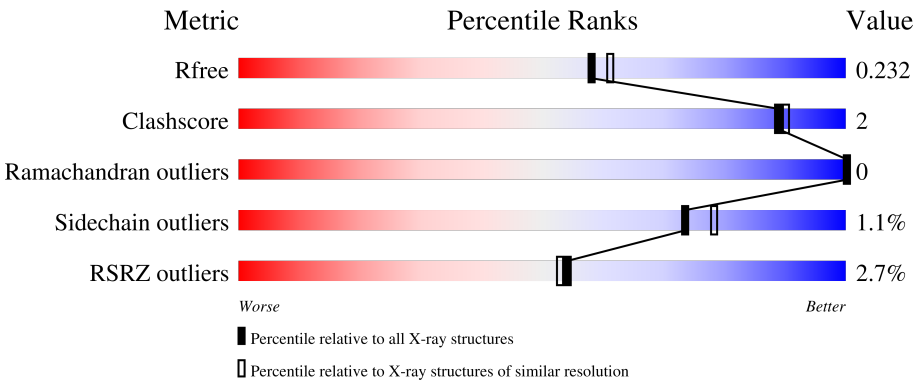
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	490	3% 92% • •
1	B	490	2% 92% 6% •
1	C	490	2% 92% • •
1	D	490	4% 89% 8% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16472 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 Asparagine–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	472	3812	2442	645	714	11	0	5	0
1	B	479	3852	2462	661	719	10	0	3	0
1	C	471	3788	2428	645	704	11	0	3	0
1	D	477	3807	2432	652	712	11	0	2	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP X5KA67
A	-6	ALA	-	expression tag	UNP X5KA67
A	-5	HIS	-	expression tag	UNP X5KA67
A	-4	HIS	-	expression tag	UNP X5KA67
A	-3	HIS	-	expression tag	UNP X5KA67
A	-2	HIS	-	expression tag	UNP X5KA67
A	-1	HIS	-	expression tag	UNP X5KA67
A	0	HIS	-	expression tag	UNP X5KA67
A	479	ASN	SER	conflict	UNP X5KA67
B	-7	MET	-	initiating methionine	UNP X5KA67
B	-6	ALA	-	expression tag	UNP X5KA67
B	-5	HIS	-	expression tag	UNP X5KA67
B	-4	HIS	-	expression tag	UNP X5KA67
B	-3	HIS	-	expression tag	UNP X5KA67
B	-2	HIS	-	expression tag	UNP X5KA67
B	-1	HIS	-	expression tag	UNP X5KA67
B	0	HIS	-	expression tag	UNP X5KA67
B	479	ASN	SER	conflict	UNP X5KA67
C	-7	MET	-	initiating methionine	UNP X5KA67
C	-6	ALA	-	expression tag	UNP X5KA67
C	-5	HIS	-	expression tag	UNP X5KA67

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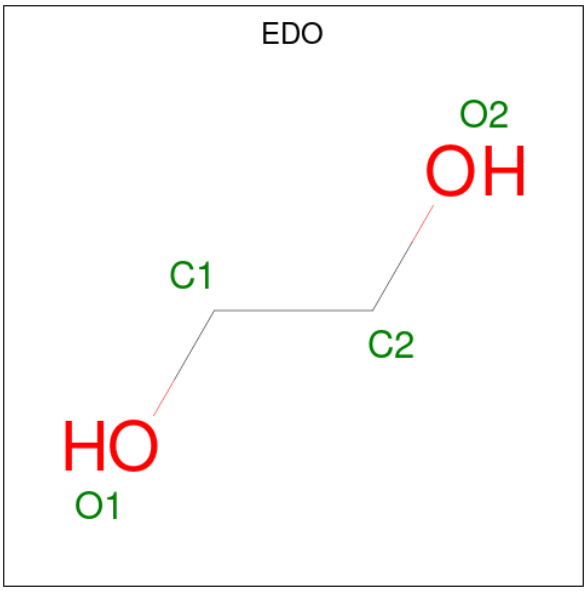
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP X5KA67
C	-3	HIS	-	expression tag	UNP X5KA67
C	-2	HIS	-	expression tag	UNP X5KA67
C	-1	HIS	-	expression tag	UNP X5KA67
C	0	HIS	-	expression tag	UNP X5KA67
C	479	ASN	SER	conflict	UNP X5KA67
D	-7	MET	-	initiating methionine	UNP X5KA67
D	-6	ALA	-	expression tag	UNP X5KA67
D	-5	HIS	-	expression tag	UNP X5KA67
D	-4	HIS	-	expression tag	UNP X5KA67
D	-3	HIS	-	expression tag	UNP X5KA67
D	-2	HIS	-	expression tag	UNP X5KA67
D	-1	HIS	-	expression tag	UNP X5KA67
D	0	HIS	-	expression tag	UNP X5KA67
D	479	ASN	SER	conflict	UNP X5KA67

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



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

- Molecule 3 is water.

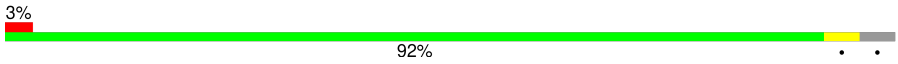
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	303	303	303	0	2
			Total	O		
3	B	366	366	366	0	1
			Total	O		
3	C	272	274	274	0	2
			Total	O		
3	D	262	262	262	0	1

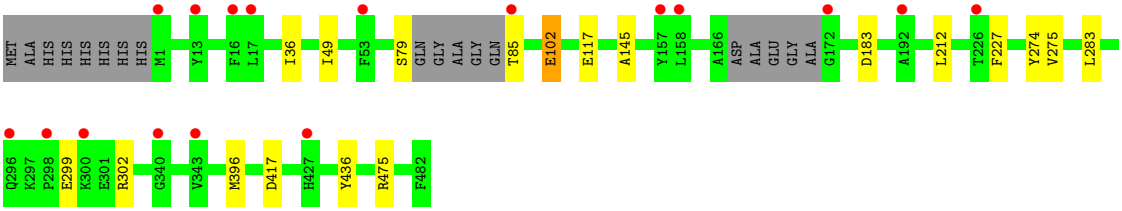
3 Residue-property plots (i)

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: Asparagine–tRNA ligase

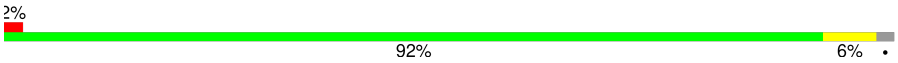
Chain A:

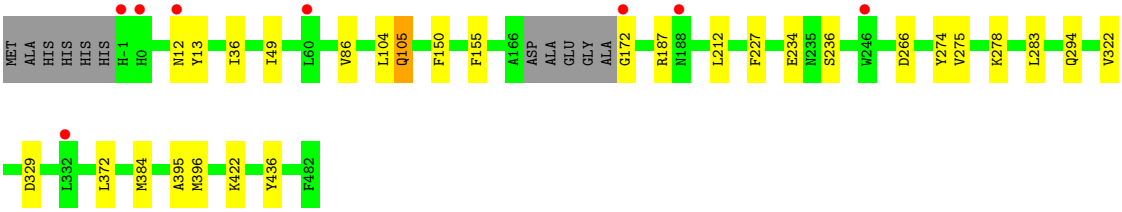




• Molecule 1: Asparagine–tRNA ligase

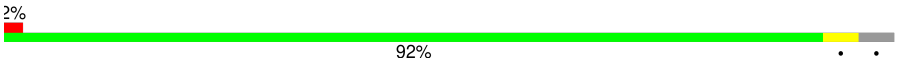
Chain B:

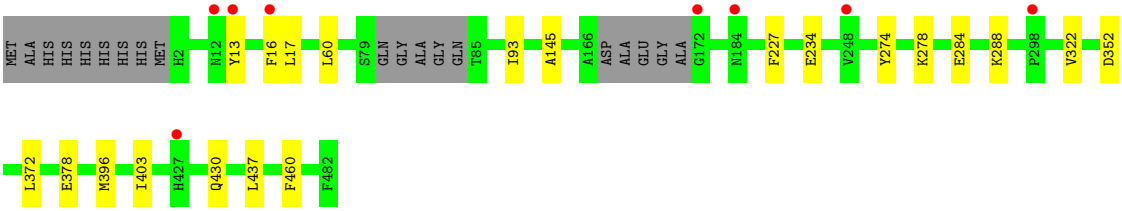




• Molecule 1: Asparagine–tRNA ligase

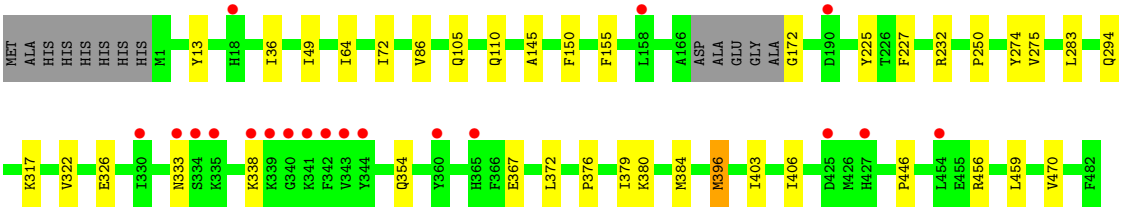
Chain C:





• Molecule 1: Asparagine–tRNA ligase

Chain D:


MET ALA HIS HIS HIS HIS HIS M1 Y13 H18 I36 I49 I64 I72 V86 Q105 Q110 A145 F150 F155 L158 A166 ASP ALA GLU GLY ALA G172 D190 Y225 T226 F227 R232 P250 Y274 V275 L283 Q294
K317 V322 E326 I330 N333 S334 K335 K338 K339 G340 K341 F342 V343 Y344 Q354 Y360 H365 F366 E367 L372 P376 I379 K380 M384 M396 I403 I406 D425 M426 H427 P446 L454 E455 R456 L459 V470 F482

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.40Å 110.75Å 137.18Å 90.00° 97.09° 90.00°	Depositor
Resolution (Å)	35.57 – 2.00 46.29 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (35.57-2.00) 99.9 (46.29-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 2.00Å)	Xtriage
Refinement program	PHENIX dev_3500	Depositor
R, R_{free}	0.181 , 0.231 0.181 , 0.232	Depositor DCC
R_{free} test set	2072 reflections (1.54%)	wwPDB-VP
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	16472	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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 56.08 % 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 2.8812e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.37	0/3906	0.53	0/5284
1	B	0.38	0/3943	0.54	0/5332
1	C	0.35	0/3878	0.52	0/5245
1	D	0.35	0/3895	0.52	0/5274
All	All	0.37	0/15622	0.53	0/21135

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	3812	0	3668	10	0
1	B	3852	0	3728	16	0
1	C	3788	0	3660	11	0
1	D	3807	0	3646	22	0
2	A	4	0	6	0	0
2	C	4	0	6	0	0
3	A	303	0	0	1	0
3	B	366	0	0	2	0
3	C	274	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	262	0	0	4	0
All	All	16472	0	14714	58	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 2.

All (58) 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:D:294:GLN:NE2	3:D:501:HOH:O	2.13	0.81
1:B:275:VAL:HG12	1:B:283:LEU:HD11	1.75	0.69
1:B:266:ASP:OD1	3:B:501:HOH:O	2.13	0.65
1:B:172:GLY:N	1:B:234:GLU:HB3	2.12	0.64
1:D:13:TYR:HB2	1:D:86:VAL:HG11	1.81	0.63
1:B:13:TYR:HB2	1:B:86:VAL:HG11	1.81	0.61
1:C:13:TYR:HA	1:C:16:PHE:HD2	1.64	0.61
1:A:79:SER:N	1:A:85:THR:O	2.28	0.61
1:B:294:GLN:NE2	3:B:510:HOH:O	2.37	0.56
1:D:354:GLN:NE2	3:D:505:HOH:O	2.33	0.55
1:A:36:ILE:HB	1:A:49:ILE:HB	1.90	0.54
1:D:333:ASN:HA	1:D:338:LYS:HE3	1.90	0.53
1:D:49:ILE:HG13	1:D:72:ILE:HD13	1.90	0.53
1:D:322:VAL:HG12	1:D:326:GLU:HB3	1.90	0.53
1:D:403:ILE:HD11	1:D:406:ILE:HB	1.91	0.53
1:C:60:LEU:HD21	1:C:93:ILE:HB	1.91	0.52
1:D:275:VAL:HG12	1:D:283:LEU:HD11	1.93	0.50
1:B:322:VAL:O	1:B:372:LEU:HA	2.12	0.50
1:B:234:GLU:HG3	1:B:236:SER:HB3	1.92	0.50
1:D:145:ALA:HB2	1:D:274:TYR:CD2	2.48	0.48
1:D:150:PHE:HB3	1:D:155:PHE:HB2	1.95	0.48
1:A:183:ASP:OD1	1:B:187:ARG:NH1	2.43	0.48
1:D:403:ILE:O	1:D:456:ARG:NH2	2.46	0.47
1:D:105:GLN:HA	1:D:110:GLN:NE2	2.29	0.47
1:C:403:ILE:HD13	1:C:460:PHE:HB2	1.97	0.47
1:C:430:GLN:HB3	1:C:437:LEU:HD11	1.97	0.47
1:C:17:LEU:HA	1:C:17:LEU:HD23	1.68	0.47
1:C:322:VAL:O	1:C:372:LEU:HA	2.15	0.46
1:D:376:PRO:HD2	1:D:379:ILE:HD11	1.98	0.45
1:D:36:ILE:HD11	1:D:64:ILE:HD13	1.99	0.45
1:A:299:GLU:HA	1:A:302:ARG:HG3	1.99	0.45
1:C:284:GLU:HG2	1:C:288:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:VAL:HG12	1:A:283:LEU:HD11	1.99	0.45
1:C:13:TYR:HA	1:C:16:PHE:CD2	2.48	0.45
1:D:225:TYR:HA	1:D:250:PRO:HA	1.98	0.45
1:A:145:ALA:HB2	1:A:274:TYR:CD2	2.52	0.44
1:D:317:LYS:NZ	3:D:530:HOH:O	2.50	0.44
1:B:212:LEU:HD22	1:B:436:TYR:CE1	2.53	0.43
1:A:117:GLU:OE2	3:A:601:HOH:O	2.21	0.43
1:B:150:PHE:HB3	1:B:155:PHE:HB2	2.00	0.43
1:B:105:GLN:H	1:B:105:GLN:HG2	1.44	0.43
1:C:234:GLU:HG2	3:C:685:HOH:O	2.17	0.43
1:D:172:GLY:HA3	1:D:232:ARG:CZ	2.48	0.43
1:B:422:LYS:HB3	1:B:422:LYS:HE2	1.81	0.43
1:B:36:ILE:HB	1:B:49:ILE:HB	1.99	0.43
1:B:274:TYR:CE2	1:B:278:LYS:HG3	2.53	0.43
1:A:212:LEU:HD22	1:A:436:TYR:CE1	2.54	0.42
1:A:102[A]:GLU:CD	1:A:102[A]:GLU:H	2.21	0.42
1:C:274:TYR:CE2	1:C:278:LYS:HG3	2.55	0.42
1:A:417:ASP:N	1:A:417:ASP:OD1	2.52	0.41
1:D:459:LEU:HG	1:D:470:VAL:HG21	2.02	0.41
1:D:322:VAL:O	1:D:372:LEU:HA	2.21	0.41
1:B:274:TYR:CZ	1:B:278:LYS:HG3	2.55	0.41
1:D:380:LYS:HB3	1:D:384:MET:SD	2.61	0.41
1:B:384:MET:SD	1:B:395:ALA:HB2	2.61	0.40
1:D:446:PRO:HA	3:D:560:HOH:O	2.22	0.40
1:C:145:ALA:HB2	1:C:274:TYR:CD2	2.56	0.40
1:D:372:LEU:O	1:D:396:MET:HA	2.21	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	471/490 (96%)	457 (97%)	14 (3%)	0	100	100
1	B	478/490 (98%)	467 (98%)	11 (2%)	0	100	100
1	C	468/490 (96%)	457 (98%)	11 (2%)	0	100	100
1	D	475/490 (97%)	462 (97%)	13 (3%)	0	100	100
All	All	1892/1960 (96%)	1843 (97%)	49 (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	402/430 (94%)	396 (98%)	6 (2%)	65	69
1	B	406/430 (94%)	399 (98%)	7 (2%)	60	65
1	C	399/430 (93%)	395 (99%)	4 (1%)	76	81
1	D	397/430 (92%)	394 (99%)	3 (1%)	81	86
All	All	1604/1720 (93%)	1584 (99%)	20 (1%)	73	76

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102[A]	GLU
1	A	102[B]	GLU
1	A	227	PHE
1	A	396	MET
1	A	475[A]	ARG
1	A	475[B]	ARG
1	B	12	ASN
1	B	104	LEU
1	B	105	GLN
1	B	227	PHE
1	B	329[A]	ASP
1	B	329[B]	ASP
1	B	396	MET

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Mol	Chain	Res	Type
1	C	227	PHE
1	C	352	ASP
1	C	378	GLU
1	C	396	MET
1	D	227	PHE
1	D	367	GLU
1	D	396	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	105	GLN
1	D	110	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)

2 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	$\#\|Z\| > 2$
2	EDO	A	501	-	3,3,3	0.48	0	2,2,2	0.44	0
2	EDO	C	501	-	3,3,3	0.44	0	2,2,2	0.34	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	EDO	A	501	-	-	0/1/1/1	-
2	EDO	C	501	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	EDO	O1-C1-C2-O2

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	472/490 (96%)	-0.05	17 (3%)	42	42	18, 32, 65, 96	0
1	B	479/490 (97%)	-0.21	8 (1%)	70	68	18, 30, 59, 94	0
1	C	471/490 (96%)	-0.13	8 (1%)	70	68	18, 33, 68, 94	0
1	D	477/490 (97%)	0.07	19 (3%)	38	37	22, 38, 69, 93	0
All	All	1899/1960 (96%)	-0.08	52 (2%)	54	53	18, 33, 66, 96	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	GLY	5.4
1	A	1	MET	4.6
1	D	360	TYR	4.2
1	A	298	PRO	4.1
1	D	342	PHE	4.0
1	C	16	PHE	3.9
1	D	333	ASN	3.7
1	D	338	LYS	3.7
1	A	192	ALA	3.7
1	C	172	GLY	3.5
1	D	334	SER	3.3
1	C	298	PRO	3.3
1	C	13	TYR	3.1
1	B	60	LEU	3.0
1	A	300	LYS	3.0
1	D	339	LYS	2.9
1	D	340	GLY	2.9
1	D	425	ASP	2.8
1	C	427	HIS	2.8
1	D	427	HIS	2.8
1	D	343	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	330	ILE	2.7
1	A	427	HIS	2.6
1	B	172	GLY	2.6
1	D	18	HIS	2.6
1	D	454	LEU	2.6
1	D	365	HIS	2.5
1	A	13	TYR	2.5
1	C	184	ASN	2.5
1	C	248	VAL	2.4
1	A	158	LEU	2.4
1	D	335	LYS	2.4
1	A	53	PHE	2.3
1	B	332	LEU	2.3
1	D	344	TYR	2.3
1	D	341	LYS	2.2
1	D	190	ASP	2.2
1	B	0	HIS	2.2
1	D	158	LEU	2.2
1	B	12	ASN	2.2
1	B	-1	HIS	2.2
1	C	12	ASN	2.2
1	A	226	THR	2.2
1	B	188	ASN	2.1
1	A	85	THR	2.1
1	A	16	PHE	2.1
1	A	17	LEU	2.0
1	A	157	TYR	2.0
1	B	246	TRP	2.0
1	A	296	GLN	2.0
1	A	340	GLY	2.0
1	A	343	VAL	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, 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	EDO	C	501	4/4	0.92	0.14	36,38,45,48	0
2	EDO	A	501	4/4	0.93	0.11	38,38,45,47	0

6.5 Other polymers (i)

There are no such residues in this entry.