



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2016 – 06:53 PM EDT

PDB ID : 5DNE  
Title : Crystal structure of the Asn-bound guinea pig L-asparaginase 1 catalytic domain active site mutant K188M  
Authors : Schalk, A.M.; Lavie, A.  
Deposited on : 2015-09-10  
Resolution : 2.39 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

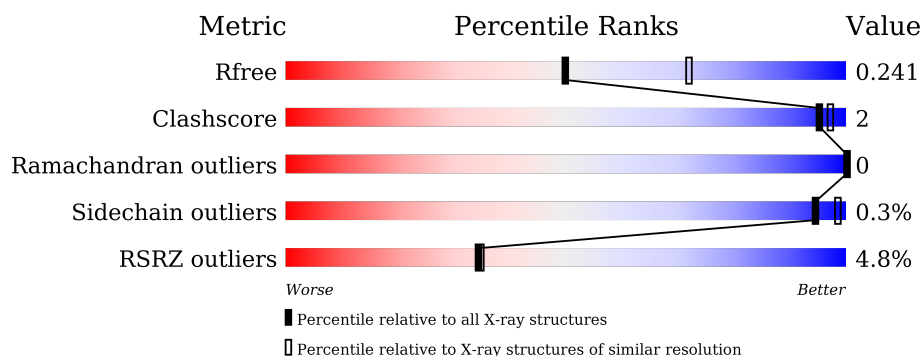
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	588	<div> <div>3%</div> <div>57%</div> <div>40%</div> </div>
1	B	588	<div> <div>3%</div> <div>58%</div> <div>39%</div> </div>
1	C	588	<div> <div>3%</div> <div>58%</div> <div>40%</div> </div>
1	D	588	<div> <div>3%</div> <div>59%</div> <div>39%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	602	-	-	-	X
3	EDO	B	602	-	-	-	X
3	EDO	B	603	-	-	X	-
3	EDO	C	602	-	-	-	X
3	EDO	C	605	-	-	-	X
3	EDO	D	602	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11260 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 L-asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	1	0
			2716	1738	469	492	17			
1	B	356	Total	C	N	O	S	0	0	0
			2722	1740	469	496	17			
1	C	354	Total	C	N	O	S	0	0	0
			2709	1733	467	492	17			
1	D	356	Total	C	N	O	S	0	0	0
			2721	1740	469	495	17			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP H0W0T5
A	-21	GLY	-	expression tag	UNP H0W0T5
A	-20	SER	-	expression tag	UNP H0W0T5
A	-19	SER	-	expression tag	UNP H0W0T5
A	-18	HIS	-	expression tag	UNP H0W0T5
A	-17	HIS	-	expression tag	UNP H0W0T5
A	-16	HIS	-	expression tag	UNP H0W0T5
A	-15	HIS	-	expression tag	UNP H0W0T5
A	-14	HIS	-	expression tag	UNP H0W0T5
A	-13	HIS	-	expression tag	UNP H0W0T5
A	-12	SER	-	expression tag	UNP H0W0T5
A	-11	SER	-	expression tag	UNP H0W0T5
A	-10	GLY	-	expression tag	UNP H0W0T5
A	-9	GLY	-	expression tag	UNP H0W0T5
A	-8	ASN	-	expression tag	UNP H0W0T5
A	-7	GLU	-	expression tag	UNP H0W0T5
A	-6	ASN	-	expression tag	UNP H0W0T5
A	-5	LEU	-	expression tag	UNP H0W0T5
A	-4	TYR	-	expression tag	UNP H0W0T5
A	-3	PHE	-	expression tag	UNP H0W0T5
A	-2	GLN	-	expression tag	UNP H0W0T5

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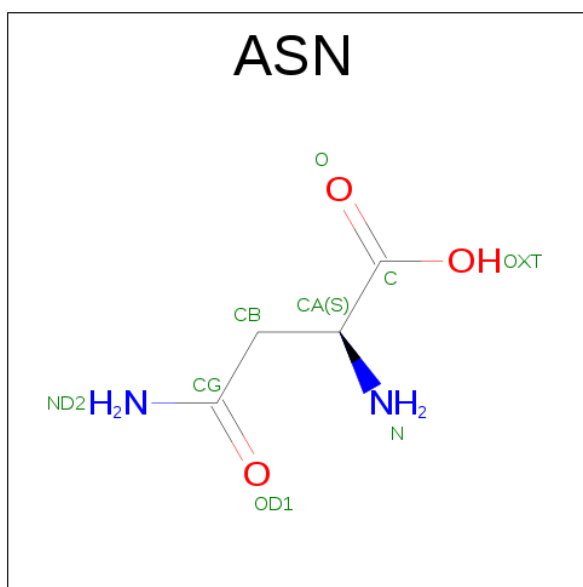
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP H0W0T5
A	0	HIS	-	expression tag	UNP H0W0T5
A	188	MET	LYS	engineered mutation	UNP H0W0T5
B	-22	MET	-	initiating methionine	UNP H0W0T5
B	-21	GLY	-	expression tag	UNP H0W0T5
B	-20	SER	-	expression tag	UNP H0W0T5
B	-19	SER	-	expression tag	UNP H0W0T5
B	-18	HIS	-	expression tag	UNP H0W0T5
B	-17	HIS	-	expression tag	UNP H0W0T5
B	-16	HIS	-	expression tag	UNP H0W0T5
B	-15	HIS	-	expression tag	UNP H0W0T5
B	-14	HIS	-	expression tag	UNP H0W0T5
B	-13	HIS	-	expression tag	UNP H0W0T5
B	-12	SER	-	expression tag	UNP H0W0T5
B	-11	SER	-	expression tag	UNP H0W0T5
B	-10	GLY	-	expression tag	UNP H0W0T5
B	-9	GLY	-	expression tag	UNP H0W0T5
B	-8	ASN	-	expression tag	UNP H0W0T5
B	-7	GLU	-	expression tag	UNP H0W0T5
B	-6	ASN	-	expression tag	UNP H0W0T5
B	-5	LEU	-	expression tag	UNP H0W0T5
B	-4	TYR	-	expression tag	UNP H0W0T5
B	-3	PHE	-	expression tag	UNP H0W0T5
B	-2	GLN	-	expression tag	UNP H0W0T5
B	-1	GLY	-	expression tag	UNP H0W0T5
B	0	HIS	-	expression tag	UNP H0W0T5
B	188	MET	LYS	engineered mutation	UNP H0W0T5
C	-22	MET	-	initiating methionine	UNP H0W0T5
C	-21	GLY	-	expression tag	UNP H0W0T5
C	-20	SER	-	expression tag	UNP H0W0T5
C	-19	SER	-	expression tag	UNP H0W0T5
C	-18	HIS	-	expression tag	UNP H0W0T5
C	-17	HIS	-	expression tag	UNP H0W0T5
C	-16	HIS	-	expression tag	UNP H0W0T5
C	-15	HIS	-	expression tag	UNP H0W0T5
C	-14	HIS	-	expression tag	UNP H0W0T5
C	-13	HIS	-	expression tag	UNP H0W0T5
C	-12	SER	-	expression tag	UNP H0W0T5
C	-11	SER	-	expression tag	UNP H0W0T5
C	-10	GLY	-	expression tag	UNP H0W0T5
C	-9	GLY	-	expression tag	UNP H0W0T5
C	-8	ASN	-	expression tag	UNP H0W0T5

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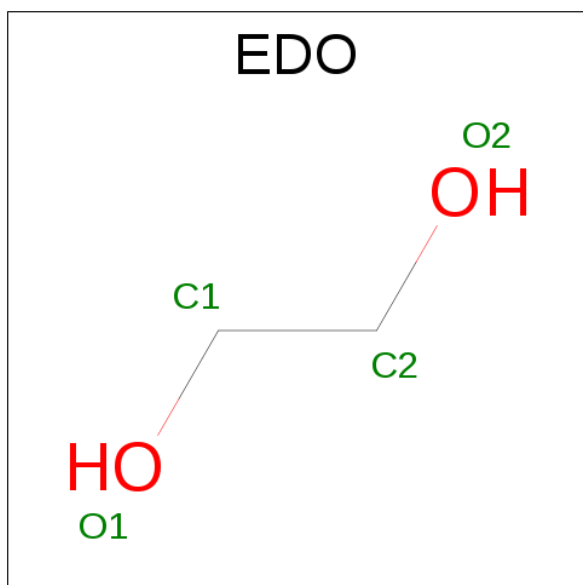
Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLU	-	expression tag	UNP H0W0T5
C	-6	ASN	-	expression tag	UNP H0W0T5
C	-5	LEU	-	expression tag	UNP H0W0T5
C	-4	TYR	-	expression tag	UNP H0W0T5
C	-3	PHE	-	expression tag	UNP H0W0T5
C	-2	GLN	-	expression tag	UNP H0W0T5
C	-1	GLY	-	expression tag	UNP H0W0T5
C	0	HIS	-	expression tag	UNP H0W0T5
C	188	MET	LYS	engineered mutation	UNP H0W0T5
D	-22	MET	-	initiating methionine	UNP H0W0T5
D	-21	GLY	-	expression tag	UNP H0W0T5
D	-20	SER	-	expression tag	UNP H0W0T5
D	-19	SER	-	expression tag	UNP H0W0T5
D	-18	HIS	-	expression tag	UNP H0W0T5
D	-17	HIS	-	expression tag	UNP H0W0T5
D	-16	HIS	-	expression tag	UNP H0W0T5
D	-15	HIS	-	expression tag	UNP H0W0T5
D	-14	HIS	-	expression tag	UNP H0W0T5
D	-13	HIS	-	expression tag	UNP H0W0T5
D	-12	SER	-	expression tag	UNP H0W0T5
D	-11	SER	-	expression tag	UNP H0W0T5
D	-10	GLY	-	expression tag	UNP H0W0T5
D	-9	GLY	-	expression tag	UNP H0W0T5
D	-8	ASN	-	expression tag	UNP H0W0T5
D	-7	GLU	-	expression tag	UNP H0W0T5
D	-6	ASN	-	expression tag	UNP H0W0T5
D	-5	LEU	-	expression tag	UNP H0W0T5
D	-4	TYR	-	expression tag	UNP H0W0T5
D	-3	PHE	-	expression tag	UNP H0W0T5
D	-2	GLN	-	expression tag	UNP H0W0T5
D	-1	GLY	-	expression tag	UNP H0W0T5
D	0	HIS	-	expression tag	UNP H0W0T5
D	188	MET	LYS	engineered mutation	UNP H0W0T5

- Molecule 2 is ASPARAGINE (three-letter code: ASN) (formula: C<sub>4</sub>H<sub>8</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	2	3		
2	B	1	Total	C	N	O	0	0
			9	4	2	3		
2	C	1	Total	C	N	O	0	0
			9	4	2	3		
2	D	1	Total	C	N	O	0	0
			9	4	2	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



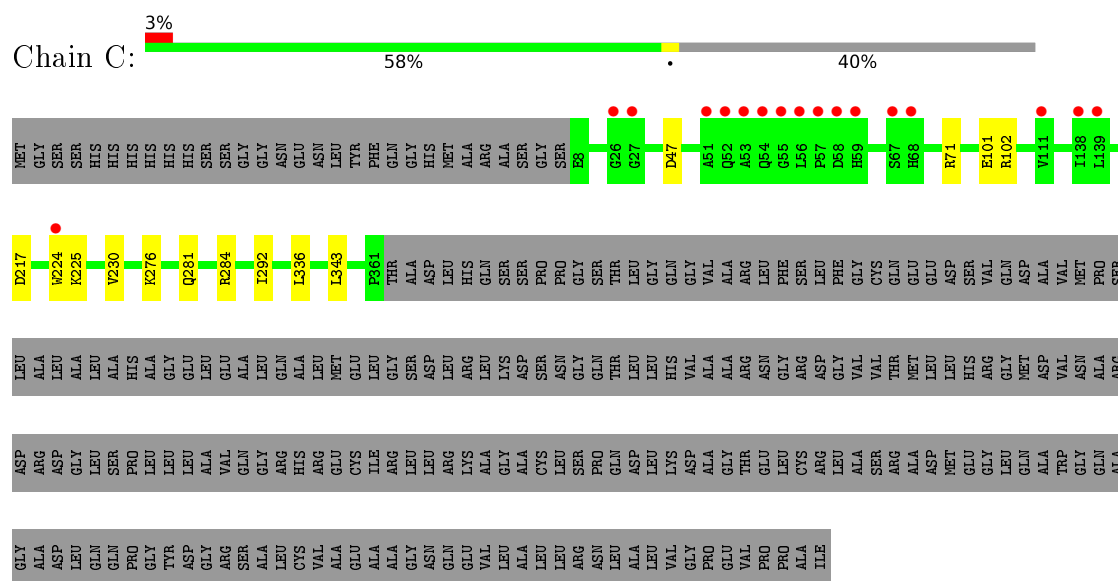
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

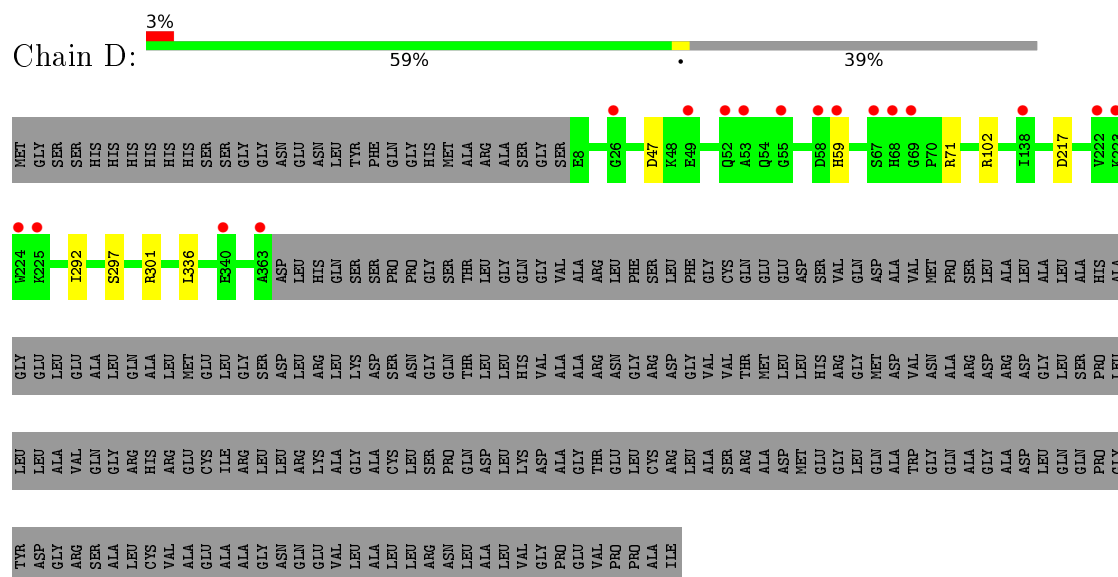
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	89	Total O 89 89	0	0
4	B	81	Total O 81 81	0	0
4	C	80	Total O 80 80	0	0
4	D	70	Total O 70 70	0	0







- Molecule 1: L-asparaginase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.91Å 154.79Å 157.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.39 28.37 – 2.39	Depositor EDS
% Data completeness (in resolution range)	94.8 (30.00-2.39) 94.9 (28.37-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.194 , 0.237 0.199 , 0.241	Depositor DCC
$R_{free}$ test set	2904 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 18.4	EDS
Estimated twinning fraction	0.012 for -h,-l,-k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 57461 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11260	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: 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	0.54	0/2777	0.68	1/3777 (0.0%)
1	B	0.54	0/2779	0.68	1/3780 (0.0%)
1	C	0.53	0/2766	0.68	0/3762
1	D	0.52	0/2778	0.68	1/3779 (0.0%)
All	All	0.53	0/11100	0.68	3/15098 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	253	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	D	102	ARG	NE-CZ-NH1	5.67	123.14	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	2716	0	2784	10	1
1	B	2722	0	2789	14	1
1	C	2709	0	2777	7	0
1	D	2721	0	2789	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	9	0	5	0	0
2	B	9	0	5	0	0
2	C	9	0	5	0	0
2	D	9	0	5	0	0
3	A	8	0	12	0	0
3	B	8	0	12	6	0
3	C	16	0	24	1	0
3	D	4	0	6	1	0
4	A	89	0	0	1	0
4	B	81	0	0	2	0
4	C	80	0	0	2	0
4	D	70	0	0	2	0
All	All	11260	0	11213	36	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 (36) 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:C:281:GLN:OE1	1:C:284:ARG:NH1	1.94	0.98
1:D:59:HIS:O	4:D:701:HOH:O	1.98	0.82
1:D:301:ARG:HD2	4:D:766:HOH:O	1.89	0.72
1:B:299:CYS:O	3:B:603:EDO:C1	2.39	0.71
3:B:603:EDO:H11	4:B:721:HOH:O	1.90	0.70
1:B:299:CYS:O	3:B:603:EDO:H12	1.93	0.69
1:A:150:TRP:NE1	1:B:208:VAL:HG11	2.11	0.65
1:B:297:SER:O	3:B:603:EDO:H12	2.01	0.60
1:C:276:LYS:HE3	4:C:712:HOH:O	2.02	0.59
1:A:150:TRP:NE1	1:B:208:VAL:CG1	2.66	0.58
1:B:323:MET:O	3:B:603:EDO:O2	2.22	0.57
1:A:40:ARG:NH2	1:A:58:ASP:O	2.34	0.56
1:B:40:ARG:NH2	1:B:58:ASP:O	2.32	0.52
1:B:297:SER:O	3:B:603:EDO:C1	2.58	0.52
1:A:289:ARG:NH1	4:A:703:HOH:O	2.43	0.51
1:B:47:ASP:OD2	1:B:71:ARG:NH2	2.44	0.51
1:B:47:ASP:HA	4:B:722:HOH:O	2.10	0.51
1:C:47:ASP:OD2	1:C:71:ARG:NH2	2.44	0.50
1:D:47:ASP:OD2	1:D:71:ARG:NH2	2.45	0.50
1:A:47:ASP:OD2	1:A:71:ARG:NH2	2.45	0.50
1:D:292:ILE:HD12	1:D:336:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:604:EDO:H11	4:C:750:HOH:O	2.14	0.46
1:A:292:ILE:HD12	1:A:336:LEU:HD21	1.98	0.46
1:C:292:ILE:HD12	1:C:336:LEU:HD21	1.98	0.46
1:B:292:ILE:HD12	1:B:336:LEU:HD21	1.97	0.45
1:A:101:GLU:HB2	1:A:230:VAL:HG21	1.99	0.45
1:D:217:ASP:N	1:D:217:ASP:OD1	2.48	0.45
1:B:101:GLU:HB2	1:B:230:VAL:HG21	1.99	0.44
1:C:224:TRP:CH2	1:C:225:LYS:HE2	2.52	0.44
1:A:217:ASP:N	1:A:217:ASP:OD1	2.49	0.43
1:C:101:GLU:HB2	1:C:230:VAL:HG21	2.00	0.43
1:A:159:GLY:HA3	1:A:175:PHE:CE2	2.55	0.41
1:C:217:ASP:N	1:C:217:ASP:OD1	2.50	0.41
1:D:297:SER:HB3	3:D:602:EDO:H12	2.02	0.41
1:B:159:GLY:HA3	1:B:175:PHE:CE2	2.56	0.40
1:A:150:TRP:HE1	1:B:208:VAL:CG1	2.34	0.40

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)
1:A:348:GLU:OE1	1:B:342:SER:OG[8_555]	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	353/588 (60%)	346 (98%)	7 (2%)	0	100	100
1	B	354/588 (60%)	347 (98%)	7 (2%)	0	100	100
1	C	352/588 (60%)	345 (98%)	7 (2%)	0	100	100
1	D	354/588 (60%)	347 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1413/2352 (60%)	1385 (98%)	28 (2%)	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	297/474 (63%)	295 (99%)	2 (1%)	88	95
1	B	298/474 (63%)	298 (100%)	0	100	100
1	C	296/474 (62%)	294 (99%)	2 (1%)	88	95
1	D	297/474 (63%)	297 (100%)	0	100	100
All	All	1188/1896 (63%)	1184 (100%)	4 (0%)	94	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	GLN
1	A	343	LEU
1	C	102	ARG
1	C	343	LEU

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 ⓘ

13 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	ASN	A	601	-	5,8,8	0.47	0	5,10,10	0.23	0
3	EDO	A	602	-	3,3,3	0.34	0	2,2,2	0.87	0
3	EDO	A	603	-	3,3,3	0.64	0	2,2,2	0.16	0
2	ASN	B	601	-	5,8,8	0.20	0	5,10,10	0.26	0
3	EDO	B	602	-	3,3,3	0.43	0	2,2,2	0.54	0
3	EDO	B	603	-	3,3,3	0.66	0	2,2,2	0.17	0
2	ASN	C	601	-	5,8,8	0.31	0	5,10,10	0.22	0
3	EDO	C	602	-	3,3,3	0.29	0	2,2,2	0.96	0
3	EDO	C	603	-	3,3,3	0.63	0	2,2,2	0.08	0
3	EDO	C	604	-	3,3,3	0.61	0	2,2,2	0.40	0
3	EDO	C	605	-	3,3,3	0.53	0	2,2,2	0.10	0
2	ASN	D	601	-	5,8,8	0.30	0	5,10,10	0.24	0
3	EDO	D	602	-	3,3,3	0.76	0	2,2,2	0.18	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	ASN	A	601	-	-	0/4/8/8	0/0/0/0
3	EDO	A	602	-	-	0/1/1/1	0/0/0/0
3	EDO	A	603	-	-	0/1/1/1	0/0/0/0
2	ASN	B	601	-	-	0/4/8/8	0/0/0/0
3	EDO	B	602	-	-	0/1/1/1	0/0/0/0
3	EDO	B	603	-	-	0/1/1/1	0/0/0/0
2	ASN	C	601	-	-	0/4/8/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	602	-	-	0/1/1/1	0/0/0/0
3	EDO	C	603	-	-	0/1/1/1	0/0/0/0
3	EDO	C	604	-	-	0/1/1/1	0/0/0/0
3	EDO	C	605	-	-	0/1/1/1	0/0/0/0
2	ASN	D	601	-	-	0/4/8/8	0/0/0/0
3	EDO	D	602	-	-	0/1/1/1	0/0/0/0

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.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	603	EDO	6	0
3	C	604	EDO	1	0
3	D	602	EDO	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

### 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<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	354/588 (60%)	-0.12	18 (5%) 32 32	21, 34, 71, 126	0
1	B	356/588 (60%)	-0.02	16 (4%) 37 38	25, 36, 71, 120	0
1	C	354/588 (60%)	-0.08	17 (4%) 34 35	24, 35, 65, 110	0
1	D	356/588 (60%)	-0.01	17 (4%) 34 35	25, 38, 75, 123	0
All	All	1420/2352 (60%)	-0.05	68 (4%) 34 35	21, 36, 71, 126	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	68	HIS	7.7
1	D	67	SER	6.0
1	C	58	ASP	5.7
1	A	67	SER	5.6
1	C	56	LEU	5.6
1	A	56	LEU	5.2
1	A	68	HIS	5.2
1	B	58	ASP	5.1
1	A	58	ASP	5.1
1	C	67	SER	4.4
1	A	66	ALA	4.4
1	D	52	GLN	4.2
1	B	362	THR	4.2
1	B	68	HIS	4.1
1	D	58	ASP	4.1
1	A	53	ALA	4.0
1	A	55	GLY	4.0
1	A	225	LYS	3.8
1	A	52	GLN	3.7
1	A	224	TRP	3.5
1	C	53	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	225	LYS	3.5
1	B	52	GLN	3.5
1	C	55	GLY	3.4
1	C	68	HIS	3.4
1	B	67	SER	3.3
1	B	224	TRP	3.3
1	B	55	GLY	3.2
1	D	224	TRP	3.2
1	D	222	VAL	3.2
1	C	54	GLN	3.1
1	A	57	PRO	3.0
1	C	52	GLN	3.0
1	D	59	HIS	3.0
1	D	49	GLU	2.9
1	C	27	GLY	2.8
1	D	69	GLY	2.8
1	D	340	GLU	2.8
1	C	59	HIS	2.8
1	A	59	HIS	2.6
1	C	26	GLY	2.6
1	B	69	GLY	2.6
1	B	138	ILE	2.6
1	C	57	PRO	2.6
1	A	69	GLY	2.6
1	B	222	VAL	2.5
1	B	139	LEU	2.5
1	C	111	VAL	2.5
1	D	363	ALA	2.5
1	D	138	ILE	2.5
1	D	55	GLY	2.4
1	C	51	ALA	2.4
1	B	53	ALA	2.4
1	A	27	GLY	2.3
1	D	53	ALA	2.3
1	A	172	VAL	2.3
1	C	138	ILE	2.2
1	D	26	GLY	2.2
1	B	56	LEU	2.1
1	B	361	PRO	2.1
1	A	361	PRO	2.1
1	D	223	LYS	2.1
1	B	137	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	70	PRO	2.1
1	B	57	PRO	2.1
1	A	138	ILE	2.0
1	C	224	TRP	2.0
1	C	139	LEU	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 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
3	EDO	B	602	4/4	0.93	0.20	5.52	54,55,56,56	0
3	EDO	A	602	4/4	0.89	0.16	4.13	39,40,40,45	0
3	EDO	C	602	4/4	0.91	0.15	2.93	37,37,39,40	0
3	EDO	C	605	4/4	0.95	0.24	2.43	35,39,42,43	0
3	EDO	D	602	4/4	0.87	0.17	2.28	40,40,41,41	0
3	EDO	A	603	4/4	0.96	0.19	1.70	42,45,45,46	0
3	EDO	B	603	4/4	0.88	0.18	1.68	36,41,42,43	0
3	EDO	C	604	4/4	0.90	0.17	1.08	46,49,49,51	0
2	ASN	A	601	9/9	0.97	0.11	0.13	23,25,31,33	0
2	ASN	B	601	9/9	0.97	0.10	0.04	29,32,34,35	0
2	ASN	D	601	9/9	0.99	0.09	-0.81	23,28,29,32	0
2	ASN	C	601	9/9	0.97	0.09	-0.83	29,33,36,37	0
3	EDO	C	603	4/4	0.95	0.09	-1.03	35,39,40,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.