



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2017 – 01:24 AM EDT

PDB ID : 5DNC
Title : Crystal structure of the Asn-bound guinea pig L-asparaginase 1 catalytic domain active site mutant T19A
Authors : Schalk, A.M.; Lavie, A.
Deposited on : unknown
Resolution : 2.01 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

<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 : rb-20030345
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) : rb-20030345

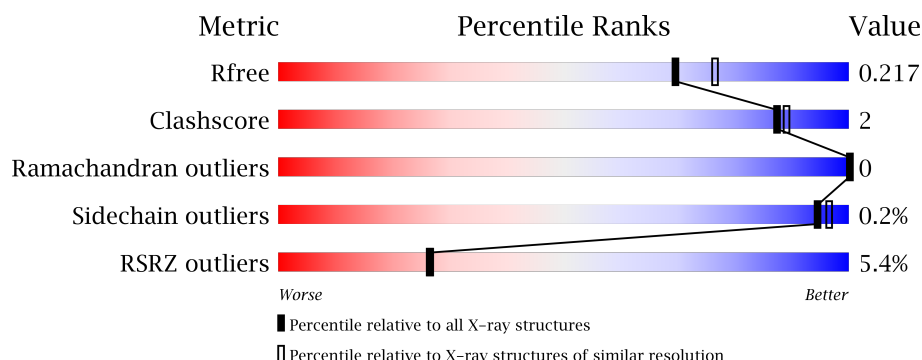
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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 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	588	<div> <div>4%</div> <div>57%</div> <div>40%</div> </div>
1	B	588	<div> <div>3%</div> <div>57%</div> <div>40%</div> </div>
1	C	588	<div> <div>3%</div> <div>56%</div> <div>40%</div> </div>
1	D	588	<div> <div>3%</div> <div>57%</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	A	603	-	-	-	X
3	EDO	B	603	-	-	-	X
3	EDO	B	604	-	-	-	X
3	EDO	C	603	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11493 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	0	0
			2708	1733	468	491	16			
1	B	355	Total	C	N	O	S	0	1	0
			2729	1748	471	494	16			
1	C	354	Total	C	N	O	S	0	1	0
			2719	1743	469	491	16			
1	D	356	Total	C	N	O	S	0	0	0
			2720	1740	470	494	16			

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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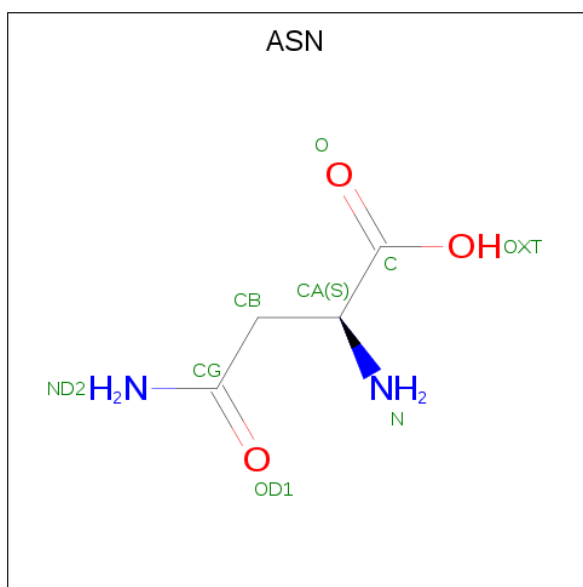
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP H0W0T5
A	0	HIS	-	expression tag	UNP H0W0T5
A	19	ALA	THR	engineered mutation	UNP H0W0T5
B	-22	MET	-	initiating methionine	UNP H0W0T5
B	-21	GLY	-	expression tag	UNP H0W0T5
B	-20	SER	-	expression tag	UNP H0W0T5
B	-19	SER	-	expression 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	19	ALA	THR	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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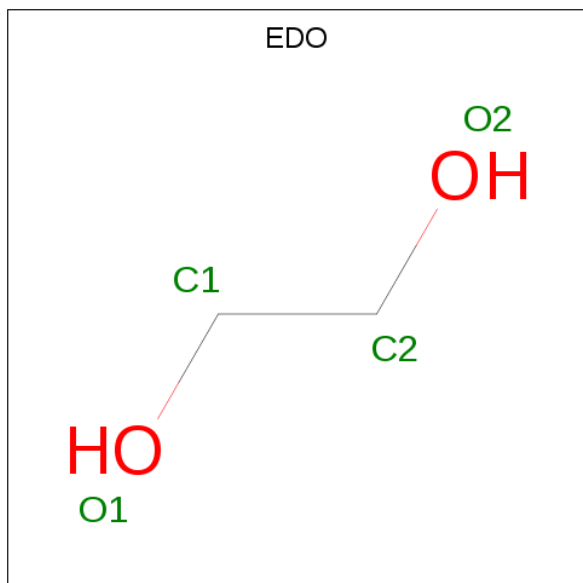
Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLU	-	expression tag	UNP H0W0T5
C	-6	ASN	-	expression tag	UNP H0W0T5
C	-5	LEU	-	expression tag	UNP H0W0T5
C	-4	TYR	-	expression tag	UNP H0W0T5
C	-3	PHE	-	expression tag	UNP H0W0T5
C	-2	GLN	-	expression tag	UNP H0W0T5
C	-1	GLY	-	expression tag	UNP H0W0T5
C	0	HIS	-	expression tag	UNP H0W0T5
C	19	ALA	THR	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	19	ALA	THR	engineered mutation	UNP H0W0T5

- Molecule 2 is ASPARAGINE (three-letter code: ASN) (formula: C₄H₈N₂O₃).



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: C₂H₆O₂).



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	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	B	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
3	D	1	Total C O 4 2 2	0	0
3	D	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	147	Total O 147 147	0	0
4	B	136	Total O 136 136	0	0
4	C	120	Total O 120 120	0	0

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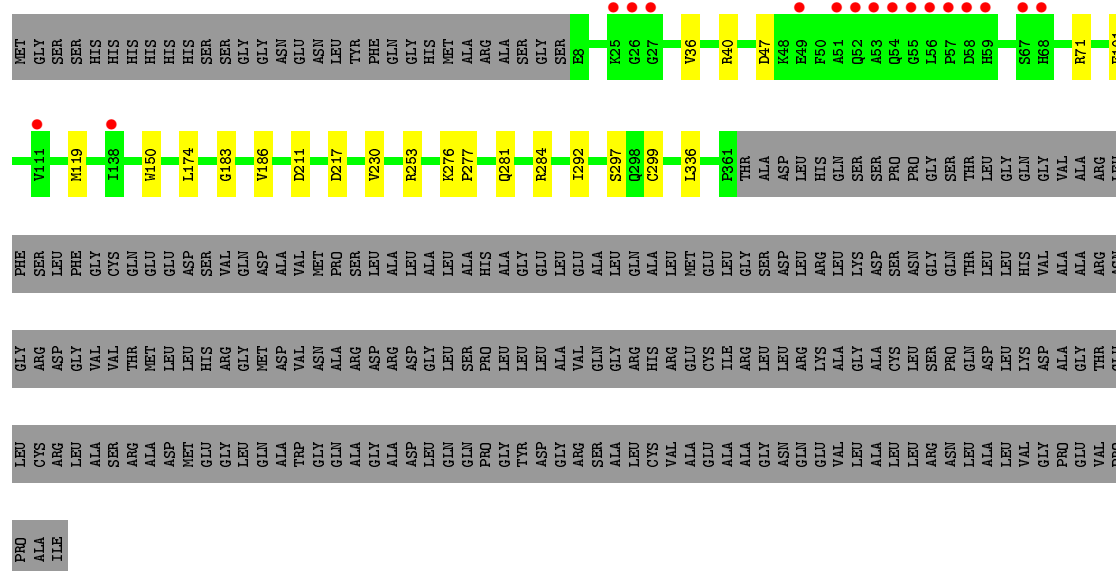
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	110	Total	O	0	0
			110	110		

TRP	GLY	GLN	ALA	GLY	ALA	ASP	GLN	GLN	PRO	GLY	TYR	ASP	GLY	ARG	SER	ALA	ALA	CYS	VAL	ALA	GLU	ALA	ALA	GLY	ASN	GLN	GLU	VAL	LEU	LEU	ALA	LEU	LEU	ARG	ASN	LEU	ALA	LEU	VAL	PRO	PRO	ALA	TYR
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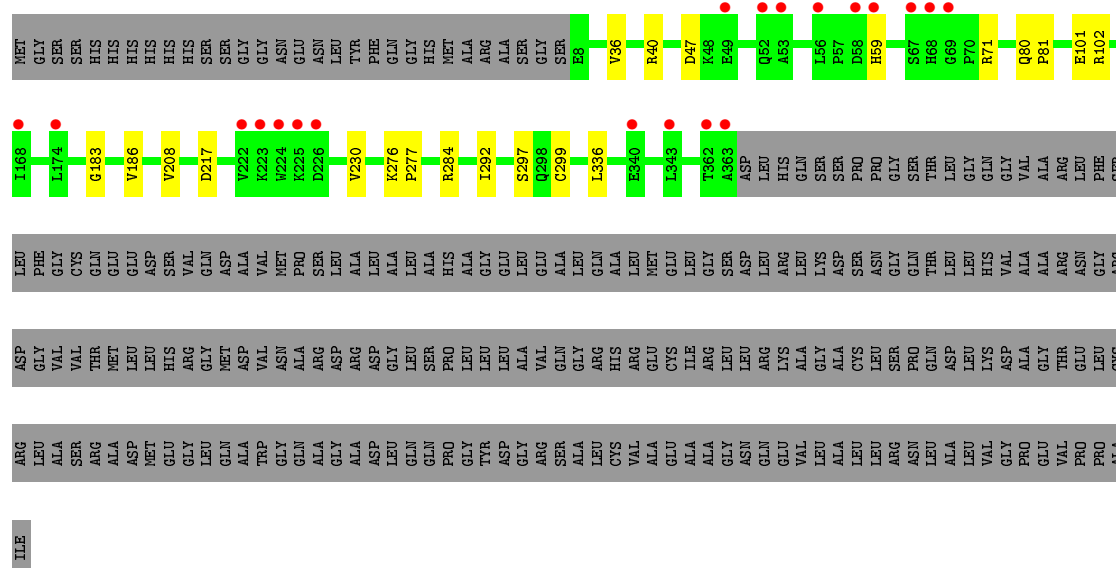
- Molecule 1: L-asparaginase

Chain C:  3% 56% 40%



- Molecule 1: L-asparaginase

Chain D:  3% 57% 39%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.19Å 155.00Å 157.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.01 29.66 – 2.01	Depositor EDS
% Data completeness (in resolution range)	96.6 (30.00-2.01) 96.7 (29.66-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.187 , 0.212 0.194 , 0.217	Depositor DCC
R_{free} test set	4817 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11493	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 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	0/2765	0.67	1/3760 (0.0%)
1	B	0.52	0/2788	0.67	2/3793 (0.1%)
1	C	0.54	0/2781	0.68	1/3783 (0.0%)
1	D	0.52	0/2777	0.68	2/3777 (0.1%)
All	All	0.53	0/11111	0.68	6/15113 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	284	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	D	102	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	301	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	253	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	B	242	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	C	253	ARG	NE-CZ-NH1	5.00	122.80	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	2708	0	2779	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2729	0	2795	13	0
1	C	2719	0	2789	18	0
1	D	2720	0	2791	17	0
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	20	0	30	1	0
3	B	16	0	24	0	0
3	C	16	0	24	3	0
3	D	16	0	24	3	0
4	A	147	0	0	1	0
4	B	136	0	0	1	0
4	C	120	0	0	0	0
4	D	110	0	0	1	0
All	All	11493	0	11276	54	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 (54) 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:NH2	2.03	0.90
1:C:150[A]:TRP:NE1	1:D:208:VAL:HG11	1.86	0.90
1:D:59:HIS:O	4:D:701:HOH:O	1.96	0.84
1:A:150:TRP:NE1	1:B:208:VAL:HG11	2.03	0.73
1:C:150[A]:TRP:NE1	1:D:208:VAL:CG1	2.53	0.71
1:A:150:TRP:NE1	1:B:208:VAL:CG1	2.54	0.70
1:C:150[A]:TRP:HE1	1:D:208:VAL:CG1	2.05	0.69
1:A:66:ALA:HA	4:A:816:HOH:O	1.93	0.67
1:C:47:ASP:OD2	1:C:71:ARG:NH2	2.31	0.63
1:B:47:ASP:OD2	1:B:71:ARG:NH2	2.31	0.63
1:A:47:ASP:OD2	1:A:71:ARG:NH2	2.32	0.63
1:D:47:ASP:OD2	1:D:71:ARG:NH2	2.31	0.62
1:A:150:TRP:HE1	1:B:208:VAL:HG12	1.67	0.59
1:C:119:MET:SD	1:C:174:LEU:HD13	2.43	0.58
1:A:119:MET:SD	1:A:174:LEU:HD13	2.46	0.56
1:A:150:TRP:HE1	1:B:208:VAL:CG1	2.20	0.51
1:C:150[A]:TRP:HE1	1:D:208:VAL:HG12	1.74	0.50
1:C:297:SER:HB3	3:C:602:EDO:H12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LYS:HE2	4:B:802:HOH:O	2.14	0.48
1:D:292:ILE:HD12	1:D:336:LEU:HD21	1.96	0.48
1:B:292:ILE:HD12	1:B:336:LEU:HD21	1.96	0.48
1:A:101:GLU:HB2	1:A:230:VAL:HG21	1.96	0.47
1:C:119:MET:SD	1:C:174:LEU:CD1	3.03	0.46
1:D:297:SER:O	3:D:605:EDO:O2	2.34	0.46
1:A:292:ILE:HD12	1:A:336:LEU:HD21	1.98	0.46
1:D:101:GLU:HB2	1:D:230:VAL:HG21	1.98	0.46
1:C:101:GLU:HB2	1:C:230:VAL:HG21	1.97	0.45
1:B:101:GLU:HB2	1:B:230:VAL:HG21	1.97	0.45
1:A:183:GLY:O	1:A:186:VAL:HG22	2.16	0.45
1:B:183:GLY:O	1:B:186:VAL:HG22	2.16	0.45
1:C:183:GLY:O	1:C:186:VAL:HG22	2.17	0.45
1:D:297:SER:HB3	3:D:605:EDO:H21	2.00	0.44
1:A:150:TRP:NE1	1:B:208:VAL:HG12	2.24	0.43
1:C:150[A]:TRP:CD1	1:D:208:VAL:HG11	2.51	0.43
1:D:217:ASP:OD1	1:D:217:ASP:N	2.52	0.43
1:D:183:GLY:O	1:D:186:VAL:HG22	2.17	0.43
1:A:217:ASP:N	1:A:217:ASP:OD1	2.52	0.43
1:A:337:GLY:HA2	3:A:605:EDO:H12	2.01	0.42
1:C:299:CYS:O	3:C:602:EDO:O1	2.36	0.42
1:D:299:CYS:O	3:D:605:EDO:O2	2.28	0.42
1:B:36:VAL:O	1:B:40:ARG:HG3	2.19	0.42
1:C:292:ILE:HD12	1:C:336:LEU:HD21	2.01	0.42
1:B:276:LYS:HA	1:B:277:PRO:HD3	1.95	0.42
1:A:119:MET:SD	1:A:174:LEU:CD1	3.06	0.42
1:A:36:VAL:O	1:A:40:ARG:HG3	2.20	0.42
1:C:36:VAL:O	1:C:40:ARG:HG3	2.20	0.42
1:B:175:PHE:O	1:B:176:MET:HG3	2.21	0.41
1:C:217:ASP:N	1:C:217:ASP:OD1	2.53	0.41
1:A:276:LYS:HA	1:A:277:PRO:HD3	1.94	0.41
1:C:276:LYS:HA	1:C:277:PRO:HD3	1.95	0.40
1:C:299:CYS:O	3:C:602:EDO:C1	2.69	0.40
1:D:36:VAL:O	1:D:40:ARG:HG3	2.21	0.40
1:D:276:LYS:HA	1:D:277:PRO:HD3	1.94	0.40
1:D:80:GLN:HA	1:D:81:PRO:HA	1.97	0.40

There are no symmetry-related clashes.

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	352/588 (60%)	346 (98%)	6 (2%)	0	100	100
1	B	354/588 (60%)	348 (98%)	6 (2%)	0	100	100
1	C	353/588 (60%)	347 (98%)	6 (2%)	0	100	100
1	D	354/588 (60%)	348 (98%)	6 (2%)	0	100	100
All	All	1413/2352 (60%)	1389 (98%)	24 (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	295/473 (62%)	294 (100%)	1 (0%)	94	96
1	B	297/473 (63%)	297 (100%)	0	100	100
1	C	296/473 (63%)	295 (100%)	1 (0%)	94	96
1	D	296/473 (63%)	296 (100%)	0	100	100
All	All	1184/1892 (63%)	1182 (100%)	2 (0%)	94	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	ASP
1	C	211	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	281	GLN
1	C	23	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

21 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	-	3,8,8	0.23	0	5,10,10	0.50	0
3	EDO	A	602	-	3,3,3	0.53	0	2,2,2	0.06	0
3	EDO	A	603	-	3,3,3	0.39	0	2,2,2	0.57	0
3	EDO	A	604	-	3,3,3	0.98	0	2,2,2	0.07	0
3	EDO	A	605	-	3,3,3	0.52	0	2,2,2	0.28	0
3	EDO	A	606	-	3,3,3	0.76	0	2,2,2	0.08	0
2	ASN	B	601	-	3,8,8	0.60	0	5,10,10	0.21	0
3	EDO	B	602	-	3,3,3	0.37	0	2,2,2	0.59	0
3	EDO	B	603	-	3,3,3	0.38	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	604	-	3,3,3	0.35	0	2,2,2	0.97	0
3	EDO	B	605	-	3,3,3	1.03	0	2,2,2	0.13	0
2	ASN	C	601	-	3,8,8	0.51	0	5,10,10	0.43	0
3	EDO	C	602	-	3,3,3	0.88	0	2,2,2	0.50	0
3	EDO	C	603	-	3,3,3	0.29	0	2,2,2	0.66	0
3	EDO	C	604	-	3,3,3	0.52	0	2,2,2	0.19	0
3	EDO	C	605	-	3,3,3	0.58	0	2,2,2	0.17	0
2	ASN	D	601	-	3,8,8	0.34	0	5,10,10	0.37	0
3	EDO	D	602	-	3,3,3	0.36	0	2,2,2	0.58	0
3	EDO	D	603	-	3,3,3	0.56	0	2,2,2	0.05	0
3	EDO	D	604	-	3,3,3	0.37	0	2,2,2	0.43	0
3	EDO	D	605	-	3,3,3	1.06	0	2,2,2	0.36	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
3	EDO	A	604	-	-	0/1/1/1	0/0/0/0
3	EDO	A	605	-	-	0/1/1/1	0/0/0/0
3	EDO	A	606	-	-	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
3	EDO	B	604	-	-	0/1/1/1	0/0/0/0
3	EDO	B	605	-	-	0/1/1/1	0/0/0/0
2	ASN	C	601	-	-	0/4/8/8	0/0/0/0
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
3	EDO	D	603	-	-	0/1/1/1	0/0/0/0
3	EDO	D	604	-	-	0/1/1/1	0/0/0/0
3	EDO	D	605	-	-	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 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	EDO	1	0
3	C	602	EDO	3	0
3	D	605	EDO	3	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, 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	354/588 (60%)	0.01	24 (6%) 18 18	22, 31, 68, 119	0
1	B	355/588 (60%)	-0.02	15 (4%) 37 37	22, 34, 66, 99	0
1	C	354/588 (60%)	-0.03	17 (4%) 31 31	22, 32, 61, 102	0
1	D	356/588 (60%)	0.11	20 (5%) 25 25	24, 37, 70, 113	0
All	All	1419/2352 (60%)	0.02	76 (5%) 26 26	22, 34, 67, 119	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	HIS	8.2
1	D	68	HIS	7.9
1	A	67	SER	7.7
1	D	225	LYS	6.2
1	D	67	SER	6.2
1	C	56	LEU	5.9
1	C	58	ASP	5.5
1	D	69	GLY	5.2
1	D	224	TRP	5.0
1	B	56	LEU	5.0
1	B	67	SER	4.7
1	A	66	ALA	4.6
1	C	57	PRO	4.5
1	B	68	HIS	4.5
1	A	56	LEU	4.4
1	A	58	ASP	4.4
1	C	52	GLN	4.4
1	A	224	TRP	4.3
1	C	68	HIS	4.2
1	C	53	ALA	4.1
1	A	69	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	362	THR	4.0
1	B	55	GLY	3.9
1	A	55	GLY	3.8
1	A	59	HIS	3.8
1	A	26	GLY	3.7
1	D	58	ASP	3.7
1	B	58	ASP	3.7
1	D	363	ALA	3.7
1	C	27	GLY	3.7
1	D	52	GLN	3.6
1	D	340	GLU	3.5
1	D	56	LEU	3.5
1	B	362	THR	3.3
1	B	52	GLN	3.3
1	A	52	GLN	3.2
1	A	138	ILE	3.2
1	D	222	VAL	3.2
1	C	54	GLN	3.0
1	C	59	HIS	3.0
1	C	55	GLY	3.0
1	D	49	GLU	2.9
1	B	69	GLY	2.9
1	A	70	PRO	2.8
1	C	26	GLY	2.8
1	B	51	ALA	2.8
1	B	53	ALA	2.7
1	A	53	ALA	2.7
1	B	225	LYS	2.7
1	C	67	SER	2.7
1	A	139	LEU	2.7
1	A	225	LYS	2.6
1	D	223	LYS	2.5
1	D	53	ALA	2.5
1	D	59	HIS	2.4
1	A	60	ALA	2.4
1	B	224[A]	TRP	2.4
1	A	49	GLU	2.3
1	C	51	ALA	2.3
1	D	226	ASP	2.3
1	A	57	PRO	2.3
1	A	54	GLN	2.2
1	B	208	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	343	LEU	2.2
1	C	111	VAL	2.2
1	C	138	ILE	2.2
1	A	112	VAL	2.2
1	C	25	LYS	2.2
1	C	49	GLU	2.2
1	B	240	LEU	2.2
1	B	54	GLN	2.1
1	A	25	LYS	2.1
1	A	27	GLY	2.1
1	D	174	LEU	2.0
1	D	168	ILE	2.0
1	A	111	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 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(Å ²)	Q<0.9
3	EDO	C	603	4/4	0.92	0.23	11.63	45,45,46,48	0
3	EDO	B	603	4/4	0.93	0.22	9.01	46,48,49,50	0
3	EDO	A	602	4/4	0.93	0.14	6.05	38,41,42,43	0
3	EDO	B	604	4/4	0.94	0.23	5.71	48,48,49,49	0
3	EDO	A	603	4/4	0.93	0.14	4.10	52,53,53,53	0
3	EDO	D	603	4/4	0.96	0.15	1.88	30,33,34,34	0
3	EDO	D	602	4/4	0.85	0.15	1.85	46,47,47,50	0
3	EDO	A	606	4/4	0.91	0.17	1.79	34,38,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	EDO	D	605	4/4	0.73	0.17	1.53	33,34,35,38	0
3	EDO	C	604	4/4	0.95	0.09	1.49	45,48,49,49	0
3	EDO	A	605	4/4	0.93	0.10	1.43	47,48,48,49	0
3	EDO	A	604	4/4	0.79	0.16	1.38	37,38,41,42	0
3	EDO	D	604	4/4	0.95	0.13	0.76	51,54,54,55	0
3	EDO	C	602	4/4	0.83	0.12	0.33	33,38,39,41	0
3	EDO	B	605	4/4	0.85	0.12	0.05	31,37,38,42	0
2	ASN	A	601	9/9	0.97	0.09	-0.48	27,28,29,33	0
2	ASN	D	601	9/9	0.97	0.08	-0.72	23,26,27,27	0
2	ASN	B	601	9/9	0.96	0.08	-0.83	26,28,29,31	0
3	EDO	B	602	4/4	0.97	0.07	-1.01	35,38,41,44	0
2	ASN	C	601	9/9	0.97	0.06	-1.18	24,26,29,30	0
3	EDO	C	605	4/4	0.89	0.14	-	45,50,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.