



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:30 AM EDT

PDB ID : 6V2C  
Title : Complex of mutant (K162M) of E. coli L-asparaginase II with L-Asp. Covalent acyl-enzyme intermediate and tetrahedral intermediate  
Authors : Lubkowski, J.; Wlodawer, A.  
Deposited on : 2019-11-22  
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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.10.1  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
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) : 2.10.1

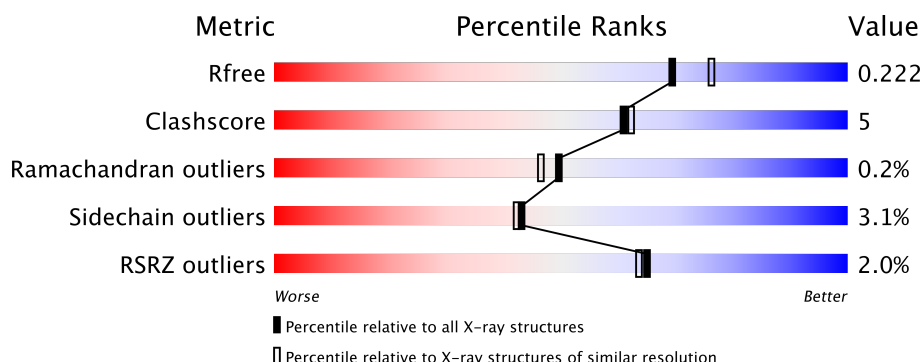
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (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  $\geq 3$ , 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	334	<div> <div style="width: 5%; background-color: red;"></div> <div style="width: 81%; background-color: green;"></div> <div style="width: 16%; background-color: yellow;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div> <div style="width: 5%; background-color: red;"></div> <div style="width: 87%; background-color: green;"></div> <div style="width: 11%; background-color: yellow;"></div> <div style="width: 1%; background-color: grey;"></div> </div>
1	B	334	<div> <div style="width: 85%; background-color: green;"></div> <div style="width: 13%; background-color: yellow;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div> <div style="width: 5%; background-color: red;"></div> <div style="width: 83%; background-color: green;"></div> <div style="width: 15%; background-color: yellow;"></div> <div style="width: 1%; background-color: grey;"></div> </div>
1	C	334	<div> <div style="width: 85%; background-color: green;"></div> <div style="width: 13%; background-color: yellow;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div> <div style="width: 5%; background-color: red;"></div> <div style="width: 83%; background-color: green;"></div> <div style="width: 15%; background-color: yellow;"></div> <div style="width: 1%; background-color: grey;"></div> </div>
1	D	334	<div> <div style="width: 5%; background-color: red;"></div> <div style="width: 81%; background-color: green;"></div> <div style="width: 16%; background-color: yellow;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div> <div style="width: 5%; background-color: red;"></div> <div style="width: 87%; background-color: green;"></div> <div style="width: 11%; background-color: yellow;"></div> <div style="width: 1%; background-color: grey;"></div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10815 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	4	0
			2471	1539	420	503	9			
1	C	327	Total	C	N	O	S	0	2	0
			2469	1537	420	503	9			
1	B	327	Total	C	N	O	S	0	2	0
			2457	1532	419	497	9			
1	D	327	Total	C	N	O	S	0	1	0
			2453	1530	418	495	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP P00805
A	-5	HIS	-	expression tag	UNP P00805
A	-4	HIS	-	expression tag	UNP P00805
A	-3	HIS	-	expression tag	UNP P00805
A	-2	HIS	-	expression tag	UNP P00805
A	-1	HIS	-	expression tag	UNP P00805
A	0	HIS	-	expression tag	UNP P00805
A	12	AEI	THR	conflict	UNP P00805
A	162	MET	LYS	engineered mutation	UNP P00805
C	-6	MET	-	expression tag	UNP P00805
C	-5	HIS	-	expression tag	UNP P00805
C	-4	HIS	-	expression tag	UNP P00805
C	-3	HIS	-	expression tag	UNP P00805
C	-2	HIS	-	expression tag	UNP P00805
C	-1	HIS	-	expression tag	UNP P00805
C	0	HIS	-	expression tag	UNP P00805
C	12	AEI	THR	conflict	UNP P00805
C	162	MET	LYS	engineered mutation	UNP P00805
B	-6	MET	-	expression tag	UNP P00805
B	-5	HIS	-	expression tag	UNP P00805
B	-4	HIS	-	expression tag	UNP P00805

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP P00805
B	-2	HIS	-	expression tag	UNP P00805
B	-1	HIS	-	expression tag	UNP P00805
B	0	HIS	-	expression tag	UNP P00805
B	12	AEI	THR	conflict	UNP P00805
B	162	MET	LYS	engineered mutation	UNP P00805
D	-6	MET	-	expression tag	UNP P00805
D	-5	HIS	-	expression tag	UNP P00805
D	-4	HIS	-	expression tag	UNP P00805
D	-3	HIS	-	expression tag	UNP P00805
D	-2	HIS	-	expression tag	UNP P00805
D	-1	HIS	-	expression tag	UNP P00805
D	0	HIS	-	expression tag	UNP P00805
D	12	AEI	THR	conflict	UNP P00805
D	162	MET	LYS	engineered mutation	UNP P00805

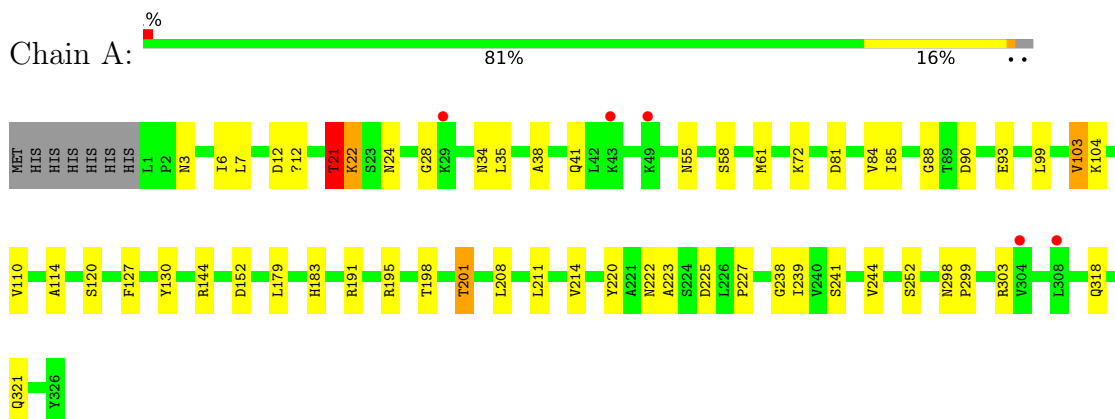
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	222	Total O 227 227	0	5
2	C	258	Total O 263 263	0	5
2	B	233	Total O 235 235	0	2
2	D	236	Total O 240 240	0	4

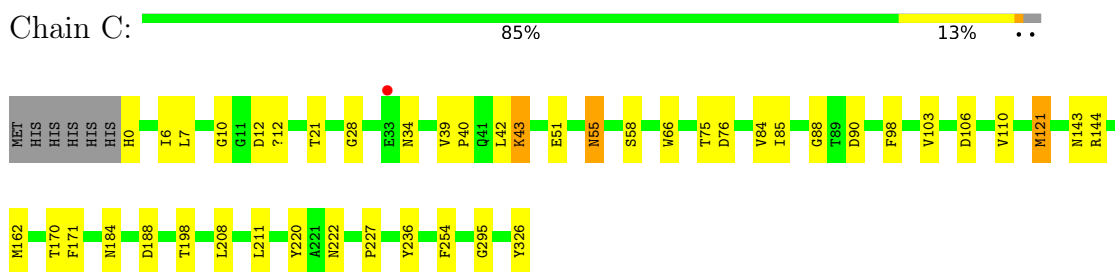
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

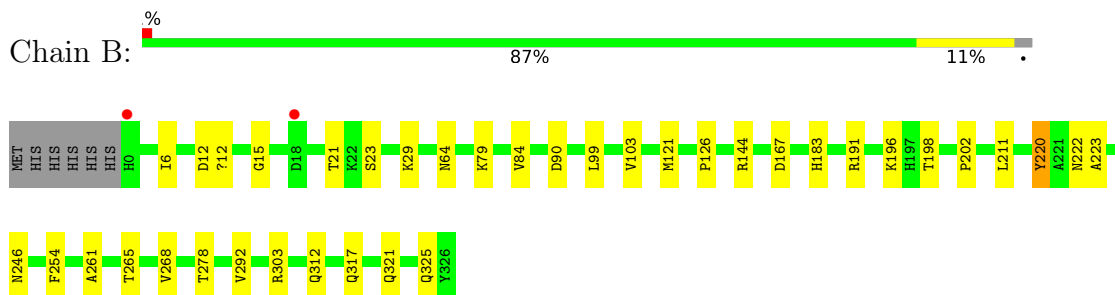
#### • Molecule 1: L-asparaginase 2



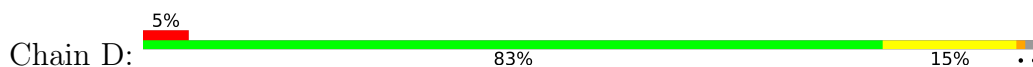
#### • Molecule 1: L-asparaginase 2

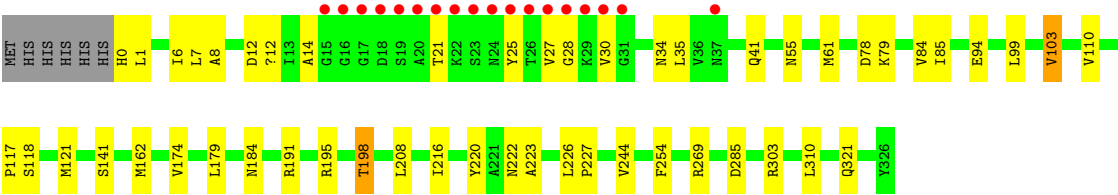


#### • Molecule 1: L-asparaginase 2



#### • Molecule 1: L-asparaginase 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.70Å 125.91Å 130.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.69 – 2.00 27.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (27.69-2.00) 95.8 (27.69-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.171 , 0.235 0.169 , 0.222	Depositor DCC
$R_{free}$ test set	2405 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10815	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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, 0.333 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: AEI, QNY

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	1.04	4/2486 (0.2%)	1.14	7/3384 (0.2%)
1	B	1.03	2/2485 (0.1%)	1.10	4/3382 (0.1%)
1	C	1.05	2/2478 (0.1%)	1.11	2/3373 (0.1%)
1	D	1.07	6/2478 (0.2%)	1.17	8/3372 (0.2%)
All	All	1.05	14/9927 (0.1%)	1.13	21/13511 (0.2%)

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	C	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	141	SER	CA-CB	-6.73	1.42	1.52
1	D	174	VAL	C-O	-6.26	1.11	1.23
1	B	15	GLY	C-O	6.06	1.33	1.23
1	C	295	GLY	C-O	6.05	1.33	1.23
1	D	94	GLU	CD-OE2	5.97	1.32	1.25
1	A	241	SER	CA-CB	-5.95	1.44	1.52
1	D	61	MET	CG-SD	5.66	1.95	1.81
1	D	8	ALA	C-O	5.46	1.33	1.23
1	B	167	ASP	C-O	-5.42	1.13	1.23
1	A	239	ILE	C-O	5.28	1.33	1.23
1	C	326	TYR	C-OXT	-5.25	1.13	1.23
1	A	93	GLU	CD-OE1	-5.15	1.20	1.25
1	D	310	LEU	C-O	-5.06	1.13	1.23
1	A	114	ALA	C-O	5.05	1.32	1.23



All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	C	144	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	A	195	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	D	269	ARG	NE-CZ-NH2	-7.57	116.51	120.30
1	D	195	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	B	191	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	195	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	A	61	MET	CG-SD-CE	6.41	110.46	100.20
1	B	191	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	21	THR	N-CA-CB	-6.04	98.83	110.30
1	D	162	MET	CG-SD-CE	5.96	109.74	100.20
1	A	144	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	188	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	D	285	ASP	CB-CG-OD2	-5.63	113.24	118.30
1	D	78	ASP	CB-CG-OD1	-5.54	113.32	118.30
1	D	269	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	144	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	B	303	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	B	144	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	D	303	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	152	ASP	CB-CG-OD2	-5.11	113.70	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	12[A]	AEI	Mainchain
1	C	12[B]	QNY	Mainchain

## 5.2 Too-close contacts

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	2471	0	2439	35	0
1	B	2457	0	2443	22	0
1	C	2469	0	2433	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2453	0	2439	25	0
2	A	227	0	0	2	0
2	B	235	0	0	3	0
2	C	263	0	0	5	0
2	D	240	0	0	3	0
All	All	10815	0	9754	94	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 5.

All (94) 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:12:AEI:CD	2:D:431:HOH:O	2.29	0.81
1:B:196:LYS:HE3	1:B:325:GLN:NE2	1.98	0.79
1:A:22:LYS:HE2	1:A:24:ASN:OD1	1.87	0.73
1:A:318:GLN:OE1	2:A:457[B]:HOH:O	2.08	0.71
1:C:220:TYR:OH	2:C:401[A]:HOH:O	2.08	0.70
1:B:183:HIS:ND1	2:B:401[A]:HOH:O	2.26	0.68
1:C:40:PRO:O	1:C:43:LYS:HG2	1.96	0.66
1:B:12:AEI:CD	2:B:481:HOH:O	2.46	0.64
1:B:196:LYS:HE3	1:B:325:GLN:HE22	1.61	0.64
2:C:531:HOH:O	1:B:21:THR:HG21	1.97	0.62
1:B:103:VAL:O	1:B:198:THR:HA	1.97	0.62
1:C:76:ASP:OD2	2:C:402:HOH:O	2.16	0.61
1:B:202:PRO:HB2	1:B:312:GLN:HE22	1.65	0.61
1:B:317:GLN:HG2	1:B:321[B]:GLN:HE21	1.66	0.61
1:A:99:LEU:O	1:A:103:VAL:HG13	2.03	0.59
1:A:318:GLN:NE2	1:A:321:GLN:OE1	2.35	0.59
1:A:21:THR:HG21	2:D:432:HOH:O	2.03	0.58
1:A:183[B]:HIS:CE1	2:A:561:HOH:O	2.57	0.57
1:A:127:PHE:HA	1:D:121[A]:MET:HE2	1.85	0.57
1:C:28:GLY:HA2	1:C:55:ASN:ND2	2.20	0.56
1:D:103:VAL:HG22	1:D:198:THR:HG22	1.88	0.55
1:A:21:THR:CG2	2:D:432:HOH:O	2.55	0.55
1:D:12:AEI:HA	1:D:27:VAL:HG12	1.87	0.55
1:C:34:ASN:ND2	2:C:409:HOH:O	2.40	0.54
1:A:22:LYS:CE	1:A:24:ASN:OD1	2.56	0.52
1:A:298:ASN:HB2	1:A:299:PRO:CD	2.40	0.52
1:C:84:VAL:HA	1:C:110:VAL:O	2.09	0.51
1:A:3:ASN:O	1:A:81:ASP:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:SER:HB3	1:C:88:GLY:HA3	1.92	0.50
1:A:225:ASP:HB3	1:A:252:SER:HB3	1.93	0.49
1:A:214:VAL:HG12	1:A:303:ARG:HG3	1.94	0.49
1:A:103:VAL:O	1:A:198:THR:HA	2.13	0.49
1:A:220:TYR:CE2	1:A:223:ALA:HA	2.48	0.49
1:C:21:THR:CG2	1:C:121:MET:HG3	2.43	0.48
1:A:227:PRO:HB3	1:C:227:PRO:HB3	1.95	0.48
1:B:99:LEU:O	1:B:103:VAL:HG13	2.13	0.48
1:A:244:VAL:HB	1:C:90:ASP:HB3	1.96	0.48
1:A:58:SER:HB3	1:A:88:GLY:HA3	1.97	0.47
1:C:121:MET:HE1	1:B:126:PRO:HB3	1.97	0.47
1:D:99:LEU:O	1:D:103:VAL:HG13	2.13	0.47
1:D:220:TYR:CZ	1:D:223:ALA:HA	2.49	0.47
1:B:317:GLN:O	1:B:321[B]:GLN:HG2	2.15	0.46
1:C:103:VAL:O	1:C:198:THR:HA	2.15	0.46
1:A:214:VAL:CG1	1:A:303:ARG:HG3	2.46	0.46
1:A:35:LEU:O	1:A:38:ALA:HB3	2.16	0.46
1:D:0:HIS:ND1	1:D:1:LEU:O	2.49	0.46
1:A:84:VAL:HA	1:A:110:VAL:O	2.15	0.45
1:A:28:GLY:HA2	1:A:55:ASN:OD1	2.16	0.45
1:B:6:ILE:HA	1:B:84:VAL:O	2.16	0.45
1:D:25:TYR:CD1	1:D:117:PRO:HG3	2.52	0.45
1:B:261:ALA:HA	1:B:265:THR:O	2.17	0.45
1:D:12:AEI:HZ	1:D:27:VAL:HG11	1.99	0.44
1:D:14:ALA:O	1:D:30:VAL:HG22	2.17	0.44
1:C:10:GLY:HA2	1:C:55:ASN:ND2	2.32	0.44
1:D:79:LYS:O	1:D:79:LYS:HG2	2.17	0.44
1:A:127:PHE:CA	1:D:121[A]:MET:HE2	2.48	0.44
1:C:106:ASP:HB3	1:C:143:ASN:HD22	1.82	0.44
1:B:220:TYR:CG	1:D:216:ILE:HD12	2.53	0.44
1:A:130:TYR:CZ	1:D:21:THR:OG1	2.68	0.44
1:A:104:LYS:NZ	1:A:201:THR:O	2.51	0.43
1:D:226:LEU:HB2	1:D:227:PRO:HD3	1.99	0.43
1:A:22:LYS:HE3	1:D:184:ASN:OD1	2.17	0.43
1:D:84:VAL:HA	1:D:110:VAL:O	2.18	0.43
1:B:90:ASP:HB3	1:D:244:VAL:HB	2.01	0.43
1:D:41:GLN:OE1	1:D:41:GLN:N	2.45	0.43
1:C:66:TRP:HB3	1:C:98:PHE:CE2	2.53	0.43
1:D:179:LEU:HA	1:D:191:ARG:HB2	2.01	0.43
1:D:7:LEU:O	1:D:85:ILE:HA	2.18	0.43
1:B:321[A]:GLN:OE1	1:B:321[A]:GLN:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ASN:ND2	2:B:600[B]:HOH:O	2.51	0.43
1:B:12:AEI:NH1	1:B:90:ASP:OD2	2.52	0.43
1:C:6:ILE:HA	1:C:84:VAL:O	2.19	0.43
1:A:12[A]:AEI:NH1	1:A:90:ASP:OD2	2.52	0.42
1:C:39:VAL:HG12	1:C:42:LEU:HG	2.01	0.42
1:A:85:ILE:HD12	1:A:85:ILE:N	2.35	0.42
1:C:170:THR:HG23	1:C:171:PHE:CD2	2.55	0.42
1:C:7:LEU:O	1:C:85:ILE:HA	2.19	0.42
1:B:220:TYR:CE2	1:B:223:ALA:HA	2.55	0.41
1:B:246:ASN:OD1	1:B:278:THR:HA	2.21	0.41
1:C:43:LYS:HD3	2:C:631:HOH:O	2.19	0.41
1:D:28:GLY:HA2	1:D:55:ASN:OD1	2.20	0.41
1:A:7:LEU:O	1:A:85:ILE:HA	2.21	0.41
1:B:268:VAL:HG22	1:B:292:VAL:HB	2.01	0.41
1:A:6:ILE:HA	1:A:84:VAL:O	2.21	0.41
1:A:41:GLN:HG2	1:D:21:THR:HB	2.03	0.41
1:C:106:ASP:HB3	1:C:143:ASN:ND2	2.35	0.41
1:C:184:ASN:HB2	1:B:23:SER:OG	2.20	0.41
1:A:214:VAL:HA	1:A:238:GLY:O	2.21	0.40
1:C:21:THR:HG23	1:C:121:MET:HG3	2.04	0.40
1:D:6:ILE:HA	1:D:84:VAL:O	2.20	0.40
1:D:321:GLN:HA	1:D:321:GLN:NE2	2.36	0.40
1:A:179:LEU:HA	1:A:191:ARG:HB2	2.03	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	326/334 (98%)	319 (98%)	7 (2%)	0	100	100
1	B	326/334 (98%)	319 (98%)	6 (2%)	1 (0%)	43	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	325/334 (97%)	319 (98%)	6 (2%)	0	100	100
1	D	325/334 (97%)	315 (97%)	8 (2%)	2 (1%)	27	21
All	All	1302/1336 (98%)	1272 (98%)	27 (2%)	3 (0%)	49	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	220	TYR
1	D	118	SER
1	D	198	THR

### 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	268/272 (98%)	259 (97%)	9 (3%)	40	38
1	B	268/272 (98%)	262 (98%)	6 (2%)	55	58
1	C	267/272 (98%)	255 (96%)	12 (4%)	30	26
1	D	267/272 (98%)	261 (98%)	6 (2%)	55	58
All	All	1070/1088 (98%)	1037 (97%)	33 (3%)	43	42

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	22	LYS
1	A	72	LYS
1	A	103	VAL
1	A	120	SER
1	A	201	THR
1	A	208	LEU
1	A	211	LEU
1	A	222	ASN

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Mol	Chain	Res	Type
1	C	0	HIS
1	C	43	LYS
1	C	51	GLU
1	C	55	ASN
1	C	75	THR
1	C	121	MET
1	C	162	MET
1	C	208	LEU
1	C	211	LEU
1	C	222	ASN
1	C	236	TYR
1	C	254	PHE
1	B	29	LYS
1	B	79	LYS
1	B	121	MET
1	B	211	LEU
1	B	222	ASN
1	B	254	PHE
1	D	34	ASN
1	D	35	LEU
1	D	103	VAL
1	D	208	LEU
1	D	222	ASN
1	D	254	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	318	GLN
1	C	47	ASN
1	C	55	ASN
1	C	64	ASN
1	C	143	ASN
1	C	321	GLN
1	B	64	ASN
1	B	325	GLN
1	D	143	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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
1	AEI	C	12[A]	1	10,14,15	1.99	1 (10%)	11,18,20	3.00	6 (54%)
1	QNY	C	12[B]	1	8,15,16	0.55	0	6,21,23	2.17	2 (33%)
1	QNY	A	12[B]	1	8,15,16	0.91	0	6,21,23	2.26	3 (50%)
1	AEI	B	12	1	10,14,15	1.68	2 (20%)	11,18,20	2.33	4 (36%)
1	AEI	D	12	1	10,14,15	2.56	4 (40%)	11,18,20	1.66	3 (27%)
1	AEI	A	12[A]	1	10,14,15	2.29	2 (20%)	11,18,20	2.42	4 (36%)

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
1	AEI	C	12[A]	1	-	5/12/18/20	-
1	QNY	C	12[B]	1	-	3/8/20/22	-
1	QNY	A	12[B]	1	-	3/8/20/22	-
1	AEI	B	12	1	-	3/12/18/20	-
1	AEI	D	12	1	-	3/12/18/20	-
1	AEI	A	12[A]	1	-	3/12/18/20	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	12[A]	AEI	OG1-CD	5.93	1.51	1.34
1	D	12	AEI	OG1-CD	5.68	1.50	1.34
1	A	12[A]	AEI	OG1-CD	4.89	1.48	1.34
1	D	12	AEI	CZ-NH1	4.53	1.57	1.47
1	A	12[A]	AEI	CE2-CD	-4.39	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	12	AEI	OG1-CD	3.96	1.45	1.34
1	B	12	AEI	CG2-CB	2.45	1.57	1.51
1	D	12	AEI	CG2-CB	2.34	1.57	1.51
1	D	12	AEI	O-C	2.20	1.28	1.19

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	12	AEI	CZ-CE2-CD	-5.63	100.95	112.85
1	C	12[A]	AEI	O-C-CA	-5.34	110.78	124.78
1	A	12[A]	AEI	OE1-CD-CE2	-5.04	113.60	124.73
1	C	12[B]	QNY	O-C-CA	-4.76	112.30	124.78
1	A	12[B]	QNY	OG1-CB-CA	4.50	117.70	106.91
1	C	12[A]	AEI	OG1-CD-CE2	4.11	119.01	111.46
1	C	12[A]	AEI	OG1-CB-CG2	3.94	116.05	108.21
1	D	12	AEI	CZ-CE2-CD	-3.73	104.96	112.85
1	C	12[A]	AEI	CZ-CE2-CD	-3.52	105.40	112.85
1	A	12[A]	AEI	OG1-CD-CE2	3.51	117.91	111.46
1	C	12[A]	AEI	OE1-CD-CE2	-3.39	117.24	124.73
1	B	12	AEI	OG1-CD-CE2	2.94	116.85	111.46
1	C	12[A]	AEI	CG2-CB-CA	2.71	118.51	113.16
1	B	12	AEI	OG1-CB-CA	2.48	111.52	105.89
1	A	12[B]	QNY	O-C-CA	-2.43	118.41	124.78
1	D	12	AEI	OG1-CB-CG2	2.36	112.91	108.21
1	A	12[A]	AEI	OG1-CB-CA	2.23	110.96	105.89
1	A	12[A]	AEI	O-C-CA	-2.20	119.00	124.78
1	B	12	AEI	OE1-CD-CE2	-2.18	119.91	124.73
1	D	12	AEI	CE2-CZ-CH2	-2.16	107.20	110.69
1	A	12[B]	QNY	CG2-CB-CA	-2.12	108.97	113.16
1	C	12[B]	QNY	OE1-CD-OE2	2.06	117.24	110.51

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	12[B]	QNY	O-C-CA-CB
1	C	12[B]	QNY	CD-CE2-CZ-NH1
1	A	12[B]	QNY	O-C-CA-CB
1	A	12[B]	QNY	CD-CE2-CZ-NH1
1	B	12	AEI	O-C-CA-CB
1	D	12	AEI	O-C-CA-CB
1	A	12[A]	AEI	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	B	12	AEI	OE1-CD-CE2-CZ
1	D	12	AEI	OE1-CD-CE2-CZ
1	C	12[B]	QNY	CD-CE2-CZ-CH2
1	A	12[B]	QNY	CD-CE2-CZ-CH2
1	C	12[A]	AEI	OE1-CD-OG1-CB
1	D	12	AEI	OG1-CD-CE2-CZ
1	C	12[A]	AEI	OE1-CD-CE2-CZ
1	C	12[A]	AEI	CE2-CD-OG1-CB
1	A	12[A]	AEI	OE1-CD-CE2-CZ
1	B	12	AEI	OG1-CD-CE2-CZ
1	C	12[A]	AEI	OG1-CD-CE2-CZ
1	A	12[A]	AEI	OG1-CD-CE2-CZ
1	C	12[A]	AEI	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	12	AEI	2	0
1	D	12	AEI	3	0
1	A	12[A]	AEI	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	325/334 (97%)	-0.18	5 (1%) 73 72	20, 31, 47, 74	0
1	B	326/334 (97%)	-0.34	2 (0%) 89 88	20, 27, 44, 54	0
1	C	326/334 (97%)	-0.34	1 (0%) 93 93	20, 27, 44, 65	0
1	D	326/334 (97%)	-0.06	18 (5%) 25 25	18, 27, 69, 147	0
All	All	1303/1336 (97%)	-0.23	26 (1%) 65 63	18, 28, 47, 147	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	26	THR	17.3
1	D	30	VAL	10.2
1	D	25	TYR	7.1
1	D	19	SER	6.5
1	D	28	GLY	6.1
1	D	24	ASN	5.9
1	D	18	ASP	4.4
1	D	29	LYS	3.6
1	D	16	GLY	3.5
1	D	17	GLY	3.4
1	D	21	THR	3.3
1	D	23	SER	3.1
1	D	22	LYS	2.7
1	B	18	ASP	2.5
1	D	37	ASN	2.5
1	D	27	VAL	2.5
1	D	15	GLY	2.4
1	D	31	GLY	2.3
1	A	308	LEU	2.3
1	A	29	LYS	2.2
1	B	0	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	20	ALA	2.2
1	C	33	GLU	2.1
1	A	43	LYS	2.1
1	A	49	LYS	2.1
1	A	304	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<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	B-factors(Å <sup>2</sup> )	Q<0.9
1	AEI	C	12[A]	15/16	0.95	0.12	22,26,30,33	15
1	AEI	D	12	15/16	0.95	0.11	22,31,45,45	0
1	QNY	C	12[B]	16/17	0.96	0.11	19,23,28,28	16
1	AEI	B	12	15/16	0.97	0.07	19,25,32,32	0
1	QNY	A	12[B]	16/17	0.97	0.09	23,25,30,31	16
1	AEI	A	12[A]	15/16	0.97	0.08	18,23,30,35	15

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.