



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:01 PM EDT

PDB ID : 6V2G
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 : 1.90 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 ⓘ symbol.

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

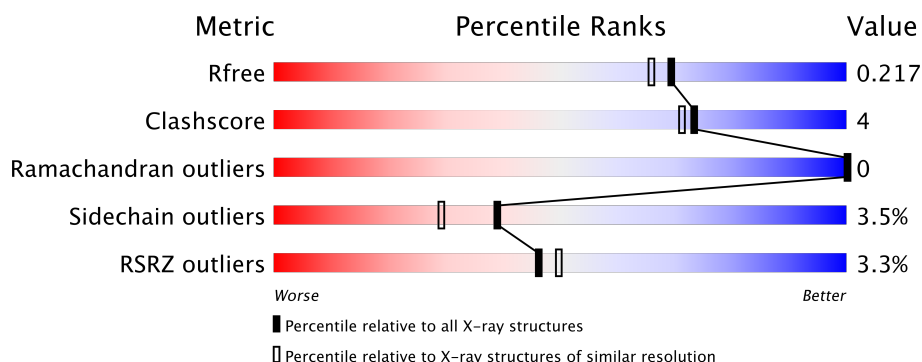
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (1.90-1.90)

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 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	
1	B	334	
1	C	334	
1	D	334	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10946 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	1	0
			2443	1524	415	494	10			
1	B	326	Total	C	N	O	S	0	2	0
			2457	1530	417	501	9			
1	C	327	Total	C	N	O	S	114	2	0
			2472	1538	421	504	9			
1	D	327	Total	C	N	O	S	0	2	0
			2458	1532	419	498	9			

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
B	-6	MET	-	expression tag	UNP P00805
B	-5	HIS	-	expression tag	UNP P00805
B	-4	HIS	-	expression tag	UNP P00805
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
C	-6	MET	-	expression tag	UNP P00805
C	-5	HIS	-	expression tag	UNP P00805
C	-4	HIS	-	expression tag	UNP P00805

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

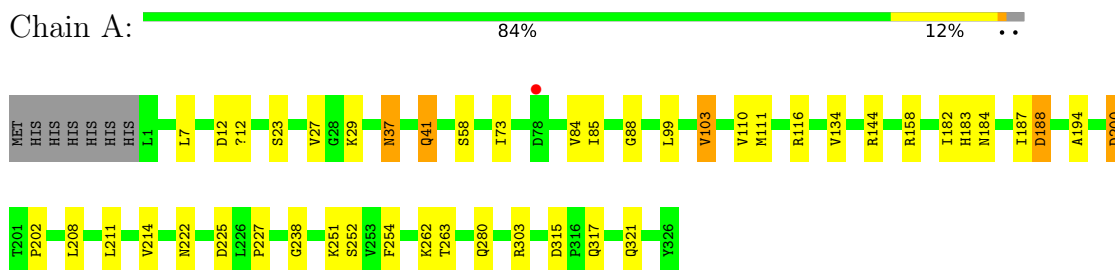
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	282	Total O 282 282	0	0
2	B	273	Total O 274 274	0	2
2	C	261	Total O 263 263	0	3
2	D	294	Total O 297 297	0	3

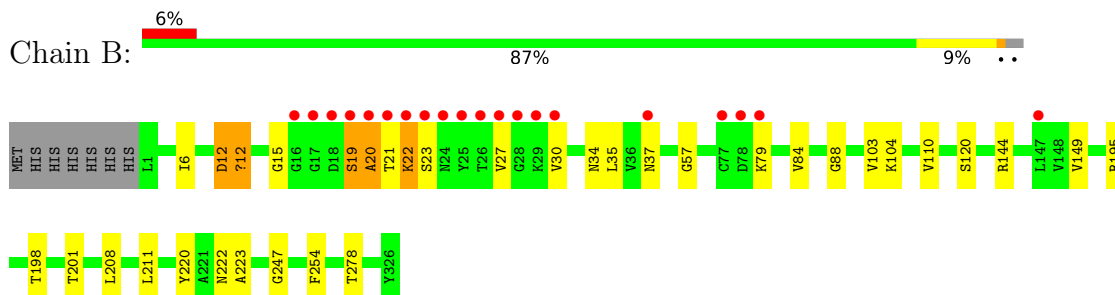
3 Residue-property plots [i](#)

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.

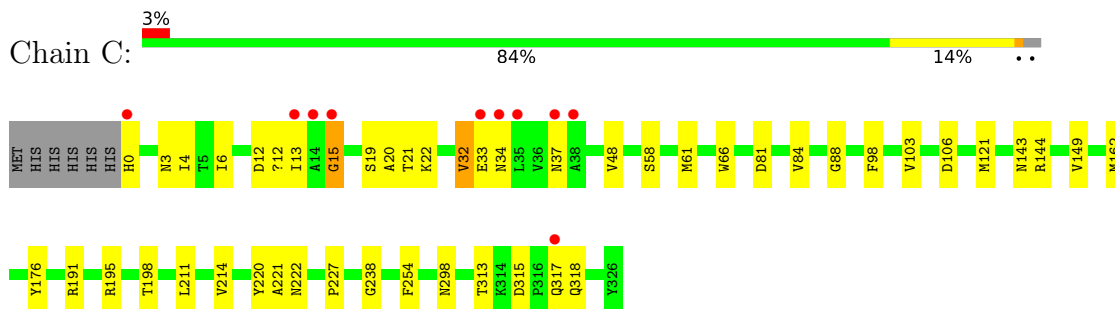
• Molecule 1: L-asparaginase 2



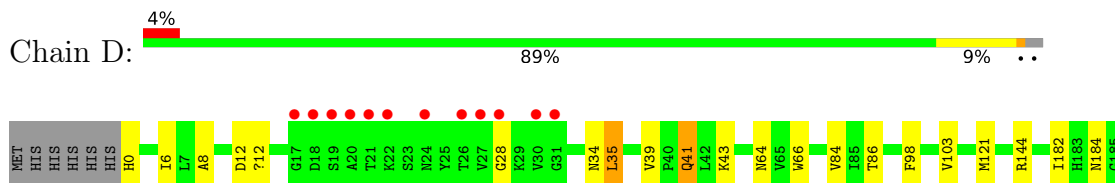
• Molecule 1: L-asparaginase 2

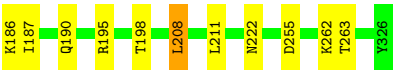


• Molecule 1: L-asparaginase 2



• Molecule 1: L-asparaginase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.10Å 125.97Å 76.38Å 90.00° 96.70° 90.00°	Depositor
Resolution (Å)	24.93 – 1.90 24.92 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.5 (24.93-1.90) 96.5 (24.92-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.149 , 0.207 0.159 , 0.217	Depositor DCC
R_{free} test set	2673 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10946	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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: 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	1.07	4/2467 (0.2%)	1.18	5/3357 (0.1%)
1	B	1.04	2/2465 (0.1%)	1.11	3/3355 (0.1%)
1	C	1.14	4/2478 (0.2%)	1.27	12/3373 (0.4%)
1	D	1.05	3/2487 (0.1%)	1.12	2/3385 (0.1%)
All	All	1.08	13/9897 (0.1%)	1.17	22/13470 (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	A	0	3
1	B	0	1
1	C	0	3
1	D	0	1
All	All	0	8

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	32	VAL	C-N	-21.84	0.83	1.34
1	C	0	HIS	N-CA	7.81	1.61	1.46
1	D	0	HIS	N-CA	7.47	1.61	1.46
1	D	186	LYS	C-O	6.01	1.34	1.23
1	A	134	VAL	C-O	5.99	1.34	1.23
1	A	111	MET	C-O	5.87	1.34	1.23
1	D	121	MET	C-O	5.67	1.34	1.23
1	A	280	GLN	C-O	5.54	1.33	1.23
1	B	144	ARG	C-O	5.46	1.33	1.23
1	B	15	GLY	C-O	5.26	1.32	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	13	ILE	N-CA	5.16	1.56	1.46
1	C	221	ALA	C-O	5.07	1.32	1.23
1	A	23	SER	CA-CB	-5.05	1.45	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	15	GLY	O-C-N	-21.48	86.69	123.20
1	C	144	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	C	32	VAL	O-C-N	-8.43	109.21	122.70
1	C	191	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	C	61	MET	CG-SD-CE	7.80	112.67	100.20
1	C	15	GLY	C-N-CA	7.76	138.59	122.30
1	A	188	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	C	15	GLY	CA-C-N	6.17	128.54	116.20
1	A	158	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	C	195	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	200	ASP	CB-CA-C	-5.81	98.78	110.40
1	B	195	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	144	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	D	144	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	C	144	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	D	195	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	B	144	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	116	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	162	MET	CG-SD-CE	5.39	108.82	100.20
1	C	195	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	20	ALA	C-N-CA	5.14	134.56	121.70
1	C	20	ALA	C-N-CA	5.13	134.53	121.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	HIS	Mainchain
1	A	27	VAL	Peptide
1	A	37	ASN	Mainchain
1	B	12[B]	QNY	Mainchain
1	C	15	GLY	Mainchain,Peptide
1	C	32	VAL	Mainchain
1	D	28	GLY	Peptide

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	2443	0	2432	18	1
1	B	2457	0	2427	15	0
1	C	2472	0	2430	20	0
1	D	2458	0	2438	18	1
2	A	282	0	0	3	0
2	B	274	0	0	2	0
2	C	263	0	0	6	0
2	D	297	0	0	4	0
All	All	10946	0	9727	65	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 4.

All (65) 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:A:188:ASP:O	2:A:401:HOH:O	2.07	0.72
1:A:12:AEI:CD	2:A:483:HOH:O	2.44	0.65
1:B:12[A]:AEI:CD	2:B:449[A]:HOH:O	2.44	0.64
1:D:41:GLN:HE21	1:D:41:GLN:H	1.47	0.61
1:D:263:THR:HG22	1:D:263:THR:O	2.02	0.59
1:C:121:MET:HE1	1:D:39:VAL:HG13	1.86	0.58
1:D:41:GLN:H	1:D:41:GLN:NE2	2.04	0.56
1:A:41:GLN:H	1:A:41:GLN:NE2	2.04	0.56
1:C:103:VAL:O	1:C:198:THR:HA	2.07	0.54
1:C:176:TYR:OH	2:C:408:HOH:O	2.17	0.54
1:C:121:MET:CE	1:D:39:VAL:HG13	2.37	0.54
1:C:58:SER:HB3	1:C:88:GLY:HA3	1.91	0.53
1:C:220:TYR:OH	2:C:496[B]:HOH:O	2.19	0.53
1:A:99:LEU:O	1:A:103:VAL:HG13	2.09	0.53
1:C:3:ASN:O	1:C:81:ASP:HB2	2.09	0.52
1:D:103:VAL:O	1:D:198:THR:HA	2.10	0.52
1:A:225:ASP:HB3	1:A:252:SER:HB3	1.94	0.50
1:B:12[A]:AEI:OT2	1:B:88:GLY:HA3	2.12	0.50
1:B:104:LYS:NZ	1:B:201:THR:O	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:GLU:O	1:C:37:ASN:ND2	2.45	0.49
1:B:103:VAL:O	1:B:198:THR:HA	2.13	0.49
1:C:121:MET:HE1	1:D:39:VAL:CG1	2.42	0.49
1:C:6:ILE:HA	1:C:84:VAL:O	2.13	0.49
1:B:19:SER:HB2	1:B:22:LYS:HE3	1.95	0.49
1:A:184:ASN:HB2	1:B:23:SER:OG	2.13	0.49
1:D:66:TRP:HB3	1:D:98:PHE:CE2	2.47	0.48
1:C:315:ASP:HB3	1:C:318:GLN:HB2	1.95	0.48
1:A:321:GLN:HG2	2:A:449:HOH:O	2.13	0.48
1:D:208:LEU:HD13	2:D:674:HOH:O	2.12	0.48
1:C:12[A]:AEI:CD	2:C:449[A]:HOH:O	2.62	0.47
1:B:84:VAL:HA	1:B:110:VAL:O	2.15	0.47
1:B:20:ALA:HA	1:B:120:SER:HA	1.98	0.46
2:C:517:HOH:O	1:D:184:ASN:HB2	2.15	0.46
1:A:58:SER:HB3	1:A:88:GLY:HA3	1.97	0.45
1:A:84:VAL:HA	1:A:110:VAL:O	2.16	0.45
1:B:27:VAL:HG11	1:B:57:GLY:HA3	1.99	0.45
1:C:66:TRP:HB3	1:C:98:PHE:CE2	2.52	0.45
1:A:194:ALA:HB3	1:D:190:GLN:HA	1.97	0.45
1:A:227:PRO:HB3	1:C:227:PRO:HB3	1.97	0.45
1:B:30:VAL:HG13	1:B:34:ASN:HB3	1.99	0.45
1:D:12:AEI:CD	2:D:522:HOH:O	2.64	0.45
1:B:6:ILE:HA	1:B:84:VAL:O	2.17	0.45
1:A:7:LEU:O	1:A:85:ILE:HA	2.16	0.45
1:C:106:ASP:HB3	1:C:143:ASN:ND2	2.32	0.44
1:B:247:GLY:HA3	1:B:278:THR:HG23	1.98	0.44
1:C:313:THR:OG1	1:C:318:GLN:NE2	2.51	0.43
1:A:214:VAL:HA	1:A:238:GLY:O	2.19	0.43
1:B:220:TYR:CE2	1:B:223:ALA:HA	2.54	0.43
1:D:6:ILE:HA	1:D:84:VAL:O	2.18	0.43
1:D:64:ASN:ND2	2:D:420:HOH:O	2.52	0.42
1:C:149:VAL:HG12	2:C:460:HOH:O	2.18	0.42
1:A:214:VAL:HG12	1:A:303:ARG:HG3	2.02	0.42
1:C:214:VAL:HA	1:C:238:GLY:O	2.20	0.42
1:B:34:ASN:ND2	1:B:34:ASN:O	2.53	0.42
1:D:8:ALA:HA	1:D:86:THR:OG1	2.20	0.42
1:A:41:GLN:H	1:A:41:GLN:HE21	1.66	0.41
1:A:315:ASP:OD2	1:A:317:GLN:NE2	2.53	0.41
1:A:182:ILE:HG12	1:A:187:ILE:HG12	2.01	0.41
1:C:4:ILE:O	1:C:48:VAL:HA	2.21	0.41
1:D:182:ILE:HG12	1:D:187:ILE:HG12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LEU:HD22	2:D:596:HOH:O	2.20	0.41
1:D:34:ASN:HA	1:D:34:ASN:HD22	1.66	0.41
1:B:149:VAL:HG12	2:B:534:HOH:O	2.21	0.40
1:A:73:ILE:HD11	1:A:85:ILE:HD11	2.03	0.40
1:C:298:ASN:HA	2:C:578:HOH:O	2.20	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:262:LYS:NZ	1:D:255:ASP:OD1[1_554]	2.19	0.01

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	324/334 (97%)	319 (98%)	5 (2%)	0	100	100
1	B	324/334 (97%)	317 (98%)	7 (2%)	0	100	100
1	C	325/334 (97%)	312 (96%)	13 (4%)	0	100	100
1	D	326/334 (98%)	321 (98%)	5 (2%)	0	100	100
All	All	1299/1336 (97%)	1269 (98%)	30 (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	266/272 (98%)	254 (96%)	12 (4%)	30	20
1	B	266/272 (98%)	256 (96%)	10 (4%)	36	26
1	C	267/272 (98%)	259 (97%)	8 (3%)	44	36
1	D	268/272 (98%)	261 (97%)	7 (3%)	49	42
All	All	1067/1088 (98%)	1030 (96%)	37 (4%)	39	29

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	37	ASN
1	A	41	GLN
1	A	103	VAL
1	A	200	ASP
1	A	202	PRO
1	A	208	LEU
1	A	211	LEU
1	A	222	ASN
1	A	251	LYS
1	A	254	PHE
1	A	263	THR
1	B	19	SER
1	B	21	THR
1	B	22	LYS
1	B	35	LEU
1	B	37	ASN
1	B	79	LYS
1	B	208	LEU
1	B	211	LEU
1	B	222	ASN
1	B	254	PHE
1	C	19	SER
1	C	21	THR
1	C	22	LYS
1	C	34	ASN
1	C	211	LEU
1	C	222	ASN
1	C	254	PHE
1	C	317	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	35	LEU
1	D	41	GLN
1	D	43	LYS
1	D	208	LEU
1	D	211	LEU
1	D	222	ASN
1	D	262	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	64	ASN
1	A	318	GLN
1	B	64	ASN
1	C	37	ASN
1	C	143	ASN
1	C	318	GLN
1	D	34	ASN
1	D	37	ASN
1	D	41	GLN
1	D	64	ASN
1	D	318	GLN

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	A	12	1	10,14,15	1.85	2 (20%)	11,18,20	1.34	2 (18%)
1	QNY	B	12[B]	1	8,15,16	1.12	0	6,21,23	2.07	2 (33%)
1	QNY	C	12[B]	1	8,15,16	1.19	0	6,21,23	2.83	2 (33%)
1	AEI	D	12	1	10,14,15	1.78	1 (10%)	11,18,20	2.64	5 (45%)
1	AEI	B	12[A]	1	10,14,15	2.22	1 (10%)	11,18,20	1.83	2 (18%)
1	AEI	C	12[A]	1	10,14,15	3.03	3 (30%)	11,18,20	2.90	5 (45%)

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	A	12	1	-	3/12/18/20	-
1	QNY	B	12[B]	1	-	3/8/20/22	-
1	QNY	C	12[B]	1	-	2/8/20/22	-
1	AEI	D	12	1	-	3/12/18/20	-
1	AEI	B	12[A]	1	-	3/12/18/20	-
1	AEI	C	12[A]	1	-	5/12/18/20	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	12[A]	AEI	OG1-CD	8.77	1.59	1.34
1	B	12[A]	AEI	OG1-CD	6.40	1.52	1.34
1	D	12	AEI	OG1-CD	4.71	1.47	1.34
1	A	12	AEI	OG1-CD	4.67	1.47	1.34
1	C	12[A]	AEI	OE1-CD	2.62	1.30	1.22
1	A	12	AEI	OG1-CB	-2.16	1.43	1.46
1	C	12[A]	AEI	O-C	2.05	1.28	1.19

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	12	AEI	CZ-CE2-CD	-6.82	98.43	112.85
1	C	12[B]	QNY	OG1-CB-CA	5.40	119.87	106.91
1	C	12[A]	AEI	CZ-CE2-CD	-5.05	102.17	112.85
1	C	12[A]	AEI	OE1-CD-CE2	-4.71	114.33	124.73
1	C	12[A]	AEI	OG1-CB-CA	4.28	115.61	105.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	12[B]	QNY	CG2-CB-CA	-4.21	104.86	113.16
1	B	12[A]	AEI	CZ-CE2-CD	-3.84	104.72	112.85
1	C	12[A]	AEI	OG1-CD-CE2	3.50	117.89	111.46
1	B	12[A]	AEI	OG1-CB-CA	3.37	113.56	105.89
1	D	12	AEI	OG1-CB-CG2	3.16	114.49	108.21
1	B	12[B]	QNY	CG2-CB-CA	-3.14	106.96	113.16
1	A	12	AEI	CZ-CE2-CD	-2.83	106.87	112.85
1	B	12[B]	QNY	OG1-CB-CA	2.76	113.54	106.91
1	D	12	AEI	OE1-CD-CE2	-2.56	119.06	124.73
1	D	12	AEI	O-C-CA	-2.27	118.82	124.78
1	C	12[A]	AEI	OG1-CB-CG2	2.24	112.67	108.21
1	A	12	AEI	OE1-CD-CE2	-2.21	119.86	124.73
1	D	12	AEI	OG1-CD-CE2	2.05	115.22	111.46

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	12	AEI	O-C-CA-CB
1	B	12[B]	QNY	O-C-CA-CB
1	C	12[B]	QNY	O-C-CA-CB
1	C	12[B]	QNY	CD-CE2-CZ-NH1
1	D	12	AEI	O-C-CA-CB
1	C	12[A]	AEI	O-C-CA-CB
1	B	12[B]	QNY	CD-CE2-CZ-NH1
1	B	12[A]	AEI	OE1-CD-CE2-CZ
1	A	12	AEI	OG1-CD-CE2-CZ
1	D	12	AEI	OG1-CD-CE2-CZ
1	B	12[A]	AEI	OG1-CD-CE2-CZ
1	A	12	AEI	OE1-CD-CE2-CZ
1	D	12	AEI	OE1-CD-CE2-CZ
1	C	12[A]	AEI	OE1-CD-CE2-CZ
1	C	12[A]	AEI	OG1-CD-CE2-CZ
1	C	12[A]	AEI	CD-CE2-CZ-NH1
1	B	12[B]	QNY	C-CA-CB-OG1
1	C	12[A]	AEI	C-CA-CB-OG1
1	B	12[A]	AEI	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	12	AEI	1	0
1	D	12	AEI	1	0
1	B	12[A]	AEI	2	0
1	C	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	32:VAL	C	33:GLU	N	0.83

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	325/334 (97%)	-0.11	1 (0%) 93 94	23, 31, 49, 80	0
1	B	325/334 (97%)	0.11	20 (6%) 20 24	22, 31, 65, 113	0
1	C	309/334 (92%)	0.10	10 (3%) 47 51	24, 34, 56, 88	0
1	D	326/334 (97%)	-0.08	12 (3%) 41 45	22, 29, 51, 73	0
All	All	1285/1336 (96%)	0.00	43 (3%) 46 50	22, 31, 54, 113	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	18	ASP	6.6
1	B	17	GLY	6.3
1	B	23	SER	6.0
1	B	29	LYS	5.8
1	B	27	VAL	4.9
1	C	15	GLY	4.9
1	B	19	SER	4.9
1	D	18	ASP	4.5
1	B	21	THR	4.0
1	C	35	LEU	4.0
1	B	22	LYS	3.9
1	B	28	GLY	3.8
1	B	16	GLY	3.8
1	B	24	ASN	3.7
1	D	24	ASN	3.6
1	D	21	THR	3.5
1	B	26	THR	3.5
1	C	0	HIS	3.4
1	D	28	GLY	3.4
1	C	14	ALA	3.4
1	D	31	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	30	VAL	3.2
1	D	19	SER	3.0
1	D	26	THR	2.9
1	B	25	TYR	2.9
1	C	34	ASN	2.9
1	B	37	ASN	2.9
1	D	17	GLY	2.7
1	A	78	ASP	2.7
1	B	77	CYS	2.5
1	C	37	ASN	2.4
1	D	20	ALA	2.4
1	D	30	VAL	2.4
1	B	20	ALA	2.2
1	C	317	GLN	2.2
1	D	27	VAL	2.2
1	B	147	LEU	2.1
1	B	78	ASP	2.1
1	C	33	GLU	2.1
1	B	79	LYS	2.1
1	D	22	LYS	2.1
1	C	38	ALA	2.0
1	C	13	ILE	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, 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
1	QNY	C	12[B]	16/17	0.93	0.12	23,31,37,40	16
1	AEI	C	12[A]	15/16	0.93	0.12	24,34,48,48	15
1	AEI	B	12[A]	15/16	0.94	0.09	22,26,42,44	15
1	QNY	B	12[B]	16/17	0.95	0.10	24,26,36,38	16
1	AEI	A	12	15/16	0.95	0.09	24,27,30,34	0
1	AEI	D	12	15/16	0.96	0.09	25,29,40,43	0

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.