



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:56 PM UTC

PDB ID : 6V2C / pdb_00006v2c
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

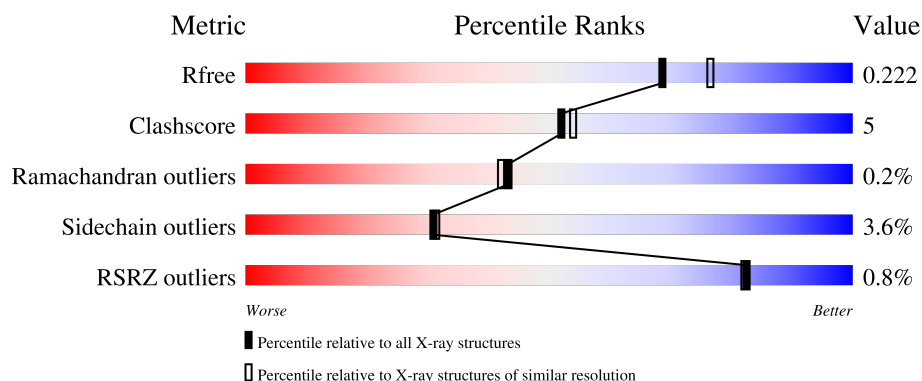
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 72% 23% ...
1	B	334	 79% 17% ..
1	C	334	 78% 18% ..
1	D	334	 78% 18% ..

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

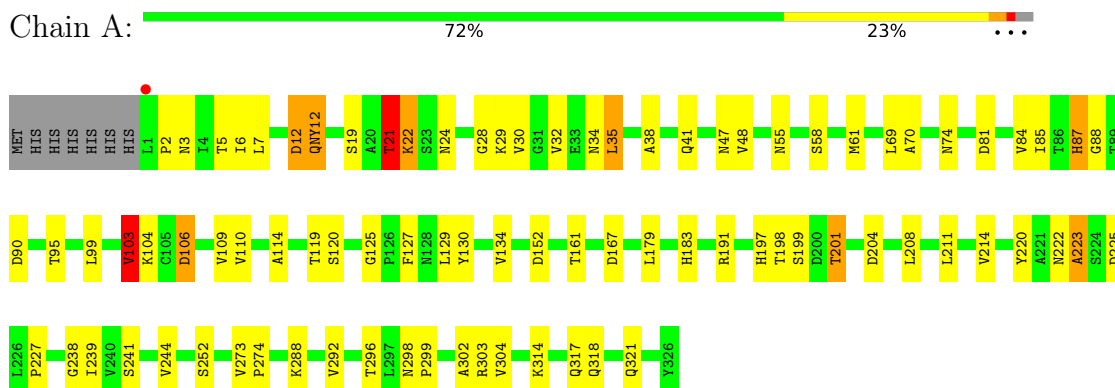
- Molecule 2 is water.

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

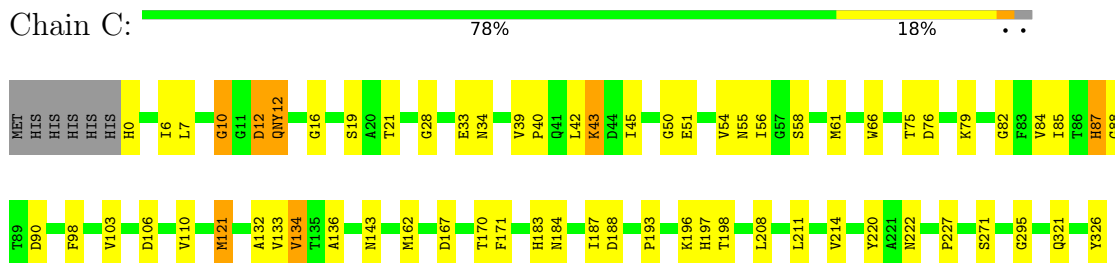
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

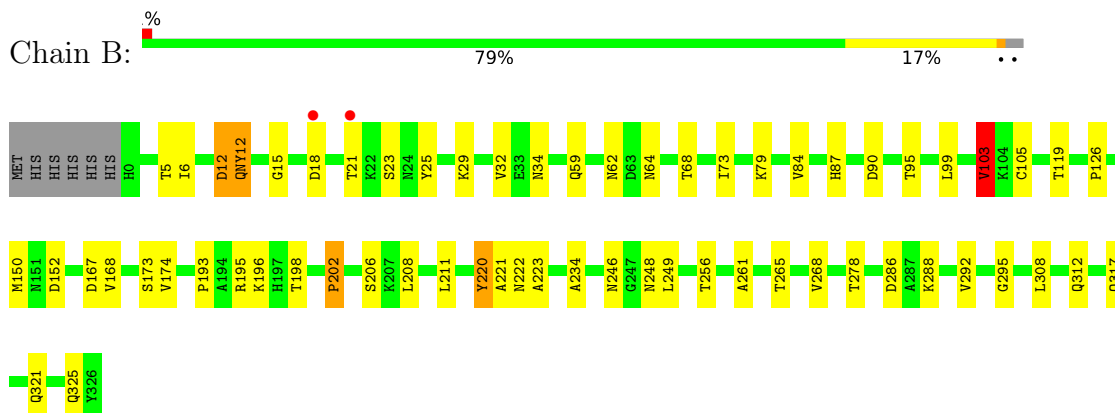
• Molecule 1: L-asparaginase 2



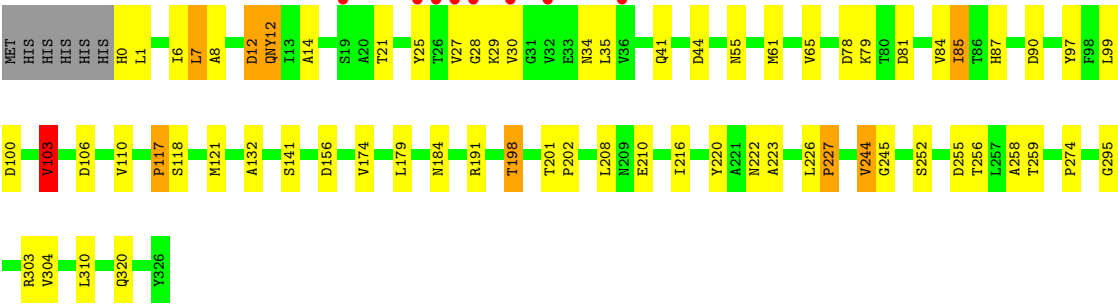
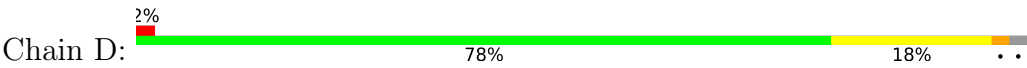
• Molecule 1: L-asparaginase 2



• 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, α , β , γ	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) 95.7 (27.69-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (2.69%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10815	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QNY, AEI

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	1.49	22/2486 (0.9%)	1.56	17/3384 (0.5%)
1	B	1.45	21/2485 (0.8%)	1.50	16/3382 (0.5%)
1	C	1.49	15/2478 (0.6%)	1.51	15/3373 (0.4%)
1	D	1.51	21/2478 (0.8%)	1.58	16/3372 (0.5%)
All	All	1.49	79/9927 (0.8%)	1.54	64/13511 (0.5%)

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 (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	174	VAL	C-O	-9.37	1.11	1.24
1	B	167	ASP	C-O	-9.07	1.13	1.23
1	A	239	ILE	C-O	8.96	1.33	1.24
1	D	202	PRO	C-O	-8.33	1.13	1.24
1	A	69	LEU	C-O	-8.07	1.14	1.24
1	D	8	ALA	C-O	8.06	1.33	1.23
1	D	310	LEU	C-O	-7.96	1.13	1.24
1	A	114	ALA	C-O	7.69	1.32	1.23
1	B	25	TYR	C-O	7.68	1.32	1.23
1	D	97	TYR	C-O	-7.65	1.15	1.24
1	C	295	GLY	C-O	7.54	1.33	1.24
1	B	174	VAL	C-O	-7.50	1.14	1.24
1	B	202	PRO	C-O	-7.23	1.15	1.24
1	D	258	ALA	C-O	-7.22	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	ASP	C-O	7.07	1.32	1.23
1	C	214	VAL	C-O	7.05	1.31	1.24
1	C	134	VAL	C-O	7.01	1.32	1.24
1	D	132	ALA	C-O	-6.97	1.16	1.24
1	C	271	SER	C-O	6.89	1.32	1.23
1	D	274	PRO	C-O	-6.89	1.15	1.24
1	B	150	MET	C-O	6.59	1.31	1.23
1	A	241	SER	CA-CB	-6.54	1.44	1.53
1	B	15	GLY	C-O	6.33	1.33	1.23
1	A	127	PHE	C-O	6.31	1.31	1.24
1	A	87	HIS	CE1-NE2	6.29	1.38	1.32
1	D	141	SER	CA-CB	-6.28	1.42	1.53
1	B	286	ASP	C-O	6.27	1.31	1.24
1	A	292	VAL	C-O	6.20	1.30	1.24
1	B	119	THR	C-O	-6.15	1.16	1.24
1	B	168	VAL	C-O	-6.14	1.16	1.24
1	A	296	THR	C-O	6.04	1.32	1.24
1	D	61	MET	CG-SD	6.04	1.95	1.80
1	A	134	VAL	C-O	5.96	1.30	1.24
1	B	68	THR	C-O	5.92	1.30	1.24
1	C	197	HIS	CE1-NE2	5.83	1.38	1.32
1	D	244	VAL	C-O	5.82	1.31	1.24
1	D	85	ILE	C-O	5.79	1.30	1.24
1	A	106	ASP	C-O	5.77	1.31	1.24
1	A	223	ALA	C-O	5.76	1.30	1.23
1	B	87	HIS	C-O	5.70	1.30	1.23
1	A	109	VAL	C-O	-5.69	1.17	1.24
1	C	56	ILE	C-O	5.69	1.29	1.23
1	A	304	VAL	C-O	5.60	1.30	1.24
1	A	48	VAL	C-O	-5.60	1.17	1.24
1	A	19	SER	C-O	5.58	1.30	1.23
1	D	256	THR	C-O	5.57	1.30	1.24
1	B	173	SER	C-O	5.53	1.31	1.23
1	D	210	GLU	C-O	5.52	1.30	1.23
1	A	2	PRO	C-O	5.48	1.30	1.23
1	C	87	HIS	C-O	5.47	1.30	1.23
1	D	106	ASP	C-O	5.46	1.31	1.24
1	C	82	GLY	C-O	5.46	1.30	1.24
1	B	256	THR	C-O	5.44	1.30	1.24
1	D	156	ASP	C-O	5.42	1.30	1.23
1	D	227	PRO	C-O	-5.42	1.16	1.24
1	C	79	LYS	C-O	5.41	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	7	LEU	C-O	5.40	1.30	1.24
1	C	188	ASP	CG-OD2	-5.38	1.15	1.25
1	D	295	GLY	C-O	5.37	1.30	1.24
1	B	62	ASN	C-O	5.33	1.30	1.23
1	C	10	GLY	C-O	5.33	1.31	1.23
1	B	195	ARG	N-CA	5.30	1.52	1.46
1	C	132	ALA	C-O	-5.29	1.17	1.24
1	A	5	THR	C-O	5.28	1.30	1.24
1	A	197	HIS	CD2-NE2	-5.26	1.32	1.37
1	B	234	ALA	C-O	-5.26	1.17	1.24
1	B	221	ALA	C-O	-5.23	1.17	1.23
1	D	255	ASP	CG-OD2	-5.23	1.15	1.25
1	D	304	VAL	C-O	5.23	1.30	1.24
1	B	248	ASN	C-O	5.21	1.30	1.23
1	A	161	THR	C-O	5.18	1.30	1.23
1	B	308	LEU	C-O	5.17	1.30	1.24
1	A	314	LYS	C-O	5.13	1.31	1.24
1	C	45	ILE	N-CA	5.13	1.50	1.46
1	C	183	HIS	C-O	5.12	1.29	1.23
1	A	152	ASP	CG-OD2	-5.12	1.15	1.25
1	B	59	GLN	C-O	5.11	1.30	1.24
1	B	193	PRO	C-O	-5.09	1.18	1.23
1	C	326	TYR	C-OXT	-5.09	1.13	1.23

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	ASP	CA-CB-CG	8.98	121.58	112.60
1	A	125	GLY	O-C-N	-7.64	118.32	121.07
1	A	21	THR	N-CA-CB	-7.50	98.83	111.27
1	B	87	HIS	CA-CB-CG	7.36	121.16	113.80
1	A	129	LEU	N-CA-C	-7.25	103.31	111.07
1	D	103	VAL	N-CA-CB	7.24	119.21	110.31
1	A	103	VAL	N-CA-CB	7.09	118.45	110.72
1	C	188	ASP	CA-CB-CG	-7.00	105.59	112.60
1	D	100	ASP	CA-CB-CG	6.75	119.35	112.60
1	D	65	VAL	N-CA-C	-6.51	103.90	111.00
1	A	204	ASP	CA-CB-CG	6.42	119.02	112.60
1	C	16	GLY	CA-C-N	6.42	128.18	122.47
1	C	16	GLY	C-N-CA	6.42	128.18	122.47
1	D	117	PRO	CA-C-N	6.37	133.71	121.54
1	D	117	PRO	C-N-CA	6.37	133.71	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	50	GLY	CA-C-O	-6.36	114.77	120.75
1	A	87	HIS	CA-CB-CG	6.30	120.10	113.80
1	D	259	THR	CA-CB-OG1	-6.29	100.16	109.60
1	B	95	THR	CA-CB-OG1	-6.21	100.28	109.60
1	D	44	ASP	CA-C-N	-6.03	115.44	122.14
1	D	44	ASP	C-N-CA	-6.03	115.44	122.14
1	C	136	ALA	N-CA-C	-6.03	104.82	111.82
1	A	32	VAL	CA-C-O	-6.01	114.80	121.05
1	C	321	GLN	N-CA-C	-6.01	104.73	111.28
1	B	167	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	274	PRO	N-CA-C	5.76	121.06	113.86
1	A	47	ASN	CA-CB-CG	-5.74	106.86	112.60
1	B	174	VAL	CA-C-O	-5.73	112.65	119.58
1	D	90	ASP	CA-CB-CG	5.72	118.33	112.60
1	D	274	PRO	N-CA-C	5.71	120.99	113.86
1	C	167	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	34	ASN	CB-CA-C	5.68	119.87	110.90
1	A	95	THR	CA-CB-OG1	-5.67	101.09	109.60
1	A	317	GLN	N-CA-C	-5.62	105.23	111.36
1	A	21	THR	CB-CA-C	5.61	119.87	110.44
1	C	183	HIS	CA-CB-CG	-5.52	108.28	113.80
1	B	105	CYS	N-CA-C	-5.52	100.29	109.46
1	D	87	HIS	CA-CB-CG	5.47	119.27	113.80
1	A	302	ALA	N-CA-C	-5.42	105.37	111.28
1	D	78	ASP	CA-CB-CG	-5.42	107.18	112.60
1	A	74	ASN	CA-C-N	5.38	127.93	120.29
1	A	74	ASN	C-N-CA	5.38	127.93	120.29
1	B	206	SER	CA-C-O	-5.36	114.84	120.63
1	C	187	ILE	CA-C-N	-5.31	115.47	122.85
1	C	187	ILE	C-N-CA	-5.31	115.47	122.85
1	C	19	SER	CA-C-N	5.30	127.91	120.28
1	C	19	SER	C-N-CA	5.30	127.91	120.28
1	B	295	GLY	CA-C-O	-5.30	114.69	122.06
1	B	103	VAL	N-CA-CB	5.27	117.48	110.26
1	B	221	ALA	N-CA-C	-5.25	102.28	110.10
1	D	252	SER	N-CA-C	-5.19	105.69	112.23
1	D	81	ASP	N-CA-C	-5.18	107.00	113.38
1	C	33	GLU	CB-CG-CD	5.17	121.39	112.60
1	C	193	PRO	CA-C-O	-5.17	115.44	121.34
1	B	73	ILE	CA-C-N	5.16	127.51	120.54
1	B	73	ILE	C-N-CA	5.16	127.51	120.54
1	D	303	ARG	N-CA-CB	5.14	117.47	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ALA	N-CA-C	-5.14	105.76	111.36
1	B	5	THR	CA-CB-OG1	-5.09	101.96	109.60
1	A	273	VAL	CB-CA-C	5.09	116.39	110.89
1	C	54	VAL	O-C-N	5.08	128.92	122.57
1	B	32	VAL	N-CA-C	-5.05	105.62	110.72
1	D	320	GLN	CB-CA-C	-5.03	102.45	110.79
1	B	18	ASP	CA-CB-CG	5.02	117.62	112.60

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	26	0
1	D	2453	0	2439	24	0
2	A	227	0	0	2	0
2	B	235	0	0	2	0
2	C	263	0	0	5	0
2	D	240	0	0	3	0
All	All	10815	0	9754	97	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 (97) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:C:121:MET:HE1	1:B:126:PRO:CB	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: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:C:103:VAL:O	1:C:198:THR:HA	2.15	0.46
1:B:317:GLN:O	1:B:321[B]:GLN:HG2	2.15	0.46
1:A:214:VAL:CG1	1:A:303:ARG:HG3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:O	1:A:38:ALA:HB3	2.16	0.46
1:A:61:MET:HE3	1:A:87:HIS:NE2	2.31	0.46
1:D:0:HIS:ND1	1:D:1:LEU:O	2.49	0.46
1:A:28:GLY:HA2	1:A:55:ASN:OD1	2.16	0.45
1:A:84:VAL:HA	1:A:110:VAL:O	2.15	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:C:61:MET:HE3	1:C:87:HIS:NE2	2.31	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:HG2	1:D:79:LYS:O	2.17	0.44
1:C:106:ASP:HB3	1:C:143:ASN:HD22	1.82	0.44
1:D:244:VAL:O	1:D:245:GLY:C	2.60	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:C:121:MET:HE1	1:B:126:PRO:HB3	1.98	0.43
1:C:133:VAL:O	1:C:134:VAL:C	2.61	0.43
1:B:90:ASP:HB3	1:D:244:VAL:HB	2.01	0.43
1:D:84:VAL:HA	1:D:110:VAL:O	2.18	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:7:LEU:O	1:D:85:ILE:HA	2.18	0.43
1:D:179:LEU:HA	1:D:191:ARG:HB2	2.01	0.43
1:B:64:ASN:ND2	2:B:600[B]:HOH:O	2.51	0.43
1:B:321[A]:GLN:HA	1:B:321[A]:GLN:OE1	2.17	0.43
1:C:6:ILE:HA	1:C:84:VAL:O	2.19	0.43
1:B:12:AEI:NH1	1:B:90:ASP:OD2	2.52	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:D:121[A]:MET:HE2	1:D:121[A]:MET:HB3	1.63	0.41
1:A:106:ASP:OD2	1:A:199:SER:OG	2.28	0.41
1:B:246:ASN:OD1	1:B:278:THR:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:179:LEU:HA	1:A:191:ARG:HB2	2.03	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	326/334 (98%)	319 (98%)	7 (2%)	0	100	100
1	B	326/334 (98%)	319 (98%)	6 (2%)	1 (0%)	36	35
1	C	325/334 (97%)	319 (98%)	6 (2%)	0	100	100
1	D	325/334 (97%)	315 (97%)	8 (2%)	2 (1%)	21	17
All	All	1302/1336 (98%)	1272 (98%)	27 (2%)	3 (0%)	43	42

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%)	255 (95%)	13 (5%)	22	20
1	B	268/272 (98%)	260 (97%)	8 (3%)	36	38
1	C	267/272 (98%)	257 (96%)	10 (4%)	30	30
1	D	267/272 (98%)	260 (97%)	7 (3%)	40	44
All	All	1070/1088 (98%)	1032 (96%)	38 (4%)	31	31

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	22	LYS
1	A	29	LYS
1	A	30	VAL
1	A	35	LEU
1	A	103	VAL
1	A	119	THR
1	A	120	SER
1	A	201	THR
1	A	208	LEU
1	A	211	LEU
1	A	222	ASN
1	A	288	LYS
1	C	0	HIS
1	C	43	LYS
1	C	51	GLU
1	C	75	THR
1	C	121	MET
1	C	162	MET
1	C	196	LYS
1	C	208	LEU
1	C	211	LEU
1	C	222	ASN
1	B	29	LYS

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Mol	Chain	Res	Type
1	B	79	LYS
1	B	103	VAL
1	B	208	LEU
1	B	211	LEU
1	B	222	ASN
1	B	249	LEU
1	B	288	LYS
1	D	29	LYS
1	D	34	ASN
1	D	35	LEU
1	D	103	VAL
1	D	201	THR
1	D	208	LEU
1	D	222	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	GLN
1	A	307	GLN
1	A	318	GLN
1	C	55	ASN
1	C	64	ASN
1	C	143	ASN
1	C	248	ASN
1	C	321	GLN
1	C	325	GLN
1	B	52	GLN
1	B	64	ASN
1	B	183	HIS
1	B	312	GLN
1	B	325	GLN
1	D	143	ASN
1	D	248	ASN
1	D	312	GLN
1	D	317	GLN
1	D	321	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	QNY	C	12[B]	1	10,15,16	0.73	0	7,21,23	1.99	1 (14%)
1	QNY	A	12[B]	1	10,15,16	0.79	0	7,21,23	2.16	3 (42%)
1	AEI	B	12	1	12,14,15	1.56	2 (16%)	12,18,20	2.16	4 (33%)
1	AEI	D	12	1	12,14,15	2.03	3 (25%)	12,18,20	1.48	2 (16%)
1	AEI	C	12[A]	1	12,14,15	1.87	1 (8%)	12,18,20	2.94	7 (58%)
1	AEI	A	12[A]	1	12,14,15	2.14	2 (16%)	12,18,20	2.23	5 (41%)

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	QNY	C	12[B]	1	-	7/12/20/22	-
1	QNY	A	12[B]	1	-	7/12/20/22	-
1	AEI	B	12	1	-	5/16/18/20	-
1	AEI	D	12	1	-	5/16/18/20	-
1	AEI	C	12[A]	1	-	7/16/18/20	-
1	AEI	A	12[A]	1	-	4/16/18/20	-

All (8) 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	5.67	1.50	1.34
1	A	12[A]	AEI	OG1-CD	4.89	1.48	1.34
1	A	12[A]	AEI	CE2-CD	-4.57	1.41	1.50
1	B	12	AEI	OG1-CD	3.96	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	12	AEI	CG2-CB	2.44	1.57	1.51
1	D	12	AEI	CG2-CB	2.33	1.57	1.51
1	D	12	AEI	O-C	2.29	1.28	1.20

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	12[A]	AEI	O-C-CA	-5.44	110.78	124.77
1	B	12	AEI	CZ-CE2-CD	-5.43	100.95	112.77
1	C	12[B]	QNY	O-C-CA	-4.85	112.30	124.77
1	A	12[A]	AEI	OE1-CD-CE2	-4.76	113.60	124.65
1	A	12[B]	QNY	OG1-CB-CA	4.65	117.70	106.93
1	C	12[A]	AEI	OG1-CD-CE2	4.23	119.01	111.43
1	C	12[A]	AEI	OG1-CB-CG2	3.92	116.05	108.20
1	A	12[A]	AEI	OG1-CD-CE2	3.62	117.91	111.43
1	D	12	AEI	CZ-CE2-CD	-3.59	104.96	112.77
1	C	12[A]	AEI	CZ-CE2-CD	-3.38	105.40	112.77
1	C	12[A]	AEI	OE1-CD-CE2	-3.19	117.24	124.65
1	B	12	AEI	OG1-CD-CE2	3.02	116.85	111.43
1	C	12[A]	AEI	CG2-CB-CA	2.69	118.51	113.26
1	B	12	AEI	OG1-CB-CA	2.60	111.52	105.80
1	A	12[B]	QNY	O-C-CA	-2.47	118.41	124.77
1	D	12	AEI	OG1-CB-CG2	2.35	112.91	108.20
1	A	12[A]	AEI	OG1-CB-CA	2.35	110.96	105.80
1	C	12[A]	AEI	OT2-CH2-OT1	-2.35	118.76	124.08
1	A	12[A]	AEI	O-C-CA	-2.24	119.00	124.77
1	A	12[B]	QNY	CG2-CB-CA	-2.20	108.97	113.26
1	A	12[A]	AEI	OG1-CD-OE1	2.05	128.49	123.70
1	B	12	AEI	OE1-CD-CE2	-2.04	119.91	124.65

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	12[A]	AEI	O-C-CA-CB
1	A	12[B]	QNY	O-C-CA-CB
1	A	12[B]	QNY	CD-CE2-CZ-NH1
1	A	12[B]	QNY	CD-CE2-CZ-CH2
1	A	12[B]	QNY	OT2-CH2-CZ-NH1
1	C	12[B]	QNY	O-C-CA-CB
1	C	12[B]	QNY	CD-CE2-CZ-NH1
1	C	12[B]	QNY	CD-CE2-CZ-CH2

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Mol	Chain	Res	Type	Atoms
1	C	12[B]	QNY	OT2-CH2-CZ-NH1
1	B	12	AEI	O-C-CA-CB
1	D	12	AEI	O-C-CA-CB
1	D	12	AEI	OT1-CH2-CZ-NH1
1	A	12[B]	QNY	OT1-CH2-CZ-NH1
1	C	12[B]	QNY	OT1-CH2-CZ-NH1
1	C	12[A]	AEI	OT2-CH2-CZ-NH1
1	D	12	AEI	OT2-CH2-CZ-NH1
1	B	12	AEI	OT2-CH2-CZ-NH1
1	C	12[A]	AEI	OT1-CH2-CZ-NH1
1	B	12	AEI	OT1-CH2-CZ-NH1
1	A	12[A]	AEI	OT2-CH2-CZ-NH1
1	A	12[B]	QNY	OT1-CH2-CZ-CE2
1	A	12[B]	QNY	OT2-CH2-CZ-CE2
1	B	12	AEI	OE1-CD-CE2-CZ
1	C	12[B]	QNY	OT1-CH2-CZ-CE2
1	C	12[B]	QNY	OT2-CH2-CZ-CE2
1	C	12[A]	AEI	OE1-CD-OG1-CB
1	D	12	AEI	OE1-CD-CE2-CZ
1	C	12[A]	AEI	CE2-CD-OG1-CB
1	C	12[A]	AEI	OE1-CD-CE2-CZ
1	B	12	AEI	OG1-CD-CE2-CZ
1	A	12[A]	AEI	OE1-CD-CE2-CZ
1	D	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	325/334 (97%)	-0.05	1 (0%) 90 89	16, 31, 47, 74	3 (0%)
1	B	326/334 (97%)	-0.25	2 (0%) 85 85	20, 27, 44, 54	2 (0%)
1	C	326/334 (97%)	-0.29	0 100 100	20, 27, 44, 65	1 (0%)
1	D	326/334 (97%)	-0.13	8 (2%) 58 58	18, 27, 69, 147	1 (0%)
All	All	1303/1336 (97%)	-0.18	11 (0%) 82 82	16, 28, 47, 147	7 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	26	THR	5.7
1	D	30	VAL	4.6
1	D	25	TYR	4.1
1	D	28	GLY	3.6
1	D	27	VAL	3.4
1	B	18	ASP	2.3
1	B	21	THR	2.3
1	D	32	VAL	2.3
1	D	19	SER	2.2
1	A	1	LEU	2.1
1	D	36	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, 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	AEI	C	12[A]	15/16	0.92	0.08	22,26,30,33	15

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	QNY	A	12[B]	16/17	-	-	23,25,30,31	16
1	AEI	D	12	15/16	0.93	0.09	22,31,45,45	0
1	QNY	C	12[B]	16/17	-	-	19,23,28,28	16
1	AEI	B	12	15/16	0.96	0.06	19,25,32,32	0
1	AEI	A	12[A]	15/16	0.97	0.06	18,23,30,35	15

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.