



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:34 PM UTC

PDB ID : 6V27 / pdb_00006v27
Title : Complex of double mutant (T89V,K162T) of E. coli L-asparaginase II with L-Asp
Authors : Lubkowski, J.; Wlodawer, A.
Deposited on : 2019-11-22
Resolution : 2.30 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 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

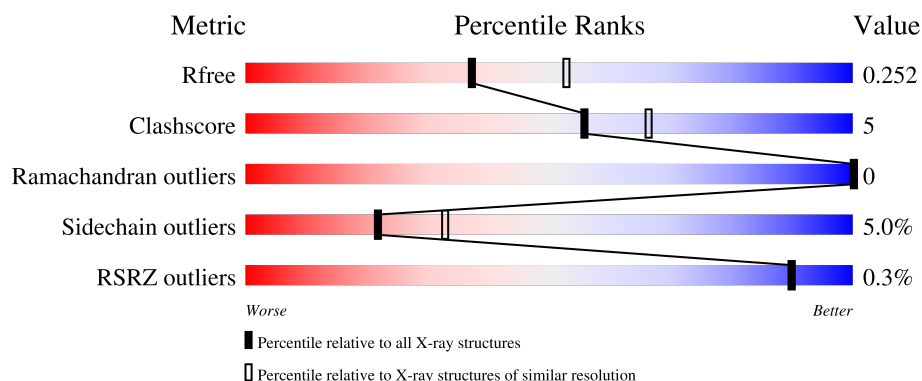
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	333	
1	B	333	
1	C	333	
1	D	333	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10153 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	2	0
			2446	1526	416	496	8			
1	B	303	Total	C	N	O	S	0	1	0
			2282	1427	387	460	8			
1	C	326	Total	C	N	O	S	0	0	0
			2437	1520	415	494	8			
1	D	315	Total	C	N	O	S	0	3	0
			2375	1484	402	481	8			

There are 40 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	89	VAL	THR	engineered mutation	UNP P00805
A	162	THR	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	89	VAL	THR	engineered mutation	UNP P00805
B	162	THR	LYS	engineered mutation	UNP P00805
C	-6	MET	-	expression tag	UNP P00805

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	89	VAL	THR	engineered mutation	UNP P00805
C	162	THR	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	89	VAL	THR	engineered mutation	UNP P00805
D	162	THR	LYS	engineered mutation	UNP P00805

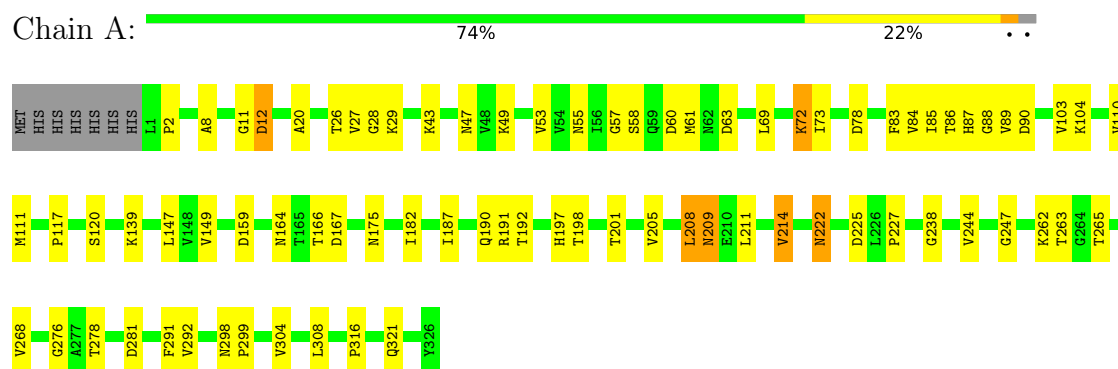
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	132	Total O 132 132	0	1
2	B	100	Total O 101 101	0	1
2	C	185	Total O 185 185	0	0
2	D	195	Total O 195 195	0	0

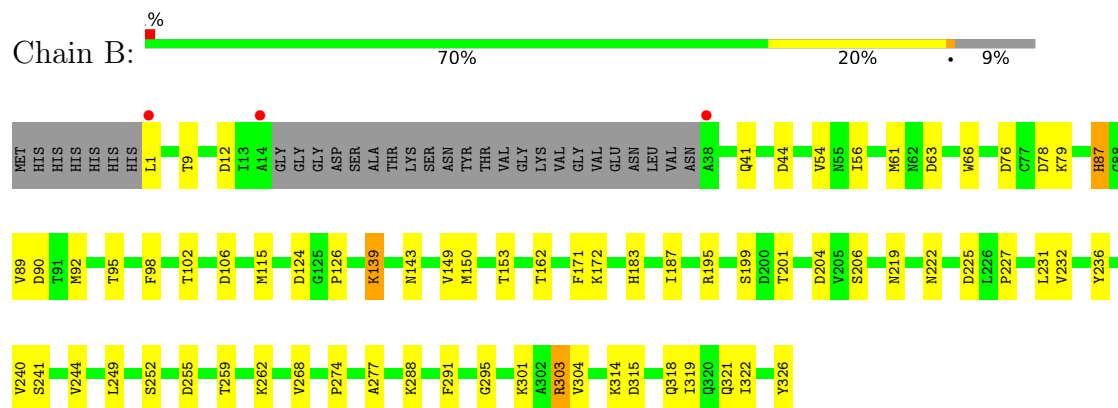
3 Residue-property plots [i](#)

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.

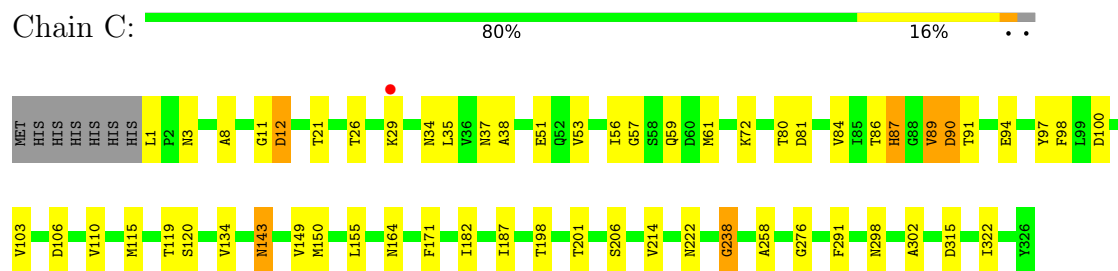
• Molecule 1: L-asparaginase 2



• Molecule 1: L-asparaginase 2

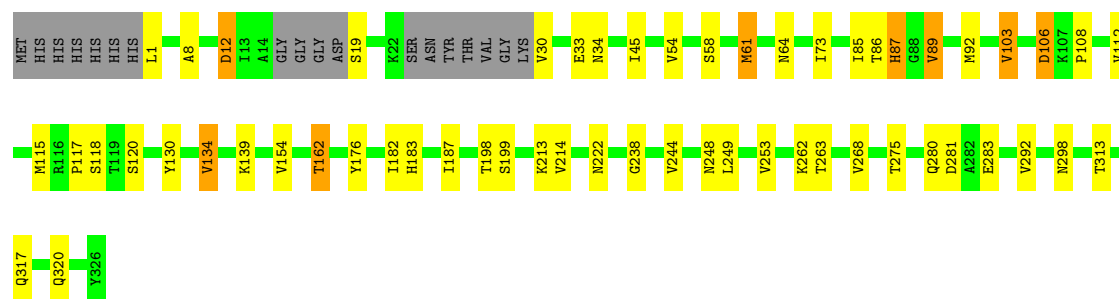


• Molecule 1: L-asparaginase 2



• Molecule 1: L-asparaginase 2

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.30Å 62.41Å 141.75Å 90.00° 117.85° 90.00°	Depositor
Resolution (Å)	26.50 – 2.30 26.50 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (26.50-2.30) 97.6 (26.50-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.160 , 0.251 0.168 , 0.252	Depositor DCC
R_{free} test set	2481 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10153	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 10.64% 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: 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	1.32	2/2473 (0.1%)	1.67	25/3368 (0.7%)
1	B	1.35	7/2304 (0.3%)	1.66	18/3137 (0.6%)
1	C	1.39	14/2458 (0.6%)	1.61	14/3347 (0.4%)
1	D	1.36	10/2402 (0.4%)	1.59	13/3269 (0.4%)
All	All	1.36	33/9637 (0.3%)	1.63	70/13121 (0.5%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	HIS	CE1-NE2	8.48	1.41	1.32
1	D	108	PRO	C-O	-7.75	1.13	1.23
1	B	274	PRO	C-O	-7.48	1.15	1.24
1	C	1	LEU	N-CA	7.33	1.60	1.46
1	C	57	GLY	C-O	7.33	1.31	1.23
1	C	238	GLY	C-O	6.88	1.31	1.24
1	A	304	VAL	C-O	6.88	1.31	1.24
1	C	56	ILE	C-O	6.34	1.30	1.24
1	B	149	VAL	C-O	6.31	1.31	1.24
1	B	56	ILE	C-O	6.21	1.31	1.23
1	D	64	ASN	C-O	6.18	1.31	1.24
1	C	91	THR	N-CA	6.14	1.52	1.46
1	D	281	ASP	CG-OD2	6.10	1.36	1.25
1	D	112	VAL	C-O	6.07	1.30	1.23
1	D	176	TYR	C-O	5.95	1.32	1.24
1	A	147	LEU	C-O	5.86	1.31	1.23
1	C	206	SER	C-O	5.86	1.31	1.24
1	B	87	HIS	CE1-NE2	5.77	1.38	1.32
1	C	91	THR	C-O	-5.71	1.15	1.24
1	B	277	ALA	C-O	5.68	1.30	1.23
1	C	258	ALA	C-O	5.65	1.30	1.24
1	B	183	HIS	CE1-NE2	5.55	1.38	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	97	TYR	C-O	5.53	1.30	1.24
1	C	155	LEU	C-O	-5.53	1.16	1.24
1	C	119	THR	C-O	5.41	1.31	1.24
1	D	320	GLN	C-O	5.41	1.30	1.24
1	C	80	THR	C-O	5.35	1.30	1.23
1	D	162	THR	C-O	-5.30	1.17	1.24
1	B	295	GLY	C-O	5.26	1.31	1.24
1	C	3	ASN	C-O	5.25	1.30	1.24
1	D	45	ILE	N-CA	5.14	1.50	1.46
1	D	1	LEU	N-CA	5.11	1.55	1.46
1	D	154	VAL	C-O	-5.09	1.18	1.24

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	GLY	CA-C-O	-9.16	113.34	121.58
1	A	276	GLY	CA-C-O	-7.49	117.06	122.23
1	B	255	ASP	CA-CB-CG	7.34	119.94	112.60
1	D	134	VAL	N-CA-C	-7.26	103.45	110.42
1	B	54	VAL	CA-C-O	-7.22	115.17	121.09
1	A	63	ASP	CA-CB-CG	7.07	119.67	112.60
1	B	259	THR	CA-CB-OG1	-6.92	99.22	109.60
1	A	281	ASP	CA-CB-CG	6.74	119.34	112.60
1	C	302	ALA	N-CA-C	-6.59	104.10	111.28
1	A	225	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	57	GLY	CA-C-O	-6.30	115.91	121.58
1	A	265	THR	CA-CB-OG1	6.05	118.68	109.60
1	A	20	ALA	CA-C-N	6.01	129.91	120.89
1	A	20	ALA	C-N-CA	6.01	129.91	120.89
1	A	192	THR	CB-CA-C	5.96	118.14	109.20
1	B	232	VAL	CA-C-O	-5.84	114.98	121.05
1	C	100	ASP	CA-CB-CG	5.83	118.44	112.60
1	D	298	ASN	CB-CA-C	5.75	122.16	110.31
1	B	162	THR	CA-CB-OG1	-5.71	101.04	109.60
1	B	236	TYR	CB-CA-C	5.69	119.38	109.65
1	B	319	ILE	CA-C-N	5.68	127.89	120.28
1	B	319	ILE	C-N-CA	5.68	127.89	120.28
1	A	291	PHE	CA-CB-CG	5.62	119.42	113.80
1	C	59	GLN	N-CA-C	-5.60	105.70	112.54
1	B	291	PHE	CA-CB-CG	5.60	119.40	113.80
1	B	304	VAL	N-CA-CB	5.59	116.71	110.62
1	A	88	GLY	CA-C-N	5.54	128.05	120.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	GLY	C-N-CA	5.54	128.05	120.46
1	D	61	MET	CA-C-O	-5.53	115.11	121.19
1	C	276	GLY	CA-C-O	-5.52	118.42	122.23
1	D	87	HIS	CA-CB-CG	5.52	119.32	113.80
1	D	183	HIS	CA-CB-CG	-5.47	108.33	113.80
1	D	280	GLN	CA-C-O	-5.38	115.75	121.94
1	C	143	ASN	CA-C-O	-5.35	114.17	120.81
1	B	231	LEU	CA-C-N	5.35	128.08	120.53
1	B	231	LEU	C-N-CA	5.35	128.08	120.53
1	B	301	LYS	N-CA-C	-5.34	105.12	111.69
1	B	303	ARG	N-CA-C	-5.31	105.49	111.28
1	B	76	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	214	VAL	CA-C-N	5.28	127.83	122.66
1	A	214	VAL	C-N-CA	5.28	127.83	122.66
1	D	106	ASP	CB-CA-C	5.28	119.48	110.56
1	D	162	THR	CA-C-O	-5.28	114.52	120.43
1	C	291	PHE	CA-CB-CG	5.26	119.06	113.80
1	A	47	ASN	CB-CA-C	5.25	120.23	111.30
1	A	53	VAL	CA-C-N	5.24	127.98	122.11
1	A	53	VAL	C-N-CA	5.24	127.98	122.11
1	A	104	LYS	N-CA-C	-5.23	105.57	112.94
1	D	253	VAL	N-CA-C	-5.22	105.44	110.72
1	D	262	LYS	N-CA-C	-5.22	106.59	113.17
1	D	19	SER	CA-C-N	5.22	129.44	120.72
1	D	19	SER	C-N-CA	5.22	129.44	120.72
1	B	76	ASP	CA-C-N	5.20	127.70	120.63
1	B	76	ASP	C-N-CA	5.20	127.70	120.63
1	A	83	PHE	CA-C-N	5.14	129.41	122.93
1	A	83	PHE	C-N-CA	5.14	129.41	122.93
1	C	90	ASP	CA-C-O	-5.12	115.13	120.55
1	D	313	THR	CA-CB-OG1	-5.11	101.94	109.60
1	B	124	ASP	CA-CB-CG	5.11	117.71	112.60
1	C	298	ASN	CB-CA-C	5.11	120.23	110.17
1	C	94	GLU	CA-C-N	5.09	127.06	120.44
1	C	94	GLU	C-N-CA	5.09	127.06	120.44
1	C	37	ASN	N-CA-C	-5.08	105.92	111.82
1	C	315	ASP	CB-CA-C	5.08	116.69	109.38
1	A	2	PRO	CA-C-N	5.06	129.53	121.99
1	A	2	PRO	C-N-CA	5.06	129.53	121.99
1	C	134	VAL	N-CA-C	-5.05	104.86	110.62
1	A	291	PHE	CA-C-N	5.04	129.44	123.19
1	A	291	PHE	C-N-CA	5.04	129.44	123.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ASN	CB-CA-C	5.01	118.64	110.17

There are no chirality outliers.

There are no planarity outliers.

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	2446	0	2436	32	0
1	B	2282	0	2273	26	0
1	C	2437	0	2423	18	0
1	D	2375	0	2370	22	0
2	A	132	0	0	3	1
2	B	101	0	0	2	0
2	C	185	0	0	1	1
2	D	195	0	0	1	1
All	All	10153	0	9502	89	3

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 (89) 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:81:ASP:OD1	2:C:401:HOH:O	2.02	0.77
1:A:28:GLY:HA2	1:A:55:ASN:OD1	1.88	0.73
1:A:72:LYS:HE3	2:A:520:HOH:O	1.91	0.71
1:D:248:ASN:C	1:D:249:LEU:HD12	2.16	0.70
1:A:159:ASP:OD1	1:A:175:ASN:HB2	1.92	0.68
1:B:106:ASP:HB3	1:B:143:ASN:ND2	2.10	0.67
1:D:263:THR:O	1:D:263:THR:HG22	1.94	0.67
1:B:89:VAL:HG11	1:B:115:MET:SD	2.35	0.65
1:D:117:PRO:HG2	1:D:120[B]:SER:OG	1.98	0.64
1:B:98:PHE:CZ	1:B:102:THR:HG21	2.33	0.64
1:A:164:ASN:HD22	1:A:167:ASP:H	1.46	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:MET:HE3	1:B:87:HIS:NE2	2.16	0.60
1:A:244:VAL:HG23	1:B:90:ASP:HB3	1.85	0.58
1:B:106:ASP:OD2	1:B:199:SER:OG	2.20	0.57
1:D:182:ILE:HG12	1:D:187:ILE:HG12	1.86	0.57
1:D:249:LEU:HD12	1:D:249:LEU:N	2.18	0.57
1:A:209:ASN:HB3	2:A:518:HOH:O	2.05	0.56
1:D:130:TYR:O	1:D:134:VAL:HG23	2.06	0.54
1:D:89:VAL:HG11	1:D:115:MET:SD	2.48	0.53
1:D:106:ASP:OD2	1:D:199:SER:OG	2.23	0.53
1:A:110:VAL:HG13	1:A:149:VAL:HG23	1.90	0.52
1:B:315:ASP:HB3	1:B:318:GLN:HB2	1.90	0.52
1:C:89:VAL:HG11	1:C:115:MET:SD	2.49	0.52
1:C:103:VAL:O	1:C:198:THR:HA	2.11	0.51
1:B:322:ILE:HG23	1:B:326:TYR:CD2	2.47	0.50
1:C:90:ASP:HB3	1:D:244:VAL:HG23	1.94	0.50
1:A:139:LYS:HD2	2:A:494:HOH:O	2.12	0.49
1:A:197:HIS:HD2	1:A:198:THR:OG1	1.96	0.49
1:B:66:TRP:NE1	1:B:95:THR:OG1	2.43	0.49
1:C:214:VAL:HA	1:C:238:GLY:O	2.12	0.49
1:C:110:VAL:HG13	1:C:149:VAL:HG23	1.95	0.49
1:A:247:GLY:HA3	1:A:278:THR:HG23	1.94	0.49
1:A:84:VAL:HA	1:A:110:VAL:O	2.13	0.48
1:A:61:MET:HE3	1:A:87:HIS:NE2	2.30	0.47
1:B:63:ASP:O	1:B:66:TRP:HB2	2.15	0.47
1:B:321:GLN:NE2	1:B:321:GLN:HA	2.30	0.47
1:A:214:VAL:HA	1:A:238:GLY:O	2.16	0.46
1:C:8:ALA:HA	1:C:86:THR:OG1	2.14	0.46
1:A:117:PRO:HG2	1:A:120:SER:HB3	1.98	0.46
1:C:182:ILE:HG12	1:C:187:ILE:HG12	1.98	0.46
1:B:225:ASP:HB3	1:B:252:SER:HB3	1.98	0.46
1:A:244:VAL:CG2	1:B:90:ASP:HB3	2.46	0.45
1:D:162:THR:HG23	1:D:162:THR:O	2.15	0.45
1:C:61:MET:HE3	1:C:87:HIS:NE2	2.31	0.45
1:B:139:LYS:HG2	2:B:484:HOH:O	2.16	0.45
1:A:11:GLY:HA2	1:A:12:AEI:OT2	2.17	0.44
1:B:41:GLN:O	1:B:44:ASP:HB2	2.17	0.44
1:B:240:VAL:HA	1:B:268:VAL:O	2.18	0.44
1:D:249:LEU:N	1:D:249:LEU:CD1	2.81	0.44
1:C:106:ASP:HB3	1:C:143:ASN:ND2	2.33	0.44
1:A:90:ASP:HB3	1:B:244:VAL:CG2	2.48	0.43
1:A:222:ASN:HB3	1:B:303:ARG:NH2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:VAL:HG22	1:D:292:VAL:HB	2.01	0.43
1:B:219:ASN:OD1	1:B:249:LEU:HA	2.19	0.43
1:A:268:VAL:HG22	1:A:292:VAL:HB	2.01	0.43
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.91	0.43
1:A:111:MET:HE2	1:A:111:MET:HB3	1.87	0.43
1:A:69:LEU:O	1:A:73:ILE:HD12	2.19	0.43
1:C:164:ASN:HA	1:D:275:THR:O	2.19	0.42
1:D:73:ILE:HD11	1:D:85:ILE:HD11	2.00	0.42
1:D:263:THR:O	1:D:263:THR:CG2	2.60	0.42
1:D:103:VAL:O	1:D:198:THR:HA	2.20	0.42
1:C:84:VAL:HA	1:C:110:VAL:O	2.19	0.42
1:C:150:MET:HG3	1:C:171:PHE:CD2	2.53	0.42
1:A:58:SER:C	1:A:60:ASP:N	2.77	0.42
1:A:205:VAL:HA	1:A:208:LEU:HD23	2.02	0.42
1:A:164:ASN:ND2	1:A:166:THR:H	2.17	0.42
1:A:190:GLN:C	1:A:191:ARG:HG2	2.45	0.42
1:C:98:PHE:CD1	1:C:98:PHE:C	2.98	0.42
1:A:298:ASN:HB2	1:A:299:PRO:CD	2.50	0.42
1:D:61:MET:HE3	1:D:87:HIS:NE2	2.35	0.42
1:B:150:MET:HG3	1:B:171:PHE:CD2	2.55	0.41
1:B:195:ARG:HD3	1:B:195:ARG:HA	1.86	0.41
1:C:35:LEU:O	1:C:38:ALA:HB3	2.19	0.41
1:A:182:ILE:HG12	1:A:187:ILE:HG12	2.03	0.41
1:B:172:LYS:NZ	2:B:409:HOH:O	2.53	0.41
1:C:11:GLY:HA2	1:C:12:AEI:OT1	2.20	0.41
1:D:8:ALA:HA	1:D:86:THR:OG1	2.21	0.41
1:A:90:ASP:HB3	1:B:244:VAL:HB	2.02	0.41
1:B:204:ASP:OD1	1:B:206:SER:OG	2.35	0.41
1:C:12:AEI:NH1	1:D:283:GLU:OE2	2.54	0.41
1:B:9:THR:OG1	1:B:87:HIS:HA	2.21	0.40
1:D:12:AEI:OT1	1:D:58:SER:OG	2.37	0.40
1:A:8:ALA:HA	1:A:86:THR:OG1	2.21	0.40
1:A:227:PRO:HB3	1:B:227:PRO:HB3	2.04	0.40
1:D:34:ASN:HB3	2:D:582:HOH:O	2.20	0.40
1:D:214:VAL:HA	1:D:238:GLY:O	2.21	0.40
1:A:73:ILE:HD11	1:A:85:ILE:HD11	2.03	0.40
1:C:51:GLU:OE1	1:C:72:LYS:CE	2.70	0.40

All (3) 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)
2:D:434:HOH:O	2:D:434:HOH:O[2_556]	0.87	1.33
2:C:434:HOH:O	2:C:434:HOH:O[2_556]	0.97	1.23
2:A:525:HOH:O	2:A:525:HOH:O[2_555]	2.17	0.03

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	325/333 (98%)	313 (96%)	12 (4%)	0	100	100
1	B	299/333 (90%)	284 (95%)	15 (5%)	0	100	100
1	C	323/333 (97%)	312 (97%)	11 (3%)	0	100	100
1	D	311/333 (93%)	304 (98%)	7 (2%)	0	100	100
All	All	1258/1332 (94%)	1213 (96%)	45 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	267/272 (98%)	249 (93%)	18 (7%)	15	21
1	B	249/272 (92%)	235 (94%)	14 (6%)	19	28
1	C	265/272 (97%)	255 (96%)	10 (4%)	29	44
1	D	261/272 (96%)	249 (95%)	12 (5%)	24	36
All	All	1042/1088 (96%)	988 (95%)	54 (5%)	22	31

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26[A]	THR
1	A	26[B]	THR
1	A	27	VAL
1	A	29	LYS
1	A	43	LYS
1	A	49	LYS
1	A	72	LYS
1	A	78	ASP
1	A	89	VAL
1	A	103	VAL
1	A	201	THR
1	A	208	LEU
1	A	211	LEU
1	A	222	ASN
1	A	262	LYS
1	A	263	THR
1	A	316	PRO
1	A	321	GLN
1	B	1	LEU
1	B	78	ASP
1	B	79	LYS
1	B	92	MET
1	B	126	PRO
1	B	139	LYS
1	B	153	THR
1	B	187	ILE
1	B	201	THR
1	B	222	ASN
1	B	241	SER
1	B	262	LYS
1	B	288	LYS
1	B	314	LYS
1	C	21	THR
1	C	26	THR
1	C	29	LYS
1	C	34	ASN
1	C	53	VAL
1	C	89	VAL
1	C	120	SER
1	C	201	THR
1	C	222	ASN
1	C	322	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	30	VAL
1	D	33	GLU
1	D	54	VAL
1	D	89	VAL
1	D	92	MET
1	D	103	VAL
1	D	118[A]	SER
1	D	118[B]	SER
1	D	139	LYS
1	D	213	LYS
1	D	222	ASN
1	D	317	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
1	A	183	HIS
1	A	190	GLN
1	A	197	HIS
1	A	312	GLN
1	A	318	GLN
1	B	64	ASN
1	B	143	ASN
1	B	183	HIS
1	B	321	GLN
1	C	37	ASN
1	C	143	ASN
1	C	183	HIS
1	C	307	GLN
1	C	312	GLN
1	D	52	GLN
1	D	183	HIS
1	D	307	GLN
1	D	317	GLN
1	D	324	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	12,14,15	1.24	1 (8%)	12,18,20	1.61	3 (25%)
1	AEI	C	12	1	12,14,15	0.99	0	12,18,20	1.79	3 (25%)
1	AEI	D	12	1	12,14,15	0.87	0	12,18,20	1.94	2 (16%)
1	AEI	B	12	1	12,14,15	1.07	1 (8%)	12,18,20	1.87	1 (8%)

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	-	5/16/18/20	-
1	AEI	C	12	1	-	5/16/18/20	-
1	AEI	D	12	1	-	7/16/18/20	-
1	AEI	B	12	1	-	4/16/18/20	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	12	AEI	OT1-CH2	2.39	1.29	1.22
1	A	12	AEI	OT1-CH2	2.19	1.28	1.22

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	12	AEI	OG1-CB-CA	5.37	117.59	105.80
1	D	12	AEI	OG1-CB-CA	4.92	116.61	105.80
1	C	12	AEI	OG1-CB-CA	3.90	114.37	105.80
1	A	12	AEI	OG1-CB-CA	3.64	113.79	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	12	AEI	CB-OG1-CD	2.70	123.18	118.36
1	C	12	AEI	CZ-CE2-CD	-2.56	107.20	112.77
1	A	12	AEI	OG1-CD-CE2	2.37	115.67	111.43
1	A	12	AEI	O-C-CA	-2.25	118.98	124.77
1	D	12	AEI	O-C-CA	-2.09	119.39	124.77

There are no chirality outliers.

All (21) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	12	AEI	1	0
1	C	12	AEI	2	0
1	D	12	AEI	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [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	325/333 (97%)	-0.18	0 100 100	23, 42, 68, 100	2 (0%)
1	B	302/333 (90%)	-0.17	3 (0%) 79 80	28, 44, 66, 97	1 (0%)
1	C	325/333 (97%)	-0.59	1 (0%) 90 90	18, 28, 52, 98	0
1	D	314/333 (94%)	-0.62	0 100 100	18, 27, 50, 87	3 (0%)
All	All	1266/1332 (95%)	-0.39	4 (0%) 90 90	18, 36, 64, 100	6 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	14	ALA	4.0
1	B	38	ALA	3.6
1	C	29	LYS	2.4
1	B	1	LEU	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	A	12	15/16	0.90	0.08	28,47,54,60	0
1	AEI	B	12	15/16	0.92	0.08	46,59,76,78	0
1	AEI	C	12	15/16	0.94	0.08	22,28,47,49	0
1	AEI	D	12	15/16	0.95	0.07	26,38,56,58	0

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.