



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 02:42 PM EDT

PDB ID : 4ECA  
Title : ASPARAGINASE FROM E. COLI, MUTANT T89V WITH COVALENTLY BOUND ASPARTATE  
Authors : Palm, G.J.; Lubkowski, J.; Wlodawer, A.  
Deposited on : 1997-02-21  
Resolution : 2.20 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 : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
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) : 2.23.2

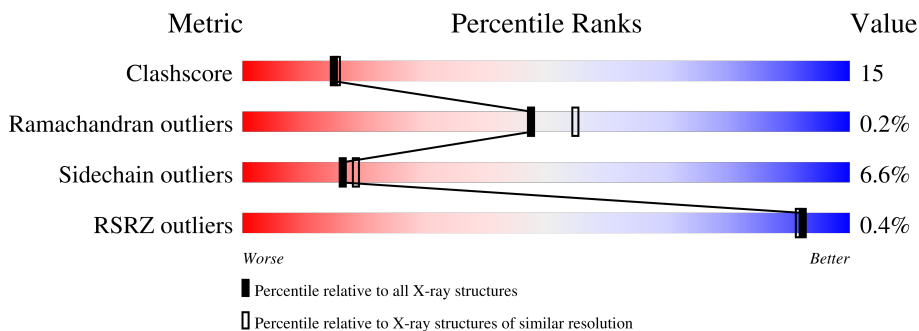
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	326	 % 64% 33% .
1	B	326	 70% 27% .
1	C	326	 68% 28% .
1	D	326	 65% 30% . .

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10476 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-ASPARAGINE AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	326	2439	1522	416	493	8	0	0	0
1	B	326	2439	1522	416	493	8	0	0	0
1	C	326	2439	1522	416	493	8	0	0	0
1	D	326	2439	1522	416	493	8	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	AEI	THR	modified residue	UNP P00805
A	89	VAL	THR	engineered mutation	UNP P00805
B	12	AEI	THR	modified residue	UNP P00805
B	89	VAL	THR	engineered mutation	UNP P00805
C	12	AEI	THR	modified residue	UNP P00805
C	89	VAL	THR	engineered mutation	UNP P00805
D	12	AEI	THR	modified residue	UNP P00805
D	89	VAL	THR	engineered mutation	UNP P00805

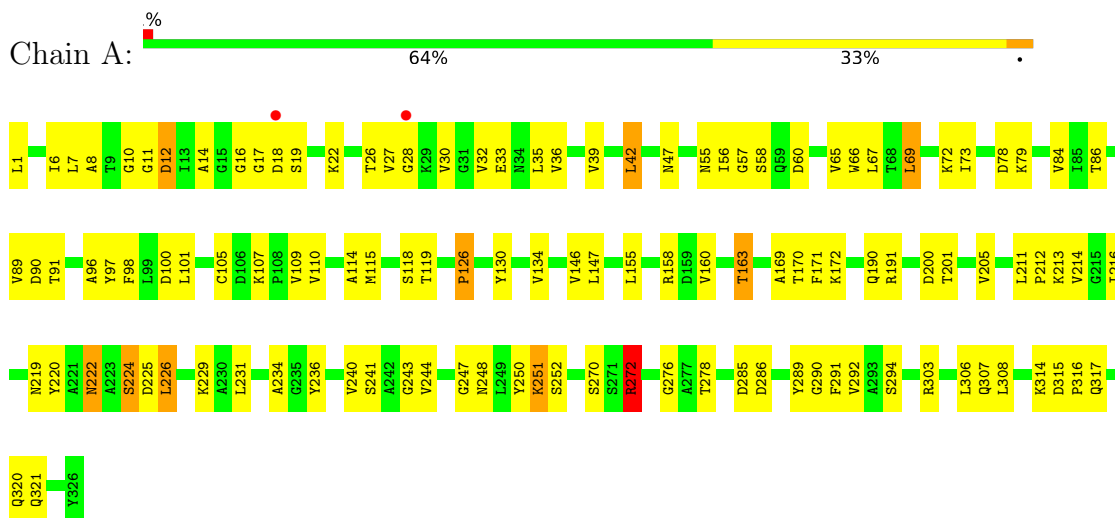
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	191	Total 191	O 191	0	0
2	B	172	Total 172	O 172	0	0
2	C	187	Total 187	O 187	0	0
2	D	170	Total 170	O 170	0	0

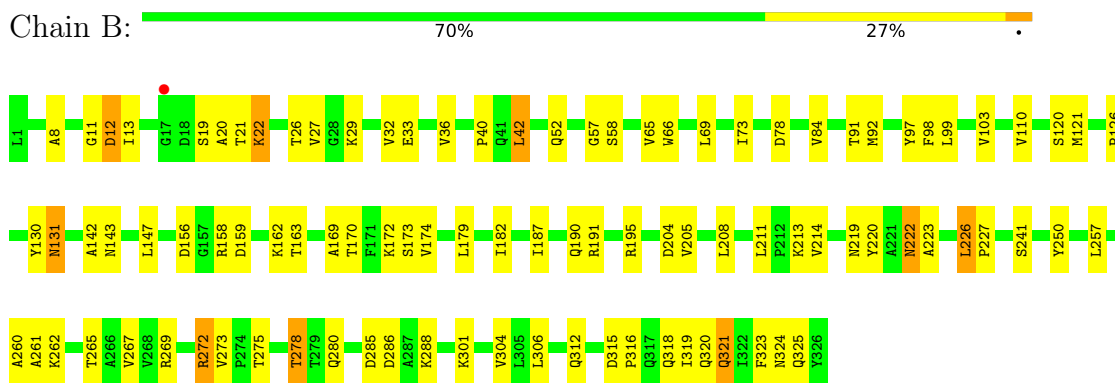
### 3 Residue-property plots [i](#)

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.

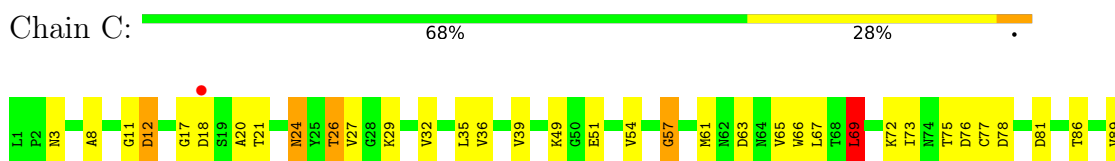
#### • Molecule 1: L-ASPARAGINE AMIDOHYDROLASE

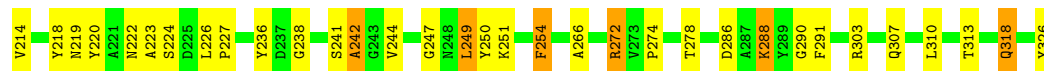


#### • Molecule 1: L-ASPARAGINE AMIDOHYDROLASE



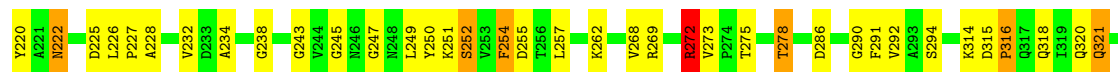
#### • Molecule 1: L-ASPARAGINE AMIDOHYDROLASE





• Molecule 1: L-ASPARAGINE AMIDOHYDROLASE

Chain D: 65% 30%



N324  
Q325  
Y326

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.00Å 126.20Å 155.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 29.29 – 2.00	Depositor EDS
% Data completeness (in resolution range)	62.4 (10.00-2.20) 53.8 (29.29-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.00Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.181 , (Not available) 0.169 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.5	Xtrriage
Anisotropy	0.448	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 78.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10476	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1105e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 i

### 5.1 Standard geometry i

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	0.71	0/2460	0.89	3/3348 (0.1%)
1	B	0.68	1/2460 (0.0%)	0.88	2/3348 (0.1%)
1	C	0.66	0/2460	0.91	3/3348 (0.1%)
1	D	0.67	0/2460	0.90	5/3348 (0.1%)
All	All	0.68	1/9840 (0.0%)	0.89	13/13392 (0.1%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	22	LYS	CE-NZ	5.49	1.62	1.49

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	B	195	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	D	272	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	A	272	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	47	ASN	N-CA-C	-5.80	95.33	111.00
1	D	272	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	C	57	GLY	N-CA-C	-5.68	98.89	113.10
1	C	69	LEU	CA-CB-CG	5.66	128.32	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	147	LEU	CA-CB-CG	5.34	127.59	115.30
1	B	278	THR	N-CA-C	-5.33	96.62	111.00
1	D	278	THR	N-CA-C	-5.15	97.09	111.00
1	C	242	ALA	N-CA-C	-5.11	97.20	111.00
1	D	57	GLY	N-CA-C	-5.07	100.44	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	326	TYR	Sidechain

## 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	2439	0	2429	81	0
1	B	2439	0	2429	73	0
1	C	2439	0	2429	76	0
1	D	2439	0	2429	81	0
2	A	191	0	0	5	0
2	B	172	0	0	12	0
2	C	187	0	0	6	0
2	D	170	0	0	3	0
All	All	10476	0	9716	294	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 15.

All (294) 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:12:AEI:HZ	1:C:27:VAL:HG21	1.53	0.90
1:D:73:ILE:HD11	1:D:85:ILE:HD11	1.54	0.87
1:C:27:VAL:HG11	1:C:57:GLY:HA2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:THR:HB	1:C:170:THR:O	1.82	0.80
2:B:421:HOH:O	1:C:183:HIS:HD2	1.65	0.80
1:D:321:GLN:O	1:D:325:GLN:HG2	1.82	0.78
1:B:26:THR:HB	1:B:29:LYS:HE3	1.66	0.77
1:C:205:VAL:HA	1:C:208:LEU:HD12	1.64	0.77
1:A:17:GLY:H	1:A:119:THR:HG21	1.50	0.77
1:D:58:SER:HB2	1:D:91:THR:OG1	1.85	0.76
1:B:227:PRO:HB3	1:D:227:PRO:HB3	1.68	0.75
1:A:19:SER:HB3	1:A:22:LYS:HB2	1.70	0.72
1:A:163:THR:HB	1:A:170:THR:O	1.90	0.71
1:C:20:ALA:HA	1:C:120:SER:HA	1.71	0.71
1:D:163:THR:HB	1:D:170:THR:O	1.90	0.71
1:D:219:ASN:ND2	1:D:250:TYR:H	1.89	0.70
1:A:32:VAL:O	1:A:36:VAL:HG23	1.93	0.69
1:A:97:TYR:CE1	1:A:158:ARG:HG3	2.28	0.69
1:D:107:LYS:HE2	2:D:477:HOH:O	1.94	0.67
1:D:19:SER:HB3	1:D:22:LYS:HB2	1.77	0.67
1:D:20:ALA:HA	1:D:120:SER:HA	1.75	0.67
1:D:205:VAL:HA	1:D:208:LEU:HD12	1.75	0.67
1:B:272:ARG:NH1	2:B:395:HOH:O	2.27	0.66
1:B:219:ASN:HD22	1:B:250:TYR:H	1.43	0.66
1:B:174:VAL:HB	1:B:275:THR:HG22	1.78	0.65
1:D:205:VAL:HG12	1:D:208:LEU:HD12	1.77	0.65
1:C:77:CYS:SG	1:C:107:LYS:HD2	2.37	0.65
1:A:214:VAL:CG1	1:A:303:ARG:HG3	2.27	0.64
1:B:222:ASN:OD1	1:D:62:ASN:HB2	1.97	0.64
1:B:205:VAL:HG12	1:B:208:LEU:HD12	1.78	0.64
1:B:163:THR:HG22	1:B:170:THR:O	1.98	0.64
1:B:32:VAL:O	1:B:36:VAL:HG23	1.98	0.64
1:A:224:SER:OG	1:A:226:LEU:HB2	1.97	0.63
1:B:69:LEU:O	1:B:73:ILE:HD12	1.98	0.63
1:B:163:THR:HG21	1:B:172:LYS:HD2	1.81	0.62
1:C:313:THR:HG21	1:C:318:GLN:HB3	1.82	0.62
1:D:30:VAL:CG1	1:D:34:ASN:HB2	2.30	0.62
1:C:12:AEI:HZ	1:C:27:VAL:CG2	2.28	0.61
1:B:321:GLN:HG2	1:B:325:GLN:HE21	1.66	0.61
1:A:224:SER:HB2	1:C:236:TYR:OH	2.00	0.61
1:A:12:AEI:HZ	1:A:27:VAL:HG11	1.82	0.61
1:B:269:ARG:O	1:B:278:THR:HG21	2.01	0.61
1:A:69:LEU:O	1:A:73:ILE:HD12	1.99	0.61
1:B:285:ASP:OD2	1:B:288:LYS:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:LYS:HD2	2:C:511:HOH:O	2.01	0.61
1:C:226:LEU:HB2	1:C:227:PRO:HD3	1.83	0.61
1:D:30:VAL:HG13	1:D:34:ASN:HB2	1.82	0.60
1:D:182:ILE:HG12	1:D:187:ILE:HG12	1.83	0.60
1:B:191:ARG:HG3	1:C:191:ARG:HD2	1.82	0.60
1:A:247:GLY:HA3	1:A:278:THR:HG23	1.83	0.59
1:C:26:THR:OG1	1:C:29:LYS:HE3	2.03	0.59
1:A:60:ASP:OD1	1:C:251:LYS:HB3	2.03	0.59
1:B:40:PRO:HA	2:B:349:HOH:O	2.03	0.58
1:B:142:ALA:O	1:B:143:ASN:HB2	2.02	0.58
1:C:63:ASP:HB3	1:C:211:LEU:HD22	1.85	0.58
1:D:110:VAL:HG13	1:D:149:VAL:HG23	1.84	0.58
1:B:22:LYS:HE3	2:B:342:HOH:O	2.03	0.57
1:A:276:GLY:HA2	2:C:418:HOH:O	2.04	0.57
1:A:243:GLY:O	1:A:272:ARG:HG2	2.03	0.57
1:D:6:ILE:HD12	1:D:48:VAL:HG11	1.86	0.57
1:C:32:VAL:O	1:C:36:VAL:HG23	2.04	0.57
1:B:169:ALA:O	1:B:172:LYS:HE3	2.04	0.57
1:C:244:VAL:HG12	1:C:272:ARG:CZ	2.35	0.57
1:D:67:LEU:HD21	1:D:211:LEU:CD1	2.35	0.56
1:B:97:TYR:CE1	1:B:158:ARG:HG3	2.40	0.56
1:B:205:VAL:HA	1:B:208:LEU:HD12	1.88	0.56
1:D:97:TYR:CE1	1:D:158:ARG:HG3	2.40	0.56
1:A:251:LYS:HD3	1:A:252:SER:N	2.21	0.56
1:A:314:LYS:HE2	2:A:435:HOH:O	2.05	0.55
1:B:65:VAL:O	1:B:69:LEU:HB2	2.06	0.55
1:D:249:LEU:HD23	1:D:257:LEU:HD12	1.88	0.55
1:C:205:VAL:HG12	1:C:208:LEU:HD12	1.89	0.55
1:C:65:VAL:HG12	1:C:69:LEU:HD23	1.88	0.55
1:D:225:ASP:HB3	1:D:252:SER:HB2	1.88	0.55
1:A:27:VAL:HG21	1:A:57:GLY:HA3	1.88	0.54
1:A:96:ALA:O	1:A:100:ASP:HB2	2.07	0.54
1:C:11:GLY:C	1:C:27:VAL:HG13	2.27	0.54
1:D:67:LEU:HD21	1:D:211:LEU:HD11	1.90	0.54
1:A:225:ASP:O	1:A:229:LYS:HG3	2.08	0.54
1:A:7:LEU:HD22	1:A:72:LYS:HD3	1.90	0.54
1:C:3:ASN:O	1:C:81:ASP:HB2	2.08	0.53
1:A:11:GLY:HA2	1:A:12:AEI:OT1	2.09	0.52
1:B:219:ASN:ND2	1:B:250:TYR:H	2.06	0.52
1:B:321:GLN:OE1	1:B:325:GLN:NE2	2.42	0.52
1:B:12:AEI:HZ	1:B:27:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:GLY:O	1:D:118:SER:OG	2.27	0.52
1:B:159:ASP:O	1:B:173:SER:HA	2.09	0.52
2:B:456:HOH:O	1:C:188:ASP:HB3	2.10	0.52
1:A:205:VAL:HG22	2:A:346:HOH:O	2.08	0.52
1:D:251:LYS:HE2	1:D:255:ASP:OD2	2.10	0.52
1:A:169:ALA:O	1:A:172:LYS:HE3	2.09	0.52
1:B:27:VAL:HG21	1:B:57:GLY:CA	2.40	0.51
1:D:62:ASN:N	1:D:62:ASN:HD22	2.09	0.51
1:A:12:AEI:HB	1:A:114:ALA:O	2.11	0.51
1:C:17:GLY:HA3	1:C:24:ASN:O	2.09	0.51
1:C:303:ARG:HD3	2:C:335:HOH:O	2.11	0.51
1:B:19:SER:HB3	1:B:22:LYS:HB3	1.93	0.51
1:C:69:LEU:O	1:C:73:ILE:HG13	2.09	0.51
1:A:286:ASP:HB3	1:A:291:PHE:O	2.11	0.51
1:B:163:THR:HG21	1:B:172:LYS:NZ	2.26	0.51
1:C:110:VAL:HG13	1:C:149:VAL:HG23	1.92	0.51
1:D:12:AEI:HZ	1:D:27:VAL:HG11	1.93	0.51
1:C:75:THR:HG22	1:C:76:ASP:OD1	2.11	0.51
1:D:219:ASN:HD22	1:D:250:TYR:H	1.57	0.51
1:C:35:LEU:O	1:C:39:VAL:HG23	2.09	0.51
1:D:66:TRP:HB3	1:D:98:PHE:CE2	2.46	0.51
1:A:8:ALA:HA	1:A:86:THR:OG1	2.11	0.50
1:A:292:VAL:HG22	1:A:320:GLN:HB2	1.91	0.50
1:B:19:SER:HB3	1:B:22:LYS:CB	2.41	0.50
1:D:320:GLN:O	1:D:324:ASN:OD1	2.29	0.50
1:B:11:GLY:HA2	1:B:12:AEI:OT2	2.11	0.50
1:D:24:ASN:O	1:D:25:TYR:HB3	2.12	0.50
1:C:220:TYR:CE2	1:C:223:ALA:HA	2.47	0.50
1:C:21:THR:HG22	1:C:121:MET:CE	2.42	0.50
1:A:190:GLN:HA	1:D:194:ALA:HB3	1.94	0.50
1:A:236:TYR:OH	1:C:224:SER:HB2	2.11	0.49
1:A:214:VAL:HG12	1:A:303:ARG:HG3	1.94	0.49
1:A:216:ILE:HA	1:A:240:VAL:O	2.12	0.49
2:A:355:HOH:O	1:C:272:ARG:HD3	2.10	0.49
1:D:6:ILE:HD12	1:D:48:VAL:CG1	2.43	0.49
1:D:174:VAL:HB	1:D:275:THR:HG22	1.95	0.49
1:C:182:ILE:HG12	1:C:187:ILE:HG12	1.93	0.49
1:D:58:SER:HB3	1:D:87:HIS:CE1	2.48	0.49
1:A:222:ASN:HB3	1:C:303:ARG:NH2	2.28	0.49
1:C:67:LEU:HD21	1:C:211:LEU:CD1	2.43	0.49
1:D:228:ALA:O	1:D:232:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD21	1:A:211:LEU:HD11	1.95	0.48
1:A:220:TYR:HA	1:A:272:ARG:NH2	2.28	0.48
1:C:8:ALA:HA	1:C:86:THR:OG1	2.13	0.48
1:D:314:LYS:O	1:D:316:PRO:HD3	2.13	0.48
1:D:147:LEU:HG	1:D:154:VAL:CG1	2.44	0.48
1:A:285:ASP:O	1:A:289:TYR:CD2	2.67	0.48
1:A:14:ALA:HA	1:A:30:VAL:HB	1.96	0.48
1:C:109:VAL:HG12	1:C:146:VAL:HG13	1.96	0.47
1:A:39:VAL:HB	1:A:42:LEU:HD22	1.95	0.47
1:A:58:SER:HB2	1:A:91:THR:OG1	2.13	0.47
1:D:32:VAL:O	1:D:36:VAL:HG23	2.14	0.47
1:D:247:GLY:HA3	1:D:278:THR:HG23	1.97	0.47
1:C:214:VAL:CG1	1:C:303:ARG:HG3	2.44	0.47
1:A:84:VAL:HA	1:A:110:VAL:O	2.14	0.47
1:C:116:ARG:HB3	1:C:120:SER:OG	2.14	0.47
1:D:196:LYS:HB2	1:D:326:TYR:CD1	2.49	0.47
1:B:42:LEU:HD11	1:B:130:TYR:HA	1.96	0.47
1:C:249:LEU:HD23	1:C:254:PHE:HA	1.95	0.47
1:B:204:ASP:HA	2:B:355:HOH:O	2.15	0.47
1:C:66:TRP:HB3	1:C:98:PHE:CE2	2.50	0.47
1:A:163:THR:O	1:C:274:PRO:HG2	2.14	0.46
1:C:49:LYS:HE2	1:C:51:GLU:OE2	2.15	0.46
1:A:248:ASN:HA	2:A:390:HOH:O	2.15	0.46
1:C:99:LEU:O	1:C:103:VAL:HB	2.14	0.46
1:D:249:LEU:CD2	1:D:257:LEU:HD12	2.45	0.46
1:B:214:VAL:CG1	1:B:306:LEU:HD23	2.45	0.46
1:C:241:SER:HB3	2:C:395:HOH:O	2.15	0.46
1:D:178:PRO:HG3	1:D:181:TYR:OH	2.16	0.46
1:A:155:LEU:HD13	1:A:160:VAL:HG23	1.98	0.46
1:D:100:ASP:HA	1:D:146:VAL:HG23	1.97	0.46
1:A:222:ASN:HB2	2:C:334:HOH:O	2.15	0.46
1:C:219:ASN:ND2	1:C:250:TYR:H	2.13	0.46
1:A:213:LYS:HE3	1:A:236:TYR:CE1	2.51	0.46
1:A:90:ASP:HB3	1:C:244:VAL:HB	1.97	0.46
1:A:100:ASP:HA	1:A:146:VAL:HG23	1.97	0.46
1:A:216:ILE:HG12	1:A:240:VAL:HB	1.98	0.45
1:C:224:SER:OG	1:C:226:LEU:HG	2.16	0.45
1:A:28:GLY:HA2	1:A:55:ASN:OD1	2.17	0.45
1:D:21:THR:HG23	1:D:121:MET:HE3	1.98	0.45
1:B:162:LYS:NZ	1:D:245:GLY:HA2	2.31	0.45
1:C:247:GLY:HA3	1:C:278:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:LEU:CD2	1:D:205:VAL:HB	2.45	0.45
1:A:89:VAL:HG21	1:A:115:MET:SD	2.57	0.45
1:A:251:LYS:HD3	1:A:252:SER:H	1.82	0.45
1:B:272:ARG:NH1	2:D:344:HOH:O	2.49	0.45
1:C:61:MET:SD	1:C:65:VAL:HG11	2.58	0.45
1:A:33:GLU:CD	1:A:33:GLU:H	2.18	0.44
1:A:42:LEU:HA	1:A:42:LEU:HD12	1.74	0.44
1:B:8:ALA:HB3	1:B:52:GLN:HA	1.98	0.44
1:B:226:LEU:HD21	1:D:234:ALA:HB2	1.98	0.44
1:D:214:VAL:HA	1:D:238:GLY:O	2.16	0.44
1:D:286:ASP:O	1:D:290:GLY:N	2.48	0.44
1:B:99:LEU:O	1:B:103:VAL:HB	2.16	0.44
1:B:174:VAL:HB	1:B:275:THR:CG2	2.47	0.44
1:A:191:ARG:NH2	1:D:156:ASP:OD1	2.51	0.44
1:A:270:SER:HA	1:A:294:SER:OG	2.17	0.44
1:B:182:ILE:HG12	1:B:187:ILE:HG12	1.99	0.44
1:C:65:VAL:O	1:C:69:LEU:HD23	2.17	0.44
1:C:212:PRO:O	1:C:307:GLN:HG2	2.17	0.44
1:A:285:ASP:O	1:A:289:TYR:HD2	1.99	0.44
1:C:288:LYS:O	1:C:288:LYS:HG3	2.17	0.44
1:D:142:ALA:O	1:D:143:ASN:HB2	2.18	0.44
1:D:174:VAL:CG2	1:D:275:THR:HG22	2.47	0.44
1:A:14:ALA:HA	1:A:35:LEU:HD21	2.00	0.44
1:A:212:PRO:O	1:A:307:GLN:HG2	2.16	0.44
1:B:315:ASP:HB3	1:B:318:GLN:HB2	2.00	0.44
1:C:249:LEU:HD12	1:C:249:LEU:N	2.32	0.44
1:A:16:GLY:HA2	1:A:119:THR:HG23	2.00	0.44
1:B:156:ASP:OD2	1:C:191:ARG:NH2	2.51	0.44
1:B:174:VAL:CB	1:B:275:THR:HG22	2.47	0.44
1:B:213:LYS:HD3	2:B:387:HOH:O	2.18	0.44
1:B:226:LEU:CB	1:B:227:PRO:HD3	2.48	0.44
1:D:292:VAL:HG13	1:D:320:GLN:HA	2.00	0.44
1:B:321:GLN:HG2	1:B:325:GLN:NE2	2.33	0.43
1:D:250:TYR:HE2	1:D:252:SER:HG	1.66	0.43
1:C:89:VAL:HG11	1:C:115:MET:SD	2.58	0.43
1:D:268:VAL:CG1	1:D:294:SER:HB3	2.48	0.43
1:A:78:ASP:OD1	1:A:79:LYS:HG3	2.18	0.43
1:B:20:ALA:HA	1:B:120:SER:HA	1.99	0.43
1:D:178:PRO:HG3	1:D:181:TYR:CZ	2.53	0.43
1:D:206:SER:OG	1:D:207:LYS:HD2	2.18	0.43
1:A:10:GLY:HA3	1:A:56:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ARG:CG	1:C:191:ARG:HD2	2.48	0.43
1:C:220:TYR:CZ	1:C:223:ALA:HA	2.53	0.43
1:A:1:LEU:N	2:A:447:HOH:O	2.42	0.43
1:B:220:TYR:CZ	1:B:223:ALA:HA	2.54	0.43
1:D:69:LEU:O	1:D:73:ILE:HG13	2.18	0.43
1:B:272:ARG:NH2	2:B:462:HOH:O	2.42	0.43
1:B:301:LYS:O	1:B:304:VAL:HB	2.18	0.43
1:C:12:AEI:HB	1:C:114:ALA:O	2.18	0.43
1:D:315:ASP:OD2	1:D:318:GLN:HG3	2.19	0.43
1:C:286:ASP:O	1:C:290:GLY:N	2.50	0.43
1:D:269:ARG:O	1:D:278:THR:HG21	2.19	0.43
1:A:101:LEU:CD1	1:A:308:LEU:HD12	2.49	0.43
1:B:214:VAL:HG13	1:B:306:LEU:HD23	2.00	0.43
1:C:286:ASP:HB3	1:C:291:PHE:O	2.18	0.43
1:A:65:VAL:HG12	1:A:69:LEU:HD22	2.01	0.42
1:A:66:TRP:HB3	1:A:98:PHE:CE2	2.54	0.42
1:C:11:GLY:CA	1:C:27:VAL:HG13	2.49	0.42
1:D:31:GLY:O	1:D:35:LEU:HB2	2.19	0.42
1:D:96:ALA:O	1:D:100:ASP:HB2	2.19	0.42
1:B:156:ASP:HB3	1:B:179:LEU:HD21	2.00	0.42
1:B:163:THR:HG21	1:B:172:LYS:CD	2.49	0.42
1:C:219:ASN:HD22	1:C:250:TYR:H	1.67	0.42
1:B:320:GLN:HE21	1:B:324:ASN:HD21	1.68	0.42
1:A:27:VAL:HG21	1:A:57:GLY:CA	2.49	0.42
1:D:8:ALA:HA	1:D:86:THR:OG1	2.19	0.42
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.92	0.42
1:A:214:VAL:HG13	1:A:306:LEU:HD23	2.02	0.42
1:A:244:VAL:HG12	1:A:272:ARG:CZ	2.50	0.42
1:C:96:ALA:O	1:C:100:ASP:HB2	2.19	0.42
1:D:151:ASN:O	1:D:152:ASP:HB2	2.19	0.42
1:A:234:ALA:HB2	1:C:226:LEU:HD13	2.02	0.42
1:D:39:VAL:CG1	1:D:42:LEU:HD13	2.50	0.42
1:B:58:SER:HB2	1:B:91:THR:OG1	2.20	0.42
2:B:354:HOH:O	1:D:222:ASN:HB2	2.20	0.42
1:A:226:LEU:HD12	1:A:226:LEU:HA	1.82	0.42
1:B:69:LEU:HB3	1:B:99:LEU:HD21	2.01	0.42
1:C:213:LYS:HE2	2:C:439:HOH:O	2.19	0.42
1:A:231:LEU:O	1:A:236:TYR:HB2	2.20	0.41
1:B:257:LEU:HB3	1:B:267:VAL:HG11	2.01	0.41
1:C:238:GLY:HA2	1:C:266:ALA:O	2.20	0.41
1:A:105:CYS:SG	1:A:107:LYS:HB2	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TYR:O	1:A:134:VAL:HG23	2.20	0.41
1:B:261:ALA:HA	1:B:265:THR:O	2.20	0.41
1:C:218:TYR:HA	1:C:242:ALA:HB3	2.03	0.41
1:A:6:ILE:HA	1:A:84:VAL:O	2.19	0.41
1:C:106:ASP:HB3	1:C:143:ASN:OD1	2.21	0.41
1:D:159:ASP:OD1	1:D:175:ASN:HB2	2.20	0.41
1:D:286:ASP:HB3	1:D:291:PHE:O	2.20	0.41
1:C:67:LEU:HD21	1:C:211:LEU:HD11	2.02	0.41
1:C:214:VAL:HG12	1:C:303:ARG:HG3	2.01	0.41
1:D:139:LYS:HD3	1:D:139:LYS:HA	1.84	0.41
1:D:196:LYS:HD3	1:D:326:TYR:CE1	2.56	0.41
1:D:243:GLY:O	1:D:272:ARG:HG2	2.19	0.41
1:B:286:ASP:HB2	2:B:408:HOH:O	2.20	0.41
1:B:163:THR:HG22	1:B:170:THR:HA	2.02	0.41
1:B:241:SER:HB3	2:B:393:HOH:O	2.20	0.41
1:A:219:ASN:ND2	1:A:250:TYR:H	2.18	0.41
1:A:286:ASP:O	1:A:290:GLY:N	2.50	0.41
1:B:273:VAL:HG11	1:D:164:ASN:C	2.40	0.41
1:D:21:THR:CG2	1:D:121:MET:HE3	2.51	0.41
1:D:72:LYS:HB2	1:D:72:LYS:HE2	1.76	0.41
1:A:315:ASP:HA	1:A:316:PRO:HD2	1.95	0.41
1:B:66:TRP:HB3	1:B:98:PHE:CD2	2.56	0.41
1:B:84:VAL:HA	1:B:110:VAL:O	2.20	0.41
1:B:131:ASN:HD22	1:B:131:ASN:HA	1.75	0.41
1:B:226:LEU:HB2	1:B:227:PRO:HD3	2.03	0.41
1:B:260:ALA:O	1:B:265:THR:HB	2.20	0.41
1:B:319:ILE:O	1:B:323:PHE:HD1	2.04	0.41
1:C:67:LEU:HD21	1:C:211:LEU:HD13	2.03	0.41
1:C:115:MET:HE1	1:C:170:THR:HG21	2.03	0.41
1:D:194:ALA:HB2	2:D:338:HOH:O	2.19	0.41
1:D:249:LEU:HD22	1:D:254:PHE:HA	2.02	0.41
1:D:249:LEU:N	1:D:249:LEU:HD12	2.36	0.41
1:A:98:PHE:CE1	1:A:211:LEU:HD21	2.55	0.41
1:C:266:ALA:HB2	1:C:310:LEU:HD21	2.02	0.41
1:A:107:LYS:O	1:A:109:VAL:HG23	2.21	0.40
1:B:21:THR:CG2	1:B:121:MET:HE3	2.52	0.40
1:D:220:TYR:HA	1:D:272:ARG:NH2	2.36	0.40
1:B:190:GLN:O	1:B:191:ARG:CD	2.69	0.40
1:C:97:TYR:CE1	1:C:158:ARG:HG3	2.57	0.40
1:D:99:LEU:O	1:D:103:VAL:HB	2.21	0.40
1:D:272:ARG:HG3	1:D:273:VAL:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:GLN:NE2	2:B:442:HOH:O	2.55	0.40
1:A:171:PHE:O	1:A:172:LYS:HG3	2.22	0.40
1:A:247:GLY:HA2	1:A:270:SER:O	2.21	0.40
1:D:7:LEU:O	1:D:85:ILE:HA	2.21	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	323/326 (99%)	311 (96%)	10 (3%)	2 (1%)	25	26
1	B	323/326 (99%)	305 (94%)	18 (6%)	0	100	100
1	C	323/326 (99%)	306 (95%)	16 (5%)	1 (0%)	41	46
1	D	323/326 (99%)	307 (95%)	16 (5%)	0	100	100
All	All	1292/1304 (99%)	1229 (95%)	60 (5%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	LYS
1	C	126	PRO
1	A	126	PRO

### 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	265/265 (100%)	248 (94%)	17 (6%)	17	20
1	B	265/265 (100%)	249 (94%)	16 (6%)	19	22
1	C	265/265 (100%)	245 (92%)	20 (8%)	13	14
1	D	265/265 (100%)	248 (94%)	17 (6%)	17	20
All	All	1060/1060 (100%)	990 (93%)	70 (7%)	16	19

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	26	THR
1	A	42	LEU
1	A	69	LEU
1	A	118	SER
1	A	126	PRO
1	A	147	LEU
1	A	163	THR
1	A	200	ASP
1	A	201	THR
1	A	222	ASN
1	A	224	SER
1	A	226	LEU
1	A	241	SER
1	A	272	ARG
1	A	317	GLN
1	A	321	GLN
1	B	13	ILE
1	B	33	GLU
1	B	42	LEU
1	B	78	ASP
1	B	92	MET
1	B	126	PRO
1	B	131	ASN
1	B	147	LEU
1	B	211	LEU
1	B	222	ASN
1	B	226	LEU
1	B	262	LYS
1	B	272	ARG
1	B	280	GLN

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Mol	Chain	Res	Type
1	B	316	PRO
1	B	321	GLN
1	C	18	ASP
1	C	24	ASN
1	C	26	THR
1	C	54	VAL
1	C	69	LEU
1	C	78	ASP
1	C	131	ASN
1	C	147	LEU
1	C	152	ASP
1	C	156	ASP
1	C	163	THR
1	C	201	THR
1	C	211	LEU
1	C	213	LYS
1	C	222	ASN
1	C	249	LEU
1	C	254	PHE
1	C	272	ARG
1	C	288	LYS
1	C	318	GLN
1	D	26	THR
1	D	34	ASN
1	D	35	LEU
1	D	58	SER
1	D	62	ASN
1	D	69	LEU
1	D	85	ILE
1	D	147	LEU
1	D	163	THR
1	D	222	ASN
1	D	226	LEU
1	D	252	SER
1	D	254	PHE
1	D	262	LYS
1	D	272	ARG
1	D	316	PRO
1	D	321	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	183	HIS
1	A	209	ASN
1	A	219	ASN
1	A	321	GLN
1	A	324	ASN
1	A	325	GLN
1	B	34	ASN
1	B	209	ASN
1	B	219	ASN
1	B	312	GLN
1	B	317	GLN
1	B	321	GLN
1	B	324	ASN
1	B	325	GLN
1	C	34	ASN
1	C	131	ASN
1	C	183	HIS
1	C	317	GLN
1	D	62	ASN
1	D	131	ASN
1	D	209	ASN
1	D	219	ASN
1	D	312	GLN
1	D	321	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	10,14,15	1.36	2 (20%)	11,18,20	1.79	3 (27%)
1	AEI	C	12	1	10,14,15	1.02	1 (10%)	11,18,20	1.54	2 (18%)
1	AEI	B	12	1	10,14,15	1.06	0	11,18,20	1.61	2 (18%)
1	AEI	D	12	1	10,14,15	1.05	0	11,18,20	1.44	2 (18%)

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	AEI	C	12	1	-	1/12/18/20	-
1	AEI	B	12	1	-	3/12/18/20	-
1	AEI	D	12	1	-	3/12/18/20	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	AEI	CB-CA	2.54	1.59	1.53
1	A	12	AEI	OG1-CD	2.47	1.41	1.34
1	C	12	AEI	OG1-CD	2.17	1.40	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	AEI	OG1-CD-CE2	4.10	118.99	111.46
1	B	12	AEI	OG1-CD-CE2	3.49	117.88	111.46
1	D	12	AEI	OG1-CD-CE2	3.48	117.85	111.46
1	C	12	AEI	OG1-CD-CE2	3.42	117.75	111.46
1	A	12	AEI	OE1-CD-CE2	-3.14	117.80	124.73
1	B	12	AEI	OE1-CD-CE2	-2.61	118.97	124.73
1	C	12	AEI	OE1-CD-CE2	-2.59	119.00	124.73
1	D	12	AEI	OE1-CD-CE2	-2.22	119.83	124.73
1	A	12	AEI	OG1-CB-CA	2.04	110.53	105.89

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 9 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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, 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	325/326 (99%)	-0.66	2 (0%) 89 88	5, 17, 39, 58	0
1	B	325/326 (99%)	-0.66	1 (0%) 94 93	5, 17, 42, 66	0
1	C	325/326 (99%)	-0.70	1 (0%) 94 93	5, 17, 42, 62	0
1	D	325/326 (99%)	-0.67	1 (0%) 94 93	6, 16, 41, 59	0
All	All	1300/1304 (99%)	-0.67	5 (0%) 92 91	5, 17, 41, 66	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	18	ASP	4.1
1	A	18	ASP	2.6
1	A	28	GLY	2.6
1	B	17	GLY	2.3
1	D	28	GLY	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	15/16	0.95	0.10	16,26,28,30	0
1	AEI	A	12	15/16	0.96	0.10	11,21,27,28	0
1	AEI	D	12	15/16	0.96	0.09	14,22,28,30	0
1	AEI	B	12	15/16	0.97	0.09	17,23,26,27	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.