



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 07:08 PM BST

PDB ID : 6V28  
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 : 1.95 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 : 2.13.1  
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) : 2.13.1

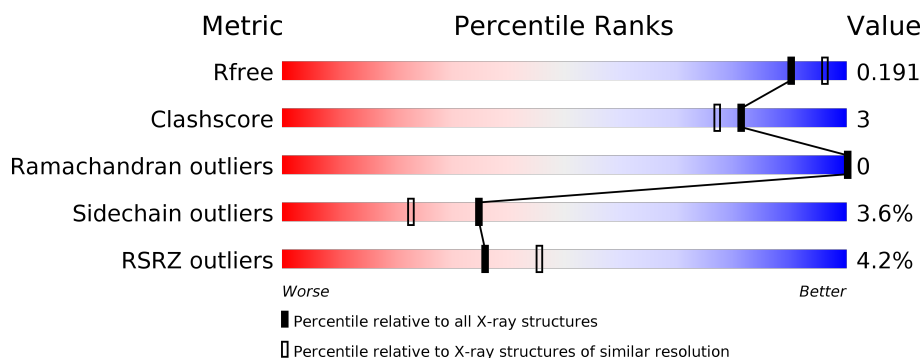
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	333	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>..</div> </div> </div>
1	B	333	<div> <div>8%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>.</div> </div> </div>
1	C	333	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>.</div> </div> </div>
1	D	333	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	901	-	-	X	X
3	GOL	D	403	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11117 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	5	0
			2462	1537	418	498	9			
1	B	326	Total	C	N	O	S	0	3	0
			2452	1531	417	496	8			
1	C	327	Total	C	N	O	S	0	3	0
			2462	1538	418	497	9			
1	D	327	Total	C	N	O	S	0	4	0
			2462	1536	418	499	9			

There are 40 discrepancies between the modelled and reference sequences:

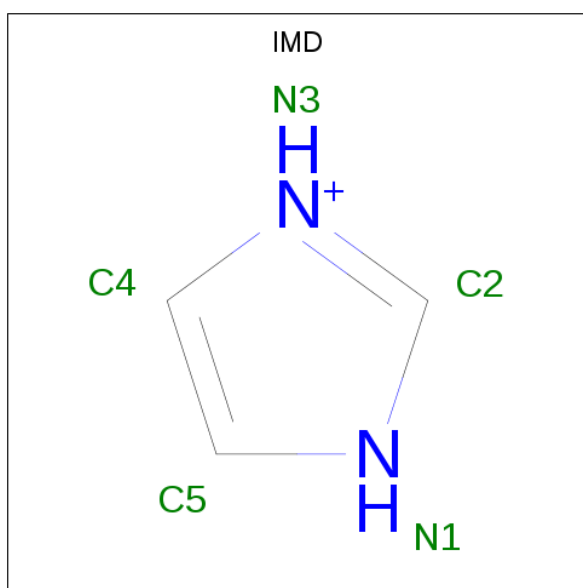
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP P00805
A	-5	HIS	-	expression tag	UNP P00805
A	-4	HIS	-	expression tag	UNP P00805
A	-3	HIS	-	expression tag	UNP P00805
A	-2	HIS	-	expression tag	UNP P00805
A	-1	HIS	-	expression tag	UNP P00805
A	0	HIS	-	expression tag	UNP P00805
A	12	AEI	THR	modified residue	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	modified residue	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

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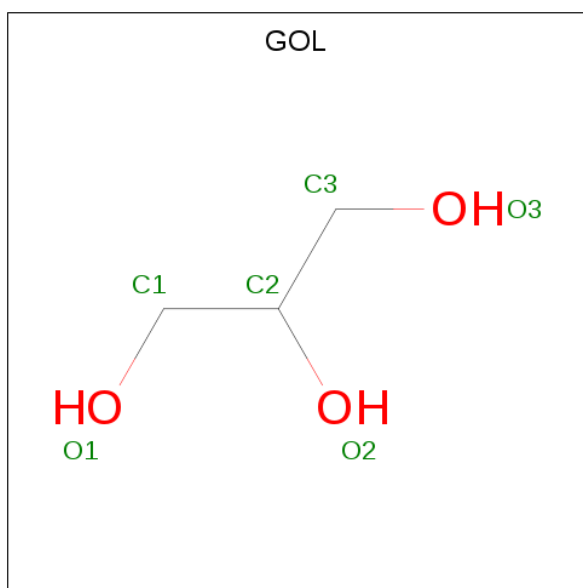
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	expression tag	UNP P00805
C	-4	HIS	-	expression tag	UNP P00805
C	-3	HIS	-	expression tag	UNP P00805
C	-2	HIS	-	expression tag	UNP P00805
C	-1	HIS	-	expression tag	UNP P00805
C	0	HIS	-	expression tag	UNP P00805
C	12	AEI	THR	modified residue	UNP 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	modified residue	UNP P00805
D	89	VAL	THR	engineered mutation	UNP P00805
D	162	THR	LYS	engineered mutation	UNP P00805

- Molecule 2 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 5 3 2	0	0
2	D	1	Total C N 5 3 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	1
			12	6	6		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			5	3	2		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			5	3	2		


- Molecule 4 is water.

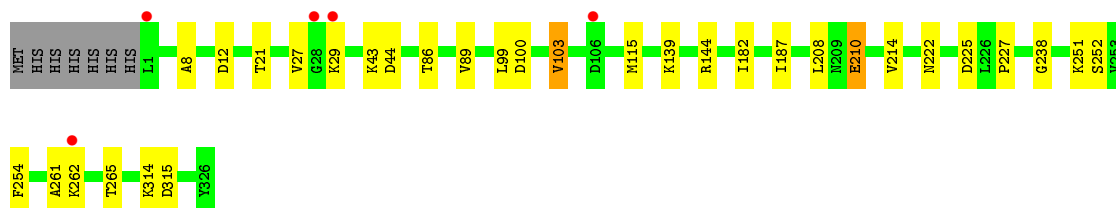
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	281	Total	O	0	0
			281	281		
4	B	235	Total	O	0	0
			235	235		
4	C	368	Total	O	0	0
			368	368		
4	D	339	Total	O	0	0
			339	339		

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

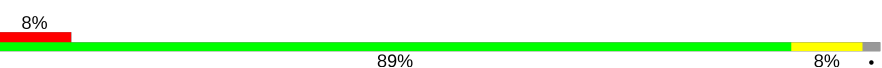
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

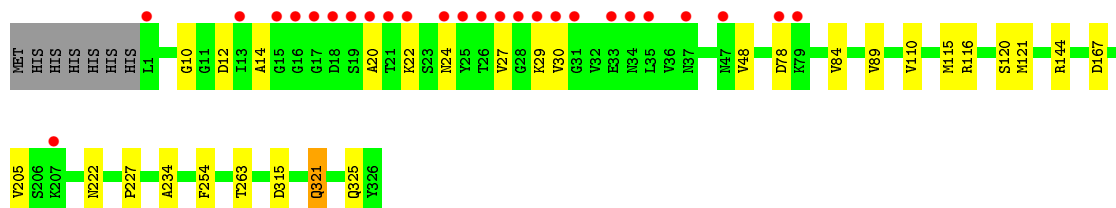
#### • Molecule 1: L-asparaginase 2

Chain A: 




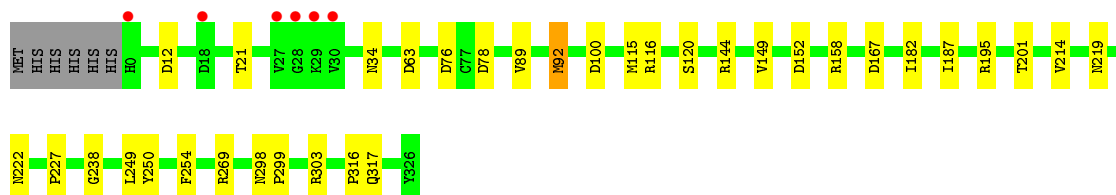
#### • Molecule 1: L-asparaginase 2

Chain B: 




#### • Molecule 1: L-asparaginase 2

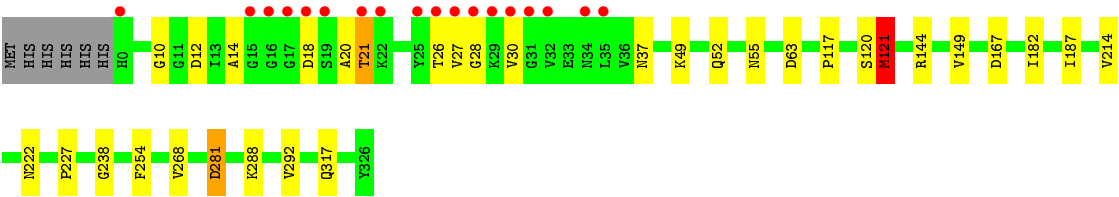
Chain C: 



#### • 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, $\alpha$ , $\beta$ , $\gamma$	151.34Å 62.54Å 141.30Å 90.00° 117.68° 90.00°	Depositor
Resolution (Å)	27.90 – 1.95 27.97 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.6 (27.90-1.95) 97.7 (27.97-1.95)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.142 , 0.186 0.153 , 0.191	Depositor DCC
$R_{free}$ test set	4018 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.3	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11117	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.88	1/2495 (0.0%)	0.92	5/3397 (0.1%)
1	B	0.86	0/2482	0.91	8/3378 (0.2%)
1	C	1.00	1/2493 (0.0%)	1.02	15/3394 (0.4%)
1	D	0.96	0/2497	1.00	9/3399 (0.3%)
All	All	0.92	2/9967 (0.0%)	0.96	37/13568 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	120	SER	CB-OG	-5.25	1.35	1.42
1	A	210	GLU	CD-OE1	5.15	1.31	1.25

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	281	ASP	CB-CG-OD2	-8.85	110.33	118.30
1	C	92	MET	CG-SD-CE	8.72	114.15	100.20
1	D	167	ASP	CB-CG-OD1	8.12	125.61	118.30
1	B	144	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	C	167	ASP	CB-CG-OD1	7.57	125.11	118.30
1	B	144	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	D	121	MET	CG-SD-CE	7.04	111.47	100.20
1	C	63	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	C	63	ASP	CB-CG-OD1	6.75	124.38	118.30
1	D	63	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	C	78	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	144	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	D	144	ARG	NE-CZ-NH2	6.59	123.59	120.30
1	C	116	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	116	ARG	NE-CZ-NH1	6.50	123.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	MET	CG-SD-CE	6.28	110.25	100.20
1	C	152	ASP	CB-CG-OD1	6.16	123.84	118.30
1	C	195	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	269	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	100	ASP	CB-CG-OD1	5.82	123.53	118.30
1	B	315	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	167	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	D	167	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	D	63	ASP	CB-CG-OD1	5.65	123.39	118.30
1	D	288	LYS	CD-CE-NZ	-5.65	98.71	111.70
1	B	116	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	158	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	303	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	C	76	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	144	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	D	281	ASP	CB-CG-OD1	5.23	123.01	118.30
1	B	167	ASP	CB-CG-OD1	5.15	122.94	118.30
1	C	100	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	A	315	ASP	CB-CG-OD1	5.11	122.89	118.30
1	A	100	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	C	249	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	A	44	ASP	CB-CG-OD2	-5.01	113.79	118.30

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	2462	0	2457	8	0
1	B	2452	0	2449	17	0
1	C	2462	0	2454	9	0
1	D	2462	0	2449	19	0
2	A	5	0	5	0	0
2	D	5	0	5	0	0
3	B	6	0	8	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	18	0	24	1	0
3	D	22	0	26	8	0
4	A	281	0	0	0	0
4	B	235	0	0	1	1
4	C	368	0	0	1	0
4	D	339	0	0	4	2
All	All	11117	0	9877	52	2

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 3.

All (52) 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:55:ASN:OD1	3:D:403:GOL:H12	1.66	0.95
1:D:52:GLN:NE2	3:D:403:GOL:O2	2.18	0.76
1:D:10:GLY:HA2	3:D:403:GOL:C1	2.18	0.74
1:D:14:ALA:HB3	3:D:403:GOL:O1	1.87	0.74
1:C:89[A]:VAL:HG21	1:C:115[A]:MET:SD	2.31	0.71
1:D:28:GLY:HA2	1:D:55:ASN:OD1	1.94	0.67
1:B:263:THR:O	1:B:263:THR:HG22	1.99	0.62
1:B:14:ALA:HB3	3:B:901:GOL:C3	2.29	0.62
1:B:14:ALA:HB1	1:B:30:VAL:HB	1.82	0.60
1:B:321[B]:GLN:HG3	1:B:325:GLN:HE21	1.66	0.60
1:A:89[A]:VAL:HG21	1:A:115[A]:MET:SD	2.42	0.59
1:D:10:GLY:HA2	3:D:403:GOL:C2	2.33	0.58
1:D:14:ALA:HB3	3:D:403:GOL:C1	2.33	0.57
1:A:182:ILE:HG12	1:A:187:ILE:HG12	1.86	0.56
1:B:14:ALA:HB3	3:B:901:GOL:H32	1.88	0.55
1:B:89:VAL:HG11	1:B:115:MET:SD	2.46	0.55
1:A:227:PRO:HB3	1:B:227:PRO:HB3	1.90	0.54
1:B:321[B]:GLN:HG3	1:B:325:GLN:NE2	2.22	0.53
1:B:10:GLY:HA2	3:B:901:GOL:O3	2.10	0.52
1:C:182:ILE:HG12	1:C:187:ILE:HG12	1.92	0.52
1:D:149:VAL:HG12	4:D:543:HOH:O	2.09	0.52
1:D:117:PRO:HG2	1:D:120[B]:SER:OG	2.10	0.52
1:A:99:LEU:O	1:A:103:VAL:HG13	2.10	0.51
1:C:219:ASN:HD22	1:C:250:TYR:H	1.59	0.51
1:D:37:ASN:HA	4:D:656:HOH:O	2.11	0.50
1:D:182:ILE:HG12	1:D:187:ILE:HG12	1.94	0.49
1:B:10:GLY:HA2	3:B:901:GOL:O2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:GLN:HA	3:D:404:GOL:H11	1.94	0.48
1:A:225:ASP:HB3	1:A:252:SER:HB3	1.94	0.48
1:D:21:THR:HG22	1:D:121:MET:HE1	1.95	0.48
1:B:14:ALA:HB1	1:B:30:VAL:CG1	2.44	0.48
1:C:317:GLN:HA	3:C:901:GOL:H11	1.97	0.47
3:D:403:GOL:H2	4:D:524:HOH:O	2.15	0.47
1:B:20:ALA:HA	1:B:120[B]:SER:HA	1.97	0.46
1:B:14:ALA:HB3	3:B:901:GOL:H31	1.98	0.45
1:C:149:VAL:HG12	4:C:1119:HOH:O	2.17	0.44
1:B:20:ALA:HA	1:B:120[A]:SER:HA	1.99	0.44
1:D:281:ASP:OD2	4:D:501:HOH:O	2.21	0.43
1:B:84:VAL:HA	1:B:110:VAL:O	2.19	0.43
1:A:261:ALA:HA	1:A:265:THR:O	2.19	0.43
1:D:14:ALA:HB1	1:D:30:VAL:HB	1.99	0.43
1:C:227:PRO:HB3	1:D:227:PRO:HB3	2.01	0.43
1:C:214:VAL:HA	1:C:238:GLY:O	2.19	0.43
1:A:214:VAL:HA	1:A:238:GLY:O	2.19	0.42
1:D:214:VAL:HA	1:D:238:GLY:O	2.20	0.42
1:D:268:VAL:HG22	1:D:292:VAL:HB	2.02	0.42
1:A:8:ALA:HA	1:A:86:THR:OG1	2.21	0.41
1:C:298:ASN:HB2	1:C:299:PRO:CD	2.50	0.41
1:B:10:GLY:HA2	3:B:901:GOL:HO2	1.84	0.41
1:B:234:ALA:O	4:B:1001:HOH:O	2.21	0.41
1:C:219:ASN:ND2	1:C:250:TYR:H	2.18	0.40
1:D:20:ALA:HA	1:D:120[A]:SER:HA	2.02	0.40

All (2) 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)
4:D:546:HOH:O	4:D:786:HOH:O[2_556]	1.95	0.25
4:B:1136:HOH:O	4:D:820:HOH:O[4_556]	2.00	0.20

## 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	328/333 (98%)	323 (98%)	5 (2%)	0	100	100
1	B	326/333 (98%)	319 (98%)	7 (2%)	0	100	100
1	C	327/333 (98%)	323 (99%)	4 (1%)	0	100	100
1	D	328/333 (98%)	322 (98%)	6 (2%)	0	100	100
All	All	1309/1332 (98%)	1287 (98%)	22 (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	270/272 (99%)	257 (95%)	13 (5%)	25	12
1	B	268/272 (98%)	257 (96%)	11 (4%)	30	18
1	C	269/272 (99%)	262 (97%)	7 (3%)	46	36
1	D	270/272 (99%)	262 (97%)	8 (3%)	41	30
All	All	1077/1088 (99%)	1038 (96%)	39 (4%)	35	23

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	27	VAL
1	A	29	LYS
1	A	43	LYS
1	A	103	VAL
1	A	139	LYS
1	A	208	LEU
1	A	210	GLU
1	A	222	ASN
1	A	251	LYS

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Mol	Chain	Res	Type
1	A	254	PHE
1	A	262	LYS
1	A	314	LYS
1	B	22	LYS
1	B	24	ASN
1	B	27	VAL
1	B	29	LYS
1	B	48	VAL
1	B	78	ASP
1	B	205	VAL
1	B	222	ASN
1	B	254	PHE
1	B	321[A]	GLN
1	B	321[B]	GLN
1	C	21	THR
1	C	34	ASN
1	C	92	MET
1	C	201	THR
1	C	222	ASN
1	C	254	PHE
1	C	316	PRO
1	D	18	ASP
1	D	21	THR
1	D	26	THR
1	D	27	VAL
1	D	49	LYS
1	D	121	MET
1	D	222	ASN
1	D	254	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	52	GLN
1	B	64	ASN
1	B	325	GLN
1	C	34	ASN
1	C	219	ASN
1	C	318	GLN
1	C	324	ASN
1	D	52	GLN
1	D	64	ASN

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Mol	Chain	Res	Type
1	D	318	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	D	12	1	10,14,15	0.91	0	11,18,20	1.63	3 (27%)
1	AEI	A	12	1	10,14,15	1.35	2 (20%)	11,18,20	1.46	3 (27%)
1	AEI	C	12	1	10,14,15	1.21	1 (10%)	11,18,20	1.11	1 (9%)
1	AEI	B	12	1	10,14,15	0.90	0	11,18,20	1.44	1 (9%)

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	D	12	1	-	3/12/18/20	-
1	AEI	A	12	1	-	3/12/18/20	-
1	AEI	C	12	1	-	3/12/18/20	-
1	AEI	B	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	OG1-CD	3.09	1.43	1.34
1	C	12	AEI	OG1-CD	2.89	1.42	1.34
1	A	12	AEI	O-C	2.09	1.28	1.19

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	12	AEI	OG1-CB-CA	3.39	113.60	105.89
1	D	12	AEI	OG1-CB-CA	3.35	113.51	105.89
1	A	12	AEI	OG1-CB-CA	2.58	111.76	105.89
1	A	12	AEI	OE1-CD-CE2	-2.50	119.20	124.73
1	D	12	AEI	CE2-CZ-CH2	-2.40	106.80	110.69
1	D	12	AEI	O-C-CA	-2.26	118.86	124.78
1	A	12	AEI	OG1-CD-OE1	2.07	128.71	123.70
1	C	12	AEI	OG1-CB-CA	2.03	110.50	105.89

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

10 ligands 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	$\# Z  > 2$
3	GOL	B	901	-	5,5,5	0.32	0	5,5,5	0.79	0
3	GOL	D	403	-	5,5,5	0.55	0	5,5,5	0.76	0
2	IMD	D	405	-	3,5,5	0.38	0	4,5,5	0.58	0
3	GOL	D	402	-	3,4,5	0.53	0	1,4,5	0.67	0
2	IMD	A	401	-	3,5,5	0.30	0	4,5,5	0.54	0
3	GOL	D	404	-	3,4,5	1.03	0	1,4,5	1.97	0
3	GOL	C	901	-	5,5,5	0.32	0	5,5,5	0.46	0
3	GOL	C	902[B]	-	5,5,5	0.36	0	5,5,5	0.49	0
3	GOL	C	902[A]	-	5,5,5	0.29	0	5,5,5	0.42	0
3	GOL	D	401	-	5,5,5	0.37	0	5,5,5	0.30	0

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
3	GOL	B	901	-	-	0/4/4/4	-
3	GOL	D	403	-	-	2/4/4/4	-
3	GOL	D	401	-	-	2/4/4/4	-
3	GOL	D	402	-	-	2/2/2/4	-
2	IMD	A	401	-	-	-	0/1/1/1
3	GOL	D	404	-	-	2/2/2/4	-
3	GOL	C	901	-	-	2/4/4/4	-
3	GOL	C	902[B]	-	-	4/4/4/4	-
3	GOL	C	902[A]	-	-	2/4/4/4	-
2	IMD	D	405	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	403	GOL	O1-C1-C2-C3
3	D	402	GOL	O1-C1-C2-O2
3	D	404	GOL	O1-C1-C2-O2
3	C	901	GOL	O1-C1-C2-C3
3	C	902[B]	GOL	O1-C1-C2-C3
3	C	902[A]	GOL	O1-C1-C2-C3
3	D	401	GOL	O1-C1-C2-C3
3	D	403	GOL	O1-C1-C2-O2
3	D	401	GOL	O1-C1-C2-O2
3	C	902[B]	GOL	C1-C2-C3-O3
3	C	901	GOL	O1-C1-C2-O2
3	C	902[B]	GOL	O1-C1-C2-O2
3	C	902[B]	GOL	O2-C2-C3-O3
3	C	902[A]	GOL	O1-C1-C2-O2
3	D	402	GOL	O1-C1-C2-C3
3	D	404	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	GOL	6	0
3	D	403	GOL	7	0
3	D	404	GOL	1	0
3	C	901	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	325/333 (97%)	-0.14	5 (1%) 73 81	19, 27, 45, 65	0
1	B	325/333 (97%)	0.13	26 (8%) 12 19	19, 29, 71, 106	0
1	C	326/333 (97%)	-0.32	6 (1%) 68 76	12, 18, 34, 55	0
1	D	326/333 (97%)	-0.17	18 (5%) 25 34	12, 18, 53, 94	0
All	All	1302/1332 (97%)	-0.12	55 (4%) 36 45	12, 24, 49, 106	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	LYS	7.1
1	B	18	ASP	7.1
1	D	26	THR	6.9
1	D	29	LYS	6.7
1	B	19	SER	6.5
1	B	26	THR	6.2
1	B	30	VAL	5.8
1	D	27	VAL	5.6
1	D	18	ASP	5.3
1	B	17	GLY	5.3
1	D	16	GLY	5.2
1	D	17	GLY	4.9
1	A	29	LYS	4.7
1	B	35	LEU	4.5
1	B	27	VAL	4.4
1	B	16	GLY	4.2
1	B	25	TYR	4.1
1	B	22	LYS	3.8
1	B	15	GLY	3.8
1	B	31	GLY	3.8
1	B	21	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	30	VAL	3.7
1	D	28	GLY	3.6
1	B	20	ALA	3.6
1	C	0	HIS	3.5
1	D	15	GLY	3.3
1	D	19	SER	3.3
1	B	34	ASN	3.3
1	D	0	HIS	3.1
1	D	25	TYR	3.0
1	B	37	ASN	2.9
1	D	31	GLY	2.8
1	D	22	LYS	2.8
1	B	33	GLU	2.7
1	C	27	VAL	2.6
1	C	29	LYS	2.5
1	D	34	ASN	2.5
1	B	24	ASN	2.5
1	D	21	THR	2.5
1	C	18	ASP	2.4
1	B	78	ASP	2.4
1	C	28	GLY	2.4
1	B	207	LYS	2.3
1	C	30	VAL	2.3
1	A	262	LYS	2.2
1	A	106	ASP	2.2
1	A	28	GLY	2.2
1	B	79	LYS	2.2
1	D	35	LEU	2.1
1	A	1	LEU	2.1
1	B	13	ILE	2.1
1	B	1	LEU	2.1
1	B	28	GLY	2.0
1	D	32	VAL	2.0
1	B	47	ASN	2.0

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

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( $\text{\AA}^2$ )	Q<0.9
1	AEI	B	12	15/16	0.87	0.12	36,40,51,53	0
1	AEI	D	12	15/16	0.93	0.11	20,26,36,37	0
1	AEI	C	12	15/16	0.95	0.09	17,19,23,24	0
1	AEI	A	12	15/16	0.95	0.08	23,25,27,29	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [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( $\text{\AA}^2$ )	Q<0.9
3	GOL	D	404	5/6	0.59	0.28	35,40,44,52	0
3	GOL	B	901	6/6	0.66	0.55	43,46,46,47	6
2	IMD	A	401	5/5	0.76	0.23	54,54,58,59	0
3	GOL	D	402	5/6	0.77	0.21	28,28,29,42	5
3	GOL	D	401	6/6	0.79	0.15	48,52,53,55	0
3	GOL	D	403	6/6	0.82	0.47	62,64,66,66	0
3	GOL	C	901	6/6	0.87	0.21	38,50,58,61	0
2	IMD	D	405	5/5	0.87	0.21	39,40,42,42	0
3	GOL	C	902[A]	6/6	0.94	0.15	26,29,32,33	6
3	GOL	C	902[B]	6/6	0.94	0.15	27,30,32,34	6

### 6.5 Other polymers [i](#)

There are no such residues in this entry.