



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 10:41 AM EDT

PDB ID : 3EUW  
Title : Crystal Structure of a Myo-inositol dehydrogenase from *Corynebacterium glutamicum* ATCC 13032  
Authors : Kumaran, D.; Mahmood, A.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2008-10-11  
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](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.

The types of validation reports are described at

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

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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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
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) : 2.37.1

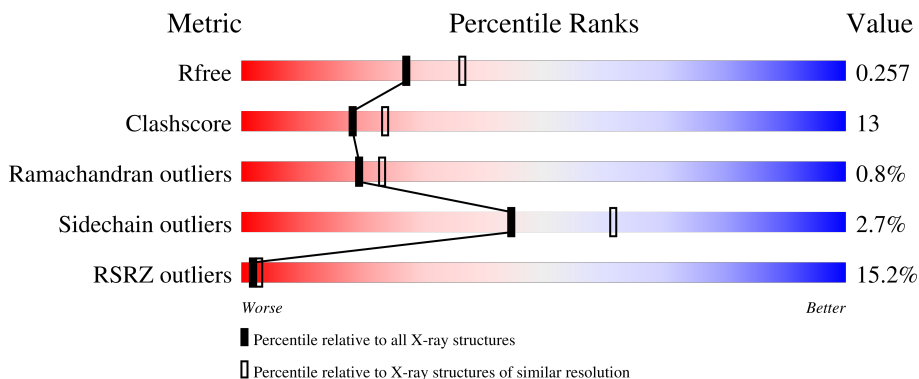
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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  $\geq 3$ , 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	344	 2% 79% 17% ..
1	B	344	 % 81% 15% ..
1	C	344	 27% 65% 30% ..
1	D	344	 28% 65% 30% ..

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 10763 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 Myo-inositol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	S				Se
1	A	333	2533	1588	445	491	4	5	0	0	0
1	B	333	2533	1588	445	491	4	5	0	0	0
1	C	333	2533	1588	445	491	4	5	0	0	0
1	D	333	2533	1588	445	491	4	5	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP Q8NL86
A	0	SER	-	expression tag	UNP Q8NL86
A	1	LEU	-	expression tag	UNP Q8NL86
A	335	GLU	-	expression tag	UNP Q8NL86
A	336	GLY	-	expression tag	UNP Q8NL86
A	337	HIS	-	expression tag	UNP Q8NL86
A	338	HIS	-	expression tag	UNP Q8NL86
A	339	HIS	-	expression tag	UNP Q8NL86
A	340	HIS	-	expression tag	UNP Q8NL86
A	341	HIS	-	expression tag	UNP Q8NL86
A	342	HIS	-	expression tag	UNP Q8NL86
B	-1	MSE	-	expression tag	UNP Q8NL86
B	0	SER	-	expression tag	UNP Q8NL86
B	1	LEU	-	expression tag	UNP Q8NL86
B	335	GLU	-	expression tag	UNP Q8NL86
B	336	GLY	-	expression tag	UNP Q8NL86
B	337	HIS	-	expression tag	UNP Q8NL86
B	338	HIS	-	expression tag	UNP Q8NL86
B	339	HIS	-	expression tag	UNP Q8NL86
B	340	HIS	-	expression tag	UNP Q8NL86
B	341	HIS	-	expression tag	UNP Q8NL86

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Chain	Residue	Modelled	Actual	Comment	Reference
B	342	HIS	-	expression tag	UNP Q8NL86
C	-1	MSE	-	expression tag	UNP Q8NL86
C	0	SER	-	expression tag	UNP Q8NL86
C	1	LEU	-	expression tag	UNP Q8NL86
C	335	GLU	-	expression tag	UNP Q8NL86
C	336	GLY	-	expression tag	UNP Q8NL86
C	337	HIS	-	expression tag	UNP Q8NL86
C	338	HIS	-	expression tag	UNP Q8NL86
C	339	HIS	-	expression tag	UNP Q8NL86
C	340	HIS	-	expression tag	UNP Q8NL86
C	341	HIS	-	expression tag	UNP Q8NL86
C	342	HIS	-	expression tag	UNP Q8NL86
D	-1	MSE	-	expression tag	UNP Q8NL86
D	0	SER	-	expression tag	UNP Q8NL86
D	1	LEU	-	expression tag	UNP Q8NL86
D	335	GLU	-	expression tag	UNP Q8NL86
D	336	GLY	-	expression tag	UNP Q8NL86
D	337	HIS	-	expression tag	UNP Q8NL86
D	338	HIS	-	expression tag	UNP Q8NL86
D	339	HIS	-	expression tag	UNP Q8NL86
D	340	HIS	-	expression tag	UNP Q8NL86
D	341	HIS	-	expression tag	UNP Q8NL86
D	342	HIS	-	expression tag	UNP Q8NL86

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	231	Total O 231 231	0	0
3	B	201	Total O 201 201	0	0
3	C	96	Total O 96 96	0	0

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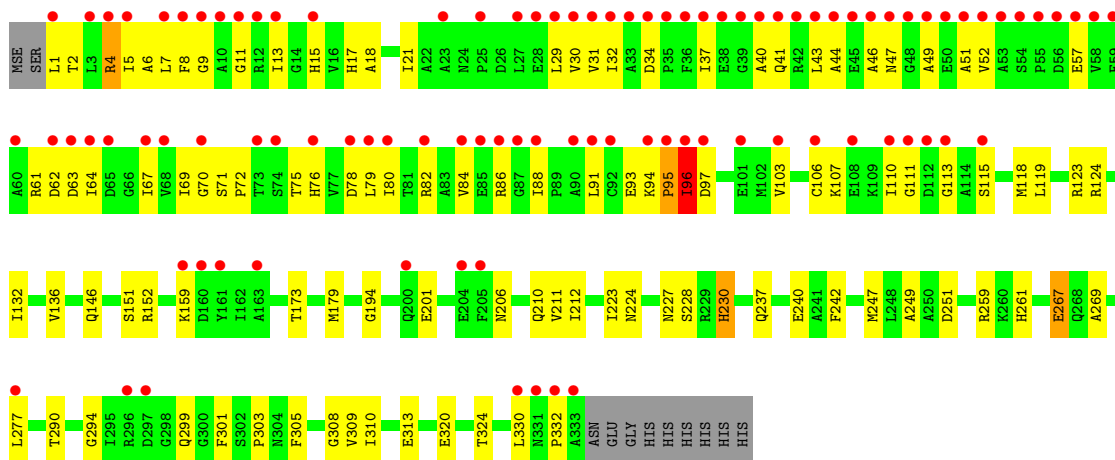
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	D	101	Total 101	O 101	0	0





- Molecule 1: Myo-inositol dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.04Å 127.59Å 87.16Å 90.00° 92.96° 90.00°	Depositor
Resolution (Å)	38.21 – 2.30 38.21 – 2.29	Depositor EDS
% Data completeness (in resolution range)	95.2 (38.21-2.30) 94.4 (38.21-2.29)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.16 (at 2.29Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.223 , 0.258 0.223 , 0.257	Depositor DCC
$R_{free}$ test set	4052 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtrriage
Anisotropy	0.349	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for l,k,-h 0.044 for h,-k,-l 0.017 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10763	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.36	0/2572	0.60	0/3481
1	B	0.38	0/2572	0.64	2/3481 (0.1%)
1	C	0.31	0/2572	0.55	0/3481
1	D	0.30	0/2572	0.56	0/3481
All	All	0.34	0/10288	0.59	2/13924 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	LYS	C-N-CD	-9.32	100.08	120.60
1	B	95	PRO	CA-N-CD	-6.31	102.66	111.50

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2533	0	2490	47	0
1	B	2533	0	2490	49	0
1	C	2533	0	2490	92	0
1	D	2533	0	2490	101	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	231	0	0	9	0
3	B	201	0	0	5	0
3	C	96	0	0	5	0
3	D	101	0	0	7	0
All	All	10763	0	9960	268	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 13.

All (268) 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)
3:A:574:HOH:O	1:B:247:MSE:HE3	1.70	0.91
1:C:29:LEU:HD21	1:C:32:ILE:HD11	1.53	0.90
1:B:240:GLU:CD	1:B:247:MSE:HE2	1.92	0.89
1:B:94:LYS:CB	1:B:95:PRO:HD2	2.04	0.86
1:C:210:GLN:NE2	1:D:146:GLN:HG3	1.91	0.86
1:C:94:LYS:HD2	1:C:95:PRO:HD2	1.57	0.85
1:C:94:LYS:HD3	1:C:175:HIS:NE2	1.99	0.78
1:C:6:ALA:HB2	1:C:64:ILE:HD12	1.67	0.77
1:D:247:MSE:CE	1:D:249:ALA:HB2	2.15	0.77
1:A:224:ASN:HD21	1:B:224:ASN:HD21	1.30	0.77
1:A:12:ARG:HE	1:A:12:ARG:HA	1.51	0.76
1:D:247:MSE:HE1	1:D:249:ALA:HB2	1.69	0.75
1:A:212:ILE:HD13	1:B:222:LEU:HD13	1.67	0.75
1:D:6:ALA:HB2	1:D:64:ILE:HG21	1.69	0.75
1:D:4:ARG:HH11	1:D:4:ARG:HB2	1.53	0.73
1:C:331:ASN:HA	3:C:414:HOH:O	1.90	0.71
1:A:4:ARG:HD2	1:A:30:VAL:HG11	1.74	0.69
1:C:261:HIS:CD2	1:C:267:GLU:H	2.11	0.69
1:A:224:ASN:HD21	1:B:224:ASN:ND2	1.91	0.69
1:A:224:ASN:ND2	1:B:224:ASN:HD21	1.92	0.68
1:C:2:THR:HG22	1:C:3:LEU:H	1.59	0.68
1:D:34:ASP:HB3	1:D:40:ALA:HB2	1.76	0.68
1:D:32:ILE:HG13	3:D:376:HOH:O	1.94	0.67
1:D:107:LYS:HE2	3:D:384:HOH:O	1.93	0.67
1:C:94:LYS:HD2	1:C:95:PRO:CD	2.25	0.67
1:A:81:THR:O	1:A:85:GLU:HG3	1.94	0.66
1:C:123:ARG:CZ	1:C:237:GLN:HE22	2.08	0.66
1:D:247:MSE:HE1	1:D:249:ALA:CB	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:HIS:CD2	1:D:267:GLU:H	2.13	0.66
1:C:332:PRO:HD2	3:C:414:HOH:O	1.95	0.65
1:D:124:ARG:HD2	1:D:303:PRO:HG3	1.78	0.65
1:C:224:ASN:ND2	1:D:224:ASN:HD21	1.94	0.65
1:B:94:LYS:HG3	1:B:95:PRO:HG2	1.79	0.65
1:C:32:ILE:HD13	1:C:44:ALA:HB2	1.79	0.65
1:C:224:ASN:HD21	1:D:224:ASN:HD21	1.45	0.65
1:C:224:ASN:HD21	1:D:224:ASN:ND2	1.95	0.64
1:B:94:LYS:HE3	1:B:171:ASP:O	1.97	0.64
1:A:82:ARG:HD3	3:A:543:HOH:O	1.97	0.63
1:C:210:GLN:HE22	1:D:146:GLN:HG3	1.63	0.63
1:D:9:GLY:HA3	1:D:70:GLY:O	1.99	0.62
1:C:54:SER:HB2	1:C:55:PRO:HD2	1.80	0.62
1:A:12:ARG:HA	1:A:12:ARG:NE	2.15	0.62
1:B:94:LYS:HB2	1:B:95:PRO:HD2	1.79	0.61
1:C:145:GLU:OE1	1:D:230:HIS:HE1	1.84	0.61
1:D:31:VAL:HG22	1:D:32:ILE:N	2.16	0.61
1:B:94:LYS:HG3	1:B:95:PRO:HD2	1.83	0.60
1:D:61:ARG:HD2	3:D:381:HOH:O	2.00	0.60
1:B:94:LYS:CG	1:B:95:PRO:HD2	2.31	0.60
1:D:67:ILE:HD11	1:D:88:ILE:HD12	1.84	0.60
1:B:241:ALA:O	1:B:247:MSE:HG2	2.01	0.59
1:D:13:ILE:HG12	1:D:93:GLU:HG3	1.84	0.59
1:C:73:THR:HA	1:C:76:HIS:CE1	2.37	0.59
1:D:118:MSE:HE1	1:D:290:THR:HG22	1.84	0.59
1:C:80:ILE:O	1:C:84:VAL:HG23	2.03	0.59
1:D:4:ARG:O	1:D:5:ILE:HD13	2.03	0.59
1:B:54:SER:HB2	3:B:402:HOH:O	2.03	0.58
1:C:3:LEU:HD12	3:C:404:HOH:O	2.02	0.58
1:C:247:MSE:CE	1:C:249:ALA:HB2	2.33	0.58
1:C:31:VAL:C	1:C:32:ILE:HD12	2.23	0.58
1:B:95:PRO:HG2	3:B:347:HOH:O	2.03	0.58
1:C:4:ARG:O	1:C:5:ILE:HD13	2.03	0.58
1:C:84:VAL:HG11	1:C:113:GLY:HA3	1.85	0.58
1:C:124:ARG:HD2	1:C:303:PRO:HG3	1.84	0.58
1:D:123:ARG:HG3	3:D:400:HOH:O	2.04	0.57
1:B:240:GLU:CG	1:B:247:MSE:HE2	2.34	0.57
1:A:42:ARG:HG2	1:A:42:ARG:HH11	1.68	0.57
1:C:26:ASP:O	1:C:27:LEU:HD23	2.05	0.57
1:D:8:PHE:HB2	1:D:69:ILE:HA	1.86	0.56
1:C:37:ILE:O	1:C:41:GLN:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:LEU:HB2	1:D:29:LEU:HD11	1.86	0.56
1:D:7:LEU:O	1:D:32:ILE:HA	2.06	0.56
1:C:17:HIS:O	1:C:21:ILE:HG13	2.06	0.56
1:D:106:CYS:O	1:D:110:ILE:HG12	2.05	0.56
1:D:247:MSE:HE3	1:D:249:ALA:HB2	1.87	0.55
1:D:63:ASP:O	1:D:64:ILE:HD13	2.07	0.55
1:A:22:ALA:HB2	3:A:481:HOH:O	2.05	0.55
1:A:123:ARG:CZ	1:A:237:GLN:HE22	2.19	0.55
1:D:30:VAL:C	1:D:49:ALA:HB1	2.27	0.55
1:A:259:ARG:HA	1:A:268:GLN:O	2.07	0.55
1:A:261:HIS:HD2	1:A:266:THR:HB	1.71	0.55
1:C:77:VAL:HG13	1:C:106:CYS:HB2	1.88	0.55
1:B:319:LEU:O	1:B:323:GLN:HG3	2.06	0.54
1:C:37:ILE:HD12	1:C:40:ALA:HB3	1.88	0.54
1:A:261:HIS:CD2	1:A:267:GLU:H	2.25	0.54
1:A:265:SER:HB2	1:C:269:ALA:O	2.07	0.54
1:B:4:ARG:HG3	1:B:4:ARG:HH11	1.73	0.54
1:C:15:HIS:CD2	1:C:43:LEU:HD13	2.42	0.54
1:D:1:LEU:HD23	1:D:2:THR:O	2.08	0.54
1:C:202:ILE:HG23	1:C:207:ASP:HB3	1.90	0.53
1:D:123:ARG:HB3	1:D:179:MSE:CE	2.38	0.53
1:A:262:ASN:HB2	3:D:409:HOH:O	2.07	0.53
1:C:94:LYS:CD	1:C:95:PRO:HD2	2.33	0.53
1:A:119:LEU:HD22	1:A:308:GLY:CA	2.39	0.53
1:C:319:LEU:O	1:C:323:GLN:HG3	2.09	0.53
1:B:202:ILE:HG23	1:B:207:ASP:HB3	1.91	0.52
1:D:123:ARG:NH2	1:D:237:GLN:HE22	2.08	0.52
1:D:94:LYS:CD	1:D:95:PRO:HD2	2.40	0.52
1:B:94:LYS:HG3	1:B:95:PRO:CD	2.39	0.52
1:D:294:GLY:HA3	1:D:301:PHE:CE1	2.45	0.52
1:C:95:PRO:HG3	1:C:174:ILE:HD13	1.92	0.52
1:D:37:ILE:HG13	1:D:41:GLN:OE1	2.09	0.52
1:D:52:VAL:HB	1:D:57:GLU:OE2	2.10	0.52
1:C:76:HIS:O	1:C:80:ILE:HG13	2.10	0.52
1:D:75:THR:O	1:D:79:LEU:HG	2.10	0.52
1:A:4:ARG:HD2	1:A:30:VAL:CG1	2.40	0.52
1:D:4:ARG:HH11	1:D:4:ARG:CB	2.23	0.52
1:D:94:LYS:HD2	1:D:95:PRO:HD2	1.91	0.52
1:A:61:ARG:HD3	1:A:64:ILE:HD11	1.90	0.51
1:D:44:ALA:CB	1:D:51:ALA:HB2	2.40	0.51
1:A:151:SER:O	1:A:227:ASN:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LYS:HG3	1:B:95:PRO:CG	2.40	0.51
1:C:146:GLN:CG	1:D:210:GLN:NE2	2.74	0.51
1:D:6:ALA:CB	1:D:64:ILE:HG21	2.38	0.51
1:B:94:LYS:HD3	1:B:175:HIS:CE1	2.46	0.51
1:D:31:VAL:HG22	1:D:32:ILE:H	1.75	0.51
1:C:96:ILE:HD12	1:C:96:ILE:H	1.76	0.50
1:D:71:SER:HB2	1:D:72:PRO:HD2	1.93	0.50
1:A:100:ILE:O	1:A:104:ARG:HG3	2.11	0.50
1:C:42:ARG:HG2	1:C:42:ARG:HH11	1.76	0.50
1:C:94:LYS:HB3	1:C:95:PRO:HD2	1.93	0.50
1:B:59:PHE:O	1:B:86:ARG:NH1	2.45	0.50
1:B:119:LEU:HD13	1:B:308:GLY:HA3	1.94	0.50
1:C:99:ASP:OD1	1:C:101:GLU:HB2	2.11	0.50
1:C:146:GLN:HB2	1:C:242:PHE:HB3	1.94	0.50
1:A:146:GLN:HE21	1:B:210:GLN:CG	2.24	0.50
1:C:222:LEU:HD12	1:D:210:GLN:HG2	1.93	0.50
1:D:96:ILE:HG21	1:D:103:VAL:HG13	1.94	0.50
1:D:118:MSE:HB2	1:D:301:PHE:CB	2.42	0.49
1:C:3:LEU:HD23	1:C:65:ASP:OD2	2.12	0.49
1:D:118:MSE:HE3	1:D:301:PHE:CD1	2.46	0.49
1:A:102:MSE:HE2	3:A:439:HOH:O	2.11	0.49
1:D:240:GLU:HG3	1:D:247:MSE:SE	2.62	0.49
1:D:247:MSE:CE	1:D:249:ALA:CB	2.86	0.49
1:B:259:ARG:HA	1:B:268:GLN:O	2.12	0.49
1:D:118:MSE:HB2	1:D:301:PHE:HB3	1.95	0.49
1:D:223:ILE:HD12	1:D:223:ILE:N	2.28	0.48
1:D:18:ALA:HB1	1:D:47:ASN:ND2	2.28	0.48
1:C:10:ALA:HB2	1:C:32:ILE:HG21	1.94	0.48
1:C:291:PHE:O	1:C:295:ILE:HG13	2.14	0.48
1:C:326:ARG:HD2	3:D:356:HOH:O	2.12	0.48
1:D:7:LEU:CB	1:D:29:LEU:HD11	2.43	0.48
3:A:574:HOH:O	1:B:247:MSE:CE	2.45	0.48
1:B:123:ARG:CZ	1:B:237:GLN:HE22	2.27	0.48
1:D:80:ILE:O	1:D:84:VAL:HG23	2.13	0.48
1:C:118:MSE:HE1	1:C:290:THR:HG22	1.95	0.48
1:B:265:SER:HB2	1:D:269:ALA:O	2.14	0.48
1:C:94:LYS:CB	1:C:95:PRO:HD2	2.43	0.48
1:D:78:ASP:O	1:D:82:ARG:HD3	2.13	0.48
1:B:94:LYS:HE2	3:B:347:HOH:O	2.14	0.48
1:D:118:MSE:HE3	1:D:301:PHE:HD1	1.79	0.48
1:B:240:GLU:HG3	1:B:247:MSE:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ASP:HB3	1:B:299:GLN:HG2	1.95	0.47
1:C:146:GLN:HE21	1:D:210:GLN:HG3	1.79	0.47
1:D:320:GLU:OE2	1:D:324:THR:HG21	2.14	0.47
1:C:309:VAL:O	1:C:313:GLU:HG3	2.14	0.47
1:D:61:ARG:NH2	1:D:63:ASP:OD1	2.46	0.47
1:C:93:GLU:HB3	1:C:94:LYS:H	1.49	0.47
1:C:277:LEU:HD12	1:C:278:GLU:N	2.29	0.47
1:D:17:HIS:O	1:D:21:ILE:HG13	2.14	0.47
1:D:76:HIS:O	1:D:80:ILE:HG13	2.15	0.47
1:D:124:ARG:HD2	1:D:303:PRO:CG	2.43	0.47
1:C:30:VAL:C	1:C:49:ALA:HB1	2.35	0.47
1:C:211:VAL:HG22	1:C:227:ASN:HB2	1.97	0.47
1:C:247:MSE:HE3	1:C:249:ALA:HB2	1.96	0.47
1:C:32:ILE:HD12	1:C:32:ILE:N	2.30	0.47
1:A:59:PHE:O	1:A:86:ARG:NH1	2.48	0.47
1:C:84:VAL:CG1	1:C:113:GLY:HA3	2.45	0.47
1:C:247:MSE:HE1	1:C:249:ALA:HB2	1.96	0.47
1:C:8:PHE:HD1	1:C:33:ALA:HB3	1.80	0.47
1:D:123:ARG:CZ	1:D:237:GLN:HE22	2.28	0.47
1:C:133:ASN:HA	1:C:183:PHE:CE1	2.50	0.46
1:A:212:ILE:HD13	1:B:222:LEU:CD1	2.43	0.46
1:C:89:PRO:HG2	1:C:295:ILE:HG23	1.96	0.46
1:C:247:MSE:HE3	1:C:248:LEU:C	2.35	0.46
1:D:146:GLN:HB2	1:D:242:PHE:HB3	1.98	0.46
1:D:37:ILE:HA	1:D:40:ALA:HB3	1.97	0.46
1:A:239:LEU:HD23	1:A:239:LEU:C	2.36	0.46
1:A:293:GLN:HE21	1:A:297:ASP:CG	2.19	0.46
1:A:293:GLN:HG3	1:A:297:ASP:OD2	2.16	0.46
1:C:67:ILE:CD1	1:C:83:ALA:HB1	2.45	0.46
1:D:4:ARG:NH1	1:D:63:ASP:O	2.48	0.46
1:C:239:LEU:C	1:C:239:LEU:HD23	2.35	0.46
1:B:301:PHE:HA	3:B:483:HOH:O	2.14	0.46
1:D:113:GLY:C	1:D:115:SER:H	2.19	0.46
1:D:15:HIS:ND1	1:D:43:LEU:HD13	2.30	0.46
1:D:84:VAL:C	1:D:86:ARG:H	2.18	0.46
1:A:240:GLU:HG3	1:A:247:MSE:SE	2.66	0.46
1:C:81:THR:O	1:C:85:GLU:HG2	2.16	0.45
1:D:91:LEU:HD13	1:D:118:MSE:SE	2.66	0.45
1:D:71:SER:HB2	1:D:72:PRO:CD	2.47	0.45
1:B:107:LYS:HE3	3:B:488:HOH:O	2.16	0.45
1:D:41:GLN:HG2	1:D:51:ALA:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:ARG:HG2	1:D:228:SER:HB3	1.98	0.45
1:A:6:ALA:HB3	1:A:67:ILE:HG12	1.99	0.45
1:A:223:ILE:HD12	1:A:223:ILE:N	2.32	0.45
1:B:159:LYS:HB2	1:B:201:GLU:OE2	2.16	0.45
1:C:219:LYS:HE2	3:C:374:HOH:O	2.16	0.45
1:D:173:THR:HA	1:D:227:ASN:HD21	1.82	0.45
1:C:274:ASN:OD1	1:C:275:PHE:CD2	2.70	0.45
1:D:96:ILE:HB	1:D:97:ASP:H	1.45	0.45
1:B:198:PHE:CE1	1:B:199:SER:HB2	2.51	0.45
3:A:519:HOH:O	1:D:259:ARG:HD2	2.17	0.44
1:D:30:VAL:HG21	1:D:64:ILE:CD1	2.47	0.44
1:D:118:MSE:CE	1:D:290:THR:HG22	2.46	0.44
1:C:187:ILE:O	1:C:330:LEU:HD12	2.18	0.44
1:D:123:ARG:HB3	1:D:179:MSE:HE2	2.00	0.44
1:D:277:LEU:O	1:D:277:LEU:HD12	2.18	0.44
1:C:293:GLN:O	1:C:297:ASP:HB2	2.17	0.44
1:A:124:ARG:HD2	1:A:303:PRO:HG3	1.99	0.44
1:B:201:GLU:O	1:B:204:GLU:HB3	2.17	0.44
1:C:81:THR:C	1:C:83:ALA:H	2.21	0.44
1:D:118:MSE:HB2	1:D:301:PHE:CG	2.53	0.44
1:A:12:ARG:HE	1:A:12:ARG:CA	2.18	0.44
1:A:64:ILE:HG12	3:A:391:HOH:O	2.18	0.44
1:A:211:VAL:O	1:A:212:ILE:HD12	2.16	0.44
1:D:151:SER:O	1:D:227:ASN:HA	2.17	0.43
1:C:95:PRO:CG	1:C:174:ILE:HD13	2.47	0.43
1:D:96:ILE:HD12	1:D:305:PHE:CE1	2.53	0.43
1:C:2:THR:HG22	1:C:3:LEU:N	2.30	0.43
1:D:159:LYS:HB2	1:D:201:GLU:OE2	2.17	0.43
1:A:146:GLN:HE21	1:B:210:GLN:HG3	1.83	0.43
1:C:67:ILE:HD13	1:C:83:ALA:HB1	2.01	0.43
1:C:3:LEU:CD2	1:C:65:ASP:HB2	2.49	0.43
1:A:41:GLN:O	1:A:45:GLU:HG2	2.19	0.43
1:C:188:VAL:HG22	1:C:216:ARG:O	2.19	0.43
1:A:152:ARG:HG2	1:A:228:SER:HB3	2.00	0.43
1:D:310:ILE:HA	1:D:313:GLU:OE1	2.19	0.43
1:A:119:LEU:HD22	1:A:308:GLY:HA3	2.00	0.42
1:D:251:ASP:HB3	3:D:367:HOH:O	2.17	0.42
1:C:104:ARG:O	1:C:108:GLU:HG3	2.19	0.42
1:D:113:GLY:C	1:D:115:SER:N	2.73	0.42
1:D:31:VAL:CG2	1:D:32:ILE:N	2.82	0.42
1:A:84:VAL:CG1	1:A:113:GLY:HA3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ARG:HD2	1:B:314:LEU:HD11	2.02	0.42
1:C:118:MSE:HB2	1:C:301:PHE:CG	2.54	0.42
1:D:43:LEU:O	1:D:46:ALA:HB3	2.19	0.42
1:D:194:GLY:HA2	1:D:211:VAL:HG12	2.01	0.42
1:C:7:LEU:HD12	1:C:8:PHE:H	1.84	0.42
1:C:199:SER:OG	1:C:202:ILE:HG13	2.20	0.42
1:D:305:PHE:O	1:D:309:VAL:HG23	2.19	0.42
1:A:132:ILE:HD11	1:A:250:ALA:HB2	2.02	0.42
1:C:69:ILE:HB	1:C:92:CYS:HA	2.00	0.42
1:B:65:ASP:O	1:B:89:PRO:HD2	2.20	0.42
1:D:132:ILE:O	1:D:136:VAL:HG23	2.20	0.42
1:B:37:ILE:O	1:B:41:GLN:HG3	2.19	0.41
1:C:234:GLY:HA3	1:C:272:ILE:HG13	2.02	0.41
1:B:81:THR:O	1:B:85:GLU:HG3	2.19	0.41
1:C:118:MSE:HE3	3:C:391:HOH:O	2.20	0.41
1:C:146:GLN:HG2	1:D:210:GLN:NE2	2.34	0.41
1:A:37:ILE:O	1:A:41:GLN:HG3	2.21	0.41
1:C:31:VAL:HG22	1:C:32:ILE:N	2.35	0.41
1:A:185:PRO:HD2	3:A:405:HOH:O	2.20	0.41
1:C:224:ASN:HB2	1:D:212:ILE:HD13	2.03	0.41
1:D:119:LEU:CD2	1:D:308:GLY:HA3	2.51	0.41
1:A:71:SER:HB2	1:A:72:PRO:CD	2.50	0.41
1:B:78:ASP:O	1:B:82:ARG:HG3	2.21	0.41
1:B:212:ILE:HD13	1:B:226:VAL:HG22	2.02	0.41
1:C:145:GLU:HB3	1:D:210:GLN:HE22	1.85	0.41
1:B:84:VAL:CG1	1:B:113:GLY:HA3	2.51	0.41
1:B:223:ILE:HD12	1:B:223:ILE:N	2.36	0.41
1:C:1:LEU:HD13	1:C:2:THR:N	2.36	0.40
1:B:151:SER:O	1:B:227:ASN:HA	2.21	0.40
1:C:8:PHE:CD2	1:C:79:LEU:HD13	2.56	0.40
1:A:299:GLN:HB2	3:A:440:HOH:O	2.21	0.40
1:C:247:MSE:HE1	1:C:249:ALA:CB	2.51	0.40
1:A:154:PRO:HG2	1:A:274:ASN:O	2.22	0.40
1:B:124:ARG:HD2	1:B:303:PRO:HG3	2.03	0.40
1:D:15:HIS:HA	1:D:43:LEU:HD11	2.03	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	331/344 (96%)	321 (97%)	9 (3%)	1 (0%)	41	50
1	B	331/344 (96%)	319 (96%)	11 (3%)	1 (0%)	41	50
1	C	331/344 (96%)	308 (93%)	20 (6%)	3 (1%)	17	20
1	D	331/344 (96%)	294 (89%)	31 (9%)	6 (2%)	8	7
All	All	1324/1376 (96%)	1242 (94%)	71 (5%)	11 (1%)	19	23

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	95	PRO
1	C	95	PRO
1	D	62	ASP
1	D	332	PRO
1	C	82	ARG
1	C	111	GLY
1	D	11	GLY
1	D	96	ILE
1	A	332	PRO
1	D	95	PRO
1	D	111	GLY

### 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	263/267 (98%)	257 (98%)	6 (2%)	50	67
1	B	263/267 (98%)	257 (98%)	6 (2%)	50	67
1	C	263/267 (98%)	254 (97%)	9 (3%)	37	51
1	D	263/267 (98%)	256 (97%)	7 (3%)	44	61
All	All	1052/1068 (98%)	1024 (97%)	28 (3%)	44	61

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	94	LYS
1	A	119	LEU
1	A	173	THR
1	A	230	HIS
1	A	320	GLU
1	B	37	ILE
1	B	95	PRO
1	B	119	LEU
1	B	173	THR
1	B	230	HIS
1	B	277	LEU
1	C	3	LEU
1	C	26	ASP
1	C	65	ASP
1	C	94	LYS
1	C	95	PRO
1	C	112	ASP
1	C	119	LEU
1	C	230	HIS
1	C	297	ASP
1	D	4	ARG
1	D	96	ILE
1	D	206	ASN
1	D	230	HIS
1	D	267	GLU
1	D	299	GLN
1	D	330	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	HIS
1	A	186	ASN
1	A	196	ASN
1	A	210	GLN
1	A	227	ASN
1	A	237	GLN
1	A	261	HIS
1	A	293	GLN
1	B	175	HIS
1	B	186	ASN
1	B	196	ASN
1	B	224	ASN
1	B	227	ASN
1	B	237	GLN
1	C	20	ASN
1	C	186	ASN
1	C	196	ASN
1	C	210	GLN
1	C	224	ASN
1	C	227	ASN
1	C	237	GLN
1	C	261	HIS
1	D	47	ASN
1	D	186	ASN
1	D	196	ASN
1	D	210	GLN
1	D	227	ASN
1	D	230	HIS
1	D	237	GLN
1	D	261	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	328/344 (95%)	-0.10	6 (1%) 68 74	10, 21, 41, 72	0
1	B	328/344 (95%)	-0.14	4 (1%) 79 83	10, 22, 43, 60	0
1	C	328/344 (95%)	1.17	93 (28%) 0 0	15, 42, 72, 76	0
1	D	328/344 (95%)	1.43	97 (29%) 0 0	14, 41, 76, 80	0
All	All	1312/1376 (95%)	0.59	200 (15%) 2 3	10, 29, 72, 80	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	51	ALA	12.2
1	D	333	ALA	10.1
1	A	333	ALA	9.4
1	D	64	ILE	9.4
1	D	49	ALA	9.2
1	D	95	PRO	8.9
1	D	39	GLY	8.6
1	C	64	ILE	8.3
1	C	51	ALA	7.7
1	D	35	PRO	7.7
1	D	31	VAL	7.6
1	D	43	LEU	7.5
1	D	32	ILE	7.5
1	D	74	SER	7.5
1	D	36	PHE	7.3
1	C	60	ALA	7.3
1	D	332	PRO	7.2
1	D	60	ALA	7.1
1	D	42	ARG	7.0
1	D	37	ILE	6.8
1	C	56	ASP	6.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	332	PRO	6.6
1	C	46	ALA	6.6
1	D	113	GLY	6.5
1	C	36	PHE	6.5
1	D	55	PRO	6.4
1	D	40	ALA	6.4
1	C	29	LEU	6.4
1	D	38	GLU	6.3
1	D	1	LEU	6.2
1	C	4	ARG	6.1
1	D	59	PHE	6.1
1	D	53	ALA	6.0
1	D	44	ALA	5.9
1	D	29	LEU	5.8
1	C	333	ALA	5.8
1	D	58	VAL	5.7
1	C	27	LEU	5.5
1	D	10	ALA	5.4
1	D	88	ILE	5.3
1	C	111	GLY	5.3
1	C	39	GLY	5.2
1	C	30	VAL	5.1
1	D	103	VAL	5.1
1	D	54	SER	5.1
1	D	48	GLY	5.1
1	D	110	ILE	5.0
1	C	49	ALA	5.0
1	C	35	PRO	5.0
1	D	73	THR	5.0
1	D	46	ALA	4.9
1	C	8	PHE	4.9
1	D	25	PRO	4.8
1	C	53	ALA	4.7
1	C	298	GLY	4.7
1	C	38	GLU	4.7
1	C	90	ALA	4.7
1	D	9	GLY	4.7
1	C	54	SER	4.7
1	D	56	ASP	4.7
1	C	95	PRO	4.5
1	D	8	PHE	4.4
1	C	58	VAL	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	52	VAL	4.4
1	C	32	ILE	4.3
1	D	330	LEU	4.3
1	D	45	GLU	4.3
1	C	33	ALA	4.2
1	D	50	GLU	4.2
1	D	4	ARG	4.2
1	C	10	ALA	4.2
1	C	45	GLU	4.1
1	C	65	ASP	4.1
1	D	67	ILE	4.1
1	C	1	LEU	4.1
1	D	33	ALA	4.0
1	C	63	ASP	4.0
1	C	42	ARG	3.8
1	C	114	ALA	3.8
1	D	23	ALA	3.8
1	C	41	GLN	3.8
1	C	67	ILE	3.7
1	C	37	ILE	3.6
1	C	113	GLY	3.6
1	C	43	LEU	3.6
1	C	12	ARG	3.6
1	C	9	GLY	3.6
1	D	15	HIS	3.5
1	B	95	PRO	3.5
1	D	70	GLY	3.4
1	D	87	GLY	3.4
1	C	59	PHE	3.4
1	D	12	ARG	3.4
1	C	77	VAL	3.4
1	C	2	THR	3.4
1	C	73	THR	3.3
1	C	86	ARG	3.3
1	D	115	SER	3.3
1	D	79	LEU	3.3
1	D	52	VAL	3.3
1	C	47	ASN	3.3
1	D	28	GLU	3.3
1	C	200	GLN	3.2
1	C	23	ALA	3.2
1	C	61	ARG	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	1	LEU	3.2
1	D	76	HIS	3.2
1	C	6	ALA	3.2
1	D	11	GLY	3.2
1	C	74	SER	3.2
1	C	3	LEU	3.1
1	D	111	GLY	3.1
1	C	163	ALA	3.1
1	D	47	ASN	3.1
1	D	7	LEU	3.1
1	D	34	ASP	3.0
1	D	3	LEU	3.0
1	C	55	PRO	3.0
1	D	205	PHE	3.0
1	D	84	VAL	3.0
1	C	112	ASP	3.0
1	C	5	ILE	3.0
1	C	88	ILE	3.0
1	D	5	ILE	3.0
1	C	57	GLU	3.0
1	C	110	ILE	3.0
1	C	332	PRO	2.9
1	D	112	ASP	2.9
1	D	108	GLU	2.9
1	D	41	GLN	2.9
1	C	78	ASP	2.9
1	C	26	ASP	2.9
1	D	96	ILE	2.9
1	C	50	GLU	2.9
1	C	25	PRO	2.9
1	C	82	ARG	2.8
1	C	296	ARG	2.8
1	D	159	LYS	2.8
1	C	159	LYS	2.8
1	C	277	LEU	2.8
1	C	34	ASP	2.8
1	D	161	TYR	2.8
1	D	296	ARG	2.7
1	C	13	ILE	2.7
1	D	13	ILE	2.7
1	D	85	GLU	2.6
1	D	90	ALA	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	161	TYR	2.6
1	D	57	GLU	2.6
1	D	331	ASN	2.6
1	D	80	ILE	2.6
1	D	160	ASP	2.6
1	D	200	GLN	2.6
1	C	204	GLU	2.6
1	D	30	VAL	2.6
1	D	92	CYS	2.6
1	C	96	ILE	2.6
1	C	160	ASP	2.5
1	D	94	LYS	2.5
1	C	85	GLU	2.5
1	D	297	ASP	2.5
1	A	108	GLU	2.5
1	C	31	VAL	2.5
1	D	78	ASP	2.5
1	D	68	VAL	2.4
1	C	108	GLU	2.4
1	D	91	LEU	2.4
1	A	331	ASN	2.4
1	C	44	ALA	2.4
1	D	86	ARG	2.3
1	D	63	ASP	2.3
1	D	65	ASP	2.3
1	C	158	PRO	2.3
1	C	292	ALA	2.3
1	D	101	GLU	2.3
1	D	62	ASP	2.3
1	C	21	ILE	2.3
1	C	105	ALA	2.3
1	C	297	ASP	2.3
1	C	87	GLY	2.3
1	D	163	ALA	2.3
1	A	48	GLY	2.3
1	D	97	ASP	2.3
1	C	109	LYS	2.2
1	D	82	ARG	2.2
1	C	40	ALA	2.2
1	D	277	LEU	2.2
1	B	332	PRO	2.2
1	D	204	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	27	LEU	2.2
1	B	333	ALA	2.1
1	C	81	THR	2.1
1	C	66	GLY	2.1
1	C	94	LYS	2.1
1	C	295	ILE	2.0
1	B	48	GLY	2.0
1	C	22	ALA	2.0
1	C	15	HIS	2.0
1	D	106	CYS	2.0
1	C	91	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 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(Å <sup>2</sup> )	Q<0.9
2	NA	B	343	1/1	0.90	0.07	42,42,42,42	0
2	NA	A	343	1/1	0.91	0.13	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.