



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 05:10 PM EST

PDB ID : 2HXG  
Title : Crystal Structure of Mn<sup>2+</sup> bound ECAI  
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Deposited on : 2006-08-03  
Resolution : 2.80 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
Xtriage (Phenix)	:	1.13
EDS	:	2.16
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)	:	2.16

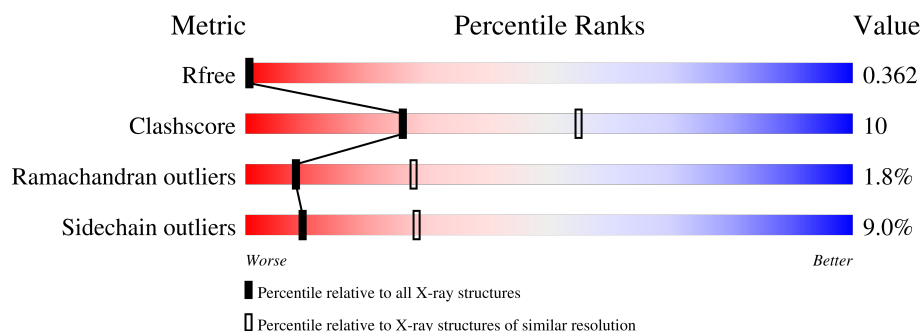
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	500	<div> <div>77%</div> <div>19%</div> <div>.</div> </div>
1	B	500	<div> <div>75%</div> <div>21%</div> <div>.</div> </div>
1	C	500	<div> <div>73%</div> <div>23%</div> <div>.</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11565 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-arabinose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3829	2431	669	705	24			
1	B	498	Total	C	N	O	S	0	0	0
			3895	2474	680	717	24			
1	C	498	Total	C	N	O	S	0	0	0
			3735	2353	650	708	24			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	PRO	ARG	SEE REMARK 999	UNP Q8FL89
B	72	PRO	ARG	SEE REMARK 999	UNP Q8FL89
C	72	PRO	ARG	SEE REMARK 999	UNP Q8FL89

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total	O	0	0
			41	41		
3	B	37	Total	O	0	0
			37	37		

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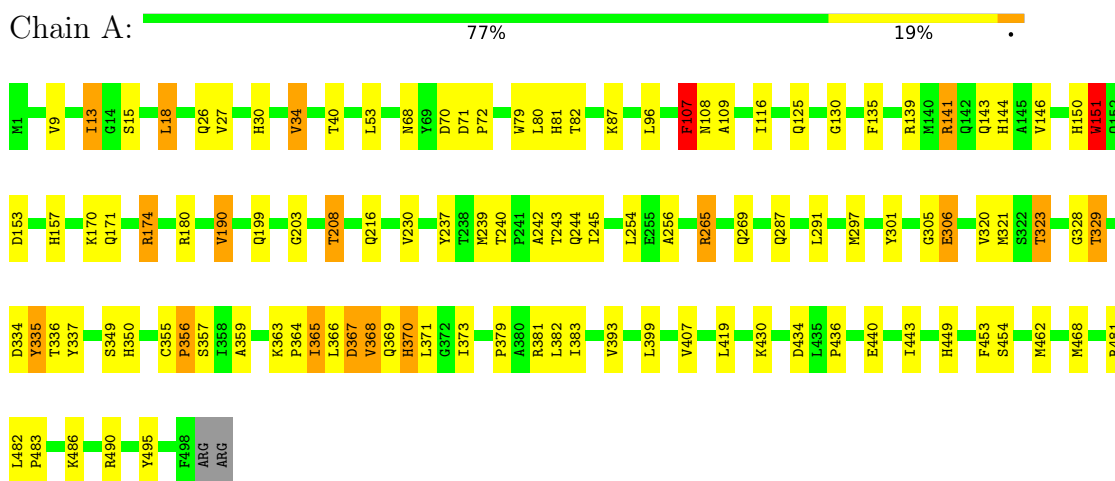
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	25	Total	O	0	0
			25	25		

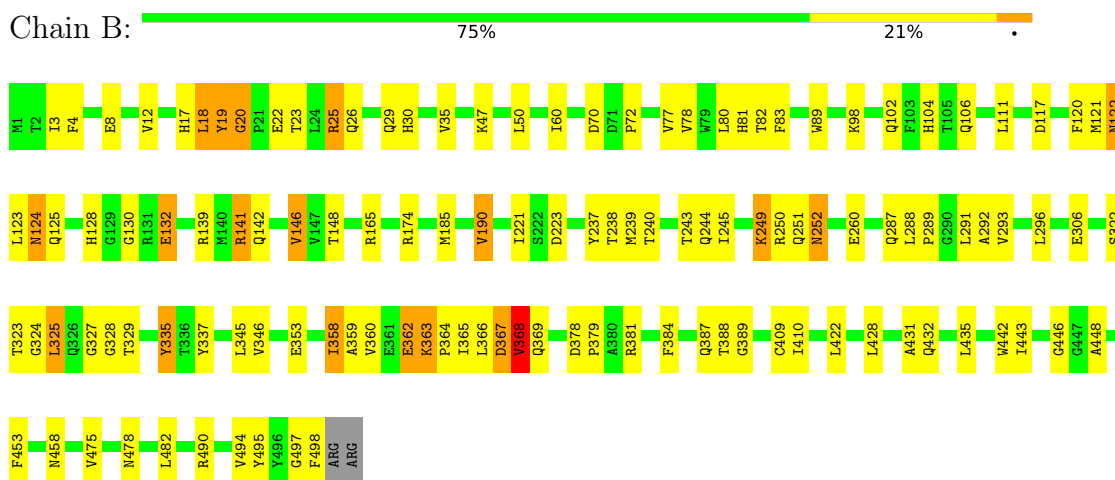
### 3 Residue-property plots [i](#)

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. 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. 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.

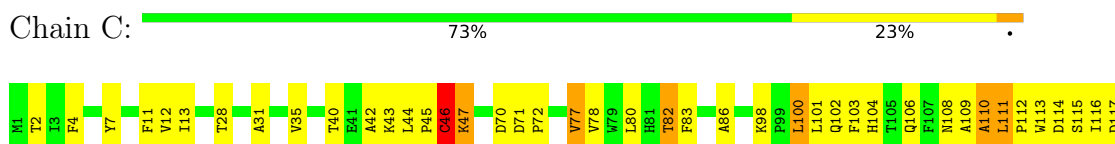
- Molecule 1: L-arabinose isomerase

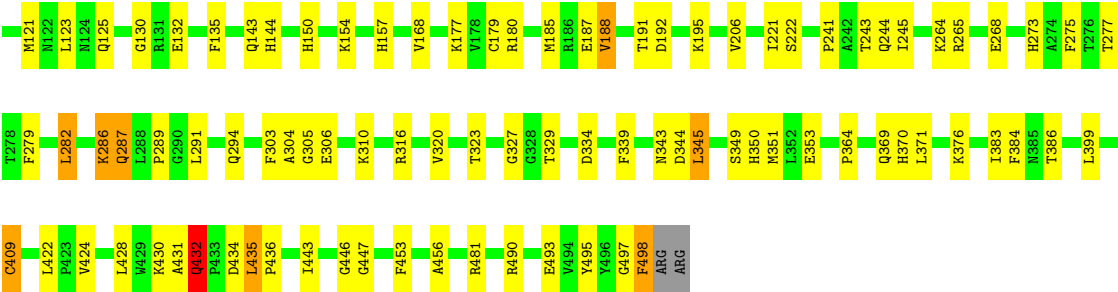


- Molecule 1: L-arabinose isomerase



- Molecule 1: L-arabinose isomerase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.87Å 116.87Å 215.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.89 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.3 (20.00-2.80) 92.3 (19.89-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.13 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.229 , 0.288 0.317 , 0.362	Depositor DCC
$R_{free}$ test set	1988 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.8	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 38.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	11565	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: MN

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	0.46	0/3922	0.63	0/5325
1	B	0.47	0/3991	0.63	0/5424
1	C	0.42	0/3826	0.59	0/5203
All	All	0.45	0/11739	0.62	0/15952

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	A	0	1
1	B	0	3
1	C	0	3
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	PHE	Peptide
1	B	327	GLY	Peptide
1	B	362	GLU	Peptide
1	B	368	VAL	Peptide
1	C	369	GLN	Peptide
1	C	431	ALA	Peptide
1	C	46	CYS	Peptide



## 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	3829	0	3686	88	0
1	B	3895	0	3783	87	0
1	C	3735	0	3440	87	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	41	0	0	3	0
3	B	37	0	0	2	0
3	C	25	0	0	0	0
All	All	11565	0	10909	235	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 10.

All (235) 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:180:ARG:HD2	1:C:195:LYS:HZ2	1.32	0.94
1:B:360:VAL:HG22	1:B:387:GLN:HG2	1.52	0.90
1:C:109:ALA:HB2	1:C:150:HIS:CG	2.12	0.85
1:A:364:PRO:HD2	1:A:383:ILE:O	1.80	0.79
1:C:180:ARG:HD2	1:C:195:LYS:NZ	1.97	0.79
1:B:102:GLN:NE2	1:B:104:HIS:HD2	1.85	0.74
1:B:165:ARG:NH2	1:B:323:THR:O	2.21	0.74
1:B:337:TYR:OH	1:C:104:HIS:HE1	1.72	0.73
1:A:366:LEU:HD11	1:A:368:VAL:HG23	1.71	0.73
1:C:112:PRO:O	1:C:116:ILE:HG13	1.88	0.73
1:A:170:LYS:HD2	1:A:468:MET:HG3	1.73	0.71
1:A:367:ASP:O	1:A:369:GLN:N	2.25	0.70
1:A:107:PHE:HB3	1:A:108:ASN:HD22	1.55	0.69
1:B:497:GLY:O	1:B:498:PHE:CD2	2.46	0.68
1:C:195:LYS:HZ3	1:C:206:VAL:CB	2.07	0.68
1:B:102:GLN:HE22	1:B:104:HIS:CD2	2.11	0.67
1:B:102:GLN:HE22	1:B:104:HIS:HD2	1.41	0.66
1:B:102:GLN:NE2	1:B:104:HIS:CD2	2.62	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ASP:O	1:A:368:VAL:C	2.34	0.66
1:A:449:HIS:HB2	1:B:128:HIS:HB2	1.76	0.66
1:A:13:ILE:H	1:A:13:ILE:HD12	1.59	0.66
1:A:107:PHE:CB	1:A:108:ASN:HD22	2.08	0.65
1:C:195:LYS:NZ	1:C:206:VAL:CB	2.60	0.65
1:B:125:GLN:HB2	1:B:128:HIS:CE1	2.31	0.65
1:C:80:LEU:HD13	1:C:130:GLY:HA2	1.78	0.63
1:C:100:LEU:HD12	1:C:101:LEU:N	2.13	0.63
1:C:109:ALA:HB2	1:C:150:HIS:CD2	2.32	0.63
1:C:82:THR:HG22	1:C:83:PHE:O	1.99	0.63
1:C:121:MET:O	1:C:125:GLN:HG2	1.98	0.63
1:C:102:GLN:HE22	1:C:104:HIS:HD2	1.46	0.63
1:A:355:CYS:SG	1:A:357:SER:HB2	2.40	0.62
1:A:13:ILE:CD1	1:A:53:LEU:HA	2.30	0.62
1:C:185:MET:HB3	1:C:188:VAL:HG21	1.80	0.62
1:C:364:PRO:HD2	1:C:383:ILE:O	1.99	0.61
1:B:252:ASN:N	1:B:252:ASN:HD22	1.98	0.61
1:A:151:TRP:O	1:A:157:HIS:NE2	2.33	0.61
1:A:436:PRO:O	1:A:440:GLU:HG3	2.00	0.61
1:B:239:MET:SD	1:B:365:ILE:HG21	2.40	0.61
1:C:46:CYS:CB	1:C:47:LYS:HB2	2.30	0.61
1:A:356:PRO:HG3	1:A:382:LEU:HD12	1.82	0.61
1:B:30:HIS:ND1	1:B:81:HIS:NE2	2.42	0.60
1:C:185:MET:HB3	1:C:188:VAL:CG2	2.31	0.60
1:B:26:GLN:HA	1:B:29:GLN:HE21	1.66	0.60
1:A:240:THR:HG21	1:A:366:LEU:HD13	1.83	0.59
1:A:237:TYR:CB	1:A:365:ILE:HG22	2.33	0.59
1:A:13:ILE:HD13	1:A:53:LEU:HA	1.83	0.59
1:C:316:ARG:O	1:C:320:VAL:HG23	2.03	0.59
1:A:337:TYR:H	1:B:106:GLN:HE22	1.51	0.58
1:B:360:VAL:HG22	1:B:387:GLN:HE21	1.69	0.58
1:A:369:GLN:O	1:A:370:HIS:C	2.40	0.58
1:B:360:VAL:HG22	1:B:387:GLN:CG	2.29	0.58
1:B:125:GLN:OE1	1:B:128:HIS:NE2	2.36	0.58
1:A:230:VAL:HG21	1:A:254:LEU:HD23	1.86	0.58
1:C:46:CYS:HB2	1:C:47:LYS:HB2	1.86	0.58
1:C:498:PHE:C	1:C:498:PHE:CD2	2.77	0.58
1:B:328:GLY:HA3	1:B:358:ILE:HG22	1.85	0.57
1:A:151:TRP:N	1:A:151:TRP:HE3	2.03	0.57
1:B:360:VAL:O	1:B:360:VAL:HG12	2.04	0.57
1:B:329:THR:HA	1:B:453:PHE:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:GLN:CB	1:B:378:ASP:HB3	2.34	0.57
1:A:87:LYS:HB2	1:C:187:GLU:O	2.05	0.57
1:C:12:VAL:O	1:C:78:VAL:HA	2.05	0.57
1:C:102:GLN:HE22	1:C:104:HIS:CD2	2.22	0.56
1:B:494:VAL:HG21	1:C:495:TYR:HA	1.88	0.56
1:A:13:ILE:HD12	1:A:13:ILE:N	2.20	0.56
1:A:369:GLN:CB	1:A:379:PRO:HD2	2.35	0.56
1:B:120:PHE:O	1:B:123:LEU:O	2.24	0.56
1:C:350:HIS:ND1	1:C:353:GLU:OE1	2.38	0.56
1:B:409:CYS:O	1:B:432:GLN:HB2	2.06	0.55
1:C:264:LYS:O	1:C:268:GLU:HG3	2.07	0.55
1:C:71:ASP:OD1	1:C:72:PRO:HD3	2.07	0.55
1:A:237:TYR:HB3	1:A:365:ILE:HG22	1.88	0.55
1:B:249:LYS:NZ	1:B:378:ASP:OD1	2.40	0.55
1:A:71:ASP:N	1:A:72:PRO:CD	2.70	0.55
1:C:409:CYS:HB2	1:C:432:GLN:HG3	1.90	0.54
1:C:2:THR:HG23	1:C:323:THR:HG21	1.88	0.54
1:A:335:TYR:CD2	1:B:121:MET:HG3	2.43	0.54
1:A:30:HIS:CD2	1:A:107:PHE:CZ	2.96	0.54
1:A:18:LEU:N	1:A:18:LEU:HD23	2.23	0.54
1:B:360:VAL:CG2	1:B:387:GLN:HG2	2.30	0.54
1:A:367:ASP:O	1:A:369:GLN:CA	2.56	0.53
1:B:367:ASP:O	1:B:368:VAL:C	2.46	0.53
1:B:368:VAL:HG12	1:B:368:VAL:O	2.09	0.53
1:B:337:TYR:H	1:C:106:GLN:HE22	1.57	0.53
1:B:70:ASP:OD1	1:B:72:PRO:HD2	2.09	0.53
1:A:151:TRP:CE3	1:A:151:TRP:N	2.77	0.53
1:B:422:LEU:HD13	1:C:116:ILE:HG22	1.90	0.53
1:B:240:THR:HG21	1:B:366:LEU:HB2	1.91	0.52
1:B:35:VAL:HG21	1:B:50:LEU:HB2	1.91	0.52
1:A:79:TRP:CZ2	1:A:81:HIS:HD2	2.27	0.52
1:A:30:HIS:CG	1:A:107:PHE:CZ	2.98	0.52
1:A:180:ARG:HB2	1:A:208:THR:HG22	1.92	0.51
1:C:180:ARG:CD	1:C:195:LYS:HZ2	2.15	0.51
1:C:195:LYS:HZ3	1:C:206:VAL:C	2.13	0.51
1:B:190:VAL:HG23	1:C:132:GLU:OE2	2.10	0.51
1:A:27:VAL:HG23	1:A:81:HIS:ND1	2.26	0.51
1:A:70:ASP:CG	1:A:72:PRO:HD2	2.30	0.51
1:A:334:ASP:O	1:B:128:HIS:HB3	2.11	0.51
1:B:322:SER:O	1:B:323:THR:C	2.50	0.51
1:B:190:VAL:HG13	1:C:135:PHE:CG	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:TYR:CZ	1:C:490:ARG:HG2	2.47	0.50
1:B:20:GLY:N	3:B:525:HOH:O	2.43	0.50
1:B:322:SER:O	1:B:325:LEU:HB2	2.12	0.50
1:C:241:PRO:HA	1:C:244:GLN:HE21	1.77	0.50
1:C:498:PHE:C	1:C:498:PHE:HD2	2.13	0.50
1:A:367:ASP:O	1:A:369:GLN:CB	2.59	0.50
1:C:108:ASN:ND2	1:C:110:ALA:O	2.39	0.50
1:A:363:LYS:HD2	1:A:363:LYS:N	2.26	0.49
1:B:324:GLY:C	1:B:325:LEU:HD23	2.32	0.49
1:A:490:ARG:HD2	1:B:495:TYR:CE2	2.46	0.49
1:A:329:THR:HA	1:A:453:PHE:O	2.12	0.49
1:C:112:PRO:HB2	1:C:115:SER:OG	2.12	0.49
1:B:365:ILE:O	1:B:365:ILE:HG12	2.13	0.49
1:B:432:GLN:HG2	1:B:478:ASN:ND2	2.27	0.48
1:C:279:PHE:HA	1:C:282:LEU:HD12	1.95	0.48
1:B:190:VAL:CG2	1:C:132:GLU:OE2	2.61	0.48
1:C:102:GLN:NE2	1:C:104:HIS:HD2	2.10	0.48
1:C:179:CYS:O	1:C:275:PHE:HA	2.12	0.48
1:C:42:ALA:O	1:C:44:LEU:HG	2.13	0.48
1:C:82:THR:CG2	1:C:83:PHE:N	2.76	0.48
1:B:490:ARG:HG2	1:C:495:TYR:CE2	2.49	0.48
1:C:279:PHE:CE2	1:C:306:GLU:HG2	2.48	0.48
1:C:329:THR:HA	1:C:453:PHE:O	2.14	0.48
1:C:77:VAL:HA	1:C:101:LEU:O	2.14	0.47
1:A:135:PHE:HA	1:C:446:GLY:HA2	1.96	0.47
1:A:141:ARG:HH22	1:C:399:LEU:HB3	1.79	0.47
1:B:22:GLU:HA	1:B:25:ARG:HG3	1.96	0.47
1:B:165:ARG:HH21	1:B:325:LEU:HG	1.79	0.47
1:B:366:LEU:HD11	1:B:368:VAL:HG23	1.97	0.47
1:B:442:TRP:O	1:B:446:GLY:O	2.32	0.47
1:B:346:VAL:HG22	1:B:435:LEU:HD21	1.96	0.47
1:A:320:VAL:O	1:A:323:THR:OG1	2.32	0.46
1:B:293:VAL:HG11	1:B:353:GLU:HG2	1.96	0.46
1:A:68:ASN:HD21	1:A:96:LEU:HA	1.80	0.46
1:A:27:VAL:CG2	1:A:81:HIS:ND1	2.79	0.46
1:A:190:VAL:HG22	1:B:132:GLU:OE2	2.16	0.46
1:C:177:LYS:H	1:C:273:HIS:HD2	1.64	0.46
1:A:321:MET:SD	1:A:462:MET:HE1	2.55	0.46
1:B:122:ASN:OD1	1:B:122:ASN:C	2.54	0.46
1:B:237:TYR:HB3	1:B:363:LYS:O	2.16	0.46
1:C:291:LEU:HG	1:C:291:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ASP:CG	1:C:72:PRO:HD2	2.37	0.45
1:A:170:LYS:HD2	1:A:468:MET:CG	2.44	0.45
1:A:239:MET:O	1:A:244:GLN:NE2	2.50	0.45
1:A:443:ILE:HG21	1:B:146:VAL:HG11	1.98	0.45
1:C:112:PRO:HG2	1:C:116:ILE:HG12	1.98	0.45
1:A:109:ALA:O	1:C:339:PHE:HB2	2.16	0.45
1:A:13:ILE:HD13	1:A:53:LEU:HD22	1.98	0.45
1:A:265:ARG:HG2	1:A:269:GLN:HE22	1.82	0.45
1:B:443:ILE:HA	3:B:524:HOH:O	2.16	0.45
1:A:141:ARG:HD3	1:C:493:GLU:OE2	2.17	0.45
1:A:80:LEU:HD13	1:A:130:GLY:HA2	1.99	0.45
1:B:345:LEU:HD13	1:B:428:LEU:HD21	1.99	0.45
1:C:185:MET:O	1:C:188:VAL:HG23	2.17	0.45
1:A:366:LEU:HD12	1:A:367:ASP:H	1.81	0.45
1:C:13:ILE:CD1	1:C:31:ALA:HB2	2.46	0.45
1:A:26:GLN:O	1:A:30:HIS:NE2	2.50	0.45
1:B:238:THR:O	1:B:364:PRO:HA	2.17	0.45
1:C:349:SER:OG	1:C:350:HIS:N	2.48	0.45
1:B:260:GLU:HA	1:B:292:ALA:HB1	1.99	0.44
1:A:239:MET:HB3	1:A:243:THR:HG22	1.98	0.44
1:A:364:PRO:HB2	3:A:520:HOH:O	2.17	0.44
1:B:80:LEU:CD1	1:B:130:GLY:HA2	2.47	0.44
1:C:101:LEU:HD23	1:C:101:LEU:C	2.38	0.44
1:A:150:HIS:O	1:A:153:ASP:N	2.36	0.44
1:A:337:TYR:OH	1:B:104:HIS:HE1	2.01	0.44
1:B:4:PHE:HD1	1:B:323:THR:HG21	1.83	0.44
1:C:46:CYS:CA	1:C:47:LYS:HB2	2.48	0.44
1:B:335:TYR:CD2	1:C:121:MET:SD	3.11	0.44
1:B:388:THR:HG22	1:B:389:GLY:N	2.33	0.44
1:C:112:PRO:HG2	1:C:116:ILE:CG1	2.48	0.43
1:C:11:PHE:CD2	1:C:35:VAL:HG23	2.52	0.43
1:A:368:VAL:HG12	1:A:368:VAL:O	2.18	0.43
1:C:435:LEU:N	1:C:436:PRO:HD2	2.33	0.43
1:A:436:PRO:HA	1:B:148:THR:HB	2.00	0.43
1:B:81:HIS:HE1	1:B:124:ASN:HD22	1.67	0.43
1:A:71:ASP:N	1:A:72:PRO:HD3	2.34	0.43
1:B:287:GLN:NE2	1:B:379:PRO:HA	2.33	0.43
1:A:30:HIS:CD2	1:A:107:PHE:HZ	2.35	0.43
1:A:329:THR:HA	1:A:454:SER:HA	2.01	0.43
1:B:83:PHE:CZ	1:B:132:GLU:HG3	2.54	0.43
1:B:324:GLY:O	1:B:325:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:LEU:HD11	1:C:430:LYS:HE2	2.00	0.43
1:C:286:LYS:O	1:C:287:GLN:CB	2.67	0.42
1:C:4:PHE:CD2	1:C:45:PRO:HB2	2.54	0.42
1:A:482:LEU:N	1:A:483:PRO:HD2	2.34	0.42
1:C:100:LEU:HD12	1:C:100:LEU:C	2.39	0.42
1:B:190:VAL:HG13	1:C:135:PHE:CD1	2.54	0.42
1:A:242:ALA:HA	3:A:531:HOH:O	2.19	0.42
1:A:199:GLN:O	1:A:203:GLY:HA2	2.20	0.42
1:A:297:MET:HA	1:A:301:TYR:O	2.19	0.42
1:A:34:VAL:CG1	1:A:151:TRP:CD1	3.03	0.42
1:B:82:THR:HB	1:B:125:GLN:HE21	1.84	0.42
1:B:288:LEU:HD12	1:B:289:PRO:HD2	2.01	0.42
1:C:154:LYS:HA	1:C:157:HIS:ND1	2.35	0.42
1:B:17:HIS:O	1:B:18:LEU:C	2.57	0.42
1:C:291:LEU:HA	1:C:294:GLN:HB2	2.02	0.42
1:A:349:SER:OG	1:A:350:HIS:N	2.52	0.42
1:A:146:VAL:HG21	1:C:443:ILE:CG2	2.50	0.42
1:A:109:ALA:N	1:A:151:TRP:HH2	2.18	0.42
1:A:171:GLN:O	1:A:174:ARG:HB2	2.20	0.42
1:A:180:ARG:HD3	1:A:208:THR:HG22	2.00	0.42
1:C:11:PHE:CD2	1:C:35:VAL:CG2	3.02	0.42
1:C:7:TYR:CD2	1:C:168:VAL:HG13	2.55	0.42
1:C:497:GLY:O	1:C:498:PHE:HB3	2.19	0.42
1:B:239:MET:HA	1:B:365:ILE:HG22	2.03	0.41
1:B:243:THR:HG21	1:B:365:ILE:HG23	2.02	0.41
1:B:185:MET:HB2	1:B:306:GLU:HB2	2.02	0.41
1:C:327:GLY:HA3	1:C:456:ALA:HB2	2.01	0.41
1:C:344:ASP:HB3	1:C:435:LEU:HD12	2.02	0.41
1:C:71:ASP:N	1:C:72:PRO:CD	2.83	0.41
1:B:19:TYR:O	1:B:20:GLY:O	2.38	0.41
1:A:256:ALA:HB2	1:A:287:GLN:NE2	2.36	0.41
1:B:125:GLN:OE1	1:B:128:HIS:CE1	2.73	0.41
1:B:190:VAL:HG11	1:B:448:ALA:HB2	2.01	0.41
1:C:82:THR:HA	1:C:125:GLN:HB2	2.03	0.41
1:A:237:TYR:HB2	1:A:365:ILE:HG22	2.02	0.41
1:C:86:ALA:HB2	1:C:132:GLU:HG3	2.03	0.41
1:C:303:PHE:CE1	1:C:304:ALA:O	2.74	0.41
1:A:305:GLY:O	1:A:306:GLU:C	2.59	0.41
1:B:60:ILE:HG21	1:B:89:TRP:HA	2.03	0.41
1:A:359:ALA:HB3	1:A:363:LYS:HE3	2.03	0.41
1:A:486:LYS:NZ	3:A:529:HOH:O	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:LEU:O	1:C:113:TRP:N	2.54	0.41
1:A:328:GLY:O	1:A:329:THR:CB	2.69	0.41
1:A:371:LEU:HD22	1:A:373:ILE:HB	2.03	0.41
1:A:399:LEU:O	1:B:141:ARG:NH2	2.54	0.40
1:B:359:ALA:HB2	1:B:384:PHE:CD2	2.56	0.40
1:A:30:HIS:CE1	1:A:107:PHE:CE1	3.09	0.40
1:B:292:ALA:O	1:B:296:LEU:HG	2.20	0.40
1:C:192:ASP:O	1:C:310:LYS:NZ	2.46	0.40
1:C:83:PHE:H	1:C:125:GLN:HE21	1.69	0.40
1:A:70:ASP:C	1:A:72:PRO:HD2	2.41	0.40
1:B:117:ASP:OD1	1:B:117:ASP:C	2.59	0.40
1:B:410:ILE:HG22	1:B:431:ALA:HA	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	496/500 (99%)	453 (91%)	36 (7%)	7 (1%)	11	34
1	B	496/500 (99%)	451 (91%)	41 (8%)	4 (1%)	19	49
1	C	496/500 (99%)	418 (84%)	62 (12%)	16 (3%)	4	13
All	All	1488/1500 (99%)	1322 (89%)	139 (9%)	27 (2%)	8	28

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	TRP
1	A	368	VAL
1	A	370	HIS
1	B	245	ILE
1	C	287	GLN

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Mol	Chain	Res	Type
1	C	370	HIS
1	C	371	LEU
1	B	20	GLY
1	C	43	LYS
1	C	376	LYS
1	C	447	GLY
1	C	40	THR
1	C	144	HIS
1	C	386	THR
1	A	143	GLN
1	C	110	ALA
1	C	143	GLN
1	C	351	MET
1	A	144	HIS
1	A	329	THR
1	B	18	LEU
1	C	47	LYS
1	C	305	GLY
1	C	432	GLN
1	A	82	THR
1	B	368	VAL
1	C	289	PRO

### 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	394/419 (94%)	361 (92%)	33 (8%)	11	31
1	B	410/419 (98%)	372 (91%)	38 (9%)	9	26
1	C	369/419 (88%)	335 (91%)	34 (9%)	9	27
All	All	1173/1257 (93%)	1068 (91%)	105 (9%)	9	28

All (105) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	9	VAL
1	A	13	ILE
1	A	15	SER
1	A	18	LEU
1	A	34	VAL
1	A	40	THR
1	A	107	PHE
1	A	116	ILE
1	A	125	GLN
1	A	139	ARG
1	A	141	ARG
1	A	151	TRP
1	A	174	ARG
1	A	190	VAL
1	A	208	THR
1	A	216	GLN
1	A	245	ILE
1	A	265	ARG
1	A	291	LEU
1	A	306	GLU
1	A	323	THR
1	A	335	TYR
1	A	336	THR
1	A	356	PRO
1	A	365	ILE
1	A	367	ASP
1	A	381	ARG
1	A	393	VAL
1	A	407	VAL
1	A	419	LEU
1	A	430	LYS
1	A	434	ASP
1	A	481	ARG
1	B	3	ILE
1	B	8	GLU
1	B	12	VAL
1	B	19	TYR
1	B	23	THR
1	B	25	ARG
1	B	47	LYS
1	B	77	VAL
1	B	78	VAL
1	B	98	LYS

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Mol	Chain	Res	Type
1	B	111	LEU
1	B	122	ASN
1	B	124	ASN
1	B	132	GLU
1	B	139	ARG
1	B	141	ARG
1	B	142	GLN
1	B	146	VAL
1	B	174	ARG
1	B	190	VAL
1	B	221	ILE
1	B	223	ASP
1	B	244	GLN
1	B	249	LYS
1	B	250	ARG
1	B	251	GLN
1	B	252	ASN
1	B	291	LEU
1	B	325	LEU
1	B	335	TYR
1	B	358	ILE
1	B	362	GLU
1	B	363	LYS
1	B	367	ASP
1	B	381	ARG
1	B	458	ASN
1	B	475	VAL
1	B	482	LEU
1	C	28	THR
1	C	46	CYS
1	C	77	VAL
1	C	82	THR
1	C	98	LYS
1	C	100	LEU
1	C	103	PHE
1	C	111	LEU
1	C	114	ASP
1	C	117	ASP
1	C	123	LEU
1	C	188	VAL
1	C	191	THR
1	C	221	ILE

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Mol	Chain	Res	Type
1	C	222	SER
1	C	243	THR
1	C	245	ILE
1	C	265	ARG
1	C	277	THR
1	C	282	LEU
1	C	286	LYS
1	C	334	ASP
1	C	343	ASN
1	C	345	LEU
1	C	384	PHE
1	C	409	CYS
1	C	422	LEU
1	C	424	VAL
1	C	428	LEU
1	C	432	GLN
1	C	434	ASP
1	C	435	LEU
1	C	481	ARG
1	C	498	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	26	GLN
1	A	108	ASN
1	A	244	GLN
1	A	251	GLN
1	A	269	GLN
1	A	343	ASN
1	A	478	ASN
1	B	6	ASN
1	B	29	GLN
1	B	102	GLN
1	B	104	HIS
1	B	106	GLN
1	B	124	ASN
1	B	142	GLN
1	B	251	GLN
1	B	252	ASN
1	B	269	GLN

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Mol	Chain	Res	Type
1	B	283	HIS
1	B	287	GLN
1	B	298	GLN
1	B	343	ASN
1	B	387	GLN
1	B	469	HIS
1	B	478	ASN
1	C	16	GLN
1	C	29	GLN
1	C	102	GLN
1	C	104	HIS
1	C	106	GLN
1	C	125	GLN
1	C	128	HIS
1	C	143	GLN
1	C	244	GLN
1	C	273	HIS
1	C	343	ASN
1	C	369	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.