



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:17 PM GMT

PDB ID : 4EAC  
Title : Crystal structure of mannonate dehydratase from Escherichia coli strain K12  
Authors : Qiu, X.; Zhu, Y.; Yuan, Y.; Zhang, Y.; Liu, H.; Gao, Y.; Teng, M.; Niu, L.  
Deposited on : 2012-03-22  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

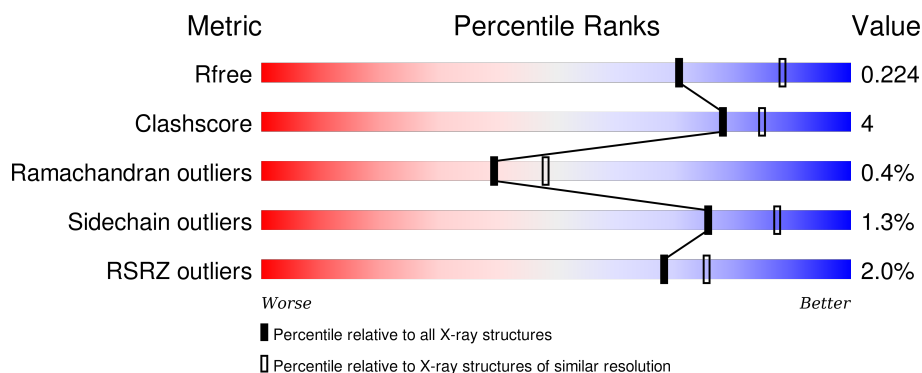
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	414	 86% 9% 5%
1	B	414	 87% 8% 5%
1	C	414	 3% 89% 6% 5%
1	D	414	 4% 88% 7% 5%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13491 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 Mannonate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3151	1991	553	590	17			
1	B	395	Total	C	N	O	S	0	0	0
			3148	1989	553	589	17			
1	C	396	Total	C	N	O	S	0	0	0
			3149	1989	554	589	17			
1	D	395	Total	C	N	O	S	0	0	0
			3146	1987	553	589	17			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P24215
A	-18	GLY	-	EXPRESSION TAG	UNP P24215
A	-17	SER	-	EXPRESSION TAG	UNP P24215
A	-16	SER	-	EXPRESSION TAG	UNP P24215
A	-15	HIS	-	EXPRESSION TAG	UNP P24215
A	-14	HIS	-	EXPRESSION TAG	UNP P24215
A	-13	HIS	-	EXPRESSION TAG	UNP P24215
A	-12	HIS	-	EXPRESSION TAG	UNP P24215
A	-11	HIS	-	EXPRESSION TAG	UNP P24215
A	-10	HIS	-	EXPRESSION TAG	UNP P24215
A	-9	SER	-	EXPRESSION TAG	UNP P24215
A	-8	SER	-	EXPRESSION TAG	UNP P24215
A	-7	GLY	-	EXPRESSION TAG	UNP P24215
A	-6	LEU	-	EXPRESSION TAG	UNP P24215
A	-5	VAL	-	EXPRESSION TAG	UNP P24215
A	-4	PRO	-	EXPRESSION TAG	UNP P24215
A	-3	ARG	-	EXPRESSION TAG	UNP P24215
A	-2	GLY	-	EXPRESSION TAG	UNP P24215
A	-1	SER	-	EXPRESSION TAG	UNP P24215
A	0	HIS	-	EXPRESSION TAG	UNP P24215
B	-19	MET	-	EXPRESSION TAG	UNP P24215

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP P24215
B	-17	SER	-	EXPRESSION TAG	UNP P24215
B	-16	SER	-	EXPRESSION TAG	UNP P24215
B	-15	HIS	-	EXPRESSION TAG	UNP P24215
B	-14	HIS	-	EXPRESSION TAG	UNP P24215
B	-13	HIS	-	EXPRESSION TAG	UNP P24215
B	-12	HIS	-	EXPRESSION TAG	UNP P24215
B	-11	HIS	-	EXPRESSION TAG	UNP P24215
B	-10	HIS	-	EXPRESSION TAG	UNP P24215
B	-9	SER	-	EXPRESSION TAG	UNP P24215
B	-8	SER	-	EXPRESSION TAG	UNP P24215
B	-7	GLY	-	EXPRESSION TAG	UNP P24215
B	-6	LEU	-	EXPRESSION TAG	UNP P24215
B	-5	VAL	-	EXPRESSION TAG	UNP P24215
B	-4	PRO	-	EXPRESSION TAG	UNP P24215
B	-3	ARG	-	EXPRESSION TAG	UNP P24215
B	-2	GLY	-	EXPRESSION TAG	UNP P24215
B	-1	SER	-	EXPRESSION TAG	UNP P24215
B	0	HIS	-	EXPRESSION TAG	UNP P24215
C	-19	MET	-	EXPRESSION TAG	UNP P24215
C	-18	GLY	-	EXPRESSION TAG	UNP P24215
C	-17	SER	-	EXPRESSION TAG	UNP P24215
C	-16	SER	-	EXPRESSION TAG	UNP P24215
C	-15	HIS	-	EXPRESSION TAG	UNP P24215
C	-14	HIS	-	EXPRESSION TAG	UNP P24215
C	-13	HIS	-	EXPRESSION TAG	UNP P24215
C	-12	HIS	-	EXPRESSION TAG	UNP P24215
C	-11	HIS	-	EXPRESSION TAG	UNP P24215
C	-10	HIS	-	EXPRESSION TAG	UNP P24215
C	-9	SER	-	EXPRESSION TAG	UNP P24215
C	-8	SER	-	EXPRESSION TAG	UNP P24215
C	-7	GLY	-	EXPRESSION TAG	UNP P24215
C	-6	LEU	-	EXPRESSION TAG	UNP P24215
C	-5	VAL	-	EXPRESSION TAG	UNP P24215
C	-4	PRO	-	EXPRESSION TAG	UNP P24215
C	-3	ARG	-	EXPRESSION TAG	UNP P24215
C	-2	GLY	-	EXPRESSION TAG	UNP P24215
C	-1	SER	-	EXPRESSION TAG	UNP P24215
C	0	HIS	-	EXPRESSION TAG	UNP P24215
D	-19	MET	-	EXPRESSION TAG	UNP P24215
D	-18	GLY	-	EXPRESSION TAG	UNP P24215
D	-17	SER	-	EXPRESSION TAG	UNP P24215

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP P24215
D	-15	HIS	-	EXPRESSION TAG	UNP P24215
D	-14	HIS	-	EXPRESSION TAG	UNP P24215
D	-13	HIS	-	EXPRESSION TAG	UNP P24215
D	-12	HIS	-	EXPRESSION TAG	UNP P24215
D	-11	HIS	-	EXPRESSION TAG	UNP P24215
D	-10	HIS	-	EXPRESSION TAG	UNP P24215
D	-9	SER	-	EXPRESSION TAG	UNP P24215
D	-8	SER	-	EXPRESSION TAG	UNP P24215
D	-7	GLY	-	EXPRESSION TAG	UNP P24215
D	-6	LEU	-	EXPRESSION TAG	UNP P24215
D	-5	VAL	-	EXPRESSION TAG	UNP P24215
D	-4	PRO	-	EXPRESSION TAG	UNP P24215
D	-3	ARG	-	EXPRESSION TAG	UNP P24215
D	-2	GLY	-	EXPRESSION TAG	UNP P24215
D	-1	SER	-	EXPRESSION TAG	UNP P24215
D	0	HIS	-	EXPRESSION TAG	UNP P24215

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

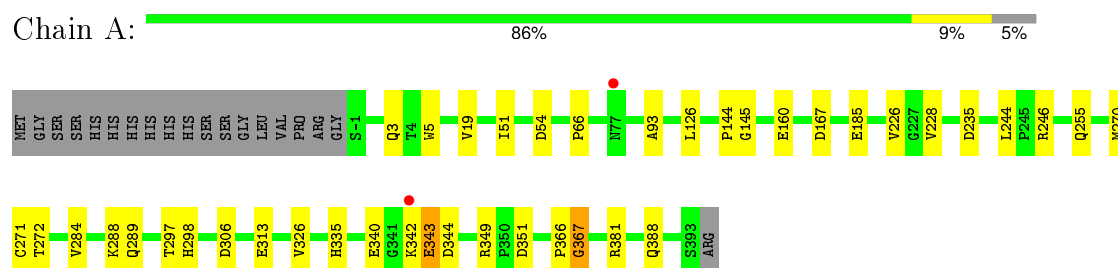
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	273	Total 273	O 273	0	0
4	B	256	Total 256	O 256	0	0
4	C	202	Total 202	O 202	0	0
4	D	158	Total 158	O 158	0	0

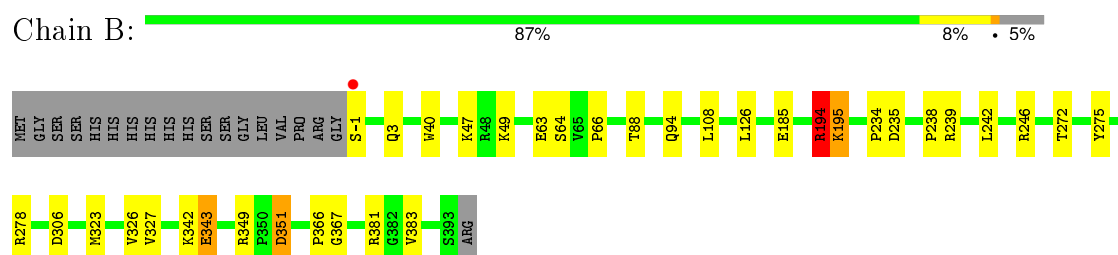
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

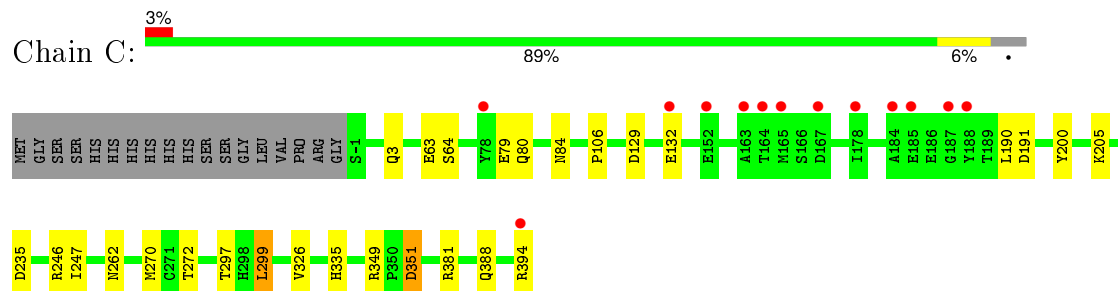
#### • Molecule 1: Mannonate dehydratase



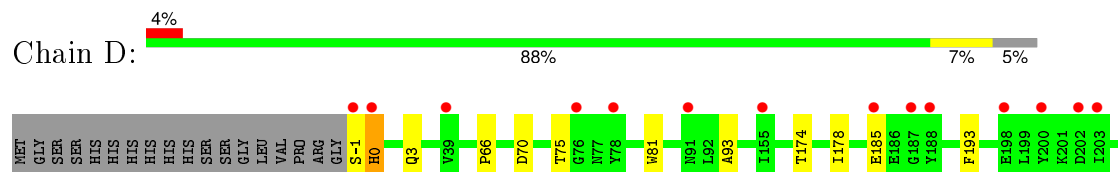
#### • Molecule 1: Mannonate dehydratase

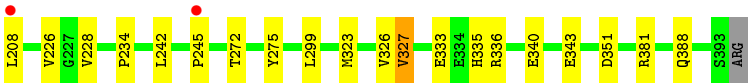


#### • Molecule 1: Mannonate dehydratase



#### • Molecule 1: Mannonate dehydratase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.96 Å   238.46 Å   54.34 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	48.42 – 2.30 48.42 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.42-2.30) 99.8 (48.42-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.18 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.183   ,   0.219 0.188   ,   0.224	Depositor DCC
$R_{free}$ test set	4630 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.2	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 34.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 92475 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13491	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MN, CL

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	0.47	0/3223	0.58	1/4369 (0.0%)
1	B	0.43	0/3220	0.60	2/4366 (0.0%)
1	C	0.44	0/3221	0.56	1/4368 (0.0%)
1	D	0.41	0/3218	0.54	0/4364
All	All	0.44	0/12882	0.57	4/17467 (0.0%)

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	2
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	ARG	N-CA-C	5.68	126.34	111.00
1	C	394	ARG	N-CA-C	-5.53	96.06	111.00
1	B	194	ARG	C-N-CA	5.16	134.59	121.70
1	A	367	GLY	N-CA-C	-5.01	100.58	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	366	PRO	Peptide
1	B	342	LYS	Peptide
1	B	366	PRO	Peptide

## 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	3151	0	3078	32	0
1	B	3148	0	3071	26	0
1	C	3149	0	3070	14	0
1	D	3146	0	3067	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	273	0	0	4	0
4	B	256	0	0	3	0
4	C	202	0	0	0	0
4	D	158	0	0	0	0
All	All	13491	0	12286	89	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 4.

All (89) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:MET:O	1:D:327:VAL:HG12	1.65	0.97
1:B:323:MET:O	1:B:327:VAL:HG12	1.80	0.80
1:A:93:ALA:CB	1:A:226:VAL:HG12	2.14	0.78
1:A:3:GLN:HE22	1:A:381:ARG:HE	1.30	0.77
1:B:327:VAL:HG11	1:B:383:VAL:CG1	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:VAL:HG11	1:B:383:VAL:HG12	1.71	0.72
1:A:289:GLN:HE22	1:B:94:GLN:HE22	1.38	0.72
1:A:255:GLN:HE21	1:B:94:GLN:HE21	1.37	0.71
1:B:3:GLN:HE22	1:B:381:ARG:HE	1.40	0.69
1:A:342:LYS:O	1:A:343:GLU:HB2	1.92	0.66
1:A:289:GLN:NE2	1:B:94:GLN:HE22	1.93	0.66
1:D:93:ALA:CB	1:D:226:VAL:HG13	2.26	0.65
1:A:367:GLY:HA2	4:A:504:HOH:O	1.96	0.64
1:D:3:GLN:HE22	1:D:381:ARG:HE	1.45	0.64
1:C:3:GLN:HE22	1:C:381:ARG:HE	1.45	0.63
1:A:93:ALA:CB	1:A:226:VAL:CG1	2.77	0.63
1:A:93:ALA:HB1	1:A:226:VAL:HG12	1.82	0.62
1:D:93:ALA:CB	1:D:226:VAL:CG1	2.78	0.62
1:C:335:HIS:HE1	1:C:388:GLN:OE1	1.84	0.61
1:B:126:LEU:HD11	1:B:367:GLY:H	1.66	0.60
1:D:-1:SER:O	1:D:0:HIS:HB2	2.03	0.59
1:A:93:ALA:HB3	1:A:226:VAL:CG1	2.34	0.58
1:A:126:LEU:HD11	1:A:367:GLY:H	1.68	0.58
1:A:66:PRO:HB3	1:A:185:GLU:HG3	1.84	0.57
1:D:335:HIS:HE1	1:D:388:GLN:OE1	1.89	0.56
1:B:272:THR:HG21	1:B:326:VAL:HG11	1.88	0.54
1:B:238:PRO:HG2	1:B:278:ARG:HG3	1.90	0.54
1:D:333:GLU:HA	1:D:336:ARG:HG2	1.90	0.53
1:B:327:VAL:HG11	1:B:383:VAL:HG11	1.88	0.53
1:A:235:ASP:HB3	1:A:246:ARG:HD3	1.91	0.53
1:D:234:PRO:HB3	1:D:275:TYR:CZ	2.45	0.52
4:A:534:HOH:O	1:B:49:LYS:HE3	2.10	0.52
1:A:93:ALA:HB3	1:A:226:VAL:HG11	1.92	0.52
1:A:3:GLN:NE2	1:A:381:ARG:HE	2.05	0.52
1:B:3:GLN:NE2	1:B:381:ARG:HE	2.08	0.52
1:C:3:GLN:NE2	1:C:381:ARG:HH21	2.09	0.51
1:C:349:ARG:NH1	1:C:351:ASP:HA	2.26	0.51
1:B:194:ARG:N	1:B:195:LYS:HB3	2.25	0.51
1:D:174:THR:O	1:D:178:ILE:HG12	2.11	0.50
1:B:66:PRO:HB3	1:B:185:GLU:HG3	1.94	0.49
1:A:226:VAL:O	1:A:226:VAL:HG12	2.12	0.49
1:B:367:GLY:HA2	4:B:745:HOH:O	2.12	0.48
1:B:126:LEU:HD11	1:B:367:GLY:N	2.27	0.48
1:B:235:ASP:HB3	1:B:246:ARG:HD3	1.95	0.48
1:D:272:THR:HG21	1:D:326:VAL:HG11	1.95	0.47
1:C:106:PRO:HB3	1:C:200:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:LEU:HD22	1:D:245:PRO:HG2	1.97	0.47
1:A:51:ILE:HG13	4:A:766:HOH:O	2.15	0.46
1:B:349:ARG:NH1	1:B:351:ASP:HA	2.31	0.46
1:C:235:ASP:HB3	1:C:246:ARG:HD3	1.97	0.46
1:C:272:THR:HG21	1:C:326:VAL:HG11	1.96	0.46
1:A:270:MET:HB3	1:A:297:THR:HG22	1.98	0.46
1:A:144:PRO:HA	1:A:145:GLY:HA2	1.78	0.46
1:C:80:GLN:HE21	1:C:84:ASN:HD21	1.63	0.46
1:B:40:TRP:HB2	1:B:88:THR:HG23	1.98	0.45
1:D:93:ALA:HB3	1:D:226:VAL:HG13	1.98	0.45
1:A:289:GLN:HE22	1:B:94:GLN:NE2	2.12	0.45
1:D:226:VAL:HG12	1:D:228:VAL:HG23	1.99	0.44
1:B:63:GLU:HA	1:B:64:SER:HA	1.76	0.44
1:A:272:THR:HG21	1:A:326:VAL:HG11	1.98	0.44
1:B:306:ASP:HB2	4:B:579:HOH:O	2.16	0.44
1:C:270:MET:HB3	1:C:297:THR:HG22	1.99	0.44
1:A:349:ARG:NH1	1:A:351:ASP:HA	2.32	0.44
1:D:70:ASP:HB2	1:D:81:TRP:CD1	2.54	0.43
1:C:205:LYS:HG3	1:C:247:ILE:HG22	2.01	0.43
1:D:3:GLN:NE2	1:D:381:ARG:HH21	2.17	0.43
1:C:297:THR:HB	1:C:299:LEU:HD13	2.01	0.43
1:A:126:LEU:HB2	1:A:313:GLU:OE1	2.18	0.43
1:A:5:TRP:CD1	1:A:19:VAL:HG22	2.54	0.43
1:A:342:LYS:HD3	1:A:344:ASP:HB2	2.00	0.42
1:A:342:LYS:HB3	1:A:343:GLU:H	1.49	0.42
1:B:239:ARG:HD3	4:B:551:HOH:O	2.19	0.42
1:D:336:ARG:O	1:D:340:GLU:HG3	2.20	0.42
1:C:63:GLU:HA	1:C:64:SER:HA	1.81	0.42
1:B:108:LEU:HD12	1:B:242:LEU:HD11	2.02	0.42
1:A:126:LEU:HD11	1:A:367:GLY:N	2.34	0.42
1:A:271:CYS:HA	1:A:298:HIS:HB2	2.02	0.41
1:B:234:PRO:HB3	1:B:275:TYR:CZ	2.56	0.41
1:A:335:HIS:HE1	1:A:388:GLN:OE1	2.03	0.41
1:A:93:ALA:HB2	1:A:228:VAL:HG23	2.02	0.41
1:A:284:VAL:HG12	1:A:288:LYS:HD2	2.01	0.41
1:D:193:PHE:HZ	1:D:242:LEU:HD13	1.85	0.41
1:D:66:PRO:HG3	1:D:185:GLU:HG2	2.03	0.41
1:D:3:GLN:NE2	1:D:381:ARG:HE	2.15	0.40
1:A:160:GLU:HG2	4:A:678:HOH:O	2.20	0.40
1:D:93:ALA:HB2	1:D:226:VAL:CG1	2.51	0.40
1:C:190:LEU:HD23	1:D:340:GLU:CD	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ASP:HB3	1:C:132:GLU:HB2	2.03	0.40
1:D:333:GLU:OE2	1:D:336:ARG:HD3	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	393/414 (95%)	379 (96%)	13 (3%)	1 (0%)	46	57
1	B	393/414 (95%)	378 (96%)	12 (3%)	3 (1%)	24	27
1	C	394/414 (95%)	383 (97%)	10 (2%)	1 (0%)	46	57
1	D	393/414 (95%)	378 (96%)	13 (3%)	2 (0%)	34	41
All	All	1573/1656 (95%)	1518 (96%)	48 (3%)	7 (0%)	39	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343	GLU
1	B	195	LYS
1	B	343	GLU
1	D	0	HIS
1	B	351	ASP
1	D	351	ASP
1	C	351	ASP

### 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	332/351 (95%)	327 (98%)	5 (2%)	72	85
1	B	331/351 (94%)	327 (99%)	4 (1%)	78	89
1	C	331/351 (94%)	327 (99%)	4 (1%)	78	89
1	D	331/351 (94%)	327 (99%)	4 (1%)	78	89
All	All	1325/1404 (94%)	1308 (99%)	17 (1%)	76	87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	167	ASP
1	A	244	LEU
1	A	306	ASP
1	A	340	GLU
1	B	-1	SER
1	B	47	LYS
1	B	194	ARG
1	B	343	GLU
1	C	79	GLU
1	C	191	ASP
1	C	262	ASN
1	C	299	LEU
1	D	75	THR
1	D	299	LEU
1	D	327	VAL
1	D	343	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	74	HIS
1	A	77	ASN
1	A	80	GLN
1	A	255	GLN
1	A	289	GLN
1	A	335	HIS
1	B	3	GLN

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Mol	Chain	Res	Type
1	B	289	GLN
1	B	335	HIS
1	C	3	GLN
1	C	80	GLN
1	C	255	GLN
1	C	289	GLN
1	C	335	HIS
1	D	3	GLN
1	D	196	HIS
1	D	335	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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 ⓘ

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	395/414 (95%)	-0.03	2 (0%) 91 94	9, 22, 42, 51	0
1	B	395/414 (95%)	-0.25	1 (0%) 94 96	9, 23, 45, 56	0
1	C	396/414 (95%)	0.03	13 (3%) 50 59	9, 27, 56, 71	0
1	D	395/414 (95%)	0.14	16 (4%) 41 50	14, 37, 65, 82	0
All	All	1581/1656 (95%)	-0.03	32 (2%) 68 75	9, 27, 57, 82	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	0	HIS	4.5
1	D	202	ASP	4.4
1	C	187	GLY	4.4
1	D	203	ILE	4.4
1	C	185	GLU	4.1
1	D	187	GLY	3.7
1	C	394	ARG	3.7
1	D	-1	SER	3.5
1	C	164	THR	3.1
1	D	185	GLU	3.0
1	B	-1	SER	3.0
1	D	155	ILE	2.8
1	D	188	TYR	2.8
1	C	165	MET	2.6
1	C	178	ILE	2.6
1	D	200	TYR	2.5
1	C	188	TYR	2.5
1	C	163	ALA	2.4
1	A	77	ASN	2.3
1	D	91	ASN	2.3
1	D	78	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	167	ASP	2.3
1	D	39	VAL	2.3
1	C	152	GLU	2.3
1	D	208	LEU	2.3
1	C	184	ALA	2.2
1	D	198	GLU	2.2
1	A	342	LYS	2.1
1	D	76	GLY	2.1
1	C	78	TYR	2.1
1	C	132	GLU	2.1
1	D	245	PRO	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MN	C	402	1/1	1.00	0.13	0.86	16,16,16,16	0
2	CL	C	401	1/1	1.00	0.12	0.78	14,14,14,14	0
2	CL	A	401	1/1	0.99	0.16	0.75	10,10,10,10	0
3	MN	A	402	1/1	1.00	0.14	0.62	11,11,11,11	0
3	MN	B	402	1/1	1.00	0.12	0.17	12,12,12,12	0
2	CL	B	401	1/1	1.00	0.11	-0.56	10,10,10,10	0
3	MN	D	402	1/1	0.99	0.09	-1.93	26,26,26,26	0
2	CL	D	401	1/1	1.00	0.10	-1.99	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.