



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:32 PM GMT

PDB ID : 4INP  
Title : The crystal structure of Helicobacter pylori Ceue (HP1561) with Ni(II) bound  
Authors : Shaik, M.M.; Cendron, L.; Zanotti, G.  
Deposited on : 2013-01-05  
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

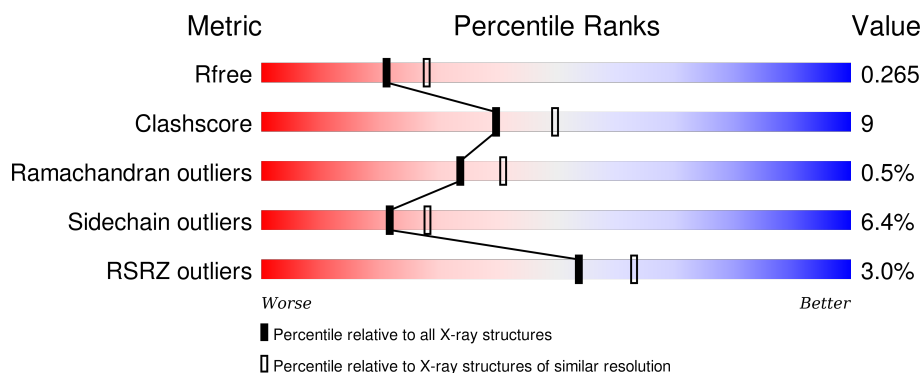
# 1 Overall quality at a glance

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	334	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>14%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	334	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>15%</div> <div>•</div> <div>10%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	404	-	-	-	X
3	ACT	A	405	-	-	-	X
3	ACT	B	404	-	-	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4996 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 Iron (III) ABC transporter, periplasmic iron-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2379	1556	386	432	5			
1	B	300	Total	C	N	O	S	0	0	0
			2379	1556	386	432	5			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	ALA	VAL	ENGINEERED MUTATION	UNP B5Z9J2
A	336	LYS	-	EXPRESSION TAG	UNP B5Z9J2
A	337	GLY	-	EXPRESSION TAG	UNP B5Z9J2
A	338	GLU	-	EXPRESSION TAG	UNP B5Z9J2
A	339	LEU	-	EXPRESSION TAG	UNP B5Z9J2
A	340	ASN	-	EXPRESSION TAG	UNP B5Z9J2
A	341	SER	-	EXPRESSION TAG	UNP B5Z9J2
A	342	LYS	-	EXPRESSION TAG	UNP B5Z9J2
A	343	LEU	-	EXPRESSION TAG	UNP B5Z9J2
A	344	GLU	-	EXPRESSION TAG	UNP B5Z9J2
A	345	GLY	-	EXPRESSION TAG	UNP B5Z9J2
A	346	LYS	-	EXPRESSION TAG	UNP B5Z9J2
A	347	PRO	-	EXPRESSION TAG	UNP B5Z9J2
A	348	ILE	-	EXPRESSION TAG	UNP B5Z9J2
A	349	PRO	-	EXPRESSION TAG	UNP B5Z9J2
A	350	ASN	-	EXPRESSION TAG	UNP B5Z9J2
A	351	PRO	-	EXPRESSION TAG	UNP B5Z9J2
A	352	LEU	-	EXPRESSION TAG	UNP B5Z9J2
A	353	LEU	-	EXPRESSION TAG	UNP B5Z9J2
A	354	GLY	-	EXPRESSION TAG	UNP B5Z9J2
A	355	LEU	-	EXPRESSION TAG	UNP B5Z9J2
A	356	ASP	-	EXPRESSION TAG	UNP B5Z9J2
A	357	SER	-	EXPRESSION TAG	UNP B5Z9J2
A	358	THR	-	EXPRESSION TAG	UNP B5Z9J2
A	359	ARG	-	EXPRESSION TAG	UNP B5Z9J2

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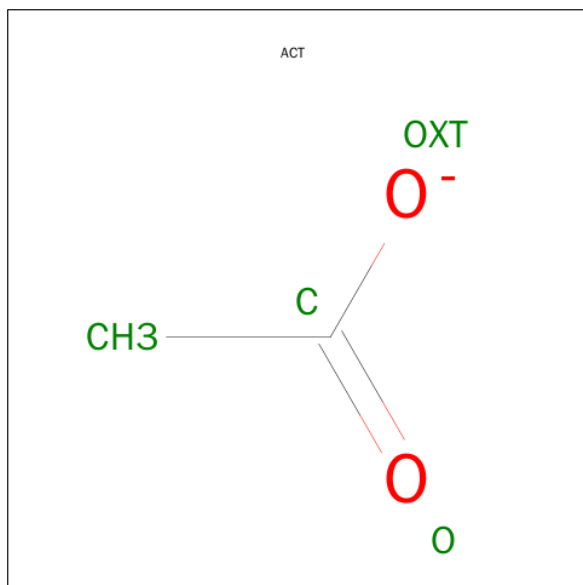
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Chain	Residue	Modelled	Actual	Comment	Reference
A	360	THR	-	EXPRESSION TAG	UNP B5Z9J2
A	361	GLY	-	EXPRESSION TAG	UNP B5Z9J2
A	362	HIS	-	EXPRESSION TAG	UNP B5Z9J2
A	363	HIS	-	EXPRESSION TAG	UNP B5Z9J2
A	364	HIS	-	EXPRESSION TAG	UNP B5Z9J2
A	365	HIS	-	EXPRESSION TAG	UNP B5Z9J2
A	366	HIS	-	EXPRESSION TAG	UNP B5Z9J2
A	367	HIS	-	EXPRESSION TAG	UNP B5Z9J2
B	104	ALA	VAL	ENGINEERED MUTATION	UNP B5Z9J2
B	336	LYS	-	EXPRESSION TAG	UNP B5Z9J2
B	337	GLY	-	EXPRESSION TAG	UNP B5Z9J2
B	338	GLU	-	EXPRESSION TAG	UNP B5Z9J2
B	339	LEU	-	EXPRESSION TAG	UNP B5Z9J2
B	340	ASN	-	EXPRESSION TAG	UNP B5Z9J2
B	341	SER	-	EXPRESSION TAG	UNP B5Z9J2
B	342	LYS	-	EXPRESSION TAG	UNP B5Z9J2
B	343	LEU	-	EXPRESSION TAG	UNP B5Z9J2
B	344	GLU	-	EXPRESSION TAG	UNP B5Z9J2
B	345	GLY	-	EXPRESSION TAG	UNP B5Z9J2
B	346	LYS	-	EXPRESSION TAG	UNP B5Z9J2
B	347	PRO	-	EXPRESSION TAG	UNP B5Z9J2
B	348	ILE	-	EXPRESSION TAG	UNP B5Z9J2
B	349	PRO	-	EXPRESSION TAG	UNP B5Z9J2
B	350	ASN	-	EXPRESSION TAG	UNP B5Z9J2
B	351	PRO	-	EXPRESSION TAG	UNP B5Z9J2
B	352	LEU	-	EXPRESSION TAG	UNP B5Z9J2
B	353	LEU	-	EXPRESSION TAG	UNP B5Z9J2
B	354	GLY	-	EXPRESSION TAG	UNP B5Z9J2
B	355	LEU	-	EXPRESSION TAG	UNP B5Z9J2
B	356	ASP	-	EXPRESSION TAG	UNP B5Z9J2
B	357	SER	-	EXPRESSION TAG	UNP B5Z9J2
B	358	THR	-	EXPRESSION TAG	UNP B5Z9J2
B	359	ARG	-	EXPRESSION TAG	UNP B5Z9J2
B	360	THR	-	EXPRESSION TAG	UNP B5Z9J2
B	361	GLY	-	EXPRESSION TAG	UNP B5Z9J2
B	362	HIS	-	EXPRESSION TAG	UNP B5Z9J2
B	363	HIS	-	EXPRESSION TAG	UNP B5Z9J2
B	364	HIS	-	EXPRESSION TAG	UNP B5Z9J2
B	365	HIS	-	EXPRESSION TAG	UNP B5Z9J2
B	366	HIS	-	EXPRESSION TAG	UNP B5Z9J2
B	367	HIS	-	EXPRESSION TAG	UNP B5Z9J2

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Ni 3 3	0	0
2	A	3	Total Ni 3 3	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

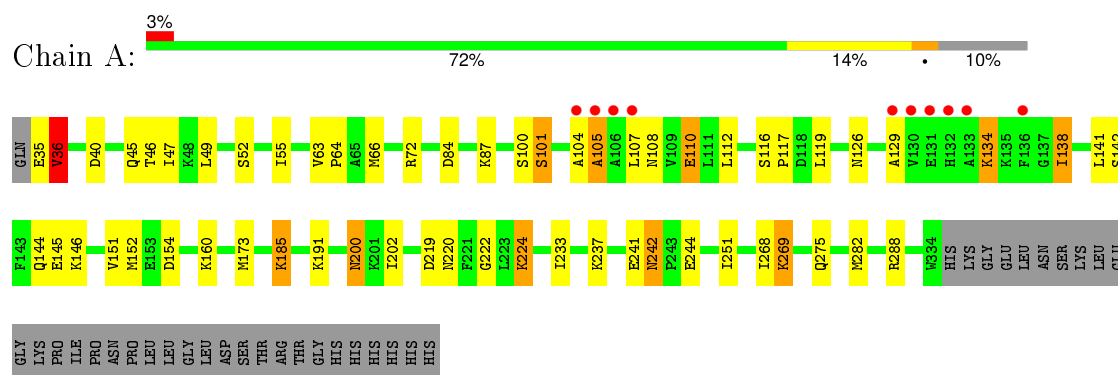
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total 114	O 114	0	0
4	B	86	Total 86	O 86	0	0

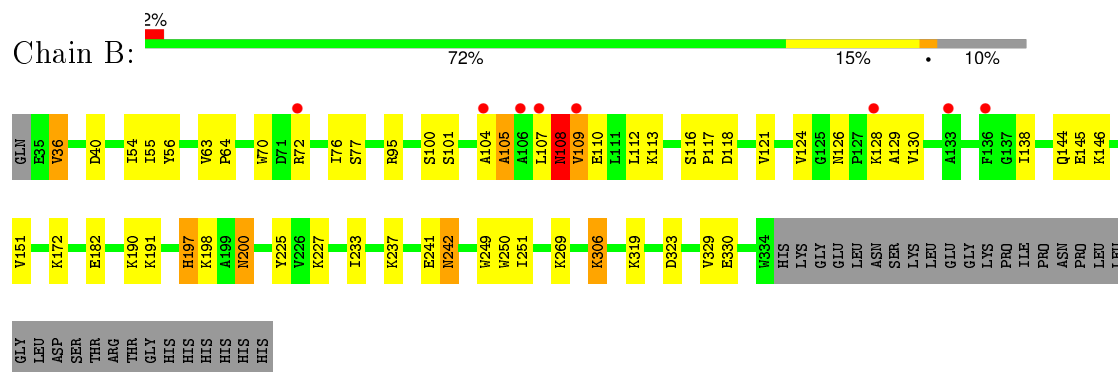
### 3 Residue-property plots

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: Iron (III) ABC transporter, periplasmic iron-binding protein



- Molecule 1: Iron (III) ABC transporter, periplasmic iron-binding protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.18Å 76.95Å 72.78Å 90.00° 94.52° 90.00°	Depositor
Resolution (Å)	52.79 – 2.30 52.79 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.7 (52.79-2.30) 91.7 (52.79-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.50 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.189 , 0.268 0.191 , 0.265	Depositor DCC
$R_{free}$ test set	1370 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.5	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 27113 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4996	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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

### 5.1 Standard geometry

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

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	0/2432	0.84	4/3283 (0.1%)
1	B	0.86	0/2432	0.84	3/3283 (0.1%)
All	All	0.87	0/4864	0.84	7/6566 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	40	ASP	CB-CG-OD1	6.80	124.42	118.30
1	A	36	VAL	CB-CA-C	-6.67	98.72	111.40
1	A	154	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	108	ASN	N-CA-C	5.64	126.24	111.00
1	A	84	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	224	LYS	CB-CA-C	5.17	120.74	110.40
1	B	36	VAL	CB-CA-C	-5.07	101.76	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	72	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2379	0	2459	46	0
1	B	2379	0	2459	39	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	16	0	12	0	0
3	B	16	0	12	2	0
4	A	114	0	0	4	0
4	B	86	0	0	3	0
All	All	4996	0	4942	86	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 9.

All (86) 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:B:108:ASN:HD22	1:B:109:VAL:H	1.10	0.99
3:B:404:ACT:H1	4:B:504:HOH:O	1.64	0.97
1:A:152:MET:HE2	1:A:173:MET:HB3	1.43	0.97
1:B:242:ASN:HD21	1:B:269:LYS:H	1.14	0.92
1:A:110:GLU:OE1	1:A:110:GLU:HA	1.77	0.85
1:B:225:TYR:HB3	1:B:233:ILE:HG21	1.62	0.79
1:A:152:MET:CE	1:A:173:MET:HB3	2.12	0.78
1:B:108:ASN:HD22	1:B:109:VAL:N	1.83	0.75
1:A:144:GLN:HE21	1:A:146:LYS:NZ	1.86	0.74
1:A:242:ASN:HD21	1:A:269:LYS:H	1.37	0.72
1:A:144:GLN:HE21	1:A:146:LYS:CE	2.04	0.70
1:A:160:LYS:NZ	4:A:588:HOH:O	2.24	0.70
1:A:100:SER:O	1:A:101:SER:CB	2.39	0.69
1:A:275:GLN:HG3	4:A:576:HOH:O	1.92	0.69
1:B:144:GLN:HE21	1:B:146:LYS:NZ	1.90	0.69
1:A:152:MET:HE2	1:A:173:MET:CB	2.18	0.69
1:B:200:ASN:HD22	1:B:200:ASN:H	1.41	0.68
1:B:249:TRP:HE1	3:B:404:ACT:H3	1.58	0.67
1:B:306:LYS:HA	1:B:306:LYS:HE3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ASN:ND2	1:A:268:ILE:HA	2.13	0.63
1:B:126:ASN:HB3	1:B:129:ALA:HB3	1.81	0.61
1:B:108:ASN:ND2	1:B:109:VAL:H	1.92	0.60
1:B:242:ASN:ND2	1:B:269:LYS:H	1.93	0.59
1:B:104:ALA:O	1:B:105:ALA:HB3	2.03	0.59
1:B:198:LYS:HE3	1:B:200:ASN:HD21	1.67	0.59
1:A:185:LYS:HE3	4:A:600:HOH:O	2.04	0.58
1:A:233:ILE:HD12	1:A:237:LYS:HB2	1.86	0.58
1:A:200:ASN:HD22	1:A:200:ASN:H	1.52	0.57
1:B:197:HIS:CE1	4:B:515:HOH:O	2.57	0.57
1:A:100:SER:O	1:A:101:SER:HB2	2.04	0.57
1:B:54:ILE:HD11	1:B:121:VAL:CG2	2.34	0.57
1:B:54:ILE:HD11	1:B:121:VAL:HG23	1.86	0.56
1:A:251:ILE:HG22	1:A:251:ILE:O	2.05	0.56
1:A:145:GLU:HG3	1:A:151:VAL:HG22	1.87	0.56
1:A:134:LYS:O	1:A:134:LYS:HG3	2.06	0.55
1:A:242:ASN:HD21	1:A:268:ILE:HA	1.72	0.54
1:A:185:LYS:CE	4:A:600:HOH:O	2.55	0.54
1:A:105:ALA:HA	1:A:108:ASN:HD21	1.73	0.54
1:B:200:ASN:HD22	1:B:200:ASN:N	2.07	0.53
1:B:144:GLN:HE21	1:B:146:LYS:HZ1	1.55	0.53
1:A:282:MET:HG2	1:A:288:ARG:CZ	2.39	0.52
1:A:55:ILE:HD12	1:A:117:PRO:HG3	1.90	0.52
1:A:244:GLU:HG3	1:A:269:LYS:HE3	1.92	0.52
1:B:250:TRP:HD1	4:B:509:HOH:O	1.94	0.50
1:A:105:ALA:HA	1:A:108:ASN:ND2	2.27	0.50
1:A:100:SER:HB2	1:A:107:LEU:HB2	1.94	0.50
1:B:56:TYR:HB2	1:B:76:ILE:HG13	1.95	0.49
1:B:55:ILE:HD12	1:B:117:PRO:HG3	1.94	0.49
1:B:242:ASN:HD21	1:B:269:LYS:N	1.96	0.49
1:B:70:TRP:O	1:B:95:ARG:NH2	2.45	0.49
1:B:108:ASN:ND2	1:B:109:VAL:N	2.58	0.48
1:B:104:ALA:O	1:B:105:ALA:CB	2.62	0.48
1:B:145:GLU:HG3	1:B:151:VAL:HG22	1.95	0.48
1:B:110:GLU:OE1	1:B:110:GLU:HA	2.13	0.48
1:A:36:VAL:HG22	1:A:49:LEU:HD11	1.97	0.47
1:B:124:VAL:HG22	1:B:130:VAL:HG21	1.97	0.46
1:B:233:ILE:HD12	1:B:237:LYS:HB2	1.98	0.46
1:B:197:HIS:CD2	1:B:198:LYS:HG2	2.51	0.46
1:A:52:SER:O	1:A:72:ARG:HD3	2.15	0.45
1:A:144:GLN:HE21	1:A:146:LYS:HE3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LYS:HB2	1:A:87:LYS:HE3	1.59	0.45
1:A:220:ASN:ND2	1:A:222:GLY:H	2.15	0.44
1:B:100:SER:HA	1:B:107:LEU:HD12	1.99	0.44
1:B:63:VAL:N	1:B:64:PRO:CD	2.80	0.44
1:A:242:ASN:ND2	1:A:269:LYS:H	2.10	0.44
1:A:104:ALA:O	1:A:105:ALA:HB3	2.18	0.44
1:B:251:ILE:O	1:B:251:ILE:HG22	2.18	0.43
1:A:40:ASP:HB2	1:A:142:SER:O	2.18	0.43
1:A:202:ILE:HD12	1:A:222:GLY:HA2	1.99	0.43
1:B:100:SER:O	1:B:101:SER:HB2	2.18	0.43
1:A:35:GLU:HA	1:A:47:ILE:O	2.18	0.43
1:B:191:LYS:HE3	1:B:241:GLU:O	2.19	0.42
1:B:249:TRP:CE2	1:B:251:ILE:HB	2.54	0.42
1:A:45:GLN:HE22	1:A:134:LYS:HE3	1.84	0.42
1:A:126:ASN:HB3	1:A:129:ALA:HB3	2.00	0.42
1:B:100:SER:CA	1:B:107:LEU:HD12	2.48	0.42
1:B:172:LYS:HE2	1:B:172:LYS:HA	2.01	0.42
1:A:105:ALA:O	1:A:108:ASN:ND2	2.50	0.42
1:A:251:ILE:CG2	1:A:251:ILE:O	2.66	0.42
1:A:200:ASN:N	1:A:200:ASN:HD22	2.11	0.42
1:A:117:PRO:O	1:A:138:ILE:HG21	2.20	0.41
1:A:191:LYS:CE	1:A:241:GLU:O	2.68	0.41
1:B:319:LYS:O	1:B:323:ASP:HA	2.21	0.41
1:A:119:LEU:HD11	1:A:141:LEU:HG	2.03	0.41
1:A:100:SER:O	1:A:101:SER:HB3	2.20	0.41
1:A:63:VAL:N	1:A:64:PRO:CD	2.84	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	298/334 (89%)	284 (95%)	13 (4%)	1 (0%)	46	57
1	B	298/334 (89%)	287 (96%)	9 (3%)	2 (1%)	26	31
All	All	596/668 (89%)	571 (96%)	22 (4%)	3 (0%)	34	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	105	ALA
1	A	105	ALA
1	B	109	VAL

### 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	259/289 (90%)	244 (94%)	15 (6%)	25	33
1	B	259/289 (90%)	241 (93%)	18 (7%)	19	24
All	All	518/578 (90%)	485 (94%)	33 (6%)	22	28

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	46	THR
1	A	66	MET
1	A	101	SER
1	A	110	GLU
1	A	112	LEU
1	A	116	SER
1	A	134	LYS
1	A	138	ILE
1	A	185	LYS
1	A	200	ASN
1	A	219	ASP
1	A	224	LYS

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Mol	Chain	Res	Type
1	A	242	ASN
1	A	269	LYS
1	B	36	VAL
1	B	77	SER
1	B	108	ASN
1	B	112	LEU
1	B	113	LYS
1	B	116	SER
1	B	118	ASP
1	B	128	LYS
1	B	138	ILE
1	B	182	GLU
1	B	190	LYS
1	B	197	HIS
1	B	200	ASN
1	B	227	LYS
1	B	242	ASN
1	B	306	LYS
1	B	329	VAL
1	B	330	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	108	ASN
1	A	144	GLN
1	A	174	GLN
1	A	200	ASN
1	A	220	ASN
1	A	242	ASN
1	A	273	ASN
1	B	108	ASN
1	B	144	GLN
1	B	200	ASN
1	B	220	ASN
1	B	242	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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	ACT	A	404	2	1,3,3	2.23	1 (100%)	0,3,3	0.00	-
3	ACT	A	405	2	1,3,3	1.54	0	0,3,3	0.00	-
3	ACT	A	406	2	1,3,3	1.83	0	0,3,3	0.00	-
3	ACT	A	407	2	1,3,3	1.47	0	0,3,3	0.00	-
3	ACT	B	404	2	1,3,3	0.33	0	0,3,3	0.00	-
3	ACT	B	405	2	1,3,3	1.67	0	0,3,3	0.00	-
3	ACT	B	406	2	1,3,3	1.37	0	0,3,3	0.00	-
3	ACT	B	407	2	1,3,3	2.21	1 (100%)	0,3,3	0.00	-

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	ACT	A	404	2	-	0/0/0/0	0/0/0/0
3	ACT	A	405	2	-	0/0/0/0	0/0/0/0
3	ACT	A	406	2	-	0/0/0/0	0/0/0/0
3	ACT	A	407	2	-	0/0/0/0	0/0/0/0
3	ACT	B	404	2	-	0/0/0/0	0/0/0/0
3	ACT	B	405	2	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	B	406	2	-	0/0/0/0	0/0/0/0
3	ACT	B	407	2	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	407	ACT	CH3-C	2.21	1.51	1.48
3	A	404	ACT	CH3-C	2.23	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	404	ACT	2	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 [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	300/334 (89%)	-0.09	10 (3%) 50 59	5, 18, 57, 68	0
1	B	300/334 (89%)	-0.08	8 (2%) 58 67	7, 20, 57, 67	0
All	All	600/668 (89%)	-0.08	18 (3%) 54 63	5, 19, 57, 68	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	LEU	12.0
1	B	107	LEU	11.3
1	B	106	ALA	9.3
1	A	106	ALA	9.1
1	A	133	ALA	5.2
1	B	104	ALA	4.9
1	A	132	HIS	4.1
1	A	129	ALA	3.6
1	A	104	ALA	3.6
1	B	128	LYS	3.0
1	B	109	VAL	2.9
1	A	105	ALA	2.6
1	A	136	PHE	2.5
1	B	136	PHE	2.5
1	A	131	GLU	2.4
1	B	72	ARG	2.1
1	A	130	VAL	2.1
1	B	133	ALA	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	ACT	A	404	4/4	0.86	0.22	8.97	25,25,27,27	0
3	ACT	A	405	4/4	0.84	0.17	7.61	17,20,20,21	0
3	ACT	B	404	4/4	0.86	0.16	2.13	27,27,27,28	0
2	NI	B	403	1/1	0.99	0.02	-	28,28,28,28	0
3	ACT	A	406	4/4	0.81	0.19	-	35,35,36,36	0
3	ACT	A	407	4/4	0.83	0.21	-	49,50,50,50	0
2	NI	A	402	1/1	0.98	0.04	-	51,51,51,51	0
3	ACT	B	405	4/4	0.69	0.26	-	48,50,50,51	0
2	NI	A	401	1/1	0.99	0.04	-	43,43,43,43	0
3	ACT	B	407	4/4	0.90	0.20	-	22,23,24,25	0
2	NI	B	401	1/1	0.94	0.06	-	46,46,46,46	0
2	NI	B	402	1/1	0.97	0.03	-	53,53,53,53	0
2	NI	A	403	1/1	0.97	0.05	-	29,29,29,29	0
3	ACT	B	406	4/4	0.83	0.18	-	54,54,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.