



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:16 AM UTC

PDB ID : 5EZ1 / pdb_00005ez1
Title : Crystal Structure of Cell Binding Factor 2 from Helicobacter pylori in complex with I2CA
Authors : Sun, Y.J.; Chu, C.H.; Tsai, Y.C.
Deposited on : 2015-11-26
Resolution : 2.40 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

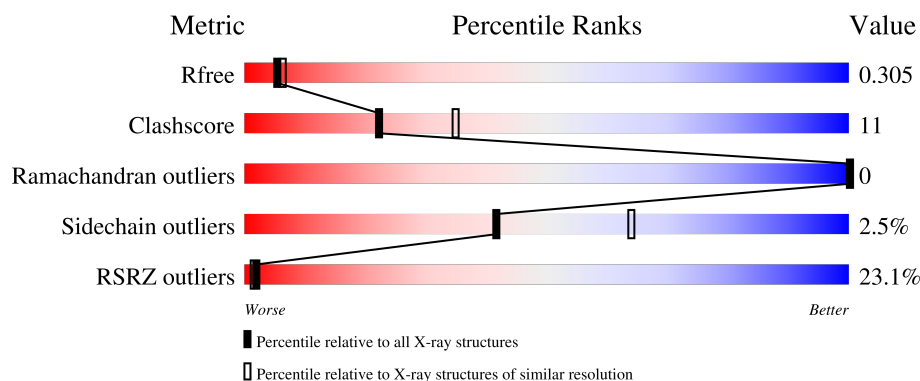
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 ≥ 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	277	5% 65% 17% • 17%
1	B	277	34% 61% 22% 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3935 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.

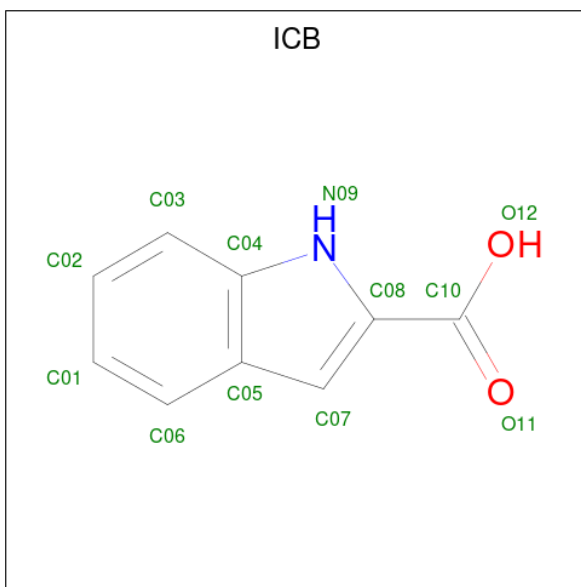
- Molecule 1 is a protein called Putative peptidyl-prolyl cis-trans isomerase HP_0175.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1876	1190	320	359	7			
1	B	232	Total	C	N	O	S	0	0	0
			1884	1196	321	360	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	expression tag	UNP P56112
A	32	GLY	-	expression tag	UNP P56112
A	300	LEU	-	expression tag	UNP P56112
A	301	GLU	-	expression tag	UNP P56112
A	302	HIS	-	expression tag	UNP P56112
A	303	HIS	-	expression tag	UNP P56112
A	304	HIS	-	expression tag	UNP P56112
A	305	HIS	-	expression tag	UNP P56112
A	306	HIS	-	expression tag	UNP P56112
A	307	HIS	-	expression tag	UNP P56112
B	31	MET	-	expression tag	UNP P56112
B	32	GLY	-	expression tag	UNP P56112
B	300	LEU	-	expression tag	UNP P56112
B	301	GLU	-	expression tag	UNP P56112
B	302	HIS	-	expression tag	UNP P56112
B	303	HIS	-	expression tag	UNP P56112
B	304	HIS	-	expression tag	UNP P56112
B	305	HIS	-	expression tag	UNP P56112
B	306	HIS	-	expression tag	UNP P56112
B	307	HIS	-	expression tag	UNP P56112

- Molecule 2 is 1H-indole-2-carboxylic acid (CCD ID: ICB) (formula: C₉H₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	9	1	2		
2	B	1	Total	C	N	O	0	0
			12	9	1	2		

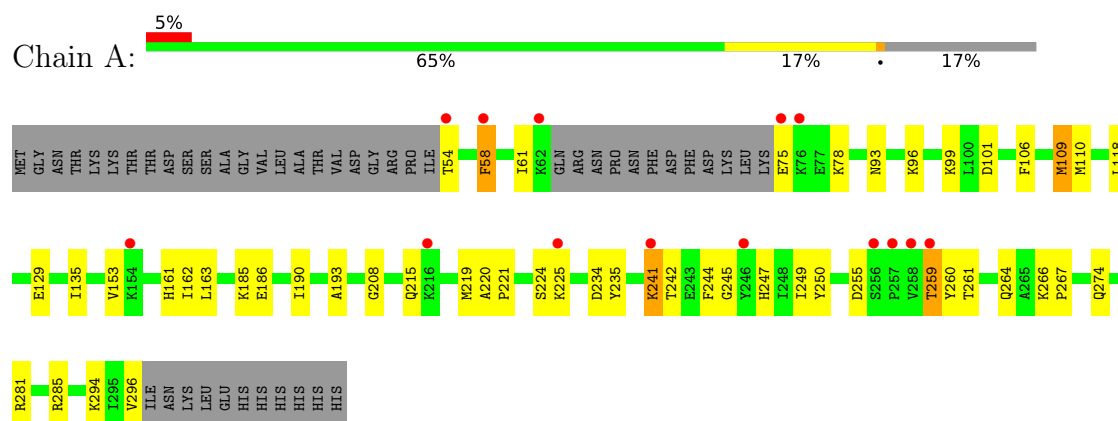
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	78	Total	O	0	0
			78	78		
3	B	73	Total	O	0	0
			73	73		

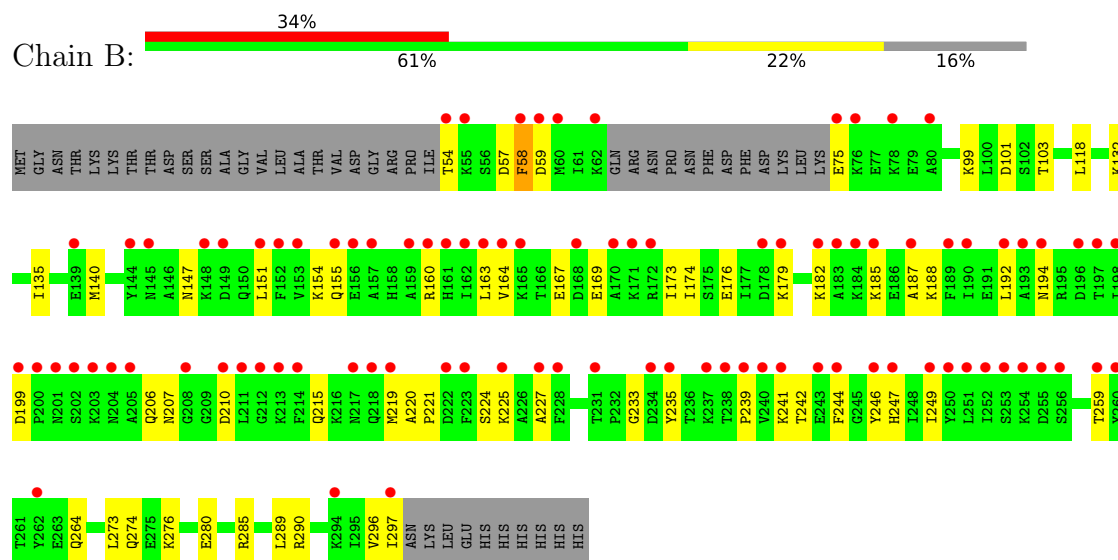
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Putative peptidyl-prolyl cis-trans isomerase HP_0175



- Molecule 1: Putative peptidyl-prolyl cis-trans isomerase HP_0175



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	62.00Å 62.00Å 366.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.67 – 2.40 26.67 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.6 (26.67-2.40) 91.5 (26.67-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.244 , 0.299 0.252 , 0.305	Depositor DCC
R_{free} test set	1571 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3935	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ICB

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	0.66	0/1906	0.95	3/2551 (0.1%)
1	B	0.57	0/1914	0.94	7/2562 (0.3%)
All	All	0.61	0/3820	0.94	10/5113 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	ASP	CA-C-N	5.89	125.44	119.19
1	B	199	ASP	C-N-CA	5.89	125.44	119.19
1	A	220	ALA	CA-C-N	5.48	124.94	119.24
1	A	220	ALA	C-N-CA	5.48	124.94	119.24
1	B	103	THR	CA-C-N	5.45	126.66	119.84
1	B	103	THR	C-N-CA	5.45	126.66	119.84
1	B	220	ALA	CA-C-N	5.16	124.60	119.24
1	B	220	ALA	C-N-CA	5.16	124.60	119.24
1	A	61	ILE	N-CA-C	5.09	115.30	107.77
1	B	167	GLU	N-CA-C	5.00	118.16	111.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1876	0	1909	39	0
1	B	1884	0	1920	48	0
2	A	12	0	0	0	0
2	B	12	0	0	0	0
3	A	78	0	0	11	1
3	B	73	0	0	16	1
All	All	3935	0	3829	81	1

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 11.

All (81) 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:206:GLN:NE2	3:B:504:HOH:O	2.04	0.91
1:A:244:PHE:O	3:A:501:HOH:O	1.92	0.87
1:B:182:LYS:HA	1:B:185:LYS:HD3	1.60	0.84
1:B:290:ARG:NH1	3:B:502:HOH:O	1.99	0.83
1:B:173:ILE:HG23	1:B:192:LEU:HD23	1.62	0.80
1:A:260:TYR:HA	3:A:507:HOH:O	1.82	0.79
1:B:54:THR:N	3:B:506:HOH:O	2.16	0.78
1:B:164:VAL:HG11	1:B:169:GLU:HB2	1.65	0.77
1:B:135:ILE:HD11	1:B:274:GLN:HG3	1.67	0.76
1:B:210:ASP:OD2	3:B:505:HOH:O	2.05	0.74
1:B:147:ASN:HB3	1:B:151:LEU:HD13	1.70	0.73
1:A:296:VAL:O	3:A:503:HOH:O	2.09	0.69
1:B:154:LYS:NZ	1:B:215:GLN:OE1	2.22	0.68
1:A:221:PRO:O	1:A:225:LYS:HG2	1.94	0.68
1:A:234:ASP:OD1	3:A:504:HOH:O	2.13	0.67
1:B:227:ALA:HB2	1:B:249:ILE:HD13	1.77	0.67
1:A:215:GLN:NE2	3:A:502:HOH:O	1.95	0.65
1:A:242:THR:HG23	1:A:244:PHE:H	1.59	0.65
1:B:155:GLN:NE2	3:B:514:HOH:O	2.30	0.64
1:A:186:GLU:OE1	3:A:505:HOH:O	2.15	0.64
1:B:221:PRO:O	1:B:225:LYS:HG2	1.97	0.63
1:A:185:LYS:HE2	3:A:506:HOH:O	1.98	0.62
1:B:182:LYS:NZ	1:B:233:GLY:O	2.33	0.62
1:A:54:THR:HG21	1:B:297:ILE:HG23	1.84	0.59
1:B:206:GLN:OE1	3:B:507:HOH:O	2.17	0.59
1:A:129:GLU:OE1	1:A:281:ARG:NH2	2.36	0.58
1:B:206:GLN:HB2	3:B:519:HOH:O	2.03	0.58
1:A:135:ILE:HD11	1:A:274:GLN:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:THR:HG23	1:A:244:PHE:N	2.20	0.57
1:B:75:GLU:N	3:B:518:HOH:O	2.38	0.56
1:B:242:THR:HG21	1:B:247:HIS:CE1	2.42	0.55
1:A:58:PHE:HE1	1:A:93:ASN:CG	2.14	0.55
1:A:118:LEU:HD21	1:B:101:ASP:HB3	1.89	0.55
1:A:242:THR:HG21	1:A:247:HIS:CE1	2.42	0.54
1:B:99:LYS:HD3	3:B:525:HOH:O	2.07	0.54
1:A:54:THR:HB	1:B:296:VAL:O	2.08	0.53
1:B:154:LYS:HG2	3:B:537:HOH:O	2.08	0.53
1:B:154:LYS:HA	3:B:537:HOH:O	2.08	0.53
1:B:185:LYS:HE3	1:B:235:TYR:CE1	2.45	0.52
1:B:187:ALA:O	3:B:508:HOH:O	2.19	0.52
1:A:96:LYS:HE3	1:B:118:LEU:HD11	1.93	0.51
1:A:259:THR:O	3:A:507:HOH:O	2.19	0.50
1:B:242:THR:HG23	1:B:244:PHE:H	1.77	0.50
1:B:176:GLU:HB3	1:B:192:LEU:HD21	1.92	0.50
1:A:250:TYR:OH	3:A:506:HOH:O	2.17	0.49
1:B:187:ALA:N	3:B:517:HOH:O	2.37	0.49
1:A:294:LYS:O	1:B:57:ASP:N	2.44	0.49
1:B:194:ASN:HB2	3:B:509:HOH:O	2.13	0.48
1:B:163:LEU:HD13	1:B:247:HIS:NE2	2.28	0.48
1:A:255:ASP:OD1	3:A:508:HOH:O	2.20	0.48
1:B:140:MET:HG2	1:B:273:LEU:HD12	1.96	0.48
1:A:296:VAL:C	1:B:54:THR:HB	2.39	0.47
1:B:206:GLN:HB3	3:B:507:HOH:O	2.15	0.47
1:A:75:GLU:N	1:A:75:GLU:OE1	2.47	0.47
1:A:163:LEU:HD13	1:A:247:HIS:NE2	2.30	0.47
1:B:176:GLU:OE2	1:B:179:LYS:NZ	2.39	0.46
1:A:109:MET:HG3	1:A:110:MET:N	2.29	0.46
1:B:160:ARG:NH2	1:B:207:ASN:O	2.48	0.46
1:A:266:LYS:HB3	1:A:267:PRO:HD3	1.97	0.46
1:B:164:VAL:CG1	1:B:169:GLU:HB2	2.41	0.46
1:B:174:ILE:HD12	1:B:239:PRO:HD3	1.97	0.46
1:B:185:LYS:HE3	1:B:235:TYR:HE1	1.81	0.46
1:A:161:HIS:HD2	1:A:247:HIS:CD2	2.33	0.46
1:A:261:THR:OG1	1:A:264:GLN:HG3	2.15	0.45
1:A:75:GLU:N	1:A:78:LYS:HE3	2.31	0.45
1:A:99:LYS:NZ	3:A:522:HOH:O	2.48	0.45
1:A:101:ASP:HA	1:A:106:PHE:CG	2.52	0.44
1:A:190:ILE:HG23	1:A:208:GLY:HA3	1.99	0.44
1:B:241:LYS:HG2	1:B:246:TYR:CE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LYS:O	1:B:192:LEU:HD13	2.20	0.42
1:B:219:MET:HB2	1:B:224:SER:OG	2.20	0.42
1:B:57:ASP:HB3	1:B:58:PHE:H	1.67	0.42
1:A:219:MET:HB2	1:A:224:SER:OG	2.21	0.41
1:A:242:THR:HG22	1:A:245:GLY:O	2.19	0.41
1:B:276:LYS:HE2	1:B:280:GLU:OE2	2.21	0.41
1:A:281:ARG:O	1:A:285:ARG:HG2	2.21	0.41
1:A:235:TYR:HA	1:A:249:ILE:O	2.20	0.41
1:A:241:LYS:HE2	1:A:241:LYS:H	1.86	0.40
1:B:264:GLN:O	3:B:510:HOH:O	2.22	0.40
1:B:285:ARG:HD3	1:B:285:ARG:HA	1.85	0.40
1:A:162:ILE:HG12	1:A:193:ALA:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:544:HOH:O	3:B:560:HOH:O[4_555]	2.18	0.02

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	227/277 (82%)	225 (99%)	2 (1%)	0	100	100
1	B	228/277 (82%)	225 (99%)	3 (1%)	0	100	100
All	All	455/554 (82%)	450 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	202/243 (83%)	197 (98%)	5 (2%)	42	64
1	B	203/243 (84%)	198 (98%)	5 (2%)	42	64
All	All	405/486 (83%)	395 (98%)	10 (2%)	42	64

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	PHE
1	A	109	MET
1	A	153	VAL
1	A	241	LYS
1	A	259	THR
1	B	58	PHE
1	B	59	ASP
1	B	132	LYS
1	B	259	THR
1	B	289	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	161	HIS
1	B	247	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ICB	A	401	-	13,13,13	1.24	1 (7%)	16,18,18	1.44	3 (18%)
2	ICB	B	401	-	13,13,13	1.24	1 (7%)	16,18,18	1.09	2 (12%)

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
2	ICB	A	401	-	-	4/4/4/4	0/2/2/2
2	ICB	B	401	-	-	4/4/4/4	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	ICB	C08-N09	-2.98	1.34	1.38
2	A	401	ICB	C08-N09	-2.83	1.34	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ICB	O12-C10-C08	3.09	120.93	114.27
2	A	401	ICB	C03-C04-C05	-2.70	119.68	122.13
2	B	401	ICB	O12-C10-C08	2.63	119.94	114.27
2	A	401	ICB	O12-C10-O11	-2.16	118.76	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	ICB	C03-C04-C05	-2.12	120.21	122.13

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ICB	C07-C08-C10-O11
2	A	401	ICB	N09-C08-C10-O11
2	A	401	ICB	C07-C08-C10-O12
2	A	401	ICB	N09-C08-C10-O12
2	B	401	ICB	C07-C08-C10-O11
2	B	401	ICB	N09-C08-C10-O11
2	B	401	ICB	C07-C08-C10-O12
2	B	401	ICB	N09-C08-C10-O12

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

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, 95th 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 ²)	Q < 0.9
1	A	231/277 (83%)	0.27	14 (6%)	27 23	15, 40, 89, 141	0
1	B	232/277 (83%)	1.80	93 (40%)	0 0	33, 75, 116, 145	0
All	All	463/554 (83%)	1.04	107 (23%)	2 1	15, 59, 105, 145	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	196	ASP	9.5
1	B	189	PHE	5.9
1	B	202	SER	5.4
1	B	193	ALA	5.3
1	B	164	VAL	5.2
1	A	58	PHE	5.1
1	B	192	LEU	5.0
1	B	203	LYS	4.8
1	B	223	PHE	4.8
1	B	60	MET	4.7
1	B	152	PHE	4.7
1	B	200	PRO	4.7
1	B	54	THR	4.7
1	B	197	THR	4.3
1	B	238	THR	4.3
1	B	153	VAL	4.2
1	A	258	VAL	4.1
1	B	227	ALA	4.1
1	B	217	ASN	4.1
1	B	244	PHE	4.0
1	B	58	PHE	4.0
1	B	241	LYS	4.0
1	B	294	LYS	3.9
1	B	219	MET	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	168	ASP	3.8
1	B	255	ASP	3.8
1	B	214	PHE	3.8
1	B	62	LYS	3.7
1	B	211	LEU	3.7
1	A	62	LYS	3.7
1	B	212	GLY	3.7
1	B	231	THR	3.7
1	B	157	ALA	3.6
1	B	145	ASN	3.5
1	B	235	TYR	3.5
1	B	161	HIS	3.4
1	B	246	TYR	3.4
1	B	172	ARG	3.4
1	B	252	ILE	3.4
1	B	78	LYS	3.4
1	B	256	SER	3.4
1	B	208	GLY	3.3
1	B	228	PHE	3.3
1	B	247	HIS	3.2
1	B	170	ALA	3.1
1	B	59	ASP	3.1
1	B	251	LEU	3.1
1	B	205	ALA	3.1
1	B	225	LYS	3.1
1	A	225	LYS	3.1
1	B	178	ASP	3.1
1	A	256	SER	3.1
1	B	155	GLN	3.0
1	B	182	LYS	3.0
1	B	194	ASN	3.0
1	B	144	TYR	3.0
1	B	198	ILE	2.9
1	B	297	ILE	2.9
1	A	76	LYS	2.8
1	B	243	GLU	2.8
1	B	165	LYS	2.8
1	A	54	THR	2.8
1	B	254	LYS	2.8
1	B	222	ASP	2.8
1	B	162	ILE	2.6
1	B	190	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	187	ALA	2.6
1	B	139	GLU	2.6
1	B	159	ALA	2.6
1	A	259	THR	2.5
1	B	75	GLU	2.5
1	B	163	LEU	2.5
1	B	184	LYS	2.5
1	B	262	TYR	2.5
1	B	249	ILE	2.5
1	A	241	LYS	2.5
1	B	218	GLN	2.5
1	A	154	LYS	2.4
1	B	76	LYS	2.4
1	B	171	LYS	2.4
1	B	239	PRO	2.4
1	B	210	ASP	2.4
1	B	240	VAL	2.4
1	B	183	ALA	2.4
1	A	246	TYR	2.3
1	B	179	LYS	2.3
1	B	80	ALA	2.3
1	B	160	ARG	2.3
1	A	216	LYS	2.2
1	B	149	ASP	2.2
1	B	234	ASP	2.2
1	A	257	PRO	2.2
1	B	204	ASN	2.2
1	B	185	LYS	2.2
1	B	201	ASN	2.2
1	B	259	THR	2.2
1	B	151	LEU	2.2
1	A	75	GLU	2.2
1	B	156	GLU	2.2
1	B	148	LYS	2.2
1	B	55	LYS	2.1
1	B	250	TYR	2.1
1	B	213	LYS	2.1
1	B	253	SER	2.1
1	B	260	TYR	2.1
1	B	237	LYS	2.0
1	B	199	ASP	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ICB	B	401	12/12	0.70	0.24	78,93,114,120	0
2	ICB	A	401	12/12	0.72	0.25	73,85,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.