



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2025 – 10:30 PM EDT

PDB ID : 1ONW  
Title : Crystal structure of Isoaspartyl Dipeptidase from E. coli  
Authors : Thoden, J.B.; Marti-Arbona, R.; Raushel, F.M.; Holden, H.M.  
Deposited on : 2003-03-02  
Resolution : 1.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

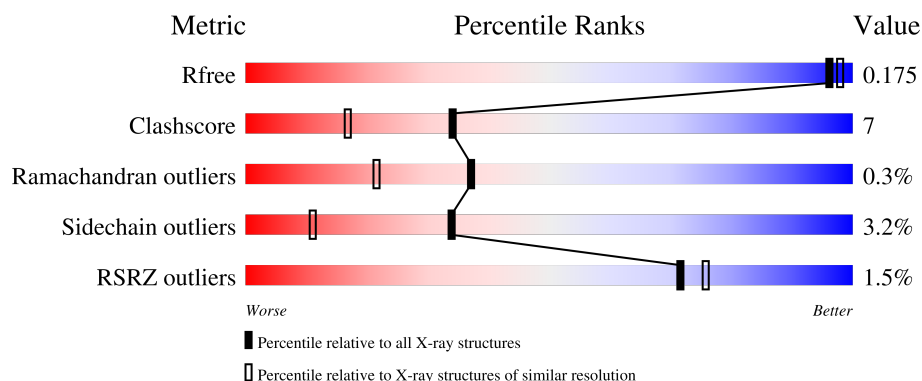
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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))
$R_{free}$	164625	2328 (1.66-1.66)
Clashscore	180529	2515 (1.66-1.66)
Ramachandran outliers	177936	2475 (1.66-1.66)
Sidechain outliers	177891	2475 (1.66-1.66)
RSRZ outliers	164620	2328 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	390	<div> <div> <div>0%</div> <div>71%</div> <div>23%</div> <div>• •</div> </div> </div>
1	B	390	<div> <div>2%</div> <div>75%</div> <div>20%</div> <div>• •</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6393 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 Isoaspartyl dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	5	0
			2795	1760	480	543	12			
1	B	380	Total	C	N	O	S	0	6	0
			2825	1778	483	552	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	KCX	LYS	modified residue	UNP P39377
B	162	KCX	LYS	modified residue	UNP P39377

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na	0	0
			1	1		

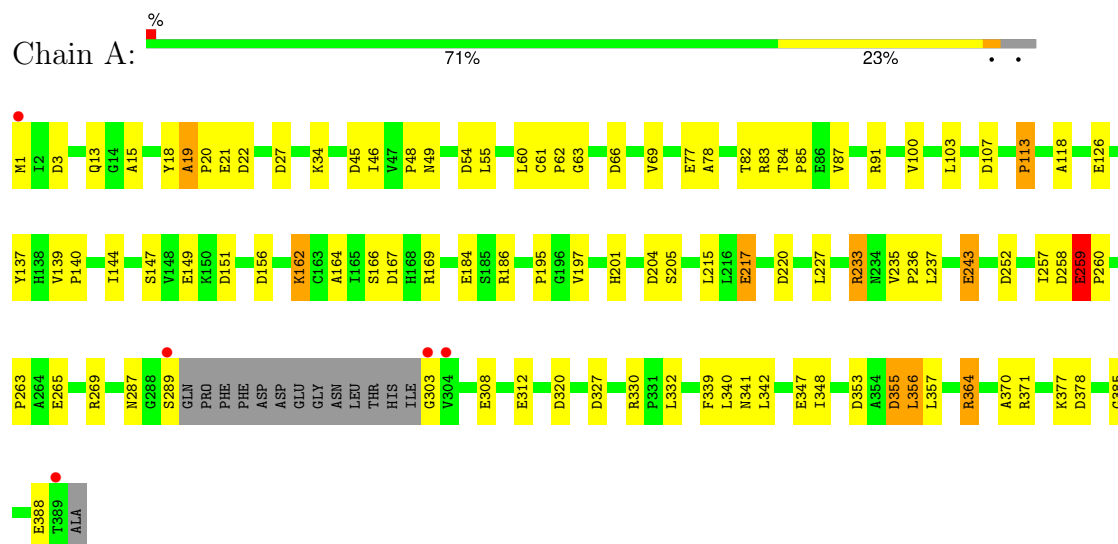
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	341	Total	O	0	1
			342	342		
7	B	409	Total	O	0	1
			410	410		

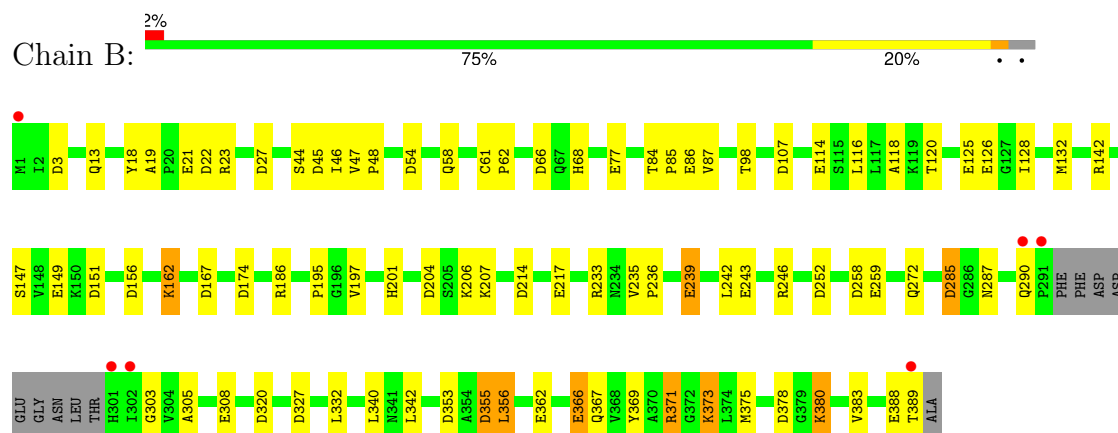
### 3 Residue-property plots [i](#)

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 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: Isoaspartyl dipeptidase



#### • Molecule 1: Isoaspartyl dipeptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.70Å 116.70Å 138.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.65 30.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-1.65) 98.0 (30.00-1.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.48 (at 1.63Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, $R_{free}$	0.178 , 0.219 0.176 , 0.175	Depositor DCC
$R_{free}$ test set	11327 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.5	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 94.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6393	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: KCX, CL, ZN, MG, NA, EDO

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	0.87	14/2847 (0.5%)	1.29	43/3871 (1.1%)
1	B	0.89	17/2882 (0.6%)	1.28	44/3920 (1.1%)
All	All	0.88	31/5729 (0.5%)	1.28	87/7791 (1.1%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	239[A]	GLU	CD-OE2	7.14	1.33	1.25
1	B	239[B]	GLU	CD-OE2	7.14	1.33	1.25
1	A	259	GLU	CD-OE2	6.51	1.32	1.25
1	A	184	GLU	CD-OE2	6.34	1.32	1.25
1	A	347	GLU	CD-OE2	6.18	1.32	1.25
1	B	388	GLU	CD-OE2	6.12	1.32	1.25
1	A	312	GLU	CD-OE2	6.09	1.32	1.25
1	B	308	GLU	CD-OE2	6.00	1.32	1.25
1	B	243	GLU	CD-OE2	5.94	1.32	1.25
1	B	259	GLU	CD-OE2	5.86	1.32	1.25
1	B	126[A]	GLU	CD-OE2	5.81	1.32	1.25
1	B	126[B]	GLU	CD-OE2	5.81	1.32	1.25
1	A	21	GLU	CD-OE2	5.81	1.32	1.25
1	A	388	GLU	CD-OE2	5.77	1.31	1.25
1	A	217	GLU	CD-OE2	5.75	1.31	1.25
1	B	21	GLU	CD-OE2	5.65	1.31	1.25
1	B	86	GLU	CD-OE2	5.63	1.31	1.25
1	A	126[A]	GLU	CD-OE2	5.62	1.31	1.25
1	A	126[B]	GLU	CD-OE2	5.62	1.31	1.25
1	B	362	GLU	CD-OE2	5.58	1.31	1.25
1	A	243	GLU	CD-OE2	5.56	1.31	1.25
1	A	77	GLU	CD-OE2	5.50	1.31	1.25
1	A	308	GLU	CD-OE2	5.47	1.31	1.25
1	B	366	GLU	CD-OE2	5.47	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	77	GLU	CD-OE2	5.47	1.31	1.25
1	A	265	GLU	CD-OE2	5.43	1.31	1.25
1	B	125	GLU	CD-OE2	5.26	1.31	1.25
1	B	114	GLU	CD-OE1	-5.24	1.19	1.25
1	B	217	GLU	CD-OE2	5.14	1.31	1.25
1	A	149	GLU	CD-OE1	-5.03	1.20	1.25
1	B	149	GLU	CD-OE2	5.00	1.31	1.25

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	ASP	CB-CG-OD2	-8.55	110.60	118.30
1	A	167	ASP	CB-CG-OD2	-8.05	111.05	118.30
1	A	167	ASP	CB-CG-OD1	8.01	125.51	118.30
1	B	214	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	B	252	ASP	CB-CG-OD1	7.76	125.29	118.30
1	A	252	ASP	CB-CG-OD1	7.60	125.14	118.30
1	B	327	ASP	CB-CG-OD2	-7.53	111.53	118.30
1	A	204	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	B	371	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	107	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	A	107	ASP	CB-CG-OD1	7.19	124.77	118.30
1	B	27	ASP	CB-CG-OD2	-7.16	111.85	118.30
1	B	156	ASP	CB-CG-OD1	7.05	124.64	118.30
1	B	355	ASP	CB-CG-OD1	7.05	124.64	118.30
1	B	214	ASP	CB-CG-OD1	7.04	124.64	118.30
1	A	320	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	B	327	ASP	CB-CG-OD1	6.84	124.46	118.30
1	A	151	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	B	107	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	A	204	ASP	CB-CG-OD1	6.74	124.36	118.30
1	A	330	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	258	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	A	156	ASP	CB-CG-OD1	6.66	124.29	118.30
1	B	378	ASP	CB-CG-OD1	6.64	124.28	118.30
1	B	320	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	151	ASP	CB-CG-OD1	6.59	124.23	118.30
1	B	142	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	B	258	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	A	233	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	B	167	ASP	CB-CG-OD1	6.45	124.10	118.30
1	B	353	ASP	CB-CG-OD2	-6.43	112.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ASP	CB-CG-OD1	6.42	124.08	118.30
1	A	320	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	233	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	378	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	22	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	54	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	B	204	ASP	CB-CG-OD1	6.36	124.03	118.30
1	A	364[A]	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	364[B]	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	22	ASP	CB-CG-OD1	6.35	124.02	118.30
1	B	156	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	B	285	ASP	CB-CG-OD1	6.34	124.01	118.30
1	A	327	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	B	285	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	B	54	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	B	22	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	A	220	ASP	CB-CG-OD1	6.28	123.95	118.30
1	B	204	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	A	233	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	45	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	B	107	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	45	ASP	CB-CG-OD1	6.06	123.75	118.30
1	B	98	THR	CA-CB-CG2	-6.05	103.92	112.40
1	B	66	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	B	151	ASP	CB-CG-OD1	5.98	123.69	118.30
1	A	27	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	A	45	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	B	23	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	320	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	A	355	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	B	233	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	A	353	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	220	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	83	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	378	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	269	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	27	ASP	CB-CG-OD1	5.84	123.56	118.30
1	B	3	ASP	CB-CG-OD1	5.83	123.54	118.30
1	A	330	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	327	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	167	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	A	19	ALA	N-CA-C	5.72	126.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	ASP	CB-CG-OD1	5.67	123.41	118.30
1	A	3	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	353	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	B	151	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	B	22	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	169	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	54	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	66	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	B	355	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	3	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	B	66	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	174	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	174	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	353	ASP	CB-CG-OD1	5.05	122.85	118.30

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	2795	0	2833	54	0
1	B	2825	0	2853	33	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	2	0	0	1	0
3	B	1	0	0	0	0
4	A	8	0	12	3	0
4	B	4	0	6	2	0
5	B	1	0	0	0	0
6	B	1	0	0	0	0
7	A	342	0	0	7	0
7	B	410	0	0	4	0
All	All	6393	0	5704	85	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 7.

All (85) 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:A:289:SER:HA	1:A:303:GLY:O	1.83	0.79
1:A:341:ASN:HB2	7:A:1140:HOH:O	1.87	0.75
1:B:342:LEU:HD23	4:B:807:EDO:H12	1.73	0.71
1:B:116:LEU:O	1:B:120[B]:THR:HG23	1.93	0.69
1:A:84:THR:HB	1:A:85:PRO:HD2	1.78	0.65
1:A:235:VAL:HB	1:A:236:PRO:HD3	1.79	0.65
1:B:342:LEU:CD2	4:B:807:EDO:H12	2.29	0.62
1:A:364[B]:ARG:NH1	7:A:891:HOH:O	2.33	0.62
1:A:259:GLU:HG2	1:A:260:PRO:HA	1.82	0.61
1:A:46:ILE:HG13	1:B:48:PRO:HG3	1.83	0.61
1:A:364[A]:ARG:NH1	7:A:987:HOH:O	2.33	0.61
1:A:364[B]:ARG:HB3	7:A:1130:HOH:O	2.01	0.61
1:A:259:GLU:HG2	1:A:260:PRO:CA	2.30	0.61
4:A:804:EDO:H21	1:B:118:ALA:HA	1.83	0.60
1:A:364[A]:ARG:HB3	7:A:1130:HOH:O	2.02	0.60
1:B:355:ASP:C	1:B:356:LEU:HG	2.20	0.59
1:B:239[A]:GLU:OE2	7:B:944:HOH:O	2.16	0.59
1:A:87[B]:VAL:HG22	1:A:287:ASN:CG	2.22	0.59
1:A:69:VAL:HG21	1:A:100[A]:VAL:HG23	1.85	0.57
1:A:85:PRO:O	1:A:287:ASN:ND2	2.31	0.57
1:B:58:GLN:NE2	1:B:366:GLU:OE1	2.40	0.55
1:B:13:GLN:NE2	7:B:1121:HOH:O	2.40	0.54
1:B:235:VAL:HB	1:B:236:PRO:HD3	1.90	0.54
1:B:195:PRO:HB2	1:B:197:VAL:HG13	1.90	0.54
1:B:290:GLN:NE2	1:B:305:ALA:HA	2.22	0.54
1:A:259:GLU:HG2	1:A:260:PRO:N	2.23	0.54
1:B:84:THR:HB	1:B:85:PRO:HD2	1.89	0.54
1:B:373:LYS:HD2	1:B:375:MET:SD	2.48	0.53
1:B:87[A]:VAL:HG23	1:B:287:ASN:ND2	2.23	0.52
1:A:69:VAL:HG21	1:A:100[A]:VAL:CG2	2.40	0.52
1:A:78:ALA:HB3	1:A:82:THR:HG21	1.92	0.52
1:A:48:PRO:HG3	1:B:46:ILE:HG13	1.92	0.51
1:A:243:GLU:HB3	7:A:1108:HOH:O	2.11	0.50
1:B:373:LYS:HD3	1:B:383:VAL:HG21	1.93	0.49
1:A:233:ARG:HG2	1:A:237:LEU:HD23	1.94	0.49
1:B:87[A]:VAL:HG23	1:B:287:ASN:CG	2.33	0.49
1:A:113:PRO:HB2	1:A:144:ILE:CG1	2.43	0.48
1:B:340:LEU:HB2	1:B:342:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:PRO:HB2	1:A:197:VAL:HG13	1.96	0.48
1:A:15:ALA:HB2	1:A:55:LEU:HB3	1.95	0.48
1:A:15:ALA:HB2	1:A:55:LEU:CB	2.44	0.48
1:A:69:VAL:CG2	1:A:100[A]:VAL:HG23	2.44	0.47
1:A:340:LEU:HB2	1:A:342:LEU:HG	1.96	0.47
1:A:162:KCX:OQ1	1:A:201:HIS:HB2	2.15	0.47
1:B:128:ILE:O	1:B:371:ARG:NH1	2.46	0.47
1:B:380:LYS:HB2	1:B:380:LYS:HE2	1.58	0.47
1:A:63:GLY:HA2	1:A:357:LEU:HG	1.97	0.47
1:A:215:LEU:C	1:A:215:LEU:HD23	2.36	0.46
1:A:257:ILE:O	1:A:263:PRO:HD3	2.15	0.46
1:B:18:TYR:O	1:B:62:PRO:HD3	2.16	0.46
1:A:355:ASP:C	1:A:356:LEU:HG	2.36	0.46
1:A:370:ALA:O	1:A:371:ARG:C	2.54	0.45
1:A:61:CYS:HB2	1:A:62:PRO:CD	2.47	0.45
1:A:18:TYR:O	1:A:62:PRO:HD3	2.17	0.45
1:B:290:GLN:O	1:B:303:GLY:N	2.40	0.45
1:A:34:LYS:HB3	7:B:1028:HOH:O	2.18	0.44
1:A:60:LEU:HD12	1:A:357:LEU:O	2.18	0.44
1:A:91:ARG:HD3	1:A:91:ARG:HA	1.80	0.44
1:A:166:SER:HB3	1:A:205:SER:HB3	2.00	0.44
1:A:87[B]:VAL:HG22	1:A:287:ASN:CB	2.47	0.43
1:A:61:CYS:HB2	1:A:62:PRO:HD2	2.00	0.43
1:A:118:ALA:HA	4:A:805:EDO:H12	1.99	0.43
1:A:139:VAL:HA	1:A:140:PRO:C	2.38	0.43
1:B:61:CYS:HB2	1:B:62:PRO:CD	2.49	0.43
1:A:87[B]:VAL:HG22	1:A:287:ASN:HB2	2.01	0.43
1:A:20:PRO:HG2	7:A:1054:HOH:O	2.19	0.43
1:A:385:GLY:HA3	3:A:802:CL:CL	2.56	0.42
1:B:162:KCX:OQ1	1:B:201:HIS:HB2	2.19	0.42
1:A:137:TYR:CG	1:A:164:ALA:HB2	2.54	0.42
1:A:340:LEU:O	1:A:341:ASN:C	2.57	0.42
1:A:48:PRO:O	1:A:49:ASN:C	2.57	0.42
1:B:242:LEU:O	1:B:246:ARG:HG3	2.20	0.42
1:A:332:LEU:HA	1:A:332:LEU:HD23	1.83	0.42
1:A:84:THR:HB	1:A:85:PRO:CD	2.50	0.42
1:A:69:VAL:CG2	1:A:100[A]:VAL:CG2	2.98	0.41
1:A:118:ALA:HA	4:A:805:EDO:C1	2.51	0.41
1:B:367:GLN:NE2	1:B:369:TYR:OH	2.54	0.41
1:B:46:ILE:HD12	1:B:46:ILE:HA	1.67	0.41
1:A:61:CYS:C	1:A:348:ILE:HD11	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:VAL:HB	1:B:48:PRO:HD2	2.04	0.40
1:B:272:GLN:NE2	7:B:924:HOH:O	2.40	0.40
1:B:68:HIS:CD2	1:B:285:ASP:HA	2.57	0.40
1:B:332:LEU:HA	1:B:332:LEU:HD23	1.83	0.40
1:A:227:LEU:HB2	1:A:339:PHE:CZ	2.57	0.40
1:B:120[B]:THR:HG21	1:B:132:MET:HB3	2.04	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	376/390 (96%)	366 (97%)	9 (2%)	1 (0%)	37	21
1	B	381/390 (98%)	373 (98%)	7 (2%)	1 (0%)	37	21
All	All	757/780 (97%)	739 (98%)	16 (2%)	2 (0%)	37	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	ALA
1	A	19	ALA

### 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	305/312 (98%)	295 (97%)	10 (3%)	33	10
1	B	309/312 (99%)	300 (97%)	9 (3%)	37	14
All	All	614/624 (98%)	595 (97%)	19 (3%)	34	12

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	13	GLN
1	A	103	LEU
1	A	113	PRO
1	A	147	SER
1	A	186	ARG
1	A	217	GLU
1	A	259	GLU
1	A	356	LEU
1	A	377	LYS
1	B	44	SER
1	B	147	SER
1	B	186	ARG
1	B	206	LYS
1	B	207	LYS
1	B	356	LEU
1	B	373	LYS
1	B	380	LYS
1	B	389	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	168	HIS
1	A	367	GLN
1	B	168	HIS
1	B	272	GLN
1	B	290	GLN
1	B	367	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	KCX	A	162	1,2	10,11,12	1.84	1 (10%)	6,12,14	3.39	1 (16%)
1	KCX	B	162	1,2	10,11,12	2.12	1 (10%)	6,12,14	2.32	1 (16%)

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
1	KCX	A	162	1,2	-	0/9/10/12	-
1	KCX	B	162	1,2	-	1/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	KCX	CX-NZ	6.35	1.46	1.35
1	A	162	KCX	CX-NZ	5.47	1.44	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	KCX	CE-NZ-CX	-8.11	108.22	121.98
1	B	162	KCX	CE-NZ-CX	-5.46	112.71	121.98

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	162	KCX	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	162	KCX	1	0
1	B	162	KCX	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	$\# Z  > 2$
4	EDO	B	807	-	3,3,3	0.34	0	2,2,2	0.13	0
4	EDO	A	805	-	3,3,3	0.42	0	2,2,2	0.33	0
4	EDO	A	804	-	3,3,3	0.43	0	2,2,2	0.22	0

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
4	EDO	B	807	-	-	1/1/1/1	-
4	EDO	A	805	-	-	1/1/1/1	-
4	EDO	A	804	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	804	EDO	O1-C1-C2-O2
4	B	807	EDO	O1-C1-C2-O2
4	A	805	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	807	EDO	2	0
4	A	805	EDO	2	0
4	A	804	EDO	1	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

### 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	375/390 (96%)	-0.53	5 (1%) 74 79	10, 21, 48, 91	5 (1%)
1	B	379/390 (97%)	-0.66	6 (1%) 70 74	10, 19, 44, 95	6 (1%)
All	All	754/780 (96%)	-0.60	11 (1%) 71 76	10, 20, 46, 95	11 (1%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	SER	6.7
1	A	303	GLY	4.8
1	B	302	ILE	4.8
1	B	389	THR	4.8
1	A	304	VAL	4.3
1	A	389	THR	3.7
1	B	301	HIS	3.6
1	B	291	PRO	3.0
1	B	1	MET	2.4
1	B	290	GLN	2.2
1	A	1	MET	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	KCX	A	162	12/13	0.98	0.06	12,15,25,36	0
1	KCX	B	162	12/13	0.99	0.04	11,15,25,29	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	A	805	4/4	0.92	0.13	15,29,30,30	0
4	EDO	A	804	4/4	0.95	0.10	19,25,29,38	0
4	EDO	B	807	4/4	0.95	0.11	28,29,32,69	0
5	MG	B	804	1/1	0.97	0.06	29,29,29,29	1
6	NA	B	805	1/1	0.97	0.06	36,36,36,36	0
3	CL	A	803	1/1	0.98	0.07	27,27,27,27	0
2	ZN	A	801	1/1	0.99	0.04	31,31,31,31	0
3	CL	A	802	1/1	0.99	0.04	24,24,24,24	0
2	ZN	A	800	1/1	1.00	0.04	29,29,29,29	0
2	ZN	B	802	1/1	1.00	0.02	25,25,25,25	0
3	CL	B	806	1/1	1.00	0.03	24,24,24,24	0
2	ZN	B	803	1/1	1.00	0.04	28,28,28,28	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.