



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:21 AM UTC

PDB ID : 4COG / pdb_00004cog
Title : Crystal structure of kynurenine formamidase from Burkholderia cenocepacia
Authors : Diaz-Saez, L.; Srikannathasan, V.; Zoltner, M.; Hunter, W.N.
Deposited on : 2014-01-28
Resolution : 1.60 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

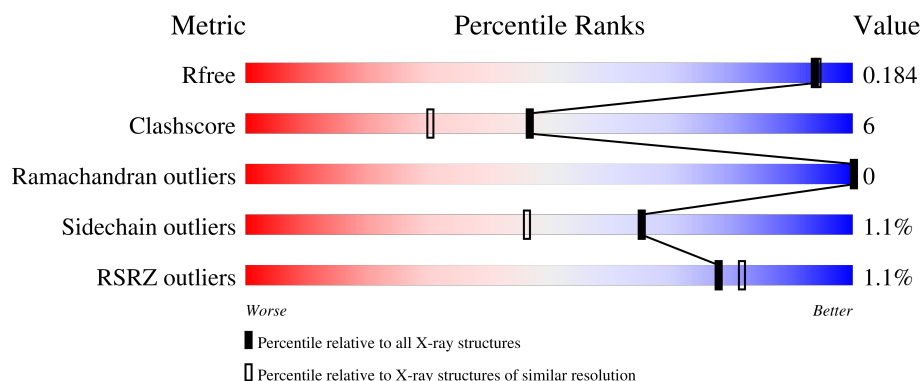
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	215	% 81% 14% . .
1	B	215	% 87% 9% .
1	C	215	86% 9% . .
1	D	215	% 85% 11% .

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
4	MG	D	1210	-	-	X	-
7	PEG	C	1215	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7700 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 KYNURENINE FORMAMIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	19	0
			1638	1050	290	289	9			
1	B	207	Total	C	N	O	S	0	13	0
			1617	1035	286	287	9			
1	C	207	Total	C	N	O	S	0	15	0
			1624	1039	285	291	9			
1	D	207	Total	C	N	O	S	0	14	0
			1622	1039	286	288	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP B4E9I9
A	0	HIS	-	expression tag	UNP B4E9I9
B	-1	GLY	-	expression tag	UNP B4E9I9
B	0	HIS	-	expression tag	UNP B4E9I9
C	-1	GLY	-	expression tag	UNP B4E9I9
C	0	HIS	-	expression tag	UNP B4E9I9
D	-1	GLY	-	expression tag	UNP B4E9I9
D	0	HIS	-	expression tag	UNP B4E9I9

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

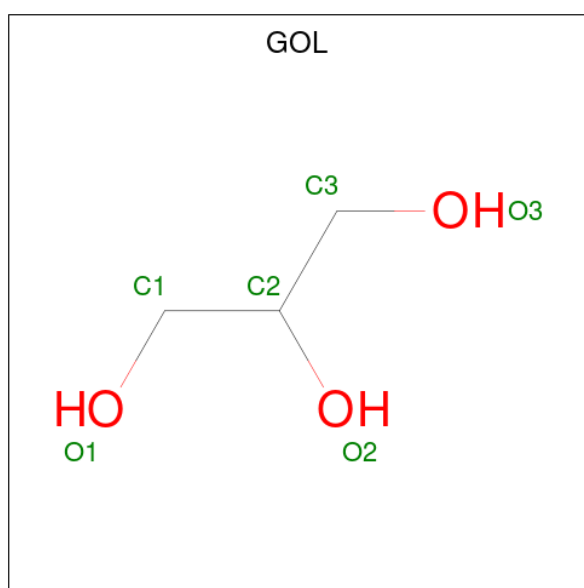
- Molecule 3 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	D	2	Total	Mg	0	0
			2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



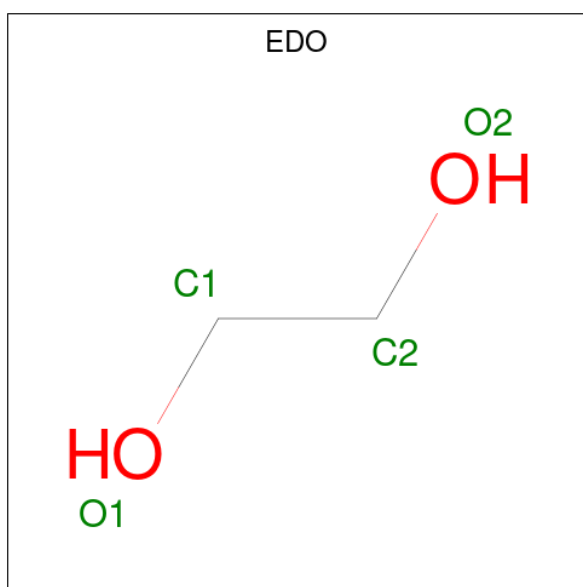
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

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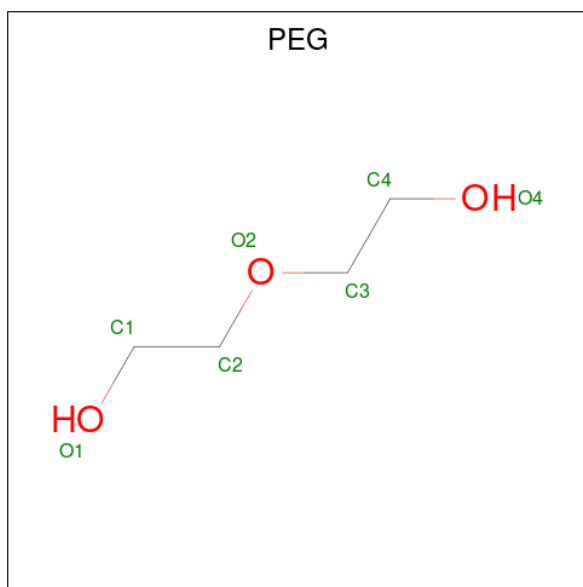
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 7 4 3	0	0

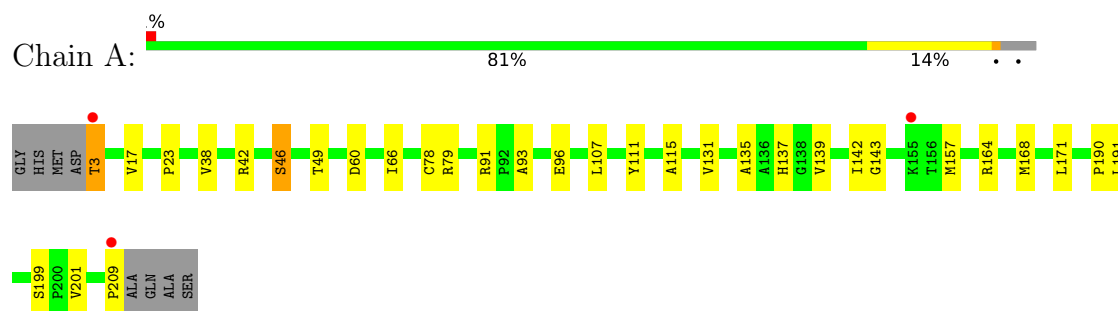
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	281	Total 281	O 281	0	0
8	B	268	Total 268	O 268	0	0
8	C	280	Total 280	O 280	0	0
8	D	239	Total 239	O 239	0	0

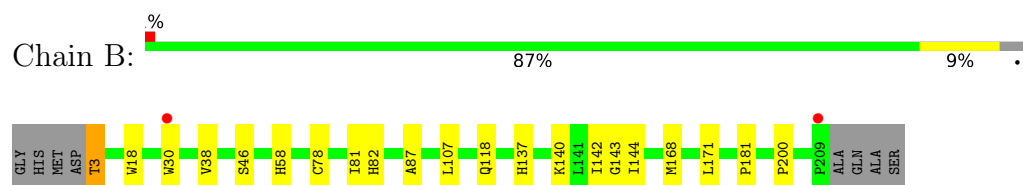
3 Residue-property plots [i](#)

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.

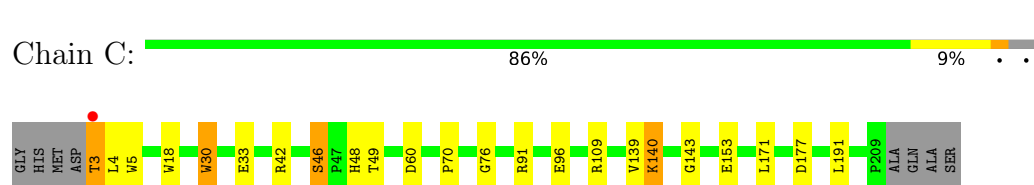
- Molecule 1: KYNURENINE FORMAMIDASE



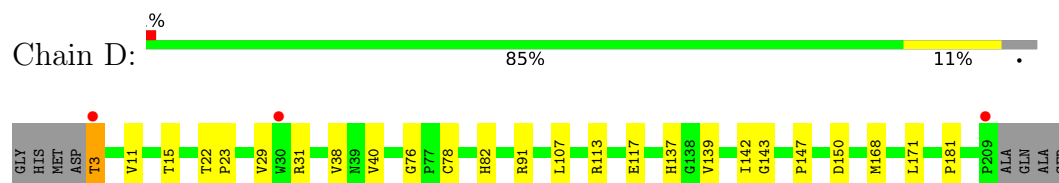
- Molecule 1: KYNURENINE FORMAMIDASE



- Molecule 1: KYNURENINE FORMAMIDASE



- Molecule 1: KYNURENINE FORMAMIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.86Å 50.12Å 135.20Å 90.00° 94.15° 90.00°	Depositor
Resolution (Å)	134.84 – 1.60 134.84 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (134.84-1.60) 99.2 (134.84-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.149 , 0.184 0.148 , 0.184	Depositor DCC
R_{free} test set	6778 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7700	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.72% 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: GOL, MG, CD, ZN, EDO, PEG

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	1.57	10/1757 (0.6%)	1.36	4/2417 (0.2%)
1	B	1.46	5/1715 (0.3%)	1.33	4/2360 (0.2%)
1	C	1.53	6/1730 (0.3%)	1.37	10/2382 (0.4%)
1	D	1.46	6/1724 (0.3%)	1.32	3/2372 (0.1%)
All	All	1.51	27/6926 (0.4%)	1.34	21/9531 (0.2%)

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	1	0

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	VAL	N-CA	7.26	1.54	1.46
1	D	38	VAL	N-CA	7.22	1.54	1.46
1	A	164[A]	ARG	N-CA	6.76	1.54	1.46
1	A	164[B]	ARG	N-CA	6.76	1.54	1.46
1	B	87	ALA	N-CA	6.52	1.55	1.46
1	C	139	VAL	N-CA	6.23	1.53	1.46
1	D	76	GLY	N-CA	6.11	1.53	1.44
1	A	79	ARG	N-CA	5.94	1.53	1.46
1	D	11	VAL	C-O	5.90	1.30	1.24
1	D	147	PRO	CA-CB	5.83	1.62	1.53
1	D	150	ASP	N-CA	5.83	1.52	1.45
1	A	66	ILE	N-CA	5.75	1.53	1.46
1	C	33	GLU	N-CA	5.60	1.53	1.46
1	B	38	VAL	N-CA	5.58	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	48	HIS	C-O	5.57	1.31	1.24
1	C	109	ARG	CD-NE	5.49	1.53	1.46
1	B	18	TRP	CA-CB	-5.43	1.45	1.53
1	A	38	VAL	N-CA	5.32	1.52	1.46
1	A	135	ALA	N-CA	5.29	1.52	1.46
1	A	199	SER	CA-C	5.24	1.57	1.52
1	B	144	ILE	C-O	5.23	1.29	1.23
1	B	81	ILE	N-CA	5.21	1.52	1.46
1	D	139	VAL	N-CA	5.18	1.52	1.46
1	C	4	LEU	N-CA	5.16	1.52	1.46
1	A	131	VAL	N-CA	5.12	1.52	1.46
1	C	76	GLY	N-CA	5.11	1.51	1.44
1	A	157	MET	N-CA	5.04	1.53	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	SER	CA-C-N	-10.01	110.62	120.83
1	C	46	SER	C-N-CA	-10.01	110.62	120.83
1	A	46	SER	CA-C-N	-8.47	111.05	120.45
1	A	46	SER	C-N-CA	-8.47	111.05	120.45
1	D	3	THR	N-CA-CB	7.05	123.49	111.50
1	B	3	THR	N-CA-CB	6.96	123.33	111.50
1	C	177	ASP	CA-C-N	-6.00	113.08	122.73
1	C	177	ASP	C-N-CA	-6.00	113.08	122.73
1	A	3	THR	CA-CB-CG2	5.84	120.43	110.50
1	B	3	THR	CA-CB-CG2	5.84	120.43	110.50
1	D	3	THR	CA-CB-CG2	5.82	120.40	110.50
1	A	3	THR	N-CA-CB	5.74	121.25	111.50
1	C	30[B]	TRP	CB-CA-C	-5.62	100.59	109.80
1	C	30[C]	TRP	CB-CA-C	-5.62	100.59	109.80
1	C	3	THR	N-CA-CB	5.52	120.88	111.50
1	C	3	THR	CA-CB-CG2	5.37	119.63	110.50
1	D	23	PRO	CB-CA-C	-5.24	104.09	110.95
1	B	46	SER	CA-C-N	-5.16	114.72	120.45
1	B	46	SER	C-N-CA	-5.16	114.72	120.45
1	C	191	LEU	CB-CG-CD2	-5.09	95.42	110.70
1	C	70	PRO	CB-CA-C	-5.05	104.95	111.46

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	3	THR	CA

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	1638	0	1672	21	0
1	B	1617	0	1629	14	0
1	C	1624	0	1634	17	0
1	D	1622	0	1636	13	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	2	0	0	2	0
4	B	2	0	0	2	0
4	C	2	0	0	2	0
4	D	2	0	0	3	0
5	A	18	0	22	0	0
5	B	18	0	22	1	0
5	C	18	0	22	5	0
5	D	18	0	22	2	0
6	A	12	0	18	4	0
6	B	12	0	18	1	0
6	D	12	0	18	3	0
7	C	7	0	10	4	0
8	A	281	0	0	13	0
8	B	268	0	0	7	0
8	C	280	0	0	11	0
8	D	239	0	0	6	1
All	All	7700	0	6723	76	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 6.

All (76) 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)
4:D:1211:MG:MG	8:D:2181:HOH:O	0.85	1.17
4:B:1211:MG:MG	8:B:2206:HOH:O	0.89	1.16
5:C:1214:GOL:H12	8:C:2186:HOH:O	1.47	1.12
4:D:1210:MG:MG	8:D:2083:HOH:O	0.98	1.06
4:C:1211:MG:MG	8:C:2116:HOH:O	0.95	1.06
4:B:1210:MG:MG	8:B:2107:HOH:O	1.01	1.04
4:A:1211:MG:MG	8:A:2131:HOH:O	1.05	0.95
4:A:1210:MG:MG	8:A:2225:HOH:O	1.13	0.92
8:A:2010:HOH:O	1:B:30[C]:TRP:CH2	2.22	0.90
1:C:5:TRP:HE1	7:C:1215:PEG:H31	1.38	0.87
8:A:2010:HOH:O	1:B:30[C]:TRP:CZ3	2.32	0.80
1:D:137:HIS:NE2	8:D:2181:HOH:O	2.17	0.76
1:C:49[B]:THR:HG23	8:C:2051:HOH:O	1.84	0.76
1:C:5:TRP:HE1	7:C:1215:PEG:C3	1.99	0.76
6:D:1216:EDO:H12	8:D:2019:HOH:O	1.85	0.76
1:C:60:ASP:OD1	8:C:2116:HOH:O	2.03	0.74
1:C:91[B]:ARG:NH2	8:C:2158:HOH:O	2.21	0.74
1:A:137:HIS:NE2	8:A:2225:HOH:O	2.20	0.74
1:B:137:HIS:NE2	8:B:2206:HOH:O	2.19	0.74
6:A:1217:EDO:O2	8:A:2278:HOH:O	2.08	0.72
6:A:1217:EDO:H21	8:A:2192:HOH:O	1.89	0.71
1:C:5:TRP:NE1	7:C:1215:PEG:H31	2.04	0.71
4:C:1210:MG:MG	8:C:2216:HOH:O	1.35	0.69
4:D:1210:MG:MG	8:D:2082:HOH:O	1.36	0.68
1:D:15:THR:OG1	6:D:1216:EDO:H22	1.95	0.67
1:A:60:ASP:OD1	8:A:2131:HOH:O	2.13	0.66
1:D:91[B]:ARG:NE	8:D:2124:HOH:O	2.29	0.65
1:A:42[B]:ARG:CZ	8:A:2107:HOH:O	2.45	0.63
1:A:91[B]:ARG:NH1	8:A:2176:HOH:O	2.32	0.62
5:C:1212:GOL:H2	1:D:40:VAL:HG21	1.86	0.57
1:A:17[B]:VAL:HG12	1:A:49[B]:THR:CG2	2.35	0.56
1:D:82:HIS:CE1	1:D:181:PRO:HD3	2.41	0.56
1:C:30[B]:TRP:HZ3	5:D:1212:GOL:H11	1.71	0.56
1:B:58:HIS:NE2	5:B:1213:GOL:O1	2.32	0.56
1:D:113:ARG:O	6:D:1217:EDO:H12	2.05	0.56
1:A:191[A]:LEU:HD23	1:B:200:PRO:HB2	1.89	0.54
1:B:82:HIS:CE1	1:B:181:PRO:HD3	2.43	0.54
1:A:78[B]:CYS:SG	1:A:107:LEU:HG	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:2083:HOH:O	1:D:29:VAL:HG11	2.07	0.54
1:C:46:SER:O	1:C:49[B]:THR:OG1	2.26	0.53
1:B:78[B]:CYS:SG	1:B:107:LEU:HG	2.50	0.52
1:B:143:GLY:HA2	1:B:171:LEU:O	2.10	0.52
1:D:143:GLY:HA2	1:D:171:LEU:O	2.10	0.52
1:A:17[B]:VAL:HG12	1:A:49[B]:THR:HG21	1.93	0.51
1:A:111:TYR:HA	6:A:1217:EDO:H11	1.92	0.51
5:C:1214:GOL:C1	8:C:2186:HOH:O	2.24	0.50
1:C:140[A]:LYS:HG2	8:C:2222:HOH:O	2.12	0.50
1:A:23:PRO:HG2	1:D:31[B]:ARG:HH12	1.77	0.50
1:C:153[B]:GLU:HG3	8:C:2232:HOH:O	2.11	0.49
1:C:30[B]:TRP:HZ3	5:D:1212:GOL:C1	2.24	0.49
1:B:118[B]:GLN:HG3	8:B:2183:HOH:O	2.13	0.49
1:A:46:SER:HB3	1:A:49[B]:THR:HG23	1.96	0.48
1:C:143:GLY:HA2	1:C:171:LEU:O	2.13	0.48
1:D:78[B]:CYS:SG	1:D:107:LEU:HG	2.53	0.48
1:A:191[A]:LEU:CD2	1:B:200:PRO:HB2	2.44	0.47
1:A:143:GLY:HA2	1:A:171:LEU:O	2.14	0.47
8:A:2010:HOH:O	1:B:30[C]:TRP:HH2	1.75	0.46
1:C:5:TRP:HE1	7:C:1215:PEG:C4	2.29	0.46
1:A:115:ALA:HB2	6:A:1215:EDO:H11	1.98	0.45
1:C:18:TRP:CG	5:C:1212:GOL:H11	2.52	0.45
1:B:140[B]:LYS:HD3	1:B:168:MET:HA	2.00	0.44
1:A:23:PRO:CG	1:D:31[B]:ARG:HH12	2.30	0.44
6:B:1217:EDO:C2	8:B:2141:HOH:O	2.65	0.44
1:C:42[A]:ARG:HG3	1:D:22:THR:HG21	1.99	0.43
5:C:1214:GOL:C2	8:C:2186:HOH:O	2.58	0.43
1:C:96[B]:GLU:HG3	8:C:2163:HOH:O	2.19	0.43
1:D:142[B]:ILE:HD11	1:D:168:MET:HE1	2.01	0.42
1:A:142[B]:ILE:HD11	1:A:168:MET:HE1	2.02	0.42
1:B:140[A]:LYS:HD2	8:B:2211:HOH:O	2.20	0.41
1:A:93:ALA:HA	1:A:96[A]:GLU:CD	2.46	0.41
1:A:190:PRO:HA	1:A:201:VAL:HG12	2.02	0.41
1:A:209:PRO:HD3	8:A:2147:HOH:O	2.20	0.41
1:A:17[B]:VAL:HG12	1:A:49[B]:THR:HG22	2.02	0.41
1:A:209:PRO:CD	8:A:2147:HOH:O	2.69	0.41
1:C:91[A]:ARG:HE	1:C:91[A]:ARG:HB2	1.63	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)
8:D:2113:HOH:O	8:D:2182:HOH:O[2_647]	1.67	0.53

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	224/215 (104%)	215 (96%)	9 (4%)	0	100	100
1	B	218/215 (101%)	210 (96%)	8 (4%)	0	100	100
1	C	220/215 (102%)	210 (96%)	10 (4%)	0	100	100
1	D	219/215 (102%)	210 (96%)	9 (4%)	0	100	100
All	All	881/860 (102%)	845 (96%)	36 (4%)	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	185/171 (108%)	184 (100%)	1 (0%)	81	70
1	B	179/171 (105%)	176 (98%)	3 (2%)	53	30
1	C	181/171 (106%)	178 (98%)	3 (2%)	53	30
1	D	180/171 (105%)	178 (99%)	2 (1%)	65	46
All	All	725/684 (106%)	716 (99%)	9 (1%)	65	43

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	B	3	THR
1	B	142[A]	ILE
1	B	142[B]	ILE
1	C	3	THR
1	C	140[A]	LYS
1	C	140[B]	LYS
1	D	3	THR
1	D	117	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	122	ASN
1	D	122	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 16 are monoatomic - leaving 22 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
5	GOL	B	1212	-	5,5,5	0.57	0	5,5,5	1.38	1 (20%)
5	GOL	C	1213	3,2	5,5,5	1.26	0	5,5,5	0.87	0
7	PEG	C	1215	-	6,6,6	0.37	0	5,5,5	1.19	0
5	GOL	B	1213	3,2	5,5,5	1.08	0	5,5,5	1.30	1 (20%)
6	EDO	D	1217	-	3,3,3	0.33	0	2,2,2	1.08	0
5	GOL	C	1214	-	5,5,5	0.84	0	5,5,5	1.72	1 (20%)
6	EDO	A	1217	-	3,3,3	0.67	0	2,2,2	1.17	0
6	EDO	D	1216	-	3,3,3	0.62	0	2,2,2	0.71	0
5	GOL	D	1214	3,2	5,5,5	0.80	0	5,5,5	0.75	0
6	EDO	B	1217	-	3,3,3	0.42	0	2,2,2	2.20	1 (50%)
6	EDO	D	1215	-	3,3,3	0.35	0	2,2,2	0.46	0
6	EDO	A	1216	-	3,3,3	0.19	0	2,2,2	0.75	0
6	EDO	B	1216	-	3,3,3	0.73	0	2,2,2	0.50	0
5	GOL	B	1214	-	5,5,5	1.03	0	5,5,5	1.47	1 (20%)
5	GOL	A	1213	3,2	5,5,5	0.69	0	5,5,5	0.95	0
5	GOL	A	1214	-	5,5,5	1.28	0	5,5,5	2.00	1 (20%)
5	GOL	D	1212	-	5,5,5	0.40	0	5,5,5	1.15	0
6	EDO	A	1215	-	3,3,3	0.43	0	2,2,2	0.39	0
5	GOL	D	1213	-	5,5,5	1.25	0	5,5,5	1.81	2 (40%)
5	GOL	A	1212	-	5,5,5	0.25	0	5,5,5	1.22	1 (20%)
6	EDO	B	1215	-	3,3,3	0.36	0	2,2,2	0.90	0
5	GOL	C	1212	-	5,5,5	0.38	0	5,5,5	0.86	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
5	GOL	B	1212	-	-	0/4/4/4	-
5	GOL	C	1213	3,2	-	0/4/4/4	-
7	PEG	C	1215	-	-	3/4/4/4	-
5	GOL	B	1213	3,2	-	0/4/4/4	-
6	EDO	D	1217	-	-	1/1/1/1	-
5	GOL	C	1214	-	-	0/4/4/4	-
6	EDO	A	1217	-	-	1/1/1/1	-
6	EDO	D	1216	-	-	0/1/1/1	-
5	GOL	D	1214	3,2	-	0/4/4/4	-
6	EDO	B	1217	-	-	1/1/1/1	-
6	EDO	D	1215	-	-	0/1/1/1	-
6	EDO	A	1216	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	1216	-	-	1/1/1/1	-
5	GOL	B	1214	-	-	2/4/4/4	-
5	GOL	A	1213	3,2	-	0/4/4/4	-
5	GOL	A	1214	-	-	2/4/4/4	-
5	GOL	D	1212	-	-	0/4/4/4	-
6	EDO	A	1215	-	-	1/1/1/1	-
5	GOL	D	1213	-	-	2/4/4/4	-
5	GOL	A	1212	-	-	0/4/4/4	-
6	EDO	B	1215	-	-	1/1/1/1	-
5	GOL	C	1212	-	-	4/4/4/4	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1214	GOL	O3-C3-C2	3.98	128.31	110.38
6	B	1217	EDO	O1-C1-C2	2.79	133.64	112.39
5	B	1214	GOL	O1-C1-C2	2.77	122.85	110.38
5	D	1213	GOL	O1-C1-C2	2.68	122.44	110.38
5	C	1214	GOL	O3-C3-C2	2.68	122.42	110.38
5	B	1212	GOL	O3-C3-C2	-2.31	99.97	110.38
5	A	1212	GOL	O1-C1-C2	-2.24	100.27	110.38
5	D	1213	GOL	O2-C2-C1	2.22	118.38	109.18
5	B	1213	GOL	O2-C2-C1	-2.14	100.33	109.18

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1214	GOL	C1-C2-C3-O3
5	C	1212	GOL	O1-C1-C2-C3
5	C	1212	GOL	C1-C2-C3-O3
5	D	1213	GOL	O1-C1-C2-O2
5	D	1213	GOL	O1-C1-C2-C3
7	C	1215	PEG	O2-C3-C4-O4
5	C	1212	GOL	O2-C2-C3-O3
7	C	1215	PEG	O1-C1-C2-O2
5	B	1214	GOL	O1-C1-C2-C3
5	A	1214	GOL	O2-C2-C3-O3
5	C	1212	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	A	1215	EDO	O1-C1-C2-O2
5	B	1214	GOL	O1-C1-C2-O2
6	B	1216	EDO	O1-C1-C2-O2
6	B	1217	EDO	O1-C1-C2-O2
6	D	1217	EDO	O1-C1-C2-O2
7	C	1215	PEG	C1-C2-O2-C3
6	B	1215	EDO	O1-C1-C2-O2
6	A	1217	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1215	PEG	4	0
5	B	1213	GOL	1	0
6	D	1217	EDO	1	0
5	C	1214	GOL	3	0
6	A	1217	EDO	3	0
6	D	1216	EDO	2	0
6	B	1217	EDO	1	0
5	D	1212	GOL	2	0
6	A	1215	EDO	1	0
5	C	1212	GOL	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, 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	207/215 (96%)	-0.45	3 (1%) 73 78	6, 15, 27, 52	25 (12%)
1	B	207/215 (96%)	-0.55	2 (0%) 79 83	6, 14, 27, 44	18 (8%)
1	C	207/215 (96%)	-0.57	1 (0%) 87 90	7, 14, 25, 48	21 (10%)
1	D	207/215 (96%)	-0.60	3 (1%) 73 78	6, 14, 25, 47	23 (11%)
All	All	828/860 (96%)	-0.54	9 (1%) 78 82	6, 14, 27, 52	87 (10%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	PRO	5.2
1	B	30[A]	TRP	3.7
1	A	209	PRO	3.1
1	D	209	PRO	3.1
1	A	3	THR	2.4
1	D	30[A]	TRP	2.3
1	C	3	THR	2.2
1	A	155	LYS	2.2
1	D	3	THR	2.1

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

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(Å ²)	Q<0.9
6	EDO	D	1217	4/4	0.83	0.13	34,43,45,45	0
6	EDO	B	1216	4/4	0.84	0.14	39,39,47,48	0
7	PEG	C	1215	7/7	0.84	0.13	35,41,45,46	0
6	EDO	B	1215	4/4	0.88	0.13	39,39,42,49	0
6	EDO	A	1216	4/4	0.90	0.14	30,42,44,48	0
5	GOL	C	1212	6/6	0.91	0.12	34,35,44,45	0
5	GOL	A	1212	6/6	0.91	0.11	35,39,42,43	0
6	EDO	B	1217	4/4	0.92	0.18	23,25,34,35	0
5	GOL	B	1212	6/6	0.93	0.09	25,26,29,30	0
5	GOL	C	1214	6/6	0.93	0.11	21,26,37,50	0
6	EDO	A	1215	4/4	0.93	0.08	38,39,40,46	0
6	EDO	D	1215	4/4	0.93	0.11	37,38,39,46	0
6	EDO	D	1216	4/4	0.93	0.13	32,33,35,41	0
5	GOL	B	1214	6/6	0.93	0.08	22,27,30,30	0
6	EDO	A	1217	4/4	0.93	0.18	20,27,32,38	0
5	GOL	A	1214	6/6	0.94	0.09	23,24,30,33	0
4	MG	A	1210	1/1	0.95	0.06	24,24,24,24	0
5	GOL	D	1212	6/6	0.96	0.07	24,27,29,30	0
5	GOL	D	1213	6/6	0.96	0.07	21,23,28,29	0
4	MG	C	1210	1/1	0.97	0.05	18,18,18,18	0
5	GOL	B	1213	6/6	0.98	0.07	11,13,16,18	0
5	GOL	C	1213	6/6	0.98	0.06	10,13,16,17	0
5	GOL	A	1213	6/6	0.98	0.06	14,17,18,20	0
4	MG	D	1210	1/1	0.99	0.02	13,13,13,13	0
4	MG	B	1210	1/1	0.99	0.02	12,12,12,12	0
4	MG	A	1211	1/1	0.99	0.02	14,14,14,14	0
4	MG	C	1211	1/1	0.99	0.03	14,14,14,14	0
5	GOL	D	1214	6/6	0.99	0.05	11,14,15,18	0
2	ZN	A	401	1/1	1.00	0.02	11,11,11,11	0
2	ZN	B	401	1/1	1.00	0.02	9,9,9,9	0
2	ZN	C	401	1/1	1.00	0.02	9,9,9,9	0
4	MG	B	1211	1/1	1.00	0.02	9,9,9,9	0
2	ZN	D	401	1/1	1.00	0.02	9,9,9,9	0
3	CD	A	402	1/1	1.00	0.01	13,13,13,13	0
3	CD	B	402	1/1	1.00	0.01	10,10,10,10	0
4	MG	D	1211	1/1	1.00	0.03	10,10,10,10	0
3	CD	C	402	1/1	1.00	0.01	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CD	D	402	1/1	1.00	0.01	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.