



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2021 – 12:06 PM EDT

PDB ID : 7LKJ
Title : Crystal structure of Helicobacter pylori aminofutalosine deaminase (AFLDA)
Authors : Harijan, R.K.; Feng, M.; Bonanno, J.B.; Almo, S.C.; Schramm, V.L.
Deposited on : 2021-02-02
Resolution : 2.79 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.20
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.20

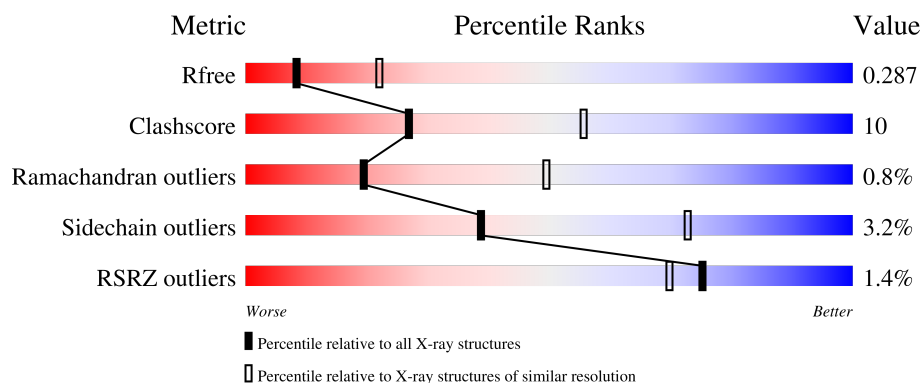
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.79 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	423	
1	B	423	
1	C	423	
1	D	423	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12742 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 Aminofutalosine deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3184	2047	531	598	8			
1	B	399	Total	C	N	O	S	0	0	0
			3087	1989	515	575	8			
1	C	409	Total	C	N	O	S	0	0	0
			3183	2046	531	598	8			
1	D	398	Total	C	N	O	S	6	1	0
			3116	2007	518	583	8			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q9ZMG8
A	-12	HIS	-	expression tag	UNP Q9ZMG8
A	-11	HIS	-	expression tag	UNP Q9ZMG8
A	-10	HIS	-	expression tag	UNP Q9ZMG8
A	-9	HIS	-	expression tag	UNP Q9ZMG8
A	-8	HIS	-	expression tag	UNP Q9ZMG8
A	-7	HIS	-	expression tag	UNP Q9ZMG8
A	-6	GLU	-	expression tag	UNP Q9ZMG8
A	-5	ASN	-	expression tag	UNP Q9ZMG8
A	-4	LEU	-	expression tag	UNP Q9ZMG8
A	-3	TYR	-	expression tag	UNP Q9ZMG8
A	-2	PHE	-	expression tag	UNP Q9ZMG8
A	-1	GLN	-	expression tag	UNP Q9ZMG8
A	0	GLY	-	expression tag	UNP Q9ZMG8
B	-13	MET	-	initiating methionine	UNP Q9ZMG8
B	-12	HIS	-	expression tag	UNP Q9ZMG8
B	-11	HIS	-	expression tag	UNP Q9ZMG8
B	-10	HIS	-	expression tag	UNP Q9ZMG8
B	-9	HIS	-	expression tag	UNP Q9ZMG8
B	-8	HIS	-	expression tag	UNP Q9ZMG8
B	-7	HIS	-	expression tag	UNP Q9ZMG8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	GLU	-	expression tag	UNP Q9ZMG8
B	-5	ASN	-	expression tag	UNP Q9ZMG8
B	-4	LEU	-	expression tag	UNP Q9ZMG8
B	-3	TYR	-	expression tag	UNP Q9ZMG8
B	-2	PHE	-	expression tag	UNP Q9ZMG8
B	-1	GLN	-	expression tag	UNP Q9ZMG8
B	0	GLY	-	expression tag	UNP Q9ZMG8
C	-13	MET	-	initiating methionine	UNP Q9ZMG8
C	-12	HIS	-	expression tag	UNP Q9ZMG8
C	-11	HIS	-	expression tag	UNP Q9ZMG8
C	-10	HIS	-	expression tag	UNP Q9ZMG8
C	-9	HIS	-	expression tag	UNP Q9ZMG8
C	-8	HIS	-	expression tag	UNP Q9ZMG8
C	-7	HIS	-	expression tag	UNP Q9ZMG8
C	-6	GLU	-	expression tag	UNP Q9ZMG8
C	-5	ASN	-	expression tag	UNP Q9ZMG8
C	-4	LEU	-	expression tag	UNP Q9ZMG8
C	-3	TYR	-	expression tag	UNP Q9ZMG8
C	-2	PHE	-	expression tag	UNP Q9ZMG8
C	-1	GLN	-	expression tag	UNP Q9ZMG8
C	0	GLY	-	expression tag	UNP Q9ZMG8
D	-13	MET	-	initiating methionine	UNP Q9ZMG8
D	-12	HIS	-	expression tag	UNP Q9ZMG8
D	-11	HIS	-	expression tag	UNP Q9ZMG8
D	-10	HIS	-	expression tag	UNP Q9ZMG8
D	-9	HIS	-	expression tag	UNP Q9ZMG8
D	-8	HIS	-	expression tag	UNP Q9ZMG8
D	-7	HIS	-	expression tag	UNP Q9ZMG8
D	-6	GLU	-	expression tag	UNP Q9ZMG8
D	-5	ASN	-	expression tag	UNP Q9ZMG8
D	-4	LEU	-	expression tag	UNP Q9ZMG8
D	-3	TYR	-	expression tag	UNP Q9ZMG8
D	-2	PHE	-	expression tag	UNP Q9ZMG8
D	-1	GLN	-	expression tag	UNP Q9ZMG8
D	0	GLY	-	expression tag	UNP Q9ZMG8

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

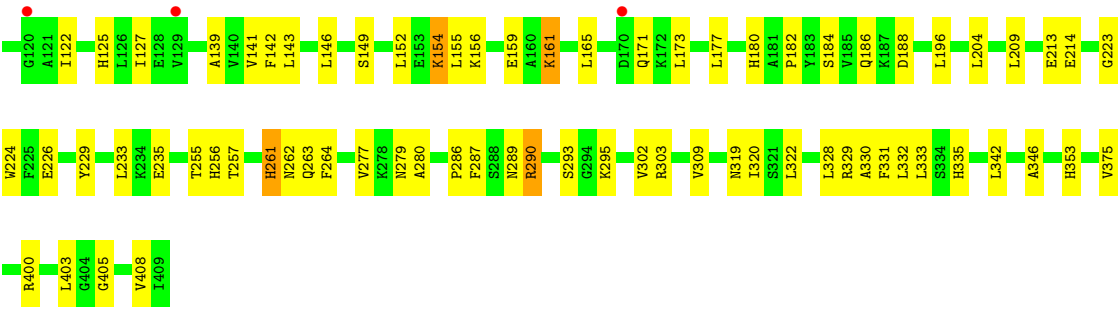
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total	O	0	0
			38	38		
4	B	34	Total	O	0	0
			34	34		
4	C	36	Total	O	0	0
			36	36		

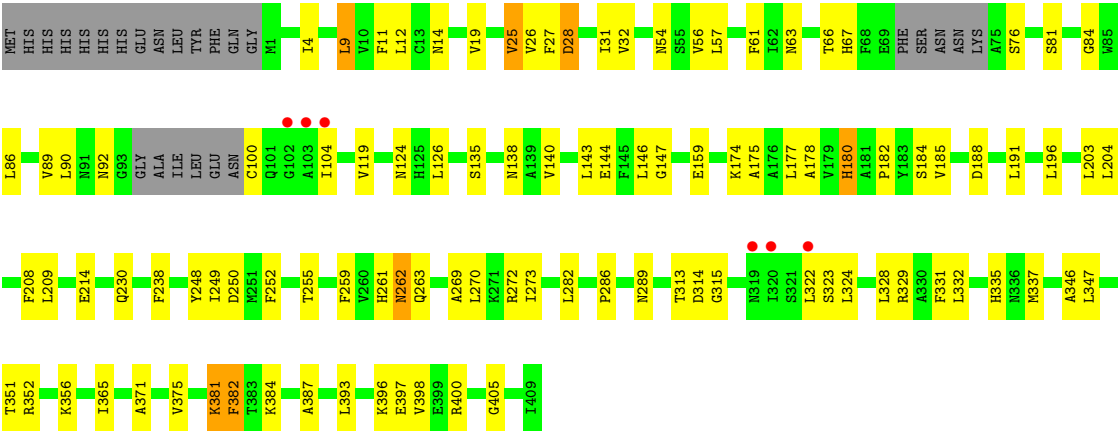
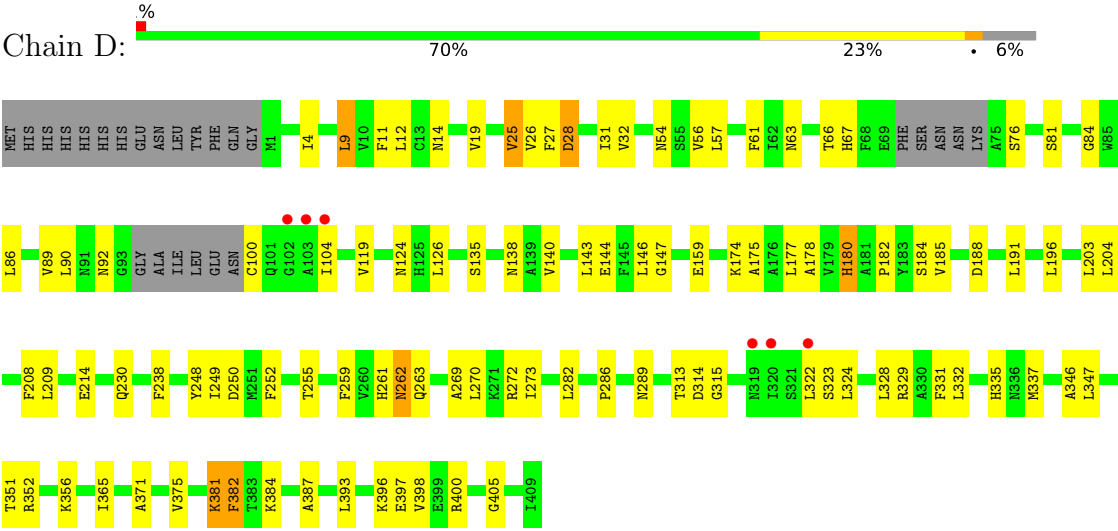
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	41	Total	O	0	0
			41	41		



● Molecule 1: Aminofutalosine deaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.30Å 73.30Å 157.50Å 90.00° 98.59° 90.00°	Depositor
Resolution (Å)	155.73 – 2.79 155.73 – 2.79	Depositor EDS
% Data completeness (in resolution range)	94.0 (155.73-2.79) 94.0 (155.73-2.79)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.253 , 0.287 0.253 , 0.287	Depositor DCC
R_{free} test set	1997 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.948	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 17.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12742	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, 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	0.33	0/3244	0.54	6/4381 (0.1%)
1	B	0.28	0/3144	0.53	6/4244 (0.1%)
1	C	0.28	0/3243	0.49	1/4380 (0.0%)
1	D	0.43	4/3174 (0.1%)	0.66	7/4283 (0.2%)
All	All	0.34	4/12805 (0.0%)	0.56	20/17288 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	396	LYS	CD-CE	8.87	1.73	1.51
1	D	25	VAL	CB-CG2	5.92	1.65	1.52
1	D	381	LYS	CB-CG	-5.50	1.37	1.52
1	D	25	VAL	CB-CG1	5.32	1.64	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	381	LYS	CA-CB-CG	-11.19	88.78	113.40
1	D	25	VAL	CG1-CB-CG2	10.61	127.87	110.90
1	B	381	LYS	CD-CE-NZ	9.90	134.47	111.70
1	A	152	LEU	CA-CB-CG	9.32	136.75	115.30
1	D	396	LYS	CG-CD-CE	-8.80	85.51	111.90
1	D	381	LYS	CG-CD-CE	-7.42	89.62	111.90
1	C	171	GLN	CA-CB-CG	-7.34	97.26	113.40
1	A	152	LEU	CB-CG-CD2	7.24	123.32	111.00
1	A	278	LYS	CB-CG-CD	-7.08	93.18	111.60
1	D	384	LYS	CB-CG-CD	-6.53	94.61	111.60
1	B	381	LYS	CG-CD-CE	-6.10	93.60	111.90
1	D	9	LEU	CA-CB-CG	5.81	128.66	115.30
1	A	278	LYS	CG-CD-CE	5.77	129.22	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	LYS	CB-CG-CD	5.74	126.53	111.60
1	A	322	LEU	CA-CB-CG	5.71	128.43	115.30
1	D	381	LYS	CD-CE-NZ	-5.64	98.73	111.70
1	B	174	LYS	CG-CD-CE	-5.58	95.16	111.90
1	B	146	LEU	CB-CG-CD2	5.41	120.19	111.00
1	A	278	LYS	CD-CE-NZ	-5.05	100.07	111.70
1	B	174	LYS	CD-CE-NZ	5.03	123.28	111.70

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	3184	0	3160	57	0
1	B	3087	0	3057	67	1
1	C	3183	0	3158	58	0
1	D	3116	0	3100	78	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	12	0	18	1	0
3	B	8	0	12	1	0
4	A	38	0	0	2	0
4	B	34	0	0	1	0
4	C	36	0	0	1	0
4	D	41	0	0	0	0
All	All	12742	0	12505	256	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 10.

All (256) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:GLN:HE21	1:D:238:PHE:HE2	1.07	1.02
1:B:8:SER:OG	1:B:381:LYS:NZ	2.05	0.89
1:D:381:LYS:HG2	1:D:382:PHE:N	1.85	0.83
1:B:270:LEU:HD22	1:B:282:LEU:HD11	1.60	0.81
1:A:256:HIS:HB2	3:A:504:EDO:H22	1.65	0.78
1:D:9:LEU:HD11	1:D:387:ALA:HB1	1.66	0.77
1:D:9:LEU:HG	1:D:381:LYS:CE	2.15	0.76
1:C:152:LEU:HG	1:C:156:LYS:HE3	1.71	0.72
1:B:146:LEU:HD21	1:B:180:HIS:CG	2.25	0.71
1:D:27:PHE:HA	1:D:32:VAL:HG23	1.74	0.70
1:B:8:SER:HG	1:B:381:LYS:HZ3	1.37	0.69
1:A:231:ARG:HB3	1:A:232:PHE:CD2	2.28	0.69
1:D:375:VAL:HB	1:D:400:ARG:HB2	1.76	0.68
1:C:27:PHE:HA	1:C:32:VAL:HG23	1.76	0.68
1:D:9:LEU:HG	1:D:381:LYS:NZ	2.11	0.65
1:B:286:PRO:HG3	1:B:331:PHE:HB2	1.79	0.65
1:D:397:GLU:HG3	1:D:398:VAL:H	1.61	0.64
1:A:5:ILE:HD11	1:A:375:VAL:HG21	1.79	0.64
1:A:143:LEU:HB3	1:A:177:LEU:HD23	1.80	0.64
1:D:230:GLN:NE2	1:D:238:PHE:HE2	1.89	0.64
1:D:9:LEU:HG	1:D:381:LYS:HE3	1.79	0.63
1:B:25:VAL:HG12	1:B:34:ILE:HG23	1.81	0.63
1:D:313:THR:HG21	1:D:322:LEU:HB3	1.82	0.62
1:A:344:LYS:NZ	4:A:602:HOH:O	2.32	0.62
1:D:314:ASP:OD1	1:D:315:GLY:N	2.29	0.62
1:B:258:LEU:HD13	1:B:283:ILE:HD11	1.82	0.62
1:C:229:TYR:HD2	1:C:233:LEU:HD12	1.64	0.61
1:C:375:VAL:HB	1:C:400:ARG:HB2	1.82	0.61
1:D:329:ARG:HA	1:D:332:LEU:HD12	1.82	0.61
1:D:397:GLU:HG3	1:D:398:VAL:N	2.16	0.61
1:B:129:VAL:HG12	1:B:141:VAL:HG21	1.81	0.60
1:D:9:LEU:CD1	1:D:387:ALA:HB1	2.31	0.60
1:C:143:LEU:HB3	1:C:177:LEU:HD23	1.83	0.60
1:C:72:ASN:ND2	1:C:99:ASN:O	2.33	0.59
1:B:4:ILE:HG12	1:B:26:VAL:HG22	1.85	0.58
1:C:332:LEU:HA	1:C:342:LEU:HD21	1.86	0.58
1:C:111:GLN:HE21	1:C:322:LEU:HB3	1.68	0.58
1:A:250:ASP:OD2	1:A:272:ARG:NH2	2.35	0.58
1:D:9:LEU:HD22	1:D:19:VAL:HG22	1.85	0.58
1:B:159:GLU:HG2	1:B:196:LEU:HD22	1.84	0.58
1:C:286:PRO:HG3	1:C:331:PHE:HB2	1.86	0.57
1:D:9:LEU:HD13	1:D:11:PHE:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:LYS:NZ	1:D:175:ALA:O	2.34	0.57
1:C:69:GLU:CB	1:C:97:LEU:HD21	2.35	0.57
1:B:328:LEU:HD22	1:B:346:ALA:HB1	1.86	0.57
1:B:108:ILE:HD11	1:B:132:LEU:HD12	1.87	0.56
1:B:14:ASN:HD21	1:B:18:GLU:HB2	1.69	0.56
1:B:326:ASP:OD2	1:B:329:ARG:NH2	2.38	0.56
1:D:140:VAL:HG13	1:D:174:LYS:HD3	1.88	0.56
1:C:69:GLU:O	1:C:97:LEU:HD23	2.05	0.56
1:B:329:ARG:HA	1:B:332:LEU:HD12	1.88	0.55
1:D:28:ASP:O	1:D:405:GLY:HA3	2.06	0.55
1:B:146:LEU:HD22	1:B:184:SER:HB2	1.87	0.55
1:A:260:VAL:HA	1:A:283:ILE:HB	1.89	0.55
1:C:25:VAL:HG23	1:C:34:ILE:HG22	1.90	0.55
1:C:122:ILE:HD13	1:C:142:PHE:HB2	1.89	0.54
1:D:286:PRO:HG3	1:D:331:PHE:HB2	1.89	0.54
1:B:250:ASP:OD1	1:B:272:ARG:NH2	2.41	0.54
1:D:9:LEU:HD22	1:D:19:VAL:CG2	2.36	0.54
1:B:332:LEU:HD23	1:B:342:LEU:HD23	1.88	0.54
1:C:4:ILE:HG12	1:C:26:VAL:HG22	1.88	0.54
1:A:286:PRO:HG3	1:A:331:PHE:HB2	1.90	0.54
1:A:316:LEU:HG	1:A:322:LEU:CD2	2.38	0.54
1:B:146:LEU:HD21	1:B:180:HIS:CB	2.38	0.54
1:A:329:ARG:HA	1:A:332:LEU:HD12	1.89	0.54
1:C:111:GLN:NE2	1:C:322:LEU:HB3	2.23	0.54
1:C:403:LEU:HD12	1:C:408:VAL:HG21	1.90	0.53
1:D:250:ASP:OD1	1:D:272:ARG:NH2	2.31	0.53
1:C:159:GLU:HG2	1:C:196:LEU:HD22	1.90	0.53
1:A:389:LEU:O	1:A:393:LEU:HD22	2.09	0.53
1:A:263:GLN:HE21	1:A:289:ASN:CG	2.13	0.53
1:A:316:LEU:HG	1:A:322:LEU:HD21	1.91	0.53
1:B:263:GLN:NE2	1:B:289:ASN:OD1	2.43	0.52
1:C:302:VAL:HG11	1:C:309:VAL:HG23	1.92	0.52
1:D:9:LEU:HD13	1:D:11:PHE:HE1	1.74	0.52
1:B:133:LYS:HE3	1:B:170:ASP:OD1	2.09	0.52
1:D:9:LEU:HD11	1:D:387:ALA:CB	2.38	0.51
1:B:258:LEU:HD22	1:B:281:PHE:HB2	1.92	0.51
1:C:277:VAL:HB	1:C:280:ALA:HB2	1.92	0.51
1:A:393:LEU:HB3	1:B:320:ILE:HG21	1.93	0.50
1:B:285:CYS:O	1:B:289:ASN:ND2	2.45	0.50
1:C:149:SER:HB3	1:C:235:GLU:OE2	2.10	0.50
1:D:146:LEU:HD22	1:D:184:SER:OG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:LEU:HD12	1:B:408:VAL:HG21	1.92	0.50
1:D:86:LEU:O	1:D:90:LEU:HG	2.10	0.50
1:B:302:VAL:HG11	1:B:309:VAL:HG13	1.93	0.50
1:B:174:LYS:HE2	1:B:175:ALA:O	2.11	0.50
1:C:141:VAL:HG23	1:C:165:LEU:HD21	1.93	0.49
1:D:208:PHE:CZ	1:D:249:ILE:HD11	2.48	0.49
1:D:182:PRO:HG3	1:D:248:TYR:CE2	2.47	0.49
1:D:209:LEU:HD23	1:D:214:GLU:HG2	1.94	0.49
1:A:122:ILE:HD13	1:A:142:PHE:HB2	1.95	0.49
1:B:347:LEU:O	1:B:351:THR:OG1	2.24	0.49
1:D:328:LEU:HD22	1:D:346:ALA:HB1	1.94	0.49
1:D:66:THR:HA	1:D:314:ASP:O	2.12	0.49
1:B:217:TRP:HE1	1:B:229:TYR:HH	1.60	0.49
1:A:75:ALA:O	1:A:77:PHE:N	2.44	0.49
1:C:146:LEU:HD23	1:C:184:SER:HB2	1.95	0.49
1:D:61:PHE:HB3	1:D:324:LEU:HD23	1.94	0.49
1:C:141:VAL:HG21	1:C:165:LEU:HD11	1.94	0.48
1:A:63:ASN:HB3	1:A:119:VAL:HG13	1.95	0.48
1:C:255:THR:OG1	1:C:256:HIS:N	2.42	0.48
1:A:326:ASP:OD1	1:A:329:ARG:NH2	2.46	0.48
1:C:290:ARG:NH2	1:D:335:HIS:O	2.47	0.48
1:D:328:LEU:O	1:D:332:LEU:HG	2.14	0.48
1:D:174:LYS:HE3	1:D:203:LEU:HD22	1.94	0.48
1:A:259:PHE:CE1	1:A:277:VAL:HG21	2.49	0.48
1:A:142:PHE:CE2	1:A:205:SER:HB3	2.48	0.48
1:A:144:GLU:HA	1:A:178:ALA:HB3	1.96	0.48
1:B:176:ALA:HA	1:B:202:SER:HB2	1.96	0.48
1:C:161:LYS:NZ	4:C:601:HOH:O	2.43	0.48
1:C:329:ARG:HA	1:C:332:LEU:HD12	1.94	0.47
1:D:14:ASN:OD1	1:D:14:ASN:N	2.43	0.47
1:D:263:GLN:NE2	1:D:289:ASN:OD1	2.47	0.47
1:A:328:LEU:HD22	1:A:346:ALA:HB1	1.96	0.47
1:B:258:LEU:HB3	1:B:283:ILE:HD11	1.95	0.47
1:D:182:PRO:HD2	1:D:214:GLU:OE1	2.14	0.47
1:C:182:PRO:HD2	1:C:214:GLU:OE1	2.13	0.47
1:B:276:GLN:O	1:B:278:LYS:HD2	2.15	0.47
1:A:28:ASP:O	1:A:405:GLY:HA3	2.15	0.47
1:C:287:PHE:HE1	1:C:320:ILE:HG23	1.80	0.47
1:C:330:ALA:HA	1:C:333:LEU:HD12	1.97	0.47
1:D:263:GLN:HE21	1:D:289:ASN:CG	2.17	0.47
1:B:174:LYS:NZ	1:B:202:SER:HA	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:LYS:HE3	1:D:203:LEU:HD13	1.95	0.47
1:B:61:PHE:HB3	1:B:324:LEU:HD23	1.96	0.47
1:C:263:GLN:NE2	1:C:289:ASN:OD1	2.48	0.47
1:D:126:LEU:HD21	1:D:143:LEU:HD13	1.96	0.47
1:D:208:PHE:HD2	1:D:262:ASN:ND2	2.13	0.47
1:D:81:SER:HB2	1:D:84:GLY:H	1.80	0.46
1:D:270:LEU:HD23	1:D:282:LEU:HD11	1.97	0.46
1:A:204:LEU:O	1:A:257:THR:HA	2.16	0.46
1:D:124:ASN:ND2	1:D:144:GLU:OE2	2.48	0.46
1:A:302:VAL:HG11	1:A:309:VAL:HG13	1.97	0.46
1:B:31:ILE:HD11	1:B:373:LEU:HD21	1.97	0.46
1:D:9:LEU:HD12	1:D:56:VAL:HG22	1.96	0.46
1:C:261:HIS:HB3	1:C:263:GLN:OE1	2.15	0.46
1:A:356:LYS:NZ	4:A:606:HOH:O	2.43	0.46
1:A:366:GLU:HB3	1:A:369:LYS:HG3	1.98	0.46
1:D:100:CYS:SG	1:D:104:ILE:HG13	2.56	0.46
1:B:122:ILE:HG13	1:B:142:PHE:HB2	1.98	0.46
1:B:59:PRO:HG3	1:B:365:ILE:HD13	1.98	0.46
1:B:14:ASN:OD1	1:B:14:ASN:N	2.37	0.45
1:B:28:ASP:OD1	1:B:29:GLU:N	2.49	0.45
1:A:28:ASP:OD1	1:A:29:GLU:N	2.49	0.45
1:D:27:PHE:CD2	1:D:371:ALA:HB1	2.51	0.45
1:D:144:GLU:OE1	1:D:180:HIS:HD2	1.98	0.45
1:A:328:LEU:O	1:A:332:LEU:HG	2.16	0.45
1:A:261:HIS:N	1:A:283:ILE:O	2.49	0.45
1:D:159:GLU:HG2	1:D:196:LEU:HD22	1.99	0.45
1:D:188:ASP:HA	1:D:191:LEU:HD12	1.98	0.45
1:B:299:LEU:HG	1:B:335:HIS:CD2	2.51	0.45
1:A:252:PHE:O	1:A:255:THR:HG22	2.17	0.45
1:C:75:ALA:O	1:C:77:PHE:N	2.50	0.45
1:C:111:GLN:NE2	1:C:322:LEU:O	2.50	0.45
1:C:155:LEU:HD23	1:C:155:LEU:HA	1.79	0.45
1:B:319:ASN:OD1	1:B:320:ILE:N	2.49	0.45
1:C:213:GLU:HG2	1:C:224:TRP:HB3	1.99	0.45
1:D:313:THR:HG21	1:D:322:LEU:CA	2.47	0.45
1:C:139:ALA:O	1:C:173:LEU:HA	2.17	0.45
1:C:319:ASN:OD1	1:C:320:ILE:N	2.50	0.45
1:A:316:LEU:HD23	1:A:319:ASN:HB3	1.99	0.44
1:C:328:LEU:O	1:C:332:LEU:HG	2.16	0.44
1:B:154:LYS:HA	1:B:154:LYS:HD3	1.68	0.44
1:C:328:LEU:HD22	1:C:346:ALA:HB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:THR:HA	1:A:327:GLU:HG2	1.98	0.44
1:B:28:ASP:O	1:B:405:GLY:HA3	2.17	0.44
1:D:230:GLN:NE2	1:D:238:PHE:CE2	2.74	0.44
1:A:277:VAL:HB	1:A:280:ALA:HB2	2.00	0.44
1:D:25:VAL:CG2	1:D:57:LEU:HD21	2.48	0.44
1:A:14:ASN:OD1	1:A:14:ASN:N	2.40	0.44
1:A:287:PHE:HB3	1:A:319:ASN:ND2	2.33	0.44
1:A:361:ASN:O	1:A:370:ARG:HG3	2.18	0.44
1:C:209:LEU:HD23	1:C:214:GLU:HG2	2.00	0.44
1:A:61:PHE:HB3	1:A:324:LEU:HD23	1.99	0.43
1:B:174:LYS:HE3	4:B:613:HOH:O	2.17	0.43
1:D:177:LEU:O	1:D:204:LEU:HA	2.19	0.43
1:A:356:LYS:HD3	1:A:356:LYS:HA	1.81	0.43
1:C:320:ILE:HG21	1:D:393:LEU:HB3	1.99	0.43
1:B:104:ILE:HD13	1:B:128:GLU:HB3	2.00	0.43
1:A:270:LEU:HD22	1:A:282:LEU:HD21	2.01	0.43
1:A:259:PHE:HE1	1:A:277:VAL:HG21	1.84	0.43
1:D:269:ALA:O	1:D:273:ILE:HG13	2.18	0.43
1:C:204:LEU:O	1:C:257:THR:HA	2.18	0.43
1:A:8:SER:HB3	1:A:381:LYS:HE3	2.00	0.42
1:A:274:LYS:NZ	1:A:306:GLY:O	2.30	0.42
1:B:252:PHE:O	1:B:255:THR:OG1	2.36	0.42
1:A:146:LEU:HD23	1:A:184:SER:HB2	2.01	0.42
1:A:313:THR:OG1	1:A:322:LEU:HD12	2.18	0.42
1:B:362:ASN:HB3	1:B:370:ARG:HB3	2.01	0.42
1:D:259:PHE:HB3	1:D:262:ASN:HD21	1.84	0.42
1:A:153:GLU:HA	1:A:156:LYS:NZ	2.34	0.42
1:C:39:ASN:OD1	1:C:40:LEU:N	2.52	0.42
1:C:186:GLN:NE2	1:C:188:ASP:OD1	2.49	0.42
1:D:12:LEU:HA	1:D:365:ILE:HB	2.01	0.42
1:B:65:HIS:NE2	1:B:67:HIS:HE1	2.17	0.42
1:D:89:VAL:O	1:D:92:ASN:HB3	2.20	0.42
1:D:144:GLU:HA	1:D:178:ALA:HB3	2.01	0.42
1:D:313:THR:CG2	1:D:322:LEU:HA	2.49	0.42
1:D:347:LEU:O	1:D:351:THR:OG1	2.25	0.42
1:A:263:GLN:HA	1:A:297:LEU:HD13	2.00	0.42
1:B:366:GLU:HB3	1:B:369:LYS:HG3	2.01	0.42
1:D:4:ILE:HG12	1:D:26:VAL:HG22	2.01	0.42
1:D:63:ASN:HD21	1:D:313:THR:HB	1.84	0.42
1:A:185:VAL:HG11	1:A:190:ALA:HB2	2.01	0.42
1:D:147:GLY:O	1:D:185:VAL:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:THR:O	1:D:313:THR:HG22	2.20	0.42
1:A:170:ASP:HB2	1:A:171:GLN:OE1	2.19	0.42
1:B:112:LEU:HB3	1:B:409:ILE:HD11	2.02	0.42
1:D:54:ASN:HA	1:D:381:LYS:HB2	2.01	0.42
1:D:313:THR:HG21	1:D:322:LEU:HA	2.01	0.42
1:A:27:PHE:HA	1:A:32:VAL:HG23	2.01	0.42
1:B:174:LYS:HZ3	1:B:202:SER:HB3	1.85	0.42
1:A:361:ASN:HB3	1:A:370:ARG:HG3	2.01	0.42
1:B:119:VAL:HG22	1:B:137:LEU:HD12	2.01	0.42
1:B:180:HIS:NE2	3:B:502:EDO:H21	2.35	0.42
1:C:335:HIS:HB2	1:C:342:LEU:HD11	2.01	0.42
1:B:58:LEU:HD21	1:B:376:PHE:CD2	2.54	0.42
1:B:187:LYS:O	1:B:191:LEU:HG	2.20	0.42
1:B:258:LEU:HB3	1:B:283:ILE:CD1	2.50	0.42
1:A:327:GLU:N	1:A:327:GLU:OE1	2.53	0.41
1:C:277:VAL:O	1:C:279:ASN:N	2.44	0.41
1:A:177:LEU:HD11	1:A:196:LEU:HD23	2.02	0.41
1:B:18:GLU:OE2	1:B:20:LEU:HD21	2.21	0.41
1:B:145:PHE:HD2	1:B:158:PHE:CD2	2.37	0.41
1:C:290:ARG:NH2	1:D:337:MET:O	2.53	0.41
1:C:229:TYR:CD2	1:C:233:LEU:HD12	2.50	0.41
1:C:264:PHE:CZ	1:C:295:LYS:HD2	2.55	0.41
1:B:133:LYS:HB3	1:B:133:LYS:HE2	1.87	0.41
1:C:125:HIS:HB2	1:C:127:ILE:HD11	2.02	0.41
1:C:152:LEU:O	1:C:156:LYS:HG3	2.20	0.41
1:D:9:LEU:CD2	1:D:381:LYS:NZ	2.84	0.41
1:D:119:VAL:N	1:D:138:ASN:O	2.51	0.41
1:B:163:LYS:HE2	1:B:163:LYS:HB3	1.80	0.41
1:C:143:LEU:HD12	1:C:143:LEU:HA	1.72	0.41
1:B:112:LEU:HD21	1:B:136:PRO:HG2	2.03	0.41
1:C:302:VAL:HG11	1:C:309:VAL:CG2	2.50	0.41
1:D:313:THR:HG21	1:D:322:LEU:CB	2.50	0.41
1:B:136:PRO:HG3	1:B:408:VAL:HG11	2.02	0.41
1:B:146:LEU:CD2	1:B:180:HIS:CB	2.99	0.41
1:B:217:TRP:CZ2	1:B:229:TYR:HE2	2.39	0.41
1:C:5:ILE:HG12	1:C:27:PHE:HE2	1.84	0.41
1:A:153:GLU:HA	1:A:156:LYS:HZ3	1.86	0.41
1:D:252:PHE:O	1:D:255:THR:OG1	2.38	0.41
1:D:352:ARG:O	1:D:356:LYS:HD3	2.20	0.41
1:B:261:HIS:HB3	1:B:263:GLN:HE21	1.87	0.40
1:B:298:ASP:O	1:B:302:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ASP:O	1:C:405:GLY:HA3	2.21	0.40
1:D:67:HIS:CD2	1:D:67:HIS:N	2.88	0.40
1:A:325:LEU:O	1:A:329:ARG:HG3	2.21	0.40
1:B:330:ALA:HA	1:B:333:LEU:HD12	2.03	0.40
1:C:154:LYS:HD2	1:C:154:LYS:HA	1.59	0.40
1:A:337:MET:HB3	1:A:342:LEU:HD13	2.02	0.40
1:C:223:GLY:O	1:C:226:GLU:HG3	2.22	0.40
1:D:27:PHE:HB3	1:D:31:ILE:HA	2.04	0.40
1:A:255:THR:OG1	1:A:256:HIS:N	2.54	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)
1:B:188:ASP:OD1	1:B:303:ARG:NE[2_655]	2.17	0.03

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	407/423 (96%)	378 (93%)	26 (6%)	3 (1%)	22	53
1	B	393/423 (93%)	371 (94%)	19 (5%)	3 (1%)	19	49
1	C	407/423 (96%)	379 (93%)	25 (6%)	3 (1%)	22	53
1	D	393/423 (93%)	369 (94%)	21 (5%)	3 (1%)	19	49
All	All	1600/1692 (95%)	1497 (94%)	91 (6%)	12 (1%)	19	49

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	SER

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Mol	Chain	Res	Type
1	C	76	SER
1	A	261	HIS
1	B	261	HIS
1	C	261	HIS
1	D	261	HIS
1	B	76	SER
1	D	76	SER
1	D	180	HIS
1	A	180	HIS
1	B	180	HIS
1	C	180	HIS

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	339/362 (94%)	329 (97%)	10 (3%)	42	76
1	B	325/362 (90%)	310 (95%)	15 (5%)	27	60
1	C	339/362 (94%)	326 (96%)	13 (4%)	33	67
1	D	333/362 (92%)	327 (98%)	6 (2%)	59	86
All	All	1336/1448 (92%)	1292 (97%)	44 (3%)	39	72

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	CYS
1	A	23	TYR
1	A	28	ASP
1	A	99	ASN
1	A	231	ARG
1	A	278	LYS
1	A	293	SER
1	A	342	LEU
1	A	353	HIS
1	A	384	LYS

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Mol	Chain	Res	Type
1	B	2	GLN
1	B	8	SER
1	B	58	LEU
1	B	66	THR
1	B	170	ASP
1	B	171	GLN
1	B	174	LYS
1	B	207	HIS
1	B	216	GLU
1	B	254	ASP
1	B	262	ASN
1	B	278	LYS
1	B	293	SER
1	B	381	LYS
1	B	406	LYS
1	C	14	ASN
1	C	17	CYS
1	C	23	TYR
1	C	28	ASP
1	C	48	LYS
1	C	53	GLU
1	C	154	LYS
1	C	161	LYS
1	C	262	ASN
1	C	290	ARG
1	C	293	SER
1	C	303	ARG
1	C	353	HIS
1	D	28	ASP
1	D	135[A]	SER
1	D	135[B]	SER
1	D	262	ASN
1	D	323	SER
1	D	382	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	ASN
1	A	353	HIS
1	B	67	HIS
1	B	263	GLN

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Mol	Chain	Res	Type
1	B	289	ASN
1	D	180	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	EDO	A	504	-	3,3,3	0.46	0	2,2,2	0.31	0
3	EDO	B	502	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	A	503	-	3,3,3	0.46	0	2,2,2	0.32	0
3	EDO	B	503	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	A	502	-	3,3,3	0.45	0	2,2,2	0.35	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
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	B	502	-	-	0/1/1/1	-
3	EDO	A	503	-	-	0/1/1/1	-
3	EDO	B	503	-	-	0/1/1/1	-
3	EDO	A	502	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	EDO	1	0
3	B	502	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, 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	409/423 (96%)	-0.28	2 (0%) 91 88	26, 39, 55, 66	0
1	B	399/423 (94%)	-0.17	8 (2%) 65 56	27, 42, 59, 69	0
1	C	409/423 (96%)	-0.16	7 (1%) 70 63	27, 39, 56, 70	0
1	D	398/423 (94%)	-0.15	6 (1%) 73 68	27, 41, 59, 71	0
All	All	1615/1692 (95%)	-0.19	23 (1%) 75 70	26, 40, 57, 71	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	322	LEU	5.9
1	D	319	ASN	5.2
1	D	103	ALA	4.8
1	A	94	GLY	4.1
1	D	102	GLY	3.4
1	C	71	SER	3.2
1	C	42	LEU	2.9
1	C	94	GLY	2.7
1	B	321	SER	2.6
1	D	104	ILE	2.6
1	B	320	ILE	2.5
1	D	320	ILE	2.5
1	A	47	LEU	2.5
1	B	126	LEU	2.5
1	B	409	ILE	2.4
1	C	170	ASP	2.4
1	C	93	GLY	2.4
1	B	146	LEU	2.2
1	C	120	GLY	2.1
1	C	129	VAL	2.1
1	B	1	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	315	GLY	2.1
1	B	206	THR	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 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, 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(\AA^2)	Q<0.9
2	FE	C	501	1/1	0.88	0.07	80,80,80,80	0
3	EDO	B	503	4/4	0.88	0.15	43,45,46,46	0
3	EDO	A	504	4/4	0.91	0.20	38,41,43,46	0
3	EDO	A	502	4/4	0.93	0.15	41,42,42,42	0
3	EDO	B	502	4/4	0.96	0.20	41,43,46,48	0
3	EDO	A	503	4/4	0.97	0.08	40,42,43,43	0
2	FE	A	501	1/1	0.97	0.08	61,61,61,61	0
2	FE	B	501	1/1	0.98	0.04	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.