



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:05 PM UTC

PDB ID : 4AD9 / pdb_00004ad9
Title : Crystal structure of human LACTB2.
Authors : Allerston, C.K.; Krojer, T.; Shrestha, B.; Burgess Brown, N.; Chalk, R.; Elkins, J.M.; Filippakopoulos, P.; Pike, A.C.W.; Muniz, J.R.C.; Vollmar, M.; Arrowsmith, C.H.; Weigelt, J.; Edwards, A.; Bountra, C.; von Delft, F.; Gileadi, O.
Deposited on : 2011-12-22
Resolution : 2.60 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

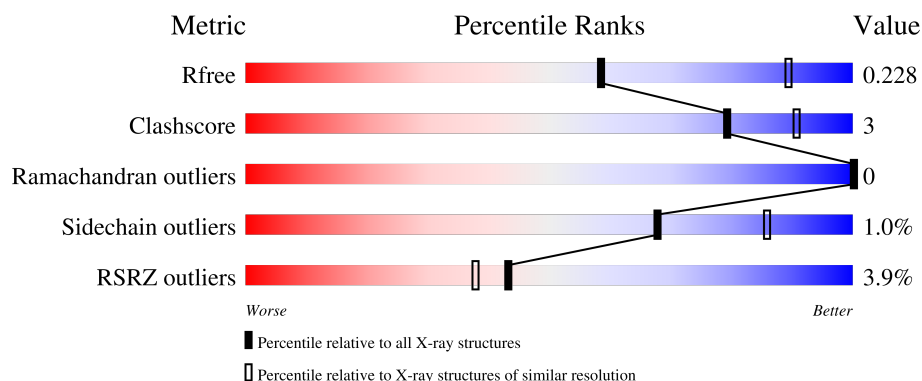
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	289	2% 90% 9%
1	B	289	9% 93% 6%
1	C	289	% 90% 9%
1	D	289	2% 93% 7%

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Mol	Chain	Length	Quality of chain
1	E	289	8% 93% 6%
1	F	289	% 88% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14225 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 BETA-LACTAMASE-LIKE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2230	1423	387	410	10			
1	B	285	Total	C	N	O	S	0	0	0
			2104	1341	363	391	9			
1	C	285	Total	C	N	O	S	0	1	0
			2242	1424	391	417	10			
1	D	288	Total	C	N	O	S	0	0	0
			2235	1423	387	415	10			
1	E	284	Total	C	N	O	S	0	0	0
			2093	1331	362	391	9			
1	F	285	Total	C	N	O	S	0	1	0
			2238	1424	387	418	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q53H82
B	0	SER	-	expression tag	UNP Q53H82
C	0	SER	-	expression tag	UNP Q53H82
D	0	SER	-	expression tag	UNP Q53H82
E	0	SER	-	expression tag	UNP Q53H82
F	0	SER	-	expression tag	UNP Q53H82

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

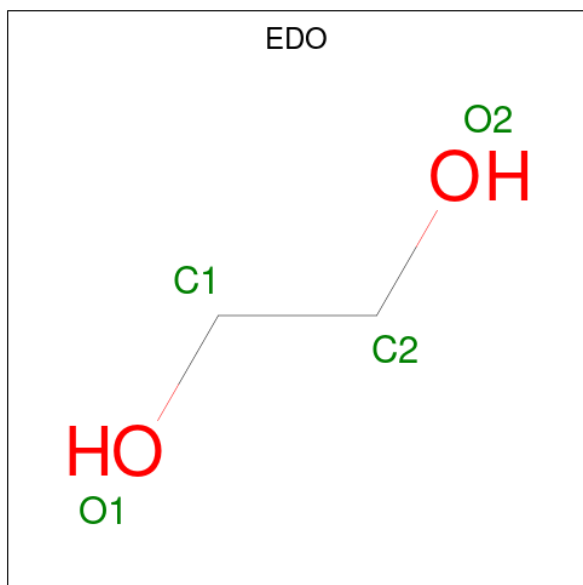
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	242	Total	O	0	0
			242	242		
4	B	94	Total	O	0	0
			94	94		

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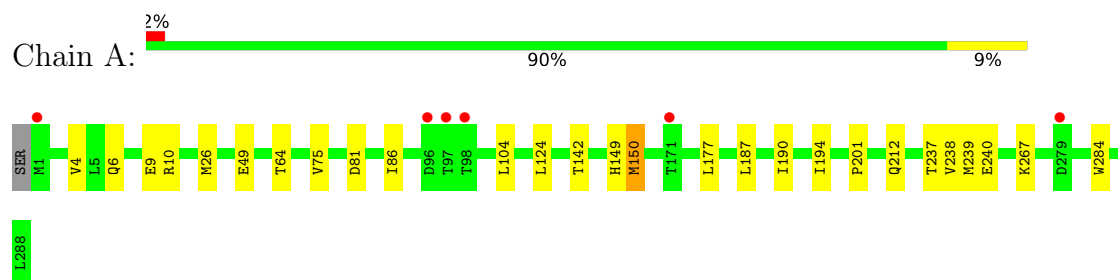
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	209	Total 209	O 209	0	0
4	D	206	Total 206	O 206	0	0
4	E	97	Total 97	O 97	0	0
4	F	207	Total 207	O 207	0	0

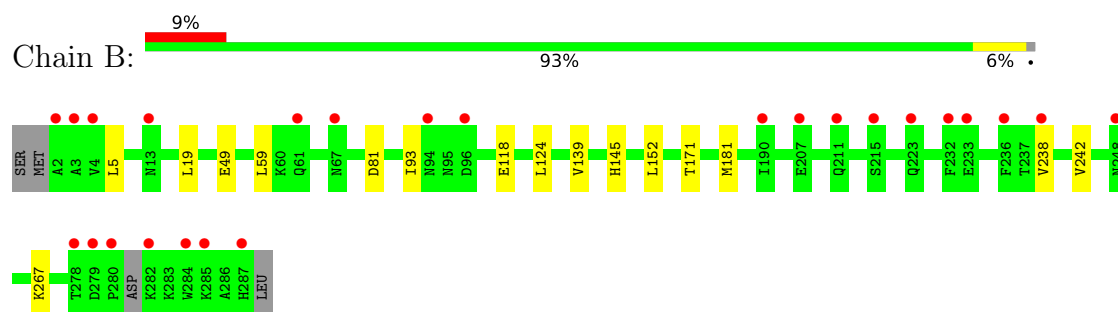
3 Residue-property plots [i](#)

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.

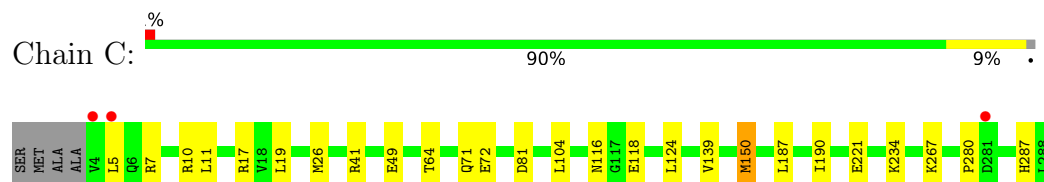
• Molecule 1: BETA-LACTAMASE-LIKE PROTEIN 2



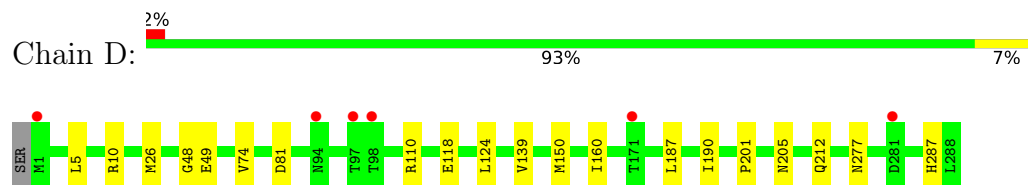
• Molecule 1: BETA-LACTAMASE-LIKE PROTEIN 2



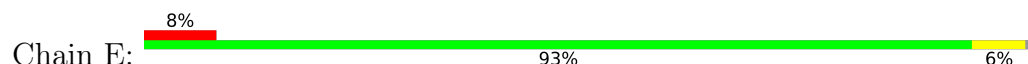
• Molecule 1: BETA-LACTAMASE-LIKE PROTEIN 2

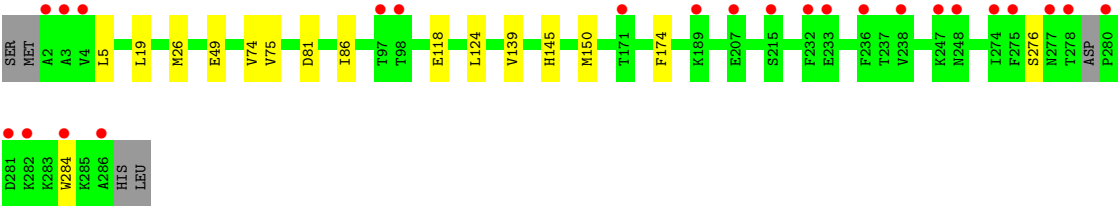


• Molecule 1: BETA-LACTAMASE-LIKE PROTEIN 2

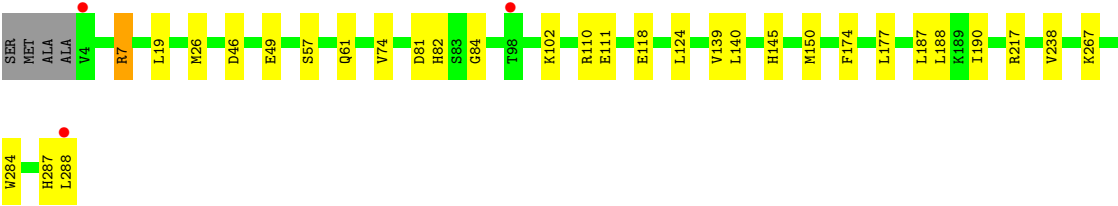
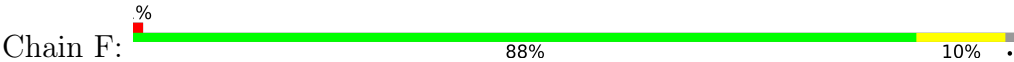


• Molecule 1: BETA-LACTAMASE-LIKE PROTEIN 2





● Molecule 1: BETA-LACTAMASE-LIKE PROTEIN 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.47Å 95.69Å 135.76Å 90.00° 112.84° 90.00°	Depositor
Resolution (Å)	46.85 – 2.60 46.85 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.85-2.60) 99.2 (46.85-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.177 , 0.224 0.184 , 0.228	Depositor DCC
R_{free} test set	1957 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14225	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.37% 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: ZN, 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	0.91	1/2275 (0.0%)	1.31	7/3088 (0.2%)
1	B	0.80	0/2143	1.28	2/2920 (0.1%)
1	C	0.89	1/2290 (0.0%)	1.28	2/3108 (0.1%)
1	D	0.90	0/2280	1.31	9/3096 (0.3%)
1	E	0.80	0/2133	1.28	0/2907
1	F	0.91	0/2286	1.30	1/3101 (0.0%)
All	All	0.87	2/13407 (0.0%)	1.29	21/18220 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	MET	SD-CE	-6.83	1.62	1.79
1	C	150	MET	SD-CE	-6.79	1.62	1.79

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	84	GLY	N-CA-C	6.20	121.68	113.37
1	D	205	ASN	CA-C-N	5.66	128.19	120.54
1	D	205	ASN	C-N-CA	5.66	128.19	120.54
1	D	212	GLN	CA-C-N	5.41	127.53	120.28
1	D	212	GLN	C-N-CA	5.41	127.53	120.28
1	A	212	GLN	CA-C-N	5.39	127.51	120.28
1	A	212	GLN	C-N-CA	5.39	127.51	120.28
1	B	145	HIS	CA-C-N	5.39	130.72	121.87
1	B	145	HIS	C-N-CA	5.39	130.72	121.87
1	D	201	PRO	CA-C-N	5.32	127.63	120.50
1	D	201	PRO	C-N-CA	5.32	127.63	120.50
1	A	9	GLU	CB-CG-CD	5.28	121.57	112.60
1	D	287	HIS	CA-C-N	5.10	130.87	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	287	HIS	C-N-CA	5.10	130.87	121.70
1	A	201	PRO	CA-C-N	5.08	127.31	120.50
1	A	201	PRO	C-N-CA	5.08	127.31	120.50
1	D	277	ASN	CA-CB-CG	5.07	117.67	112.60
1	C	64	THR	CA-C-N	5.06	127.06	120.28
1	C	64	THR	C-N-CA	5.06	127.06	120.28
1	A	64	THR	CA-C-N	5.04	127.28	120.38
1	A	64	THR	C-N-CA	5.04	127.28	120.38

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	2230	0	2177	15	0
1	B	2104	0	1967	8	0
1	C	2242	0	2199	14	0
1	D	2235	0	2180	10	0
1	E	2093	0	1948	11	0
1	F	2238	0	2186	19	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	4	0	6	0	0
3	D	8	0	12	0	0
3	F	4	0	6	1	0
4	A	242	0	0	1	0
4	B	94	0	0	1	0
4	C	209	0	0	2	0
4	D	206	0	0	1	0
4	E	97	0	0	0	0
4	F	207	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14225	0	12681	69	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 3.

All (69) 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:124:LEU:HD12	1:A:150:MET:HE1	1.54	0.89
1:F:287:HIS:O	1:F:288:LEU:CB	2.38	0.71
1:C:124:LEU:HD12	1:C:150:MET:HE1	1.74	0.68
1:C:104:LEU:HG	1:C:150:MET:HE3	1.76	0.67
1:A:26:MET:HE2	1:C:118:GLU:HB3	1.78	0.65
1:D:48:GLY:HA3	4:D:2025:HOH:O	2.03	0.57
1:F:110:ARG:HD2	4:F:2103:HOH:O	2.05	0.56
1:D:26:MET:HE2	1:F:118:GLU:HB3	1.87	0.56
1:E:5:LEU:HB2	1:E:19:LEU:HD11	1.86	0.56
1:B:118:GLU:HB3	1:C:26:MET:HE2	1.89	0.55
1:E:118:GLU:HB3	1:F:26:MET:HE2	1.88	0.55
1:F:124:LEU:HD13	1:F:139:VAL:HG21	1.89	0.55
1:E:145:HIS:HA	1:E:174:PHE:HA	1.90	0.54
1:B:181:MET:HG3	1:B:267:LYS:HE3	1.90	0.53
1:A:177:LEU:HG	1:A:267:LYS:HD2	1.89	0.53
1:A:124:LEU:HD12	1:A:150:MET:CE	2.35	0.52
1:C:124:LEU:HD13	1:C:139:VAL:HG21	1.92	0.51
1:F:74:VAL:CG1	1:F:150:MET:HE1	2.40	0.51
1:F:238:VAL:HG23	1:F:284:TRP:CZ3	2.45	0.51
1:A:239:MET:HE1	4:A:2223:HOH:O	2.10	0.51
1:D:187:LEU:HA	1:D:190:ILE:HD12	1.92	0.51
1:C:11:LEU:HD11	1:C:17:ARG:HB2	1.93	0.51
1:E:276:SER:OG	1:E:284:TRP:NE1	2.43	0.51
1:A:104:LEU:HG	1:A:150:MET:HE3	1.93	0.51
1:E:276:SER:HG	1:E:284:TRP:CD1	2.29	0.50
1:D:74:VAL:CG1	1:D:150:MET:HE1	2.43	0.49
1:A:237:THR:HG23	1:A:240:GLU:H	1.77	0.49
1:C:187:LEU:HA	1:C:190:ILE:HD12	1.95	0.49
1:A:187:LEU:HA	1:A:190:ILE:HD12	1.95	0.48
1:C:49:GLU:HG3	1:C:81:ASP:HA	1.94	0.48
1:D:49:GLU:HG3	1:D:81:ASP:HA	1.95	0.48
1:F:49:GLU:HG3	1:F:81:ASP:HA	1.96	0.48
1:F:187:LEU:HA	1:F:190:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:VAL:HG12	1:E:150:MET:HE1	1.96	0.48
1:E:124:LEU:HD13	1:E:139:VAL:HG21	1.96	0.47
1:F:7:ARG:HA	1:F:19:LEU:HD12	1.96	0.47
1:A:6:GLN:OE1	1:F:57:SER:HB3	2.14	0.47
1:A:238:VAL:HG23	1:A:284:TRP:CZ3	2.48	0.47
1:A:238:VAL:HG23	1:A:284:TRP:HZ3	1.78	0.47
1:E:74:VAL:CG1	1:E:150:MET:HE1	2.45	0.47
1:A:142:THR:O	1:A:149:HIS:HB3	2.15	0.46
1:F:238:VAL:HG23	1:F:284:TRP:HZ3	1.79	0.46
1:E:49:GLU:HG3	1:E:81:ASP:HA	1.97	0.46
1:B:5:LEU:HB2	1:B:19:LEU:HD11	1.98	0.46
1:B:124:LEU:HD13	1:B:139:VAL:HG21	1.97	0.46
1:B:59:LEU:HD23	1:B:93:ILE:HD13	1.99	0.44
1:D:118:GLU:HB3	1:E:26:MET:HE2	1.98	0.44
1:B:49:GLU:HG3	1:B:81:ASP:HA	1.98	0.44
1:D:124:LEU:HD13	1:D:139:VAL:HG21	1.99	0.44
1:C:221:GLU:OE1	1:C:267:LYS:HD3	2.18	0.43
1:E:75:VAL:HG21	1:E:86:ILE:HD11	2.00	0.43
1:C:5:LEU:HB2	1:C:19:LEU:HD11	2.00	0.43
1:A:49:GLU:HG3	1:A:81:ASP:HA	2.01	0.42
1:C:71:GLN:HG2	1:C:72:GLU:HG2	2.00	0.42
1:C:280:PRO:HD2	4:C:2203:HOH:O	2.18	0.42
1:B:118:GLU:OE2	4:B:2064:HOH:O	2.21	0.42
1:D:74:VAL:HG13	1:D:150:MET:HE1	2.01	0.42
1:C:41[A]:ARG:HB3	1:C:71:GLN:HB2	2.02	0.42
1:F:145:HIS:HA	1:F:174:PHE:HA	2.01	0.42
1:C:116:ASN:HB2	4:C:2110:HOH:O	2.19	0.41
1:F:217:ARG:HD3	3:F:1289:EDO:H22	2.03	0.41
1:D:110:ARG:HH22	1:F:111:GLU:CD	2.28	0.41
1:F:46:ASP:CG	1:F:82:HIS:HD1	2.29	0.41
1:F:102:LYS:HD3	1:F:124:LEU:HD21	2.02	0.41
1:A:75:VAL:HG21	1:A:86:ILE:HD11	2.02	0.40
1:D:160:ILE:HD13	1:D:187:LEU:HD22	2.02	0.40
1:B:238:VAL:O	1:B:242:VAL:HG23	2.22	0.40
1:F:177:LEU:HG	1:F:267:LYS:HD2	2.02	0.40
1:A:4:VAL:HB	1:F:61:GLN:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	286/289 (99%)	279 (98%)	7 (2%)	0	100	100
1	B	281/289 (97%)	274 (98%)	7 (2%)	0	100	100
1	C	284/289 (98%)	276 (97%)	8 (3%)	0	100	100
1	D	286/289 (99%)	278 (97%)	8 (3%)	0	100	100
1	E	280/289 (97%)	271 (97%)	9 (3%)	0	100	100
1	F	284/289 (98%)	275 (97%)	9 (3%)	0	100	100
All	All	1701/1734 (98%)	1653 (97%)	48 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	229/256 (90%)	227 (99%)	2 (1%)	70	87
1	B	200/256 (78%)	198 (99%)	2 (1%)	68	86
1	C	238/256 (93%)	234 (98%)	4 (2%)	53	78
1	D	232/256 (91%)	230 (99%)	2 (1%)	70	87
1	E	199/256 (78%)	199 (100%)	0	100	100
1	F	235/256 (92%)	232 (99%)	3 (1%)	61	82
All	All	1333/1536 (87%)	1320 (99%)	13 (1%)	68	86

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	194	ILE
1	B	152	LEU
1	B	171	THR
1	C	7	ARG
1	C	10	ARG
1	C	234	LYS
1	C	287	HIS
1	D	5	LEU
1	D	10	ARG
1	F	7	ARG
1	F	140	LEU
1	F	188	LEU

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

Mol	Chain	Res	Type
1	A	259	HIS
1	A	260	ASN
1	B	231	ASN
1	C	109	GLN
1	C	120	GLN
1	C	260	ASN
1	D	120	GLN
1	D	259	HIS
1	D	260	ASN
1	E	260	ASN
1	F	204	HIS
1	F	231	ASN
1	F	260	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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	F	1289	-	3,3,3	0.45	0	2,2,2	0.31	0
3	EDO	A	1289	-	3,3,3	0.32	0	2,2,2	0.65	0
3	EDO	D	1290	-	3,3,3	0.37	0	2,2,2	0.62	0
3	EDO	D	1289	-	3,3,3	0.33	0	2,2,2	0.61	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	F	1289	-	-	1/1/1/1	-
3	EDO	A	1289	-	-	0/1/1/1	-
3	EDO	D	1290	-	-	0/1/1/1	-
3	EDO	D	1289	-	-	0/1/1/1	-

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	F	1289	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1289	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	288/289 (99%)	-0.19	6 (2%) 63 58	16, 36, 66, 86	0
1	B	285/289 (98%)	0.46	25 (8%) 15 12	30, 64, 96, 124	0
1	C	285/289 (98%)	-0.22	3 (1%) 78 74	16, 35, 64, 91	1 (0%)
1	D	288/289 (99%)	-0.13	6 (2%) 63 58	18, 40, 68, 85	0
1	E	284/289 (98%)	0.43	24 (8%) 16 13	31, 62, 106, 140	0
1	F	285/289 (98%)	-0.27	3 (1%) 78 74	13, 33, 60, 82	1 (0%)
All	All	1715/1734 (98%)	0.01	67 (3%) 43 38	13, 43, 90, 140	2 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	278	THR	5.8
1	E	280	PRO	4.3
1	F	288	LEU	4.3
1	B	287	HIS	4.1
1	B	280	PRO	3.9
1	A	98	THR	3.8
1	B	3	ALA	3.5
1	A	97	THR	3.3
1	E	97	THR	3.3
1	E	281	ASP	3.2
1	D	98	THR	3.2
1	C	4	VAL	3.1
1	B	232	PHE	3.1
1	B	279	ASP	3.1
1	E	286	ALA	3.1
1	E	284	TRP	3.0
1	B	94	ASN	3.0
1	A	96	ASP	3.0
1	E	277	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	284	TRP	2.9
1	E	248	ASN	2.9
1	E	238	VAL	2.8
1	C	5	LEU	2.7
1	E	2	ALA	2.7
1	F	98	THR	2.7
1	E	282	LYS	2.6
1	B	96	ASP	2.6
1	B	223	GLN	2.6
1	B	278	THR	2.6
1	E	171	THR	2.6
1	B	236	PHE	2.6
1	F	4	VAL	2.5
1	A	279	ASP	2.5
1	E	207	GLU	2.5
1	E	233	GLU	2.5
1	E	4	VAL	2.5
1	B	215	SER	2.4
1	A	1	MET	2.4
1	E	232	PHE	2.4
1	B	233	GLU	2.4
1	B	238	VAL	2.4
1	B	2	ALA	2.4
1	E	274	ILE	2.3
1	B	282	LYS	2.3
1	D	97	THR	2.3
1	D	94	ASN	2.3
1	D	281	ASP	2.3
1	B	211	GLN	2.3
1	E	275	PHE	2.3
1	E	215	SER	2.2
1	D	1	MET	2.2
1	E	189	LYS	2.2
1	B	248	ASN	2.1
1	E	3	ALA	2.1
1	B	285	LYS	2.1
1	B	190	ILE	2.1
1	B	67	ASN	2.1
1	E	236	PHE	2.1
1	E	247	LYS	2.1
1	D	171	THR	2.1
1	B	4	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	281	ASP	2.0
1	E	98	THR	2.0
1	B	61	GLN	2.0
1	B	207	GLU	2.0
1	A	171	THR	2.0
1	B	13	ASN	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
3	EDO	F	1289	4/4	0.94	0.12	42,46,48,49	0
3	EDO	D	1290	4/4	0.97	0.08	31,34,37,42	0
3	EDO	A	1289	4/4	0.97	0.08	34,35,35,38	0
3	EDO	D	1289	4/4	0.98	0.07	39,39,40,43	0
2	ZN	B	1000	1/1	0.99	0.04	50,50,50,50	0
2	ZN	C	1001	1/1	1.00	0.01	31,31,31,31	0
2	ZN	D	1000	1/1	1.00	0.03	37,37,37,37	0
2	ZN	D	1001	1/1	1.00	0.04	31,31,31,31	0
2	ZN	E	1000	1/1	1.00	0.02	55,55,55,55	0
2	ZN	E	1001	1/1	1.00	0.03	54,54,54,54	0
2	ZN	F	1000	1/1	1.00	0.03	33,33,33,33	0
2	ZN	F	1001	1/1	1.00	0.04	30,30,30,30	0
2	ZN	A	1001	1/1	1.00	0.02	30,30,30,30	0
2	ZN	A	1000	1/1	1.00	0.02	28,28,28,28	0
2	ZN	B	1001	1/1	1.00	0.03	48,48,48,48	0
2	ZN	C	1000	1/1	1.00	0.04	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.