



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2026 – 04:24 am BST

PDB ID : 9H60 / pdb\_00009h60  
Title : Leishmania braziliensis ISP2 in complex with bovine alpha-chymotrypsin  
Authors : Freitag-Pohl, S.; Pohl, E.  
Deposited on : 2024-10-23  
Resolution : 1.90 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	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
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

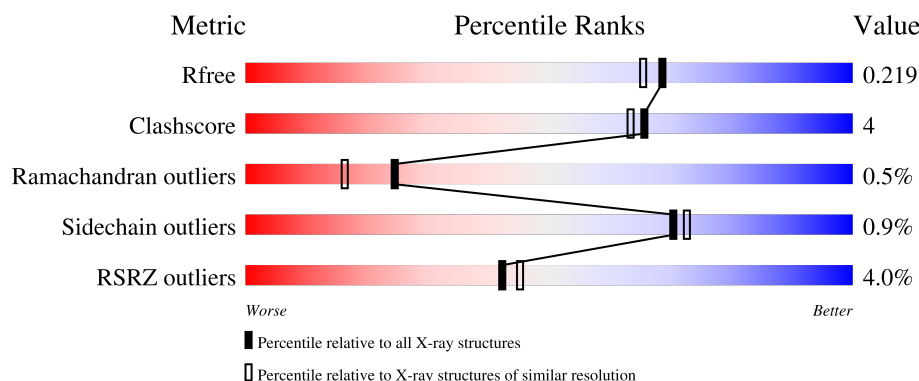
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	158	<div> <div>7%</div> <div> <div></div> <div>75%</div> <div>10%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	158	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>•</div> <div>11%</div> </div> </div>
2	B	245	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div>•</div> </div> </div>
2	D	245	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>•</div> </div> </div>

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	ACT	D	307	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11975 atoms, of which 5826 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 Ecotin-like protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	137	Total	C	H	N	O	S	55	1	0
			2098	683	1045	177	190	3			
1	C	141	Total	C	H	N	O	S	54	0	0
			2153	702	1072	182	195	2			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A4H823
A	2	PRO	-	expression tag	UNP A4H823
A	3	ALA	-	expression tag	UNP A4H823
A	4	GLY	-	expression tag	UNP A4H823
A	112	ARG	HIS	conflict	UNP A4H823
C	1	MET	-	initiating methionine	UNP A4H823
C	2	PRO	-	expression tag	UNP A4H823
C	3	ALA	-	expression tag	UNP A4H823
C	4	GLY	-	expression tag	UNP A4H823
C	112	ARG	HIS	conflict	UNP A4H823

- Molecule 2 is a protein called Chymotrypsinogen A.

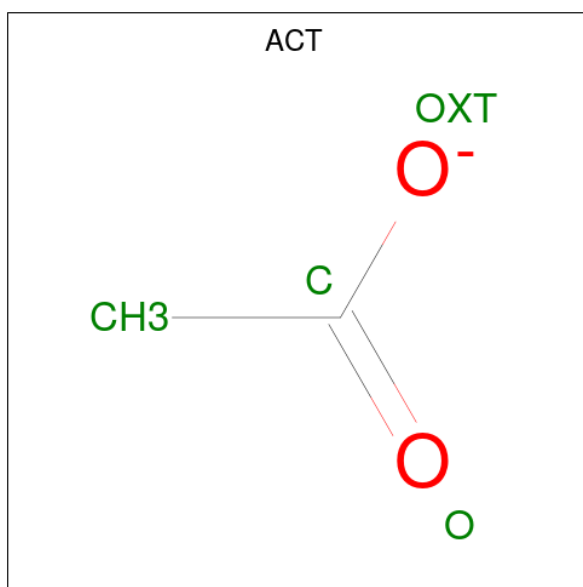
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	239	Total	C	H	N	O	S	69	3	0
			3466	1095	1722	293	344	12			
2	D	240	Total	C	H	N	O	S	68	4	0
			3504	1109	1742	294	346	13			

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	4	1
			34	8	20	6		
3	A	1	Total	C	H	O	2	0
			17	4	10	3		
3	B	1	Total	C	H	O	2	0
			17	4	10	3		
3	D	1	Total	C	H	O	2	0
			17	4	10	3		
3	D	1	Total	C	H	O	2	0
			17	4	10	3		
3	D	1	Total	C	H	O	2	0
			17	4	10	3		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



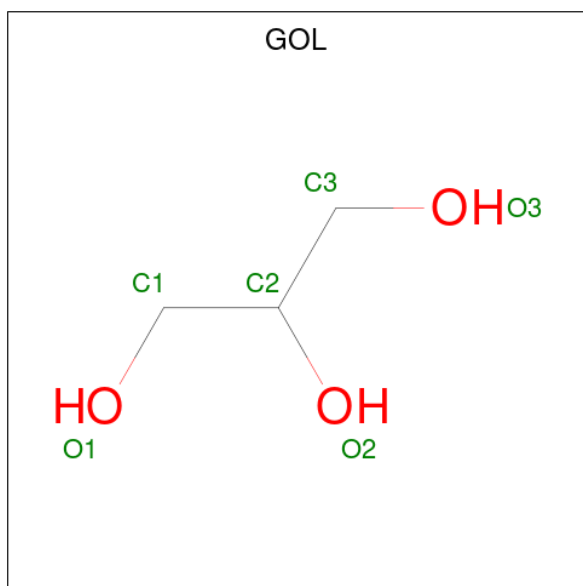
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	3	0
			7	2	3	2		
4	A	1	Total	C	H	O	3	0
			7	2	3	2		
4	A	1	Total	C	H	O	3	0
			7	2	3	2		
4	B	1	Total	C	H	O	3	0
			7	2	3	2		
4	B	1	Total	C	H	O	3	0
			7	2	3	2		
4	B	1	Total	C	H	O	3	0
			7	2	3	2		
4	B	1	Total	C	H	O	3	0
			7	2	3	2		
4	C	1	Total	C	H	O	3	0
			7	2	3	2		
4	C	1	Total	C	H	O	3	0
			7	2	3	2		
4	C	1	Total	C	H	O	3	0
			7	2	3	2		
4	C	1	Total	C	H	O	3	0
			7	2	3	2		
4	D	1	Total	C	H	O	3	0
			7	2	3	2		
4	D	1	Total	C	H	O	3	0
			7	2	3	2		
4	D	1	Total	C	H	O	3	0
			7	2	3	2		

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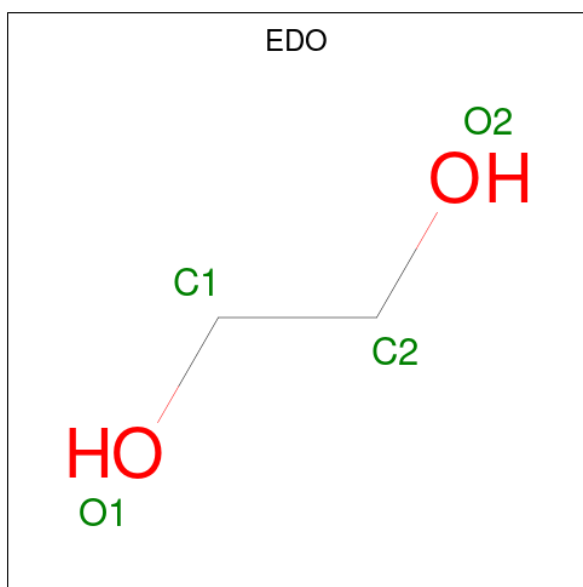
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	H	O	3	0
			7	2	3	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	3	0
			14	3	8	3		
5	B	1	Total	C	H	O	3	0
			14	3	8	3		
5	B	1	Total	C	H	O	3	0
			14	3	8	3		
5	B	1	Total	C	H	O	3	0
			14	3	8	3		
5	B	1	Total	C	H	O	3	0
			14	3	8	3		
5	C	1	Total	C	H	O	3	0
			14	3	8	3		
5	D	1	Total	C	H	O	3	0
			14	3	8	3		
5	D	1	Total	C	H	O	3	0
			14	3	8	3		
5	D	1	Total	C	H	O	3	0
			14	3	8	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	2	0
			10	2	6	2		
6	A	1	Total	C	H	O	2	0
			10	2	6	2		
6	B	1	Total	C	H	O	2	0
			10	2	6	2		
6	B	1	Total	C	H	O	2	0
			10	2	6	2		
6	D	1	Total	C	H	O	2	0
			10	2	6	2		
6	D	1	Total	C	H	O	2	0
			10	2	6	2		
6	D	1	Total	C	H	O	2	0
			10	2	6	2		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Cl	0	0
			1	1		

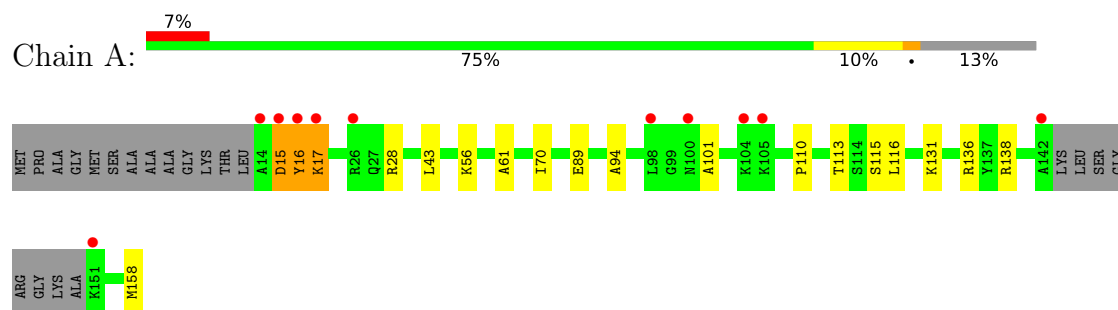
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	28	Total 28	O 28	0	0
8	B	110	Total 110	O 110	0	0
8	C	50	Total 50	O 50	0	0
8	D	118	Total 118	O 118	0	0

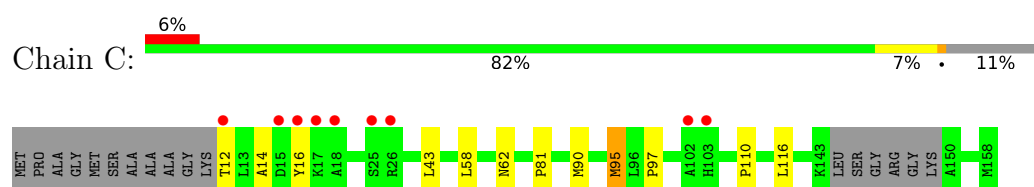
### 3 Residue-property plots [i](#)

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.

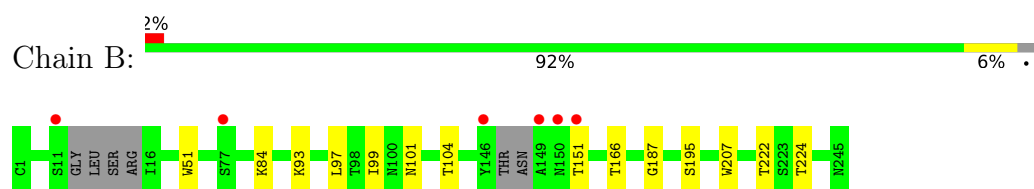
- Molecule 1: Ecotin-like protein 2



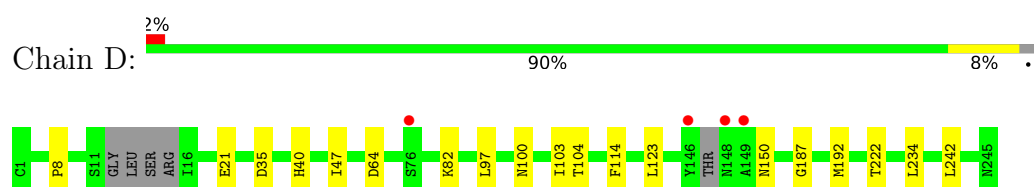
- Molecule 1: Ecotin-like protein 2



- Molecule 2: Chymotrypsinogen A



- Molecule 2: Chymotrypsinogen A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.28Å 92.09Å 96.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.87 – 1.90 53.87 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (53.87-1.90) 100.0 (53.87-1.90)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.181 , 0.217 0.184 , 0.219	Depositor DCC
$R_{free}$ test set	3275 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11975	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, PEG, CL, GOL, 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	0.55	0/1083	0.98	0/1478
1	C	0.57	0/1109	0.96	1/1515 (0.1%)
2	B	0.61	0/1787	0.94	1/2438 (0.0%)
2	D	0.63	0/1808	0.94	0/2467
All	All	0.60	0/5787	0.95	2/7898 (0.0%)

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	A	0	3
1	C	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	95	MET	CG-SD-CE	-7.98	83.35	100.90
2	B	166	THR	CA-CB-OG1	-6.02	100.57	109.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	PRO	Peptide
1	A	136	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	138	ARG	Sidechain
1	C	110	PRO	Peptide

## 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	1053	1045	1011	12	0
1	C	1081	1072	1041	11	0
2	B	1744	1722	1703	9	0
2	D	1762	1742	1728	19	0
3	A	21	30	30	2	0
3	B	7	10	10	2	0
3	D	28	40	40	3	0
4	A	12	9	9	0	0
4	B	16	12	12	0	0
4	C	16	12	12	1	0
4	D	16	12	12	3	0
5	A	6	8	8	1	0
5	B	24	32	32	0	0
5	C	6	8	8	0	0
5	D	18	24	24	2	0
6	A	8	12	12	1	0
6	B	8	12	11	2	0
6	D	16	24	24	2	0
7	C	1	0	0	0	0
8	A	28	0	0	0	0
8	B	110	0	0	1	0
8	C	50	0	0	0	0
8	D	118	0	0	3	0
All	All	6149	5826	5727	44	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 4.

All (44) 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)
2:D:123:LEU:HD12	4:D:308:ACT:H3	1.43	0.99
2:B:51:TRP:HE1	3:B:301:PEG:H31	1.28	0.95
2:D:100:ASN:HD22	6:D:315:EDO:H21	1.32	0.93
1:A:28:ARG:NH1	1:A:131:LYS:O	2.09	0.86
4:C:203:ACT:H1	8:D:498:HOH:O	1.83	0.77
2:B:51:TRP:HE1	3:B:301:PEG:C3	2.04	0.70
1:C:95:MET:HE1	5:D:309:GOL:O3	1.93	0.68
2:D:21:GLU:O	3:D:303:PEG:H21	1.98	0.63
1:A:89[A]:GLU:OE1	2:B:224:THR:HG21	1.99	0.63
2:D:8:PRO:HD2	3:D:301:PEG:H11	1.81	0.61
1:C:62:ASN:ND2	2:D:192[B]:MET:HE3	2.19	0.57
1:A:116:LEU:H	3:A:201[A]:PEG:H12	1.70	0.56
1:A:16:TYR:O	1:A:17:LYS:CB	2.55	0.55
3:A:201[A]:PEG:H11	1:C:116:LEU:HG	1.87	0.55
1:C:97:PRO:HD3	2:D:192[B]:MET:HE1	1.88	0.55
2:D:150:ASN:ND2	8:D:403:HOH:O	2.37	0.54
1:C:97:PRO:HD3	2:D:192[B]:MET:CE	2.37	0.54
2:D:103:ILE:HD12	2:D:234:LEU:HD12	1.89	0.54
4:D:307:ACT:O	8:D:401:HOH:O	2.18	0.54
6:B:310:EDO:H12	8:B:450:HOH:O	2.08	0.52
2:B:93:LYS:HE2	2:B:101[A]:ASN:HD21	1.75	0.51
1:A:15:ASP:O	1:A:16:TYR:C	2.54	0.50
2:D:82:LYS:O	3:D:304:PEG:H12	2.12	0.49
2:B:93:LYS:HD2	1:C:81:PRO:HD3	1.93	0.49
1:C:62:ASN:HD21	2:D:192[B]:MET:HE3	1.79	0.47
2:B:207:TRP:HE1	6:B:310:EDO:H11	1.79	0.46
1:C:58:LEU:HD21	1:C:90:MET:HE1	1.98	0.46
1:C:14:ALA:C	1:C:16:TYR:H	2.24	0.45
2:D:47:ILE:CD1	2:D:242:LEU:HD21	2.47	0.44
1:A:16:TYR:O	5:A:206:GOL:O3	2.27	0.44
1:A:61:ALA:HB2	1:A:101:ALA:HB1	2.01	0.43
2:D:40:HIS:HB3	6:D:312:EDO:H12	2.00	0.43
1:A:43:LEU:HD21	2:D:97:LEU:HG	2.00	0.43
1:A:94:ALA:C	2:B:195:SER:OG	2.62	0.43
1:A:70:ILE:HD12	1:A:113:THR:HG21	2.01	0.42
1:A:158:MET:HE1	1:C:12:THR:HA	2.02	0.41
2:B:187:GLY:C	2:B:222:THR:HB	2.45	0.41
2:D:187:GLY:C	2:D:222:THR:HB	2.45	0.41
1:A:115:SER:HB3	6:A:208:EDO:H21	2.03	0.41
2:D:114:PHE:HD2	4:D:307:ACT:H2	1.86	0.41
2:D:103:ILE:CD1	2:D:234:LEU:HD12	2.51	0.41
2:B:97:LEU:HG	1:C:43:LEU:HG	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:ASP:HA	2:D:64:ASP:OD1	2.22	0.40
2:D:64:ASP:OD1	5:D:309:GOL:H12	2.21	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	134/158 (85%)	129 (96%)	2 (2%)	3 (2%)	5	1
1	C	137/158 (87%)	135 (98%)	2 (2%)	0	100	100
2	B	236/245 (96%)	230 (98%)	5 (2%)	1 (0%)	30	22
2	D	238/245 (97%)	232 (98%)	6 (2%)	0	100	100
All	All	745/806 (92%)	726 (97%)	15 (2%)	4 (0%)	24	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	TYR
1	A	17	LYS
1	A	15	ASP
2	B	99	ILE

### 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	102/128 (80%)	101 (99%)	1 (1%)	68	70
1	C	105/128 (82%)	105 (100%)	0	100	100
2	B	192/200 (96%)	189 (98%)	3 (2%)	55	54
2	D	195/200 (98%)	194 (100%)	1 (0%)	81	84
All	All	594/656 (90%)	589 (99%)	5 (1%)	70	75

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
2	B	84	LYS
2	B	104	THR
2	B	151	THR
2	D	104	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	63	HIS
2	B	50	ASN
2	B	116	GLN
1	C	44	ASN
1	C	103	HIS
2	D	50	ASN
2	D	100	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 41 ligands modelled in this entry, 1 is monoatomic - leaving 40 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	ACT	D	305	-	3,3,3	0.89	0	3,3,3	0.95	0
6	EDO	B	311	-	3,3,3	1.97	1 (33%)	2,2,2	1.06	0
3	PEG	A	202	-	6,6,6	0.29	0	5,5,5	0.17	0
4	ACT	A	205	-	3,3,3	0.92	0	3,3,3	1.02	0
6	EDO	A	207	-	3,3,3	0.33	0	2,2,2	0.46	0
6	EDO	D	314	-	3,3,3	0.27	0	2,2,2	0.40	0
4	ACT	B	303	-	3,3,3	0.96	0	3,3,3	0.84	0
4	ACT	C	204	-	3,3,3	1.06	0	3,3,3	0.63	0
4	ACT	C	203	-	3,3,3	0.93	0	3,3,3	1.06	0
6	EDO	A	208	-	3,3,3	0.07	0	2,2,2	0.13	0
5	GOL	D	310	-	5,5,5	0.09	0	5,5,5	0.30	0
4	ACT	C	205	-	3,3,3	0.95	0	3,3,3	0.80	0
5	GOL	B	306	-	5,5,5	0.17	0	5,5,5	0.44	0
5	GOL	D	311	-	5,5,5	0.06	0	5,5,5	0.36	0
3	PEG	D	303	-	6,6,6	0.33	0	5,5,5	0.20	0
3	PEG	A	201[A]	-	6,6,6	0.30	0	5,5,5	0.21	0
6	EDO	D	313	-	3,3,3	0.17	0	2,2,2	0.16	0
4	ACT	B	305	-	3,3,3	1.20	0	3,3,3	0.68	0
3	PEG	A	201[B]	-	6,6,6	0.16	0	5,5,5	0.11	0
3	PEG	D	301	-	6,6,6	0.21	0	5,5,5	0.21	0
4	ACT	A	203	-	3,3,3	1.03	0	3,3,3	0.73	0
4	ACT	B	304	-	3,3,3	0.84	0	3,3,3	1.08	0
5	GOL	C	206	-	5,5,5	0.13	0	5,5,5	0.57	0
4	ACT	D	307	-	3,3,3	1.74	1 (33%)	3,3,3	0.95	0
3	PEG	B	301	-	6,6,6	0.38	0	5,5,5	0.44	0
6	EDO	D	315	-	3,3,3	0.22	0	2,2,2	1.23	0
4	ACT	D	308	-	3,3,3	0.70	0	3,3,3	1.11	0
5	GOL	B	308	-	5,5,5	0.28	0	5,5,5	0.60	0
3	PEG	D	304	-	6,6,6	0.24	0	5,5,5	0.23	0
4	ACT	C	202	-	3,3,3	1.06	0	3,3,3	0.77	0
4	ACT	D	306	-	3,3,3	1.06	0	3,3,3	0.79	0
5	GOL	D	309	-	5,5,5	0.14	0	5,5,5	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ACT	B	302	-	3,3,3	1.02	0	3,3,3	1.06	0
3	PEG	D	302	-	6,6,6	0.58	0	5,5,5	0.41	0
4	ACT	A	204	-	3,3,3	1.04	0	3,3,3	0.86	0
5	GOL	B	307	-	5,5,5	0.07	0	5,5,5	0.34	0
6	EDO	D	312	-	3,3,3	0.42	0	2,2,2	0.92	0
6	EDO	B	310	-	3,3,3	0.56	0	2,2,2	0.06	0
5	GOL	A	206	-	5,5,5	0.11	0	5,5,5	0.29	0
5	GOL	B	309	-	5,5,5	0.10	0	5,5,5	0.32	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
6	EDO	B	311	-	-	1/1/1/1	-
3	PEG	A	202	-	-	1/4/4/4	-
6	EDO	A	207	-	-	1/1/1/1	-
6	EDO	D	314	-	-	0/1/1/1	-
6	EDO	A	208	-	-	0/1/1/1	-
5	GOL	D	310	-	-	3/4/4/4	-
5	GOL	B	306	-	-	2/4/4/4	-
5	GOL	D	311	-	-	2/4/4/4	-
3	PEG	D	303	-	-	2/4/4/4	-
3	PEG	A	201[A]	-	-	1/4/4/4	-
6	EDO	D	313	-	-	1/1/1/1	-
3	PEG	A	201[B]	-	-	2/4/4/4	-
3	PEG	D	301	-	-	0/4/4/4	-
5	GOL	C	206	-	-	0/4/4/4	-
3	PEG	B	301	-	-	2/4/4/4	-
6	EDO	D	315	-	-	1/1/1/1	-
5	GOL	B	308	-	-	0/4/4/4	-
3	PEG	D	304	-	-	2/4/4/4	-
3	PEG	D	302	-	-	2/4/4/4	-
5	GOL	B	307	-	-	0/4/4/4	-
6	EDO	D	312	-	-	1/1/1/1	-
6	EDO	B	310	-	-	1/1/1/1	-
5	GOL	A	206	-	-	2/4/4/4	-
5	GOL	B	309	-	-	4/4/4/4	-
5	GOL	D	309	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	311	EDO	O1-C1	-3.25	1.25	1.42
4	D	307	ACT	OXT-C	-2.44	1.19	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	306	GOL	O1-C1-C2-C3
5	D	310	GOL	O1-C1-C2-C3
3	A	201[B]	PEG	O1-C1-C2-O2
3	A	201[B]	PEG	O2-C3-C4-O4
3	D	302	PEG	O1-C1-C2-O2
3	D	303	PEG	O2-C3-C4-O4
3	B	301	PEG	O2-C3-C4-O4
5	B	309	GOL	O1-C1-C2-C3
5	D	309	GOL	O1-C1-C2-C3
5	D	311	GOL	O1-C1-C2-C3
5	B	306	GOL	O1-C1-C2-O2
5	B	309	GOL	O1-C1-C2-O2
5	D	309	GOL	O1-C1-C2-O2
5	D	310	GOL	O1-C1-C2-O2
6	B	311	EDO	O1-C1-C2-O2
3	D	303	PEG	O1-C1-C2-O2
3	D	304	PEG	O2-C3-C4-O4
5	D	310	GOL	O2-C2-C3-O3
5	D	311	GOL	O1-C1-C2-O2
6	B	310	EDO	O1-C1-C2-O2
6	D	312	EDO	O1-C1-C2-O2
3	D	302	PEG	O2-C3-C4-O4
5	A	206	GOL	O1-C1-C2-O2
5	B	309	GOL	O2-C2-C3-O3
3	B	301	PEG	O1-C1-C2-O2
6	A	207	EDO	O1-C1-C2-O2
3	A	202	PEG	O2-C3-C4-O4
6	D	313	EDO	O1-C1-C2-O2
6	D	315	EDO	O1-C1-C2-O2
5	A	206	GOL	O2-C2-C3-O3
3	A	201[A]	PEG	C4-C3-O2-C2
5	B	309	GOL	C1-C2-C3-O3
3	D	304	PEG	O1-C1-C2-O2

There are no ring outliers.

14 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	203	ACT	1	0
6	A	208	EDO	1	0
3	D	303	PEG	1	0
3	A	201[A]	PEG	2	0
3	D	301	PEG	1	0
4	D	307	ACT	2	0
3	B	301	PEG	2	0
6	D	315	EDO	1	0
4	D	308	ACT	1	0
3	D	304	PEG	1	0
5	D	309	GOL	2	0
6	D	312	EDO	1	0
6	B	310	EDO	2	0
5	A	206	GOL	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	137/158 (86%)	0.78	11 (8%) 18 19	24, 45, 67, 81	1 (0%)
1	C	141/158 (89%)	0.61	9 (6%) 25 27	27, 40, 63, 73	0
2	B	239/245 (97%)	-0.07	6 (2%) 58 62	16, 33, 49, 81	4 (1%)
2	D	240/245 (97%)	-0.00	4 (1%) 69 72	16, 33, 49, 86	4 (1%)
All	All	757/806 (93%)	0.23	30 (3%) 42 45	16, 36, 58, 86	9 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	149	ALA	5.7
1	A	15	ASP	5.5
2	D	148	ASN	5.4
1	A	16	TYR	5.4
1	C	12	THR	5.3
2	B	150	ASN	5.1
1	A	14	ALA	5.0
2	D	149	ALA	4.7
1	C	18	ALA	4.4
1	C	15	ASP	3.9
2	D	76	SER	3.8
1	C	17	LYS	3.8
2	B	77	SER	3.8
1	A	105	LYS	3.2
1	C	16	TYR	3.2
1	C	26	ARG	3.1
2	D	146	TYR	3.1
2	B	151	THR	2.9
1	C	102	ALA	2.8
1	A	17	LYS	2.5
1	A	98	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	142	ALA	2.4
1	C	25	SER	2.4
1	A	104	LYS	2.4
1	A	100	ASN	2.4
1	A	26	ARG	2.3
2	B	11	SER	2.3
2	B	146	TYR	2.1
1	A	151	LYS	2.1
1	C	103	HIS	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 [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	ACT	D	306	4/4	0.61	0.24	61,61,69,76	3
3	PEG	A	201[B]	7/7	0.70	0.34	35,41,48,48	17
3	PEG	A	201[A]	7/7	0.70	0.34	30,43,51,52	17
4	ACT	C	204	4/4	0.74	0.28	62,68,71,77	3
6	EDO	D	312	4/4	0.77	0.20	47,54,58,62	2
6	EDO	A	207	4/4	0.80	0.17	55,61,63,63	2
3	PEG	B	301	7/7	0.80	0.18	43,58,63,66	2
3	PEG	D	304	7/7	0.81	0.17	40,54,65,66	2
3	PEG	D	303	7/7	0.82	0.19	59,68,70,75	2
4	ACT	A	203	4/4	0.83	0.20	48,63,64,65	3
4	ACT	A	204	4/4	0.84	0.20	52,56,59,63	3
4	ACT	C	202	4/4	0.84	0.20	60,61,68,71	3
3	PEG	D	302	7/7	0.84	0.15	34,57,62,64	2
5	GOL	D	309	6/6	0.85	0.13	49,59,65,65	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	D	310	6/6	0.85	0.17	68,73,75,75	3
3	PEG	A	202	7/7	0.85	0.17	66,71,73,73	2
4	ACT	C	203	4/4	0.85	0.20	51,59,60,69	3
6	EDO	D	314	4/4	0.85	0.17	62,66,68,68	2
4	ACT	C	205	4/4	0.87	0.19	66,66,67,78	3
5	GOL	B	308	6/6	0.87	0.14	49,58,61,64	3
5	GOL	B	309	6/6	0.87	0.15	65,71,75,77	3
4	ACT	D	305	4/4	0.87	0.15	66,69,70,73	3
4	ACT	D	308	4/4	0.88	0.17	58,65,67,68	3
6	EDO	D	313	4/4	0.88	0.15	44,55,57,58	2
3	PEG	D	301	7/7	0.88	0.15	57,62,75,76	2
6	EDO	A	208	4/4	0.89	0.14	68,71,72,73	2
4	ACT	A	205	4/4	0.89	0.18	54,55,72,76	3
4	ACT	B	305	4/4	0.90	0.17	54,66,66,74	3
4	ACT	D	307	4/4	0.90	0.25	20,58,58,69	3
4	ACT	B	302	4/4	0.90	0.15	48,63,63,65	3
4	ACT	B	304	4/4	0.91	0.17	52,67,68,71	3
5	GOL	B	306	6/6	0.91	0.10	37,44,57,57	3
6	EDO	B	310	4/4	0.91	0.11	39,48,51,52	2
5	GOL	A	206	6/6	0.92	0.11	49,61,64,64	3
6	EDO	D	315	4/4	0.92	0.12	26,30,33,37	2
6	EDO	B	311	4/4	0.93	0.15	16,26,34,41	2
5	GOL	C	206	6/6	0.94	0.09	47,49,52,52	3
4	ACT	B	303	4/4	0.95	0.10	41,58,60,60	3
7	CL	C	201	1/1	0.95	0.10	56,56,56,56	0
5	GOL	D	311	6/6	0.96	0.07	33,39,44,44	3
5	GOL	B	307	6/6	0.96	0.07	36,45,56,56	3

## 6.5 Other polymers [i](#)

There are no such residues in this entry.