



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:47 AM UTC

PDB ID : 2BJG / pdb_00002bjg
Title : Crystal Structure of Conjugated Bile Acid Hydrolase from *Clostridium perfringens* in Complex with Reaction Products Taurine and Deoxycholate
Authors : Rossocha, M.; Schultz-Heienbrok, R.; Von Moeller, H.; Coleman, J.P.; Saenger, W.
Deposited on : 2005-02-02
Resolution : 2.10 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

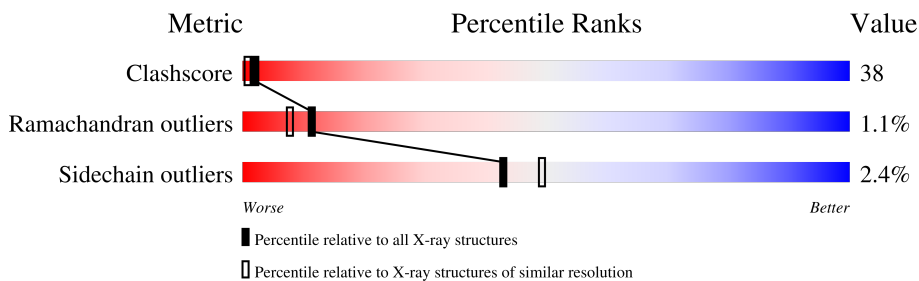
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	329	 82% 14% . .
1	B	329	 83% 13% . .

2 Entry composition [i](#)

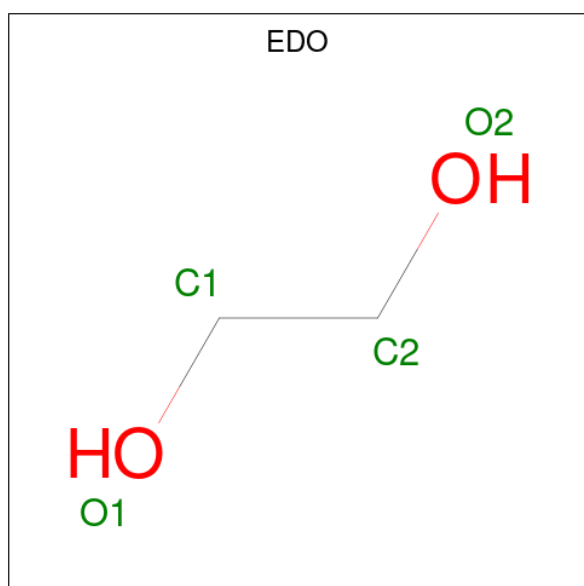
There are 3 unique types of molecules in this entry. The entry contains 5627 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CHOLYLGLYCINE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2608	1660	430	505	13			
1	B	328	Total	C	N	O	S	0	0	0
			2608	1660	430	505	13			

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



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

- Molecule 3 is water.

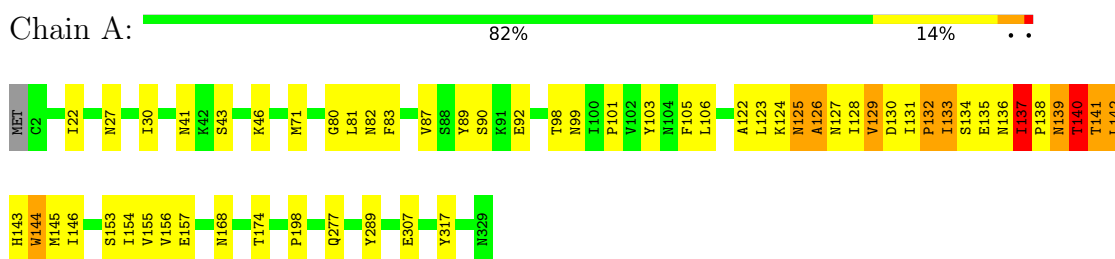
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	206	Total 206	O 206	0	0
3	B	197	Total 197	O 197	0	0

3 Residue-property plots

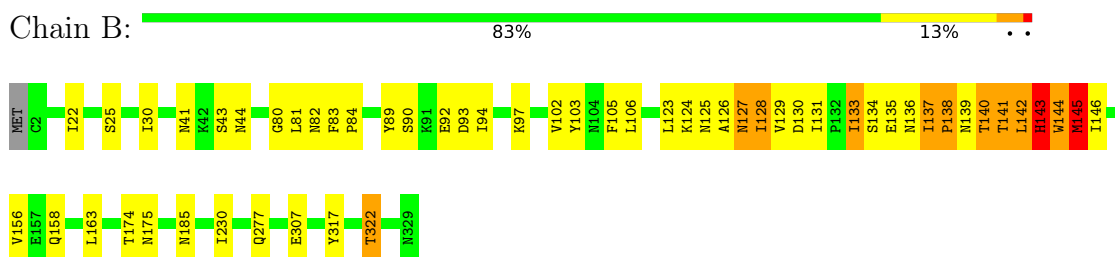
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: CHOLYLGLYCINE HYDROLASE



• Molecule 1: CHOLYLGLYCINE HYDROLASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	63.78Å 63.78Å 341.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10	Depositor
% Data completeness (in resolution range)	81.1 (50.00-2.10)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5627	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.51	0/2658	0.78	3/3597 (0.1%)
1	B	0.53	1/2659 (0.0%)	1.32	8/3600 (0.2%)
All	All	0.52	1/5317 (0.0%)	1.08	11/7197 (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	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	145	MET	C-N	-7.68	1.23	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	MET	O-C-N	-49.62	57.92	122.43
1	B	145	MET	CA-C-N	26.91	156.56	123.19
1	B	145	MET	C-N-CA	26.91	156.56	123.19
1	A	144	TRP	N-CA-C	7.52	121.64	110.52
1	B	137	ILE	CA-C-N	7.46	129.17	119.84
1	B	137	ILE	C-N-CA	7.46	129.17	119.84
1	A	137	ILE	CA-C-N	7.39	129.08	119.84
1	A	137	ILE	C-N-CA	7.39	129.08	119.84
1	B	143	HIS	N-CA-C	-6.59	99.17	109.72
1	B	141	THR	N-CA-C	-5.78	106.07	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	THR	N-CA-C	5.31	118.23	109.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	145	MET	Mainchain

5.2 Too-close contacts [i](#)

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	2608	0	2559	200	3
1	B	2608	0	2562	189	3
2	A	8	0	12	1	0
3	A	206	0	0	6	0
3	B	197	0	0	11	0
All	All	5627	0	5133	389	3

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 38.

All (389) 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:B:89:TYR:CD1	1:B:128:ILE:HD12	1.23	1.67
1:A:101:PRO:HB3	1:A:131:ILE:CG2	1.28	1.61
1:A:87:VAL:CG1	1:A:141:THR:HG21	1.23	1.60
1:A:81:LEU:N	1:A:142:LEU:CD2	1.68	1.52
1:A:87:VAL:HG11	1:A:141:THR:CG2	1.48	1.44
1:A:145:MET:HE2	1:A:168:ASN:ND2	1.34	1.38
1:B:83:PHE:CB	1:B:141:THR:O	1.71	1.37
1:A:145:MET:C	1:A:154:ILE:O	1.68	1.35
1:B:89:TYR:CD1	1:B:128:ILE:CD1	2.11	1.34
1:A:132:PRO:HG2	3:A:2027:HOH:O	1.25	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLY:C	1:A:142:LEU:HD21	1.55	1.31
1:B:89:TYR:CE1	1:B:128:ILE:HD12	1.65	1.30
1:A:81:LEU:N	1:A:142:LEU:HD21	0.97	1.30
1:B:83:PHE:C	1:B:141:THR:HB	1.56	1.29
1:A:46:LYS:HE3	1:A:131:ILE:CD1	1.63	1.28
1:B:102:VAL:CB	1:B:139:ASN:OD1	1.81	1.28
1:B:94:ILE:HD12	1:B:127:ASN:OD1	1.34	1.27
1:A:43:SER:HB2	1:A:134:SER:O	1.30	1.27
1:B:81:LEU:O	1:B:142:LEU:HA	1.17	1.26
1:B:89:TYR:HD1	1:B:128:ILE:CD1	1.47	1.26
1:B:142:LEU:HD21	3:B:2050:HOH:O	1.29	1.26
1:A:145:MET:CG	1:A:154:ILE:O	1.84	1.26
1:A:81:LEU:O	1:A:142:LEU:HD23	1.35	1.25
1:B:103:TYR:CZ	1:B:133:ILE:HB	1.72	1.25
1:A:99:ASN:OD1	1:A:127:ASN:ND2	1.68	1.24
1:A:144:TRP:CB	1:A:156:VAL:HB	1.66	1.24
1:A:101:PRO:CB	1:A:131:ILE:HG21	1.66	1.24
1:A:89:TYR:OH	1:A:141:THR:CA	1.83	1.23
1:A:145:MET:CE	1:A:168:ASN:ND2	2.03	1.22
1:A:101:PRO:CB	1:A:131:ILE:CG2	2.19	1.21
1:A:145:MET:CE	1:A:168:ASN:HD22	1.51	1.21
1:A:89:TYR:CD1	1:A:128:ILE:HG22	1.75	1.20
1:A:43:SER:CB	1:A:134:SER:O	1.88	1.20
1:A:145:MET:HA	1:A:155:VAL:CA	1.71	1.19
1:B:82:ASN:OD1	1:B:141:THR:OG1	1.59	1.19
1:B:83:PHE:HB3	1:B:141:THR:O	1.02	1.18
1:A:145:MET:CA	1:A:154:ILE:O	1.90	1.18
1:B:144:TRP:CZ3	1:B:156:VAL:HG11	1.77	1.18
1:B:82:ASN:O	1:B:143:HIS:CE1	1.97	1.17
1:A:145:MET:CA	1:A:155:VAL:HA	1.75	1.16
1:B:94:ILE:CD1	1:B:127:ASN:OD1	1.94	1.15
1:A:46:LYS:CE	1:A:131:ILE:HD11	1.75	1.15
1:A:89:TYR:OH	1:A:141:THR:HA	0.99	1.15
1:A:122:ALA:O	1:A:125:ASN:HA	1.47	1.14
1:B:127:ASN:ND2	3:B:2072:HOH:O	1.81	1.14
1:A:89:TYR:CZ	1:A:141:THR:HG22	1.83	1.13
1:B:82:ASN:O	1:B:143:HIS:HE1	1.30	1.13
1:A:89:TYR:CE2	1:A:140:THR:O	2.02	1.13
1:A:101:PRO:HB3	1:A:131:ILE:HG22	1.21	1.12
1:B:102:VAL:HB	1:B:139:ASN:CG	1.73	1.12
1:B:92:GLU:C	1:B:129:VAL:HG21	1.74	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:VAL:HG21	1:B:130:ASP:OD2	1.48	1.11
1:A:87:VAL:CG1	1:A:141:THR:CG2	2.17	1.11
1:B:128:ILE:HG12	1:B:158:GLN:CD	1.73	1.11
1:A:89:TYR:HE2	1:A:140:THR:O	1.30	1.09
1:A:103:TYR:CE2	1:A:132:PRO:O	2.06	1.09
1:B:124:LYS:C	1:B:125:ASN:N	2.12	1.07
1:A:144:TRP:HB2	1:A:156:VAL:HB	1.33	1.05
1:A:101:PRO:HB3	1:A:131:ILE:HG21	1.09	1.05
1:A:87:VAL:HG13	1:A:141:THR:HG21	1.33	1.04
1:A:101:PRO:CG	1:A:131:ILE:HG21	1.87	1.04
1:A:81:LEU:CA	1:A:142:LEU:HD21	1.86	1.04
1:B:43:SER:OG	1:B:133:ILE:O	1.76	1.04
1:B:89:TYR:CG	1:B:130:ASP:OD1	2.10	1.04
1:B:81:LEU:O	1:B:142:LEU:CA	2.04	1.03
1:B:102:VAL:HB	1:B:139:ASN:OD1	0.85	1.03
1:A:135:GLU:HB3	3:A:2069:HOH:O	1.58	1.02
1:B:138:PRO:HB3	3:B:2074:HOH:O	1.55	1.02
1:B:84:PRO:N	1:B:141:THR:HB	1.75	1.02
1:A:103:TYR:HE2	1:A:132:PRO:O	1.37	1.01
1:A:144:TRP:HB3	1:A:156:VAL:HB	1.36	1.01
1:A:144:TRP:N	1:A:156:VAL:O	1.92	1.01
1:A:89:TYR:CE1	1:A:128:ILE:CG2	2.43	1.01
1:A:145:MET:HG3	1:A:154:ILE:O	1.54	1.01
1:A:87:VAL:HG11	1:A:141:THR:CB	1.89	1.00
1:A:89:TYR:CZ	1:A:141:THR:HA	1.97	0.99
1:B:89:TYR:HD1	1:B:128:ILE:CG1	1.75	0.99
1:B:128:ILE:HG12	1:B:158:GLN:NE2	1.77	0.99
1:A:124:LYS:C	1:A:125:ASN:HB2	1.88	0.98
1:A:99:ASN:HA	1:A:127:ASN:HD22	1.25	0.98
1:A:89:TYR:CE1	1:A:128:ILE:HG22	1.97	0.98
1:B:43:SER:OG	1:B:133:ILE:C	2.09	0.95
1:B:126:ALA:HB3	1:B:163:LEU:CD2	1.96	0.95
1:B:143:HIS:NE2	1:B:174:THR:O	2.00	0.95
1:A:89:TYR:CE2	1:A:141:THR:CG2	2.49	0.94
1:B:80:GLY:C	1:B:142:LEU:HG	1.93	0.93
1:A:81:LEU:O	1:A:142:LEU:CD2	2.16	0.93
1:B:138:PRO:CB	3:B:2074:HOH:O	2.14	0.93
1:B:102:VAL:HG11	1:B:139:ASN:HB3	1.50	0.92
1:A:143:HIS:NE2	1:A:174:THR:O	2.01	0.92
1:A:145:MET:C	1:A:146:ILE:N	2.28	0.92
1:B:126:ALA:O	1:B:163:LEU:HD22	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:THR:HG1	1:A:125:ASN:N	1.68	0.91
1:A:89:TYR:CE2	1:A:141:THR:HG23	2.06	0.90
1:B:102:VAL:CG1	1:B:139:ASN:HB3	2.01	0.90
1:B:81:LEU:N	1:B:142:LEU:HG	1.87	0.90
1:A:89:TYR:HH	1:A:141:THR:HA	1.11	0.89
1:B:124:LYS:O	1:B:125:ASN:N	2.06	0.89
1:A:89:TYR:CZ	1:A:141:THR:CG2	2.56	0.88
1:B:83:PHE:N	1:B:141:THR:OG1	2.07	0.88
1:B:102:VAL:CG2	1:B:130:ASP:CG	2.47	0.87
1:B:133:ILE:O	1:B:133:ILE:HD13	1.73	0.87
1:B:92:GLU:C	1:B:129:VAL:CG2	2.47	0.87
1:A:89:TYR:HE1	1:A:128:ILE:HG21	1.40	0.87
1:B:124:LYS:C	1:B:125:ASN:HB2	2.00	0.87
1:A:145:MET:CB	1:A:154:ILE:O	2.23	0.86
1:B:89:TYR:CB	1:B:130:ASP:OD1	2.24	0.85
1:A:81:LEU:N	1:A:142:LEU:HD22	1.90	0.85
1:B:43:SER:HG	1:B:133:ILE:C	1.84	0.84
1:A:41:ASN:ND2	1:A:133:ILE:HG12	1.92	0.84
1:B:102:VAL:HG21	1:B:130:ASP:CG	2.01	0.84
1:A:145:MET:C	1:A:154:ILE:C	2.45	0.84
1:A:145:MET:HG2	1:A:154:ILE:O	1.77	0.84
1:B:81:LEU:C	1:B:142:LEU:HA	2.02	0.83
1:B:83:PHE:H	1:B:141:THR:CB	1.90	0.83
1:B:126:ALA:HB3	1:B:163:LEU:HD21	1.60	0.83
1:A:80:GLY:C	1:A:142:LEU:CD2	2.31	0.83
1:A:87:VAL:HG11	1:A:141:THR:HG21	0.84	0.83
1:A:129:VAL:HG22	1:A:130:ASP:H	1.42	0.83
1:B:80:GLY:HA3	1:B:142:LEU:HD23	1.60	0.83
1:A:89:TYR:CE1	1:A:128:ILE:HG21	2.14	0.83
1:A:99:ASN:CA	1:A:127:ASN:HD22	1.92	0.83
1:B:82:ASN:CG	1:B:141:THR:OG1	2.20	0.82
1:B:83:PHE:C	1:B:141:THR:CB	2.48	0.82
1:B:84:PRO:HA	1:B:141:THR:CG2	2.09	0.82
1:B:105:PHE:CE2	1:B:144:TRP:CD2	2.48	0.81
1:A:105:PHE:CD2	1:A:144:TRP:CE2	2.68	0.81
1:B:102:VAL:CG2	1:B:130:ASP:OD2	2.27	0.81
1:B:128:ILE:CD1	1:B:158:GLN:HB3	2.10	0.81
1:B:83:PHE:CA	1:B:141:THR:O	2.29	0.81
1:B:103:TYR:CE2	1:B:133:ILE:HB	2.16	0.81
1:A:99:ASN:CG	1:A:127:ASN:ND2	2.38	0.80
1:A:101:PRO:HG3	1:A:131:ILE:HG21	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:THR:HB	1:A:125:ASN:N	1.96	0.80
1:B:105:PHE:CD1	1:B:144:TRP:CH2	2.45	0.80
1:A:89:TYR:CD1	1:A:128:ILE:CG2	2.62	0.79
1:B:81:LEU:O	1:B:143:HIS:N	2.15	0.79
1:A:81:LEU:C	1:A:142:LEU:CD2	2.56	0.79
1:A:41:ASN:HD21	1:A:133:ILE:HG12	1.48	0.79
1:B:144:TRP:CZ3	1:B:156:VAL:CG1	2.65	0.79
1:B:90:SER:OG	1:B:129:VAL:HB	1.82	0.79
1:A:87:VAL:HG21	1:A:141:THR:CG2	2.13	0.78
1:A:89:TYR:CE2	1:A:141:THR:HG22	2.14	0.78
1:A:43:SER:HB3	1:A:134:SER:O	1.82	0.78
1:A:81:LEU:C	1:A:142:LEU:HD23	2.08	0.78
1:A:99:ASN:HA	1:A:127:ASN:ND2	1.99	0.77
1:A:87:VAL:CB	1:A:141:THR:HG21	2.13	0.77
1:B:128:ILE:CG1	1:B:158:GLN:NE2	2.47	0.77
1:B:41:ASN:OD1	1:B:133:ILE:O	2.03	0.76
1:B:128:ILE:HD13	1:B:158:GLN:HB3	1.68	0.76
1:A:90:SER:O	1:A:130:ASP:HB2	1.86	0.76
1:A:128:ILE:HG22	1:A:128:ILE:O	1.84	0.75
1:B:102:VAL:HG11	1:B:139:ASN:CB	2.15	0.75
1:A:81:LEU:CA	1:A:142:LEU:CD2	2.56	0.75
1:A:90:SER:O	1:A:129:VAL:HG22	1.86	0.74
1:B:89:TYR:CD2	1:B:130:ASP:OD1	2.40	0.74
1:B:97:LYS:HD3	1:B:125:ASN:OD1	1.87	0.74
1:A:41:ASN:OD1	1:A:133:ILE:O	2.06	0.74
1:B:144:TRP:CE3	1:B:156:VAL:HB	2.23	0.74
1:B:83:PHE:H	1:B:141:THR:C	1.97	0.73
1:A:145:MET:HE2	1:A:168:ASN:HD22	0.65	0.72
1:B:105:PHE:CD1	1:B:144:TRP:CZ2	2.78	0.72
1:B:83:PHE:HB2	1:B:143:HIS:ND1	2.04	0.72
1:A:87:VAL:CG2	1:A:141:THR:CG2	2.68	0.72
1:A:123:LEU:O	1:A:126:ALA:CB	2.37	0.72
1:B:80:GLY:C	1:B:142:LEU:CG	2.63	0.72
1:B:83:PHE:N	1:B:141:THR:C	2.48	0.72
1:A:87:VAL:HG21	1:A:141:THR:HG22	1.70	0.72
1:B:90:SER:OG	1:B:129:VAL:CB	2.37	0.72
1:B:89:TYR:CE1	1:B:128:ILE:CD1	2.57	0.72
1:A:89:TYR:HD1	1:A:128:ILE:HG22	1.50	0.71
1:A:101:PRO:CB	1:A:131:ILE:HG22	2.07	0.71
1:A:145:MET:O	1:A:154:ILE:HG13	1.88	0.71
1:B:80:GLY:HA3	1:B:142:LEU:CD2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:TYR:CZ	1:B:133:ILE:CB	2.65	0.71
1:B:102:VAL:CG1	1:B:139:ASN:CB	2.69	0.70
1:B:105:PHE:CG	1:B:144:TRP:CZ2	2.78	0.70
1:A:98:THR:CB	1:A:125:ASN:N	2.54	0.69
1:A:90:SER:O	1:A:130:ASP:N	2.25	0.69
1:A:105:PHE:HD2	1:A:144:TRP:CE2	2.08	0.69
1:A:145:MET:CB	1:A:146:ILE:N	2.56	0.69
1:A:123:LEU:C	1:A:126:ALA:H	2.00	0.69
1:A:122:ALA:O	1:A:125:ASN:CA	2.36	0.69
1:A:145:MET:HB3	1:A:146:ILE:N	2.07	0.69
1:B:105:PHE:CD2	1:B:144:TRP:CE2	2.81	0.69
1:B:139:ASN:HA	3:B:2075:HOH:O	1.92	0.68
1:A:133:ILE:HD13	1:A:133:ILE:C	2.19	0.68
1:B:142:LEU:CD2	3:B:2050:HOH:O	2.07	0.68
1:A:46:LYS:HE3	1:A:131:ILE:HD11	0.79	0.68
1:A:145:MET:HA	1:A:155:VAL:HA	0.82	0.68
1:A:83:PHE:CG	1:A:143:HIS:HB3	2.28	0.68
1:B:102:VAL:HG23	1:B:130:ASP:CG	2.18	0.68
1:B:138:PRO:CG	3:B:2074:HOH:O	2.40	0.68
1:B:97:LYS:HA	1:B:125:ASN:OD1	1.95	0.67
1:B:89:TYR:HB3	1:B:130:ASP:OD1	1.93	0.67
1:A:145:MET:HG3	1:A:154:ILE:C	2.20	0.67
1:A:123:LEU:O	1:A:126:ALA:HB2	1.94	0.66
1:A:80:GLY:HA3	1:A:142:LEU:HD13	1.77	0.66
1:A:129:VAL:HG13	1:A:130:ASP:N	2.10	0.66
1:B:84:PRO:CA	1:B:141:THR:HB	2.26	0.66
1:A:80:GLY:HA3	1:A:142:LEU:CD1	2.24	0.66
1:A:89:TYR:CD1	1:A:128:ILE:O	2.47	0.66
1:B:103:TYR:CE1	1:B:133:ILE:HB	2.29	0.66
1:A:41:ASN:HD21	1:A:133:ILE:CG1	2.09	0.66
1:A:92:GLU:O	1:A:129:VAL:HG21	1.96	0.65
1:B:140:THR:HB	1:B:142:LEU:HB2	1.77	0.65
1:A:82:ASN:O	1:A:143:HIS:CE1	2.48	0.65
1:B:307:GLU:OE2	1:B:317:TYR:OH	2.15	0.65
1:A:43:SER:HB3	1:A:134:SER:HA	1.79	0.64
1:A:145:MET:HE1	1:A:168:ASN:ND2	2.06	0.64
1:B:140:THR:HG22	1:B:141:THR:N	2.13	0.64
1:A:133:ILE:HG23	1:A:134:SER:N	2.13	0.64
1:A:144:TRP:HB3	1:A:156:VAL:CB	2.21	0.64
1:A:123:LEU:O	1:A:126:ALA:N	2.30	0.64
1:B:93:ASP:N	1:B:129:VAL:HG21	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:TRP:CE3	1:B:156:VAL:HG11	2.29	0.64
1:A:144:TRP:HB2	1:A:156:VAL:CB	2.20	0.63
1:B:89:TYR:HA	1:B:128:ILE:HG13	1.80	0.63
1:B:140:THR:HG22	1:B:141:THR:H	1.62	0.63
1:B:144:TRP:CE3	1:B:156:VAL:CB	2.81	0.63
1:B:136:ASN:C	1:B:137:ILE:HD12	2.23	0.63
1:A:90:SER:H	1:A:129:VAL:HA	1.63	0.63
1:B:80:GLY:C	1:B:142:LEU:CD2	2.72	0.63
1:B:84:PRO:N	1:B:141:THR:CB	2.58	0.63
1:A:80:GLY:HA2	1:A:142:LEU:HD22	1.81	0.62
1:B:94:ILE:HD12	1:B:127:ASN:CG	2.21	0.62
1:A:105:PHE:CD2	1:A:144:TRP:CZ2	2.87	0.62
1:A:105:PHE:HD2	1:A:144:TRP:CZ2	2.18	0.61
1:A:307:GLU:OE2	1:A:317:TYR:OH	2.17	0.61
1:B:105:PHE:CE2	1:B:144:TRP:CE2	2.89	0.61
1:B:90:SER:OG	1:B:129:VAL:HA	2.00	0.61
1:A:123:LEU:HA	1:A:126:ALA:H	1.65	0.60
1:A:140:THR:OG1	1:A:141:THR:N	2.30	0.60
1:B:102:VAL:CG2	1:B:130:ASP:OD1	2.49	0.60
1:B:105:PHE:CD2	1:B:144:TRP:CZ2	2.89	0.60
1:B:138:PRO:HG3	3:B:2074:HOH:O	1.99	0.60
1:B:145:MET:O	1:B:146:ILE:HG13	2.00	0.60
1:A:87:VAL:CG2	1:A:141:THR:HG22	2.31	0.60
1:B:94:ILE:HB	1:B:127:ASN:OD1	2.02	0.60
1:B:144:TRP:CE3	1:B:156:VAL:CG1	2.84	0.60
1:A:43:SER:CB	1:A:134:SER:C	2.72	0.60
1:B:92:GLU:O	1:B:129:VAL:CG2	2.49	0.60
1:B:139:ASN:CB	3:B:2075:HOH:O	2.50	0.60
1:B:90:SER:OG	1:B:129:VAL:CA	2.51	0.59
1:A:87:VAL:CG2	1:A:141:THR:HG21	2.33	0.59
1:B:139:ASN:CA	3:B:2075:HOH:O	2.50	0.58
1:A:80:GLY:CA	1:A:142:LEU:CD2	2.80	0.58
1:B:83:PHE:N	1:B:141:THR:CB	2.64	0.58
1:B:83:PHE:N	1:B:141:THR:O	2.37	0.58
1:B:124:LYS:C	1:B:125:ASN:CB	2.74	0.58
1:A:99:ASN:CG	1:A:127:ASN:HD22	2.12	0.57
1:B:89:TYR:CD1	1:B:128:ILE:CG1	2.68	0.57
1:A:133:ILE:HG23	1:A:134:SER:H	1.69	0.57
1:A:83:PHE:HB2	1:A:143:HIS:ND1	2.20	0.57
1:B:128:ILE:HD11	1:B:158:GLN:HB3	1.85	0.57
1:A:128:ILE:CG2	1:A:128:ILE:O	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:MET:CA	1:A:154:ILE:C	2.77	0.56
1:B:80:GLY:CA	1:B:142:LEU:HD23	2.33	0.56
1:B:84:PRO:HB3	1:B:141:THR:HG21	1.87	0.56
1:B:94:ILE:HD13	1:B:127:ASN:OD1	1.98	0.56
1:B:80:GLY:CA	1:B:142:LEU:CD2	2.83	0.56
1:A:128:ILE:O	1:A:129:VAL:O	2.24	0.56
1:B:83:PHE:O	1:B:141:THR:HB	1.98	0.56
1:B:81:LEU:O	1:B:142:LEU:C	2.49	0.56
1:A:98:THR:OG1	1:A:125:ASN:N	2.36	0.56
1:B:89:TYR:HB3	1:B:128:ILE:O	2.06	0.55
1:A:81:LEU:C	1:A:142:LEU:HD21	2.27	0.55
1:B:84:PRO:CA	1:B:141:THR:CG2	2.83	0.55
1:B:81:LEU:O	1:B:143:HIS:ND1	2.39	0.55
1:A:125:ASN:O	1:A:126:ALA:C	2.49	0.55
1:A:87:VAL:HG11	1:A:141:THR:OG1	2.06	0.55
1:A:123:LEU:CA	1:A:126:ALA:H	2.18	0.55
1:A:80:GLY:CA	1:A:142:LEU:CD1	2.85	0.55
1:A:101:PRO:HG3	1:A:131:ILE:HD13	1.88	0.55
1:B:89:TYR:CD2	1:B:130:ASP:CG	2.85	0.55
1:A:145:MET:C	1:A:154:ILE:HG13	2.33	0.54
1:A:143:HIS:HB2	1:A:157:GLU:HG2	1.90	0.54
1:B:129:VAL:HG13	1:B:129:VAL:O	2.05	0.54
1:A:134:SER:HA	3:A:2068:HOH:O	2.07	0.54
1:A:98:THR:O	1:A:127:ASN:HB3	2.08	0.54
1:A:98:THR:H	1:A:125:ASN:ND2	2.06	0.53
1:B:44:ASN:ND2	1:B:133:ILE:HA	2.23	0.53
1:A:80:GLY:CA	1:A:142:LEU:HD22	2.38	0.53
1:A:145:MET:O	1:A:156:VAL:HG23	2.08	0.53
1:A:145:MET:HG2	1:A:146:ILE:N	2.24	0.53
1:A:145:MET:SD	1:A:153:SER:HB3	2.48	0.53
1:A:89:TYR:CE2	1:A:141:THR:HA	2.44	0.53
1:B:81:LEU:CA	1:B:142:LEU:HG	2.38	0.53
1:B:92:GLU:O	1:B:129:VAL:HG21	2.06	0.53
1:B:105:PHE:CD2	1:B:144:TRP:CD2	2.95	0.53
1:A:90:SER:C	1:A:129:VAL:HG22	2.33	0.52
1:B:84:PRO:HA	1:B:141:THR:HG21	1.90	0.52
1:B:84:PRO:HA	1:B:141:THR:HG22	1.92	0.52
1:A:89:TYR:HE2	1:A:140:THR:C	2.14	0.52
1:B:84:PRO:HA	1:B:141:THR:HB	1.92	0.52
1:B:84:PRO:HA	1:B:141:THR:CB	2.39	0.51
1:B:84:PRO:CA	1:B:141:THR:HG21	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:TYR:HH	1:A:141:THR:CA	1.98	0.51
1:A:43:SER:HB3	1:A:134:SER:C	2.34	0.51
1:A:145:MET:HA	1:A:154:ILE:C	2.36	0.51
1:B:102:VAL:HB	1:B:139:ASN:CB	2.39	0.50
1:B:102:VAL:CB	1:B:139:ASN:CG	2.62	0.50
1:A:89:TYR:OH	1:A:141:THR:C	2.53	0.50
1:B:94:ILE:CB	1:B:127:ASN:OD1	2.59	0.50
1:B:84:PRO:CA	1:B:141:THR:CB	2.90	0.49
1:B:82:ASN:C	1:B:143:HIS:CE1	2.85	0.49
1:B:127:ASN:O	1:B:129:VAL:N	2.40	0.49
1:A:43:SER:HB3	1:A:134:SER:CA	2.43	0.49
1:B:322:THR:HG23	3:B:2184:HOH:O	2.12	0.49
1:B:137:ILE:HD12	1:B:137:ILE:N	2.28	0.48
1:A:145:MET:CE	1:A:168:ASN:HD21	2.16	0.48
1:B:92:GLU:CA	1:B:129:VAL:CG2	2.92	0.48
1:A:46:LYS:CE	1:A:131:ILE:CD1	2.58	0.48
1:A:142:LEU:O	3:A:2073:HOH:O	2.20	0.48
1:B:143:HIS:N	1:B:143:HIS:ND1	2.61	0.48
1:A:136:ASN:C	1:A:137:ILE:HG12	2.39	0.47
1:B:105:PHE:CG	1:B:144:TRP:CH2	2.97	0.47
1:A:89:TYR:OH	1:A:141:THR:CB	2.58	0.47
1:B:105:PHE:CE2	1:B:144:TRP:CZ2	2.98	0.47
1:A:133:ILE:CG2	1:A:134:SER:N	2.78	0.47
1:A:145:MET:HA	1:A:154:ILE:O	1.88	0.47
1:B:80:GLY:O	1:B:142:LEU:HD21	2.15	0.47
1:B:97:LYS:CD	1:B:125:ASN:OD1	2.59	0.47
1:A:105:PHE:HB3	1:A:144:TRP:CH2	2.51	0.46
1:B:81:LEU:C	1:B:143:HIS:CE1	2.93	0.46
1:B:102:VAL:CB	1:B:139:ASN:CB	2.94	0.46
1:B:127:ASN:C	1:B:129:VAL:H	2.23	0.46
1:B:144:TRP:CD1	1:B:144:TRP:N	2.83	0.46
1:B:30:ILE:HB	1:B:317:TYR:HB2	1.98	0.46
1:A:133:ILE:C	1:A:133:ILE:CD1	2.87	0.46
1:B:89:TYR:OH	1:B:140:THR:O	2.26	0.46
1:B:103:TYR:CE1	1:B:133:ILE:HG13	2.50	0.46
1:A:30:ILE:HB	1:A:317:TYR:HB2	1.97	0.46
1:A:137:ILE:HA	1:A:138:PRO:HD3	1.70	0.45
1:B:22:ILE:HG13	1:B:277:GLN:HG3	1.98	0.45
1:A:134:SER:C	3:A:2069:HOH:O	2.59	0.45
1:B:90:SER:O	1:B:129:VAL:HA	2.16	0.45
1:A:90:SER:C	1:A:129:VAL:CG2	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LYS:C	1:A:125:ASN:CB	2.75	0.45
1:A:133:ILE:CG2	1:A:134:SER:H	2.30	0.45
1:B:128:ILE:CD1	1:B:158:GLN:CB	2.90	0.45
1:A:144:TRP:O	1:A:155:VAL:CG1	2.64	0.45
1:A:43:SER:CB	1:A:134:SER:HA	2.45	0.45
1:A:144:TRP:CA	1:A:156:VAL:O	2.65	0.44
1:A:145:MET:CG	1:A:146:ILE:N	2.80	0.44
1:B:143:HIS:CE1	1:B:175:ASN:HA	2.52	0.44
1:B:84:PRO:CB	1:B:141:THR:HG21	2.47	0.44
1:B:102:VAL:CA	1:B:139:ASN:OD1	2.60	0.44
1:B:124:LYS:C	1:B:125:ASN:CA	2.90	0.44
1:B:126:ALA:C	1:B:163:LEU:HD22	2.39	0.44
1:A:41:ASN:HD21	1:A:133:ILE:HA	1.82	0.44
1:B:140:THR:C	1:B:142:LEU:H	2.25	0.44
1:B:81:LEU:C	1:B:142:LEU:HG	2.43	0.43
1:A:81:LEU:HB2	1:A:143:HIS:CE1	2.53	0.43
1:B:123:LEU:O	1:B:125:ASN:N	2.51	0.43
1:B:126:ALA:HB3	1:B:163:LEU:HD22	1.91	0.43
1:A:22:ILE:HG13	1:A:277:GLN:HG3	1.99	0.43
1:A:41:ASN:ND2	1:A:133:ILE:CG1	2.71	0.43
1:A:82:ASN:O	1:A:143:HIS:HE1	2.00	0.43
1:A:198:PRO:HD2	3:A:2106:HOH:O	2.17	0.43
1:A:80:GLY:C	1:A:142:LEU:HD11	2.44	0.43
1:B:89:TYR:CD1	1:B:128:ILE:HB	2.53	0.43
1:B:126:ALA:CB	1:B:163:LEU:CD2	2.84	0.43
1:A:80:GLY:HA3	1:A:142:LEU:HD11	1.98	0.43
1:A:99:ASN:CB	1:A:127:ASN:HD22	2.31	0.43
1:A:129:VAL:HG22	1:A:130:ASP:N	2.20	0.43
1:A:139:ASN:HD22	1:A:139:ASN:HA	1.59	0.43
1:A:83:PHE:CD1	1:A:143:HIS:HB3	2.54	0.43
1:A:71:MET:HE1	1:A:289:TYR:HB2	2.00	0.43
2:A:331:EDO:H21	1:B:84:PRO:HG3	2.01	0.42
1:A:80:GLY:CA	1:A:142:LEU:HD13	2.44	0.42
1:B:140:THR:CG2	1:B:141:THR:N	2.82	0.42
1:B:103:TYR:CE1	1:B:133:ILE:CB	3.01	0.42
1:B:43:SER:CB	1:B:134:SER:HA	2.50	0.42
1:B:43:SER:HB3	1:B:134:SER:HA	2.01	0.42
1:B:83:PHE:H	1:B:141:THR:CA	2.32	0.42
1:A:41:ASN:HD21	1:A:133:ILE:CA	2.33	0.42
1:A:144:TRP:O	1:A:155:VAL:HG13	2.20	0.42
1:A:131:ILE:O	1:A:139:ASN:OD1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:MET:CA	1:A:146:ILE:N	2.83	0.41
1:B:140:THR:HG21	1:B:142:LEU:HD13	2.02	0.41
1:B:103:TYR:HE2	1:B:131:ILE:O	2.04	0.41
1:B:137:ILE:O	1:B:137:ILE:HG22	2.21	0.41
1:A:43:SER:CB	1:A:134:SER:CA	2.98	0.41
1:B:80:GLY:C	1:B:142:LEU:HD21	2.45	0.41
1:A:81:LEU:CB	1:A:143:HIS:CE1	3.04	0.40
1:B:140:THR:C	1:B:142:LEU:N	2.80	0.40
1:B:102:VAL:HG12	1:B:139:ASN:HB3	1.95	0.40
1:B:185:ASN:ND2	1:B:230:ILE:HD11	2.37	0.40

All (3) 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:A:135:GLU:OE2	1:B:25:SER:O[1_455]	1.13	1.07
1:A:27:ASN:CB	1:B:135:GLU:OE2[1_455]	1.57	0.63
1:A:135:GLU:OE2	1:B:25:SER:C[1_455]	2.02	0.18

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	322/329 (98%)	303 (94%)	14 (4%)	5 (2%)	7	4
1	B	324/329 (98%)	309 (95%)	13 (4%)	2 (1%)	21	18
All	All	646/658 (98%)	612 (95%)	27 (4%)	7 (1%)	11	8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	VAL

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Mol	Chain	Res	Type
1	B	128	ILE
1	B	138	PRO
1	A	126	ALA
1	A	140	THR
1	A	132	PRO
1	A	137	ILE

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	292/293 (100%)	285 (98%)	7 (2%)	43	49
1	B	292/293 (100%)	285 (98%)	7 (2%)	43	49
All	All	584/586 (100%)	570 (98%)	14 (2%)	43	49

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	LEU
1	A	125	ASN
1	A	133	ILE
1	A	139	ASN
1	A	140	THR
1	A	141	THR
1	A	142	LEU
1	B	106	LEU
1	B	127	ASN
1	B	133	ILE
1	B	142	LEU
1	B	143	HIS
1	B	144	TRP
1	B	322	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	112	ASN
1	A	125	ASN
1	A	127	ASN
1	A	139	ASN
1	A	242	ASN
1	A	305	ASN
1	A	326	ASN
1	B	112	ASN
1	B	185	ASN
1	B	212	GLN
1	B	242	ASN
1	B	305	ASN
1	B	326	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	A	331	-	3,3,3	0.44	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	A	330	-	3,3,3	0.33	0	2,2,2	0.58	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
2	EDO	A	331	-	-	1/1/1/1	-
2	EDO	A	330	-	-	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
2	A	331	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
2	A	331	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	124:LYS	C	125:ASN	N	5.09
1	A	145:MET	C	146:ILE	N	2.28
1	B	124:LYS	C	125:ASN	N	2.12

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.