



Full wwPDB X-ray Structure Validation Report ⓘ

May 4, 2016 – 07:50 PM EDT

PDB ID : 5E6Y
Title : Crystal structure of E.Coli branching enzyme in complex with alpha cyclodextrin
Authors : Feng, L.; Nosrati, M.; Geiger, J.H.
Deposited on : 2015-10-11
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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

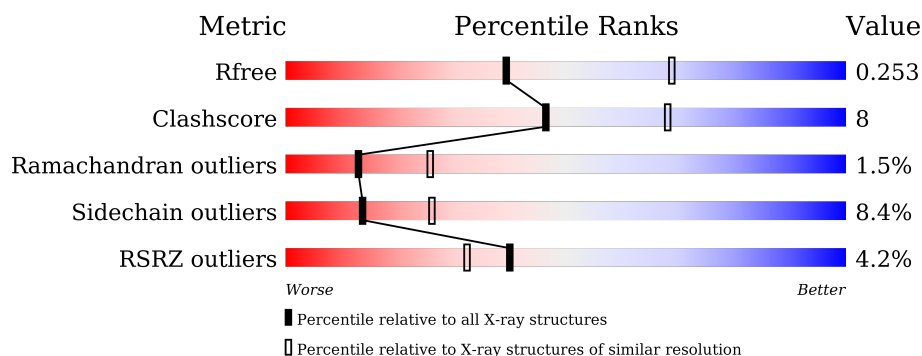
1 Overall quality at a glance

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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	612	
1	B	612	
1	C	612	
1	D	612	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACX	B	801	-	-	-	X
2	ACX	D	801	-	-	-	X
3	GOL	A	803	-	-	-	X

2 Entry composition ⓘ

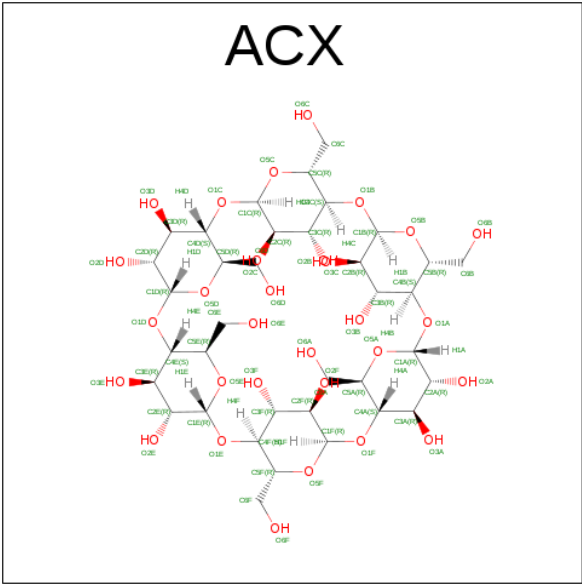
There are 4 unique types of molecules in this entry. The entry contains 20457 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1,4-alpha-glucan branching enzyme GlgB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4729	3025	831	860	13			
1	B	594	Total	C	N	O	S	0	0	0
			4873	3116	861	880	16			
1	C	584	Total	C	N	O	S	0	1	0
			4814	3079	855	864	16			
1	D	589	Total	C	N	O	S	0	0	0
			4836	3090	860	870	16			

- Molecule 2 is ALPHA-CYCLODEXTRIN (CYCLOHEXA-AMYLOSE) (three-letter code: ACX) (formula: C₃₆H₆₀O₃₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			66	36	30		
2	A	1	Total	C	O	0	0
			66	36	30		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			66	36	30		
2	C	1	Total	C	O	0	0
			66	36	30		
2	C	1	Total	C	O	0	0
			66	36	30		
2	C	1	Total	C	O	0	0
			66	36	30		
2	D	1	Total	C	O	0	0
			66	36	30		
2	D	1	Total	C	O	0	0
			66	36	30		
2	D	1	Total	C	O	0	0
			66	36	30		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

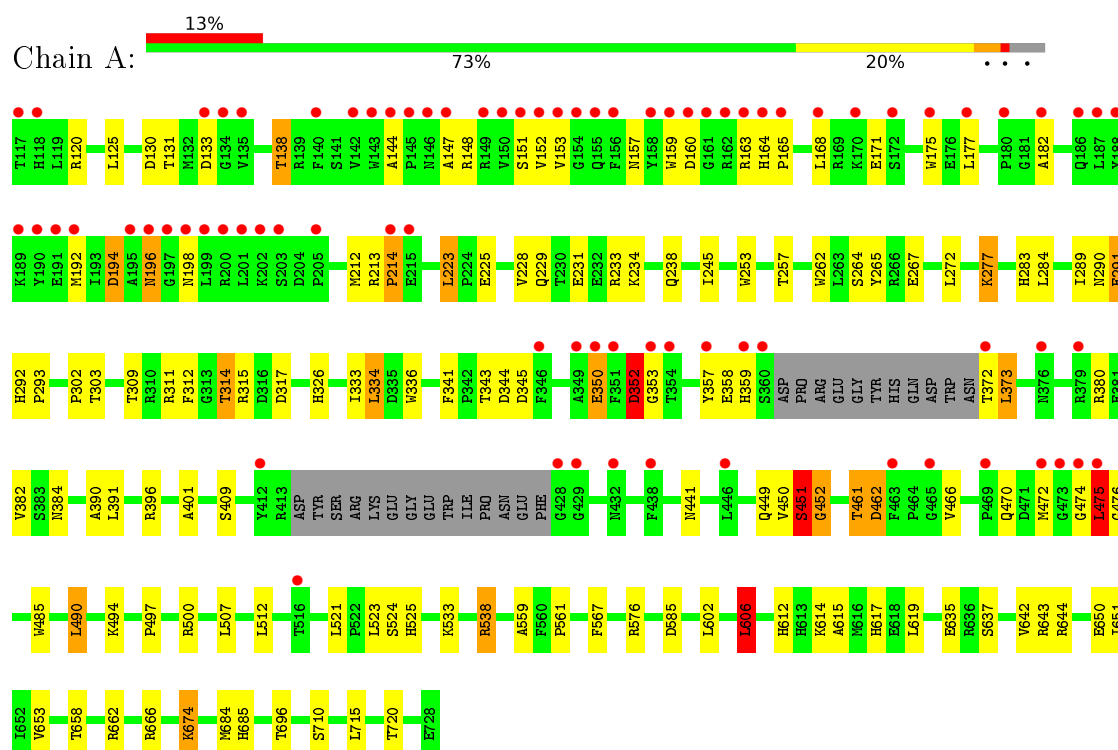
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	128	Total	O	0	0
			128	128		
4	B	188	Total	O	0	0
			188	188		
4	C	72	Total	O	0	0
			72	72		
4	D	193	Total	O	0	0
			193	193		

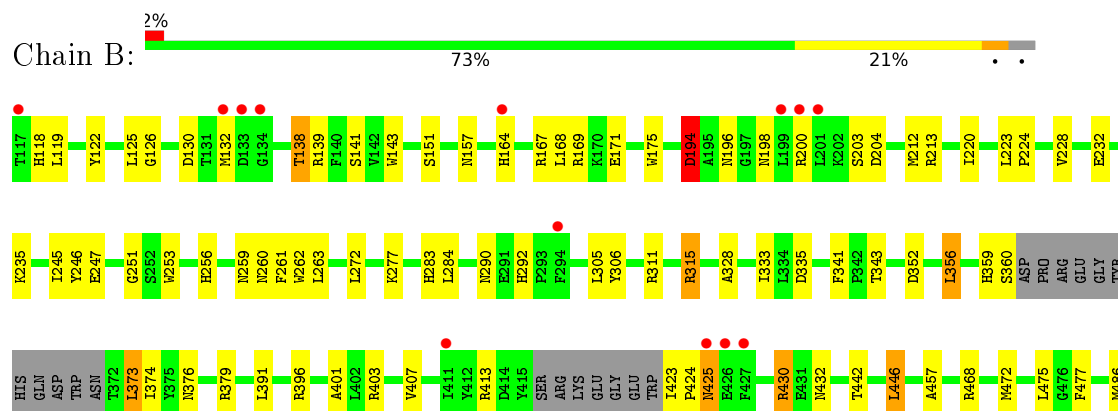
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 1,4-alpha-glucan branching enzyme GlgB



- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.02Å 103.81Å 186.08Å 90.00° 91.97° 90.00°	Depositor
Resolution (Å)	42.43 – 2.60 45.32 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.2 (42.43-2.60) 95.2 (45.32-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.190 , 0.256 0.187 , 0.253	Depositor DCC
R_{free} test set	10334 reflections (10.05%)	DCC
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20457	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACX

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	0.40	0/4882	0.56	1/6644 (0.0%)
1	B	0.48	0/5029	0.61	0/6832
1	C	0.43	0/4970	0.59	1/6748 (0.0%)
1	D	0.51	0/4989	0.67	0/6774
All	All	0.46	0/19870	0.61	2/26998 (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	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	723	LEU	CA-CB-CG	5.43	127.78	115.30
1	A	606	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	473	GLY	Peptide
1	D	289	ILE	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	4729	0	4365	78	0
1	B	4873	0	4580	85	0
1	C	4814	0	4554	64	0
1	D	4836	0	4567	65	0
2	A	132	0	120	2	0
2	B	66	0	60	1	0
2	C	198	0	180	2	0
2	D	198	0	180	5	0
3	A	12	0	16	0	0
3	B	12	0	16	1	0
3	D	6	0	8	0	0
4	A	128	0	0	3	0
4	B	188	0	0	8	0
4	C	72	0	0	2	0
4	D	193	0	0	5	0
All	All	20457	0	18646	291	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 8.

All (291) 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:157:ASN:HD21	1:A:164:HIS:HB2	1.37	0.90
1:C:149:ARG:HH12	1:C:151:SER:HB2	1.38	0.88
1:C:470:GLN:HA	1:C:474:GLY:HA2	1.57	0.86
1:B:292:HIS:O	1:B:311:ARG:NH1	2.15	0.80
1:A:644:ARG:NH2	1:A:650:GLU:OE1	2.15	0.79
1:A:292:HIS:O	1:A:311:ARG:NH1	2.16	0.77
1:C:149:ARG:NH1	1:C:151:SER:HB2	2.00	0.77
1:C:310:ARG:HH11	1:C:310:ARG:HG3	1.52	0.75
1:B:277:LYS:HD2	1:B:328:ALA:HB1	1.70	0.74
1:B:194:ASP:HB3	1:B:196:ASN:H	1.51	0.73
1:C:658:THR:HG23	1:C:660:VAL:H	1.53	0.73
1:C:250:LEU:HD22	1:C:268:LEU:HD13	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:ASP:HB3	1:D:196:ASN:H	1.54	0.72
1:B:224:PRO:HG2	1:B:396:ARG:HB3	1.70	0.72
1:B:373:LEU:HD23	1:B:373:LEU:H	1.55	0.72
1:C:527:GLU:O	1:C:538:ARG:NH1	2.22	0.69
1:A:533:LYS:O	1:A:538:ARG:NH2	2.24	0.69
1:B:658:THR:HG22	1:B:660:VAL:H	1.58	0.69
1:D:492:TYR:CZ	1:D:500:ARG:HG2	2.28	0.68
1:C:292:HIS:CD2	1:C:311:ARG:HH11	2.11	0.68
1:D:527:GLU:O	1:D:538:ARG:NH2	2.27	0.68
1:D:250:LEU:HD22	1:D:268:LEU:HD13	1.76	0.67
1:A:262:TRP:CZ3	1:A:311:ARG:HG2	2.30	0.67
1:A:138:THR:OG1	1:A:182:ALA:O	2.12	0.66
1:B:262:TRP:CZ3	1:B:311:ARG:HG2	2.30	0.66
1:A:194:ASP:N	1:A:194:ASP:OD1	2.29	0.66
1:C:511:ILE:HG22	2:C:803:ACX:H6F2	1.77	0.65
1:A:160:ASP:HB3	1:A:163:ARG:HH12	1.62	0.65
1:D:602:LEU:HG	1:D:606:LEU:HD22	1.78	0.65
1:D:549:ASN:HA	4:D:1034:HOH:O	1.96	0.65
1:D:152:VAL:O	1:D:157:ASN:ND2	2.31	0.64
1:D:403:ARG:NH1	4:D:903:HOH:O	2.31	0.63
1:C:297:SER:HB2	1:C:301:GLN:HG3	1.81	0.62
1:A:194:ASP:HB2	1:A:353:GLY:HA3	1.80	0.62
1:A:262:TRP:CH2	1:A:311:ARG:HG2	2.34	0.62
1:B:157:ASN:HD21	1:B:164:HIS:HB2	1.64	0.61
1:B:492:TYR:CZ	1:B:500:ARG:HG2	2.35	0.61
1:A:662:ARG:HB2	1:A:715:LEU:HB2	1.82	0.61
1:D:292:HIS:O	1:D:311:ARG:NH1	2.34	0.60
1:A:291:GLU:HG2	1:A:309:THR:HA	1.82	0.59
1:B:138:THR:HG21	1:B:220:ILE:HD13	1.84	0.59
1:D:232:GLU:H	1:D:232:GLU:CD	2.05	0.59
1:C:685:HIS:CE1	1:D:685:HIS:HD2	2.19	0.59
1:B:130:ASP:OD2	1:B:139:ARG:NH1	2.30	0.59
1:C:403:ARG:NH1	4:C:902:HOH:O	2.32	0.59
1:B:247:GLU:HG2	1:B:567:PHE:HD1	1.68	0.58
1:C:262:TRP:CH2	1:C:311:ARG:HD3	2.38	0.58
1:A:153:VAL:HB	1:A:159:TRP:HA	1.86	0.58
1:A:466:VAL:HG13	1:A:475:LEU:HD23	1.85	0.58
1:C:667:PHE:HE1	1:C:713:LEU:HD11	1.69	0.57
1:B:572:PHE:HB2	1:B:589:LEU:HD21	1.85	0.57
1:C:153:VAL:HB	1:C:159:TRP:HA	1.85	0.57
1:A:350:GLU:N	1:A:358:GLU:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:TRP:O	1:C:604:ARG:HD2	2.05	0.57
1:B:260:ASN:ND2	4:B:912:HOH:O	2.38	0.56
1:D:215:GLU:HB2	2:D:801:ACX:H5C	1.86	0.56
1:A:576:ARG:NH2	4:A:902:HOH:O	2.26	0.56
1:A:196:ASN:N	1:A:196:ASN:OD1	2.38	0.56
1:A:130:ASP:OD1	1:A:131:THR:N	2.39	0.56
1:A:293:PRO:HD3	1:A:303:THR:HG23	1.87	0.56
1:B:651:ILE:CD1	1:B:722:TRP:HB3	2.36	0.56
1:B:512:LEU:HD13	2:B:801:ACX:H6B2	1.88	0.55
1:B:593:ASP:OD2	1:B:687:HIS:NE2	2.36	0.55
1:B:616:MET:SD	1:B:651:ILE:HG12	2.46	0.55
1:A:461:THR:OG1	1:A:462:ASP:N	2.35	0.55
1:B:413:ARG:HE	1:B:432:ASN:HA	1.72	0.55
1:C:651:ILE:CD1	1:C:722:TRP:HB3	2.37	0.55
1:D:145:PRO:HD2	1:D:356:LEU:HD11	1.89	0.55
1:A:290:ASN:O	1:A:292:HIS:ND1	2.39	0.54
1:A:585:ASP:OD1	4:A:901:HOH:O	2.18	0.54
1:C:194:ASP:HB3	1:C:197:GLY:H	1.72	0.54
1:B:527:GLU:O	1:B:538:ARG:NH2	2.37	0.54
1:A:152:VAL:O	1:A:157:ASN:ND2	2.39	0.54
1:A:615:ALA:HB3	1:A:651:ILE:HD12	1.89	0.54
1:A:497:PRO:HA	1:A:500:ARG:HD2	1.90	0.54
1:C:471:ASP:OD1	1:C:471:ASP:N	2.41	0.54
1:C:556:TRP:HE3	1:C:655:SER:HG	1.56	0.54
1:A:559:ALA:HB1	1:A:653:VAL:HG21	1.88	0.54
1:C:490:LEU:O	1:C:494:LYS:HG3	2.08	0.53
1:D:676:ARG:NE	1:D:726:GLU:OE1	2.23	0.53
1:B:232:GLU:N	1:B:232:GLU:OE1	2.35	0.53
1:B:256:HIS:NE2	1:B:263:LEU:HD23	2.23	0.53
1:D:319:ARG:NH2	1:D:396:ARG:O	2.42	0.53
1:B:552:ALA:HA	1:B:720:THR:HG23	1.91	0.53
1:B:494:LYS:HG2	1:B:538:ARG:HG2	1.91	0.52
1:D:120:ARG:NH2	1:D:449:GLN:OE1	2.41	0.52
1:A:151:SER:HB2	1:A:165:PRO:HA	1.90	0.52
1:B:315:ARG:HD3	4:B:915:HOH:O	2.08	0.52
1:C:551:ARG:NH1	1:C:681:THR:O	2.43	0.52
1:A:157:ASN:ND2	1:A:164:HIS:HB2	2.16	0.52
1:C:309:THR:OG1	1:C:311:ARG:HG3	2.09	0.52
1:B:341:PHE:HD1	1:B:373:LEU:HD12	1.74	0.52
1:C:681:THR:HB	1:C:720:THR:H	1.74	0.52
1:B:138:THR:HG21	1:B:220:ILE:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:PHE:CD1	2:D:802:ACX:H3A	2.45	0.51
1:B:335:ASP:OD1	1:B:403:ARG:HD3	2.11	0.51
1:A:602:LEU:HG	1:A:606:LEU:HD22	1.92	0.51
1:D:651:ILE:HD13	1:D:722:TRP:HB3	1.91	0.51
1:A:470:GLN:HA	1:A:474:GLY:HA2	1.91	0.51
1:A:685:HIS:HD2	4:A:1009:HOH:O	1.93	0.51
1:B:508:THR:O	1:B:511:ILE:HG22	2.10	0.51
1:C:296:GLY:HA2	1:C:580:HIS:CE1	2.45	0.51
1:A:635:GLU:CD	1:A:635:GLU:H	2.13	0.51
1:D:558:TRP:HA	1:D:564:LYS:HE3	1.92	0.50
1:B:376:ASN:OD1	1:B:379:ARG:HB2	2.11	0.50
1:D:509:PHE:HA	2:D:803:ACX:H6D2	1.94	0.50
1:A:168:LEU:HD13	1:A:175:TRP:CE2	2.45	0.50
1:A:168:LEU:HB2	1:A:175:TRP:CZ3	2.47	0.49
1:C:138:THR:HG21	1:C:220:ILE:HD13	1.93	0.49
1:C:470:GLN:N	1:C:470:GLN:OE1	2.38	0.49
1:B:430:ARG:CD	1:B:430:ARG:H	2.26	0.49
1:D:194:ASP:HB2	1:D:198:ASN:H	1.76	0.49
1:A:614:LYS:HA	1:A:617:HIS:NE2	2.28	0.49
1:B:486:MET:O	1:B:490:LEU:HB2	2.12	0.49
1:B:658:THR:CG2	1:B:660:VAL:H	2.24	0.49
1:C:407:VAL:HG21	1:C:457:ALA:HB1	1.94	0.49
1:C:651:ILE:HD13	1:C:722:TRP:HB3	1.94	0.49
1:A:314:THR:HG23	1:A:317:ASP:OD2	2.13	0.48
1:C:148:ARG:NH2	1:C:196:ASN:O	2.46	0.48
1:B:407:VAL:HG21	1:B:457:ALA:HB1	1.95	0.48
1:D:372:THR:O	1:D:372:THR:OG1	2.32	0.48
1:C:574:GLN:HG2	1:C:576:ARG:O	2.12	0.48
1:C:620:ASP:OD1	1:C:643:ARG:NH2	2.42	0.48
1:A:194:ASP:OD1	1:A:198:ASN:N	2.47	0.48
1:C:494:LYS:HD3	1:C:538:ARG:HG2	1.94	0.48
1:D:693:ASN:OD1	1:D:713:LEU:HB2	2.14	0.47
1:A:450:VAL:O	1:A:452:GLY:N	2.47	0.47
1:A:474:GLY:O	1:A:476:GLY:N	2.47	0.47
1:B:168:LEU:HB2	1:B:175:TRP:CH2	2.50	0.47
1:C:292:HIS:O	1:C:311:ARG:NH1	2.47	0.47
1:C:310:ARG:NH1	1:C:310:ARG:HG3	2.22	0.47
1:C:297:SER:C	1:C:299:GLY:H	2.18	0.47
1:B:585:ASP:OD2	4:B:901:HOH:O	2.20	0.47
1:D:497:PRO:HA	1:D:500:ARG:HD3	1.97	0.47
1:C:685:HIS:NE2	1:D:685:HIS:HD2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:HB2	1:A:175:TRP:CE3	2.50	0.46
1:A:262:TRP:CZ3	2:A:801:ACX:H6D2	2.49	0.46
1:B:430:ARG:H	1:B:430:ARG:HD2	1.78	0.46
1:B:708:GLN:O	4:B:902:HOH:O	2.21	0.46
1:D:211:GLN:O	1:D:212:MET:HG2	2.14	0.46
1:D:492:TYR:CE2	1:D:500:ARG:HG2	2.51	0.46
1:D:652:ILE:HB	1:D:723:LEU:HB2	1.97	0.46
1:C:437:GLU:O	1:C:441:ASN:HB2	2.15	0.46
1:C:511:ILE:HG12	1:C:626:PHE:CE1	2.50	0.46
1:D:428:GLY:HA2	1:D:429:GLY:HA3	1.60	0.46
1:D:568:MET:HB2	1:D:584:LEU:HD11	1.98	0.46
1:A:277:LYS:HD3	4:B:1006:HOH:O	2.13	0.46
1:B:602:LEU:HG	1:B:606:LEU:HD22	1.97	0.46
1:C:559:ALA:HB1	1:C:653:VAL:HG21	1.98	0.46
1:C:610:TYR:O	1:C:617:HIS:HD2	1.99	0.46
1:D:139:ARG:HD2	4:D:1074:HOH:O	2.15	0.46
1:A:253:TRP:CH2	1:A:272:LEU:HA	2.50	0.46
1:B:126:GLY:HA2	1:B:204:ASP:OD2	2.16	0.46
1:C:680:ASN:HA	1:C:721:ILE:HG22	1.98	0.46
1:C:334:LEU:HB3	1:C:399:ILE:HD13	1.98	0.46
1:A:233:ARG:HD3	1:A:326:HIS:CD2	2.51	0.45
1:A:451:SER:OG	1:A:451:SER:O	2.31	0.45
1:B:679:LEU:HG	1:B:680:ASN:N	2.32	0.45
1:B:719:ALA:HB2	4:B:960:HOH:O	2.16	0.45
1:D:646:LYS:HE2	1:D:646:LYS:HB3	1.73	0.45
1:D:242:PRO:HD3	1:D:617:HIS:CE1	2.52	0.45
1:A:644:ARG:HD3	1:A:650:GLU:HG2	1.98	0.45
1:C:155:GLN:HB2	4:C:956:HOH:O	2.16	0.45
1:D:192:MET:SD	1:D:352:ASP:HA	2.56	0.45
1:A:380:ARG:O	1:A:384:ASN:ND2	2.34	0.45
1:B:490:LEU:HA	1:B:490:LEU:HD12	1.77	0.45
1:C:618:GLU:OE1	1:C:645:ASP:HB2	2.16	0.45
1:D:170:LYS:HE2	4:D:944:HOH:O	2.16	0.45
1:A:666:ARG:NH1	1:A:710:SER:OG	2.47	0.45
1:C:616:MET:SD	1:C:651:ILE:HG12	2.56	0.45
1:A:292:HIS:HB3	1:A:302:PRO:HA	1.97	0.45
1:B:245:ILE:HG12	1:B:283:HIS:HB2	1.99	0.45
1:D:341:PHE:CZ	1:D:358:GLU:HB3	2.52	0.45
1:D:616:MET:SD	1:D:651:ILE:HG12	2.57	0.45
1:A:265:TYR:CE2	1:A:312:PHE:HB2	2.52	0.45
1:B:457:ALA:HB2	1:B:477:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:ASP:OD2	1:B:649:ASN:HB2	2.17	0.45
1:D:429:GLY:HA2	1:D:430:ARG:HA	1.56	0.45
2:D:801:ACX:O3A	2:D:801:ACX:O2F	2.32	0.45
1:A:264:SER:OG	1:A:267:GLU:HG3	2.17	0.44
1:B:359:HIS:CG	1:B:360:SER:N	2.85	0.44
1:B:551:ARG:HB3	1:B:681:THR:HB	1.99	0.44
1:C:298:TRP:HE1	1:C:580:HIS:CD2	2.35	0.44
1:B:122:TYR:HB3	1:B:306:TYR:CE2	2.53	0.44
1:B:343:THR:HG22	1:B:373:LEU:HD11	1.98	0.44
1:D:523:LEU:HD22	1:D:557:MET:SD	2.57	0.44
1:A:223:LEU:HB3	1:A:396:ARG:NH2	2.33	0.44
2:A:801:ACX:O6A	2:A:801:ACX:O6B	2.30	0.44
1:B:169:ARG:HD3	1:B:171:GLU:OE2	2.18	0.44
1:B:341:PHE:CD1	1:B:373:LEU:HD12	2.53	0.44
1:D:264:SER:HB2	4:D:937:HOH:O	2.18	0.44
1:D:437:GLU:O	1:D:441:ASN:HB2	2.17	0.44
1:B:558:TRP:HA	1:B:564:LYS:HE3	2.00	0.44
1:D:627:GLU:HB3	1:D:642:VAL:HG12	2.00	0.43
1:B:413:ARG:CZ	1:B:425:ASN:HB3	2.49	0.43
1:A:284:LEU:HD12	1:A:284:LEU:HA	1.88	0.43
1:A:333:ILE:HG12	1:A:401:ALA:HB3	2.01	0.43
1:A:637:SER:HB2	1:A:658:THR:HG23	2.00	0.43
1:B:143:TRP:CH2	1:B:356:LEU:HD22	2.53	0.43
1:B:373:LEU:CD2	1:B:373:LEU:H	2.30	0.43
1:B:568:MET:O	4:B:903:HOH:O	2.21	0.43
1:B:658:THR:HG23	1:B:659:PRO:HD2	1.99	0.43
1:A:485:TRP:CD2	1:A:521:LEU:HD22	2.54	0.43
1:B:560:PHE:CG	1:B:561:PRO:HD2	2.54	0.43
1:C:140:PHE:HZ	1:C:220:ILE:HD11	1.84	0.43
1:C:391:LEU:HA	1:C:391:LEU:HD12	1.91	0.43
1:B:442:THR:HG22	1:B:446:LEU:HD22	2.00	0.43
1:D:314:THR:O	1:D:317:ASP:HB2	2.18	0.43
1:A:336:TRP:CH2	1:A:390:ALA:HB2	2.54	0.42
1:B:251:GLY:N	4:B:917:HOH:O	2.45	0.42
1:C:512:LEU:HD13	2:C:803:ACX:H6C2	2.01	0.42
1:B:632:ASP:N	1:B:632:ASP:OD1	2.52	0.42
1:C:566:LEU:HG	1:C:570:ASN:HB2	2.00	0.42
1:D:290:ASN:HD22	1:D:290:ASN:HA	1.47	0.42
1:B:198:ASN:HB3	1:B:200:ARG:NH1	2.33	0.42
1:B:468:ARG:NH2	1:B:515:TYR:O	2.52	0.42
1:D:168:LEU:HB2	1:D:175:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:ARG:HD2	1:D:313:GLY:O	2.20	0.42
1:B:716:PRO:HB2	1:B:719:ALA:HB3	2.01	0.42
1:C:667:PHE:CE1	1:C:713:LEU:HD11	2.53	0.42
1:C:676:ARG:HD2	1:C:726:GLU:OE2	2.20	0.42
1:D:457:ALA:HB2	1:D:477:PHE:CD1	2.54	0.42
1:C:277:LYS:HD2	1:C:328:ALA:HB1	2.02	0.42
1:C:571:GLU:O	1:C:599:VAL:HG12	2.20	0.42
1:A:212:MET:C	1:A:214:PRO:HD2	2.39	0.42
1:B:253:TRP:CH2	1:B:272:LEU:HA	2.54	0.42
1:B:490:LEU:O	1:B:494:LYS:HG3	2.19	0.42
1:D:264:SER:OG	1:D:267:GLU:HG3	2.19	0.42
1:C:510:GLY:HA2	1:C:513:TYR:CE2	2.55	0.42
1:C:658:THR:HA	1:C:659:PRO:HD3	1.90	0.42
1:D:120:ARG:HG2	1:D:122:TYR:CZ	2.55	0.42
1:A:357:TYR:HD1	1:A:382:VAL:HG22	1.84	0.42
1:A:674:LYS:NZ	1:A:696:THR:HG21	2.34	0.42
1:B:141:SER:HA	1:B:175:TRP:O	2.20	0.42
1:B:284:LEU:HA	1:B:284:LEU:HD12	1.90	0.42
1:A:341:PHE:O	1:A:343:THR:HG23	2.19	0.41
1:B:157:ASN:OD1	1:B:164:HIS:CD2	2.73	0.41
1:B:644:ARG:HG2	1:B:650:GLU:HG2	2.02	0.41
1:D:292:HIS:CG	1:D:299:GLY:HA2	2.55	0.41
1:D:317:ASP:O	1:D:320:TYR:HB3	2.20	0.41
1:D:564:LYS:HE2	1:D:610:TYR:CE1	2.54	0.41
1:A:229:GLN:HG2	1:A:234:LYS:HG3	2.01	0.41
1:A:466:VAL:HG22	1:A:475:LEU:HD23	2.02	0.41
1:C:359:HIS:CG	1:C:360:SER:H	2.38	0.41
1:A:265:TYR:CZ	1:A:312:PHE:HB2	2.55	0.41
1:B:356:LEU:HA	1:B:356:LEU:HD23	1.92	0.41
1:B:521:LEU:HA	1:B:522:PRO:HD3	1.83	0.41
1:A:245:ILE:HG12	1:A:283:HIS:HB2	2.02	0.41
1:A:561:PRO:HA	1:A:643:ARG:NH2	2.34	0.41
1:B:651:ILE:HD13	1:B:722:TRP:HB3	2.03	0.41
1:D:143:TRP:CH2	1:D:356:LEU:HD22	2.55	0.41
1:D:523:LEU:HD12	1:D:523:LEU:HA	1.98	0.41
1:A:120:ARG:NH1	1:A:449:GLN:OE1	2.34	0.41
1:C:685:HIS:CD2	1:D:685:HIS:CD2	3.08	0.41
1:D:156:PHE:HD1	1:D:157:ASN:OD1	2.03	0.41
1:A:160:ASP:HB3	1:A:163:ARG:NH1	2.31	0.41
1:A:373:LEU:H	1:A:373:LEU:HG	1.65	0.41
1:C:643:ARG:HA	1:C:643:ARG:HD2	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:TYR:CD1	1:A:382:VAL:HG22	2.55	0.41
1:A:289:ILE:HG13	1:A:334:LEU:HD11	2.01	0.41
1:B:563:LYS:HE2	1:B:621:PHE:CZ	2.56	0.41
1:B:613:HIS:HB3	3:B:802:GOL:H32	2.01	0.41
1:D:468:ARG:O	1:D:474:GLY:HA3	2.21	0.41
1:B:333:ILE:HG12	1:B:401:ALA:HB3	2.02	0.41
1:B:666:ARG:HA	1:B:711:LEU:O	2.21	0.41
1:A:494:LYS:HD3	1:A:538:ARG:HG2	2.03	0.41
1:B:495:LEU:HD11	1:B:503:HIS:CD2	2.56	0.41
1:D:671:GLN:HA	1:D:672:PRO:HD2	1.98	0.41
1:D:677:GLU:HA	1:D:723:LEU:HD13	2.01	0.41
1:A:525:HIS:HB3	1:A:567:PHE:CE1	2.56	0.40
1:A:144:ALA:HB1	1:A:352:ASP:HB2	2.02	0.40
1:A:490:LEU:HD12	1:A:490:LEU:HA	1.83	0.40
1:B:125:LEU:HA	1:B:141:SER:HB2	2.03	0.40
1:B:246:TYR:OH	1:B:571:GLU:OE1	2.27	0.40
1:C:466:VAL:HG22	1:C:475:LEU:HD12	2.04	0.40
1:C:716:PRO:HB2	1:C:719:ALA:HB3	2.03	0.40
1:D:170:LYS:H	1:D:170:LYS:CD	2.33	0.40
1:D:642:VAL:CG2	1:D:650:GLU:HB3	2.51	0.40
1:A:192:MET:HE1	1:A:352:ASP:HA	2.02	0.40
1:B:168:LEU:HB2	1:B:175:TRP:CZ3	2.55	0.40
1:B:259:ASN:HB2	1:B:261:PHE:CE1	2.55	0.40
1:B:423:ILE:HA	1:B:424:PRO:HD2	1.96	0.40
1:B:606:LEU:HA	1:B:606:LEU:HD12	1.91	0.40
1:C:246:TYR:HB2	1:C:281:PHE:CG	2.57	0.40
1:D:293:PRO:HD3	1:D:303:THR:HG23	2.02	0.40
1:A:265:TYR:HB2	1:A:317:ASP:HB3	2.03	0.40
1:A:358:GLU:H	1:A:358:GLU:CD	2.20	0.40
1:C:480:LYS:HG2	1:C:481:TRP:O	2.20	0.40
1:D:574:GLN:HG2	1:D:576:ARG:O	2.22	0.40
1:D:587:HIS:O	1:D:590:GLU:HB2	2.22	0.40
1:D:260:ASN:HB3	2:D:802:ACX:O2B	2.22	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	581/612 (95%)	506 (87%)	62 (11%)	13 (2%)	8	15
1	B	588/612 (96%)	546 (93%)	38 (6%)	4 (1%)	26	51
1	C	579/612 (95%)	532 (92%)	41 (7%)	6 (1%)	19	39
1	D	583/612 (95%)	543 (93%)	29 (5%)	11 (2%)	10	19
All	All	2331/2448 (95%)	2127 (91%)	170 (7%)	34 (2%)	13	26

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	ARG
1	A	225	GLU
1	A	451	SER
1	B	194	ASP
1	B	212	MET
1	C	194	ASP
1	C	213	ARG
1	D	149	ARG
1	D	194	ASP
1	D	214	PRO
1	D	290	ASN
1	A	612	HIS
1	D	259	ASN
1	A	125	LEU
1	A	177	LEU
1	A	475	LEU
1	B	585	ASP
1	A	147	ALA
1	A	148	ARG
1	C	197	GLY
1	C	522	PRO
1	D	257	THR

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Mol	Chain	Res	Type
1	D	413	ARG
1	D	522	PRO
1	A	133	ASP
1	A	214	PRO
1	A	352	ASP
1	C	226	LYS
1	D	211	GLN
1	D	709	HIS
1	A	452	GLY
1	B	522	PRO
1	C	497	PRO
1	D	213	ARG

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	475/521 (91%)	434 (91%)	41 (9%)	13	25
1	B	502/521 (96%)	462 (92%)	40 (8%)	15	29
1	C	498/521 (96%)	451 (91%)	47 (9%)	11	20
1	D	499/521 (96%)	462 (93%)	37 (7%)	17	34
All	All	1974/2084 (95%)	1809 (92%)	165 (8%)	14	26

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	THR
1	A	171	GLU
1	A	194	ASP
1	A	196	ASN
1	A	223	LEU
1	A	228	VAL
1	A	231	GLU
1	A	238	GLN
1	A	257	THR

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Mol	Chain	Res	Type
1	A	277	LYS
1	A	291	GLU
1	A	314	THR
1	A	315	ARG
1	A	334	LEU
1	A	344	ASP
1	A	345	ASP
1	A	350	GLU
1	A	352	ASP
1	A	359	HIS
1	A	372	THR
1	A	373	LEU
1	A	391	LEU
1	A	409	SER
1	A	441	ASN
1	A	451	SER
1	A	461	THR
1	A	462	ASP
1	A	472	MET
1	A	475	LEU
1	A	490	LEU
1	A	507	LEU
1	A	512	LEU
1	A	523	LEU
1	A	524	SER
1	A	538	ARG
1	A	606	LEU
1	A	619	LEU
1	A	642	VAL
1	A	674	LYS
1	A	684	MET
1	A	720	THR
1	B	118	HIS
1	B	119	LEU
1	B	132	MET
1	B	138	THR
1	B	151	SER
1	B	167	ARG
1	B	194	ASP
1	B	203	SER
1	B	213	ARG
1	B	223	LEU

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Mol	Chain	Res	Type
1	B	228	VAL
1	B	235	LYS
1	B	290	ASN
1	B	305	LEU
1	B	315	ARG
1	B	352	ASP
1	B	356	LEU
1	B	373	LEU
1	B	374	ILE
1	B	391	LEU
1	B	425	ASN
1	B	430	ARG
1	B	446	LEU
1	B	472	MET
1	B	475	LEU
1	B	490	LEU
1	B	507	LEU
1	B	512	LEU
1	B	523	LEU
1	B	538	ARG
1	B	558	TRP
1	B	581	ASP
1	B	606	LEU
1	B	618	GLU
1	B	619	LEU
1	B	651	ILE
1	B	658	THR
1	B	666	ARG
1	B	720	THR
1	B	723	LEU
1	C	119	LEU
1	C	132	MET
1	C	138	THR
1	C	141	SER
1	C	149	ARG
1	C	156	PHE
1	C	168	LEU
1	C	171	GLU
1	C	212	MET
1	C	213	ARG
1	C	219	LEU
1	C	223	LEU

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Mol	Chain	Res	Type
1	C	257	THR
1	C	258	ASP
1	C	290	ASN
1	C	310	ARG
1	C	315	ARG
1	C	319	ARG
1	C	352	ASP
1	C	356	LEU
1	C	380	ARG
1	C	383	SER
1	C	391	LEU
1	C	441	ASN
1	C	446	LEU
1	C	471	ASP
1	C	472	MET
1	C	475	LEU
1	C	490	LEU
1	C	505	ASP
1	C	507	LEU
1	C	511	ILE
1	C	512	LEU
1	C	523	LEU
1	C	595	TRP
1	C	619	LEU
1	C	635	GLU
1	C	642	VAL
1	C	643	ARG
1	C	647	GLU
1	C	651	ILE
1	C	658	THR
1	C	679	LEU
1	C	681	THR
1	C	713	LEU
1	C	720	THR
1	C	723	LEU
1	D	119	LEU
1	D	138	THR
1	D	141	SER
1	D	148	ARG
1	D	155	GLN
1	D	163	ARG
1	D	170	LYS

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Mol	Chain	Res	Type
1	D	171	GLU
1	D	213	ARG
1	D	223	LEU
1	D	225	GLU
1	D	232	GLU
1	D	258	ASP
1	D	270	ASP
1	D	290	ASN
1	D	295	ASP
1	D	315	ARG
1	D	344	ASP
1	D	352	ASP
1	D	356	LEU
1	D	372	THR
1	D	373	LEU
1	D	391	LEU
1	D	430	ARG
1	D	475	LEU
1	D	490	LEU
1	D	507	LEU
1	D	523	LEU
1	D	581	ASP
1	D	606	LEU
1	D	614	LYS
1	D	619	LEU
1	D	632	ASP
1	D	646	LYS
1	D	651	ILE
1	D	679	LEU
1	D	720	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	164	HIS
1	B	157	ASN
1	B	164	HIS
1	B	425	ASN
1	B	525	HIS
1	C	580	HIS
1	C	617	HIS

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Mol	Chain	Res	Type
1	D	164	HIS
1	D	290	ASN
1	D	617	HIS
1	D	685	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

14 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	ACX	A	801	-	72,72,72	1.07	2 (2%)	108,108,108	1.46	19 (17%)
2	ACX	A	802	-	72,72,72	1.11	2 (2%)	108,108,108	1.26	16 (14%)
3	GOL	A	803	-	5,5,5	0.38	0	5,5,5	0.29	0
3	GOL	A	804	-	5,5,5	0.35	0	5,5,5	0.21	0
2	ACX	B	801	-	72,72,72	1.06	3 (4%)	108,108,108	1.30	14 (12%)
3	GOL	B	802	-	5,5,5	0.39	0	5,5,5	0.20	0
3	GOL	B	803	-	5,5,5	0.35	0	5,5,5	0.27	0
2	ACX	C	801	-	72,72,72	1.01	2 (2%)	108,108,108	1.12	10 (9%)
2	ACX	C	802	-	72,72,72	1.08	2 (2%)	108,108,108	1.25	15 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACX	C	803	-	72,72,72	1.03	2 (2%)	108,108,108	1.22	12 (11%)
2	ACX	D	801	-	72,72,72	1.09	2 (2%)	108,108,108	1.47	19 (17%)
2	ACX	D	802	-	72,72,72	1.08	2 (2%)	108,108,108	1.22	14 (12%)
2	ACX	D	803	-	72,72,72	1.03	2 (2%)	108,108,108	1.17	10 (9%)
3	GOL	D	804	-	5,5,5	0.23	0	5,5,5	0.41	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	ACX	A	801	-	-	0/36/156/156	0/0/7/7
2	ACX	A	802	-	-	0/36/156/156	0/0/7/7
3	GOL	A	803	-	-	0/4/4/4	0/0/0/0
3	GOL	A	804	-	-	0/4/4/4	0/0/0/0
2	ACX	B	801	-	-	0/36/156/156	0/0/7/7
3	GOL	B	802	-	-	0/4/4/4	0/0/0/0
3	GOL	B	803	-	-	0/4/4/4	0/0/0/0
2	ACX	C	801	-	-	0/36/156/156	0/0/7/7
2	ACX	C	802	-	-	0/36/156/156	0/0/7/7
2	ACX	C	803	-	-	0/36/156/156	0/0/7/7
2	ACX	D	801	-	-	0/36/156/156	0/0/7/7
2	ACX	D	802	-	-	0/36/156/156	0/0/7/7
2	ACX	D	803	-	-	0/36/156/156	0/0/7/7
3	GOL	D	804	-	-	0/4/4/4	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ACX	O1E-C1E	-3.24	1.32	1.41
2	C	802	ACX	O1E-C1E	-3.05	1.33	1.41
2	D	803	ACX	O1E-C1E	-3.01	1.33	1.41
2	A	802	ACX	O1E-C1E	-2.99	1.33	1.41
2	C	801	ACX	O1E-C1E	-2.92	1.33	1.41
2	A	801	ACX	O1E-C1E	-2.89	1.33	1.41
2	C	803	ACX	O1E-C1E	-2.87	1.33	1.41
2	D	801	ACX	O1E-C1E	-2.74	1.34	1.41
2	D	802	ACX	O1E-C1E	-2.63	1.34	1.41
2	B	801	ACX	O5D-C1D	2.01	1.47	1.41
2	C	801	ACX	O5E-C1E	5.38	1.55	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ACX	O5E-C1E	5.48	1.55	1.41
2	D	803	ACX	O5E-C1E	5.61	1.56	1.41
2	A	801	ACX	O5E-C1E	5.77	1.56	1.41
2	C	803	ACX	O5E-C1E	5.79	1.56	1.41
2	C	802	ACX	O5E-C1E	5.90	1.57	1.41
2	D	802	ACX	O5E-C1E	5.90	1.57	1.41
2	D	801	ACX	O5E-C1E	6.00	1.57	1.41
2	A	802	ACX	O5E-C1E	6.09	1.57	1.41

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	ACX	C1F-O1F-C4A	-3.09	109.78	118.00
2	D	803	ACX	C1D-O1D-C4E	-3.05	109.90	118.00
2	D	803	ACX	C1B-O1B-C4C	-2.96	110.13	118.00
2	A	801	ACX	C1B-O1B-C4C	-2.88	110.35	118.00
2	C	801	ACX	C1E-O5E-C5E	-2.87	108.10	113.74
2	A	801	ACX	C1F-O1F-C4A	-2.74	110.72	118.00
2	C	802	ACX	C1C-O5C-C5C	-2.69	108.47	113.74
2	C	802	ACX	C1B-O1B-C4C	-2.67	110.89	118.00
2	C	802	ACX	C1D-O5D-C5D	-2.66	108.52	113.74
2	C	803	ACX	C1F-O1F-C4A	-2.58	111.14	118.00
2	C	802	ACX	C1D-O1D-C4E	-2.55	111.23	118.00
2	D	802	ACX	C1F-O5F-C5F	-2.54	108.75	113.74
2	A	801	ACX	C1E-O1E-C4F	-2.49	111.38	118.00
2	A	801	ACX	C1F-O5F-C5F	-2.49	108.86	113.74
2	D	801	ACX	C1D-O1D-C4E	-2.48	111.40	118.00
2	A	801	ACX	C1A-O5A-C5A	-2.48	108.87	113.74
2	B	801	ACX	C1E-O5E-C5E	-2.47	108.89	113.74
2	C	802	ACX	C1F-O5F-C5F	-2.43	108.98	113.74
2	A	802	ACX	C1E-O1E-C4F	-2.34	111.77	118.00
2	B	801	ACX	C1B-O1B-C4C	-2.29	111.91	118.00
2	C	803	ACX	C1E-O1E-C4F	-2.29	111.92	118.00
2	C	802	ACX	C1A-O5A-C5A	-2.28	109.26	113.74
2	C	801	ACX	C1F-O5F-C5F	-2.28	109.27	113.74
2	A	802	ACX	C1F-O1F-C4A	-2.27	111.95	118.00
2	A	802	ACX	C1F-O5F-C5F	-2.27	109.29	113.74
2	A	801	ACX	C1C-O1C-C4D	-2.26	111.99	118.00
2	B	801	ACX	C1C-O1C-C4D	-2.26	112.00	118.00
2	A	801	ACX	C1D-C2D-C3D	-2.24	105.53	109.98
2	B	801	ACX	O1E-C1E-O5E	-2.22	104.90	110.69
2	D	802	ACX	C1F-O1F-C4A	-2.22	112.11	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	802	ACX	C1C-O1C-C4D	-2.21	112.13	118.00
2	A	802	ACX	C1B-O1B-C4C	-2.18	112.21	118.00
2	D	802	ACX	C1D-O5D-C5D	-2.16	109.51	113.74
2	D	801	ACX	C1E-O1E-C4F	-2.15	112.29	118.00
2	C	803	ACX	C1C-O1C-C4D	-2.13	112.33	118.00
2	D	803	ACX	C1E-O5E-C5E	-2.13	109.56	113.74
2	A	801	ACX	C1C-O5C-C5C	-2.10	109.62	113.74
2	D	801	ACX	C6F-C5F-C4F	-2.10	107.09	113.25
2	C	803	ACX	C1E-O5E-C5E	-2.09	109.64	113.74
2	D	803	ACX	C1B-O5B-C5B	-2.06	109.70	113.74
2	D	802	ACX	C1E-O5E-C5E	-2.05	109.72	113.74
2	C	801	ACX	O5D-C5D-C4D	2.01	114.07	109.78
2	D	802	ACX	O5F-C5F-C4F	2.02	114.08	109.78
2	C	802	ACX	O5C-C5C-C4C	2.02	114.08	109.78
2	A	801	ACX	O5D-C1D-C2D	2.02	114.48	110.28
2	D	803	ACX	C2E-C3E-C4E	2.03	114.12	109.63
2	A	802	ACX	C3E-C4E-C5E	2.04	115.51	110.85
2	D	801	ACX	O5A-C5A-C4A	2.05	114.15	109.78
2	C	801	ACX	O5F-C5F-C4F	2.05	114.15	109.78
2	C	802	ACX	C2A-C3A-C4A	2.07	114.21	109.63
2	C	802	ACX	C1F-C2F-C3F	2.10	114.14	109.98
2	C	802	ACX	O5F-C5F-C4F	2.10	114.25	109.78
2	A	802	ACX	O5D-C5D-C4D	2.11	114.29	109.78
2	D	802	ACX	C2C-C3C-C4C	2.12	114.30	109.63
2	C	803	ACX	O5E-C5E-C4E	2.12	114.29	109.78
2	D	801	ACX	C1D-C2D-C3D	2.12	114.19	109.98
2	D	802	ACX	C2E-C3E-C4E	2.14	114.37	109.63
2	C	803	ACX	O5F-C5F-C4F	2.15	114.36	109.78
2	D	801	ACX	O1B-C1B-C2B	2.15	113.47	108.12
2	C	803	ACX	O5B-C5B-C4B	2.16	114.38	109.78
2	A	802	ACX	C1A-O1A-C4B	2.16	123.76	118.00
2	B	801	ACX	C3A-C4A-C5A	2.18	115.83	110.85
2	C	801	ACX	O5C-C5C-C4C	2.19	114.44	109.78
2	A	802	ACX	O5B-C5B-C4B	2.19	114.46	109.78
2	C	801	ACX	O5A-C5A-C4A	2.20	114.48	109.78
2	C	803	ACX	C1A-O1A-C4B	2.22	123.92	118.00
2	B	801	ACX	O5D-C1D-C2D	2.22	114.90	110.28
2	A	801	ACX	C2B-C3B-C4B	2.25	114.60	109.63
2	C	803	ACX	C2C-C3C-C4C	2.27	114.64	109.63
2	C	802	ACX	C1D-C2D-C3D	2.28	114.50	109.98
2	A	802	ACX	O5C-C5C-C4C	2.28	114.64	109.78
2	C	801	ACX	O5E-C5E-C4E	2.31	114.70	109.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	802	ACX	O5E-C5E-C4E	2.31	114.71	109.78
2	D	803	ACX	C2B-C3B-C4B	2.33	114.78	109.63
2	D	801	ACX	C3E-C4E-C5E	2.34	116.19	110.85
2	D	801	ACX	C2A-C3A-C4A	2.35	114.81	109.63
2	C	803	ACX	O5C-C5C-C4C	2.37	114.83	109.78
2	D	802	ACX	O5B-C5B-C4B	2.37	114.84	109.78
2	D	802	ACX	C2F-C3F-C4F	2.42	114.97	109.63
2	A	802	ACX	O5F-C5F-C4F	2.42	114.95	109.78
2	C	801	ACX	C2F-C3F-C4F	2.42	114.98	109.63
2	C	801	ACX	O5B-C5B-C4B	2.43	114.97	109.78
2	C	803	ACX	C2E-C3E-C4E	2.44	115.02	109.63
2	B	801	ACX	O5E-C5E-C4E	2.50	115.11	109.78
2	D	801	ACX	C1C-O5C-C5C	2.53	118.70	113.74
2	D	803	ACX	O5F-C5F-C4F	2.53	115.18	109.78
2	A	802	ACX	C2F-C3F-C4F	2.57	115.30	109.63
2	D	801	ACX	C1E-C2E-C3E	2.58	115.10	109.98
2	D	801	ACX	O5E-C5E-C4E	2.59	115.30	109.78
2	A	801	ACX	C1F-C2F-C3F	2.59	115.12	109.98
2	B	801	ACX	O5F-C5F-C4F	2.63	115.38	109.78
2	D	801	ACX	O5B-C5B-C4B	2.64	115.42	109.78
2	C	802	ACX	C1A-O1A-C4B	2.68	125.14	118.00
2	A	802	ACX	C1E-C2E-C3E	2.73	115.39	109.98
2	D	801	ACX	C2F-C3F-C4F	2.73	115.66	109.63
2	D	801	ACX	C2D-C3D-C4D	2.78	115.77	109.63
2	B	801	ACX	O5A-C5A-C4A	2.79	115.73	109.78
2	D	802	ACX	O5E-C5E-C4E	2.80	115.75	109.78
2	C	802	ACX	C2D-C3D-C4D	2.81	115.83	109.63
2	D	803	ACX	O5D-C5D-C4D	2.81	115.78	109.78
2	A	801	ACX	C2F-C3F-C4F	2.83	115.87	109.63
2	D	802	ACX	C2B-C3B-C4B	2.83	115.88	109.63
2	B	801	ACX	O5C-C5C-C4C	2.83	115.83	109.78
2	D	801	ACX	C3F-C4F-C5F	2.86	117.38	110.85
2	D	802	ACX	O5A-C5A-C4A	2.88	115.91	109.78
2	A	801	ACX	C1D-O5D-C5D	2.90	119.43	113.74
2	A	801	ACX	C3E-C4E-C5E	2.90	117.48	110.85
2	B	801	ACX	C1D-O5D-C5D	2.90	119.44	113.74
2	C	802	ACX	C2F-C3F-C4F	2.95	116.15	109.63
2	C	801	ACX	C1A-O1A-C4B	2.96	125.87	118.00
2	A	801	ACX	C2C-C3C-C4C	2.97	116.19	109.63
2	D	801	ACX	C1A-O1A-C4B	3.05	126.13	118.00
2	A	801	ACX	O5E-C5E-C4E	3.06	116.31	109.78
2	D	802	ACX	C1A-O1A-C4B	3.08	126.20	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	802	ACX	C1D-C2D-C3D	3.10	116.13	109.98
2	D	803	ACX	C1A-O1A-C4B	3.12	126.30	118.00
2	A	801	ACX	C2E-C3E-C4E	3.15	116.59	109.63
2	C	803	ACX	O5D-C5D-C4D	3.17	116.55	109.78
2	B	801	ACX	C1A-O1A-C4B	3.19	126.49	118.00
2	A	802	ACX	C2D-C3D-C4D	3.20	116.69	109.63
2	D	803	ACX	O5A-C5A-C4A	3.23	116.67	109.78
2	D	801	ACX	C2E-C3E-C4E	3.37	117.06	109.63
2	A	801	ACX	C1C-C2C-C3C	3.40	116.72	109.98
2	C	802	ACX	O5E-C5E-C4E	3.48	117.19	109.78
2	A	802	ACX	C2E-C3E-C4E	3.69	117.79	109.63
2	B	801	ACX	O5D-C5D-C4D	4.31	118.96	109.78
2	A	801	ACX	O5D-C5D-C4D	4.74	119.89	109.78
2	D	801	ACX	O5C-C5C-C4C	4.94	120.32	109.78
2	D	801	ACX	O5F-C5F-C4F	5.11	120.68	109.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ACX	2	0
2	B	801	ACX	1	0
3	B	802	GOL	1	0
2	C	803	ACX	2	0
2	D	801	ACX	2	0
2	D	802	ACX	2	0
2	D	803	ACX	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	587/612 (95%)	0.35	80 (13%) 4 2	33, 64, 136, 151	2 (0%)
1	B	594/612 (97%)	-0.24	13 (2%) 65 59	34, 53, 84, 104	2 (0%)
1	C	584/612 (95%)	-0.26	5 (0%) 85 83	35, 55, 79, 96	0
1	D	589/612 (96%)	-0.39	1 (0%) 95 95	30, 43, 69, 97	3 (0%)
All	All	2354/2448 (96%)	-0.13	99 (4%) 40 32	30, 53, 106, 151	7 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	TYR	6.4
1	A	201	LEU	6.2
1	A	159	TRP	6.2
1	A	475	LEU	6.1
1	B	133	ASP	5.4
1	A	187	LEU	5.3
1	A	145	PRO	4.9
1	A	349	ALA	4.8
1	A	214	PRO	4.8
1	A	146	ASN	4.7
1	A	359	HIS	4.6
1	A	134	GLY	4.5
1	A	153	VAL	4.5
1	A	175	TRP	4.4
1	A	429	GLY	4.4
1	A	165	PRO	4.4
1	A	158	TYR	4.4
1	A	428	GLY	4.3
1	A	473	GLY	4.3
1	A	192	MET	4.3
1	A	150	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	411	ILE	4.2
1	A	196	ASN	4.0
1	A	351	PHE	4.0
1	A	350	GLU	3.9
1	A	472	MET	3.9
1	A	202	LYS	3.8
1	B	427	PHE	3.8
1	A	144	ALA	3.8
1	A	346	PHE	3.7
1	A	160	ASP	3.7
1	A	180	PRO	3.7
1	A	162	ARG	3.7
1	A	118	HIS	3.5
1	A	188	TYR	3.4
1	A	353	GLY	3.4
1	B	199	LEU	3.4
1	A	215	GLU	3.4
1	A	172	SER	3.3
1	A	163	ARG	3.3
1	A	195	ALA	3.2
1	A	143	TRP	3.2
1	A	140	PHE	3.2
1	A	372	THR	3.2
1	A	438	PHE	3.1
1	A	147	ALA	3.1
1	A	197	GLY	3.1
1	A	151	SER	3.0
1	B	426	GLU	3.0
1	A	117	THR	3.0
1	A	164	HIS	3.0
1	A	474	GLY	3.0
1	A	191	GLU	2.9
1	A	168	LEU	2.9
1	A	465	GLY	2.9
1	A	142	VAL	2.9
1	A	152	VAL	2.9
1	B	117	THR	2.8
1	A	360	SER	2.7
1	A	155	GLN	2.7
1	C	360	SER	2.7
1	A	200	ARG	2.6
1	A	156	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	133	ASP	2.6
1	A	161	GLY	2.6
1	A	469	PRO	2.6
1	A	446	LEU	2.6
1	A	357	TYR	2.6
1	A	135	VAL	2.5
1	A	376	ASN	2.5
1	A	198	ASN	2.5
1	A	199	LEU	2.5
1	B	200	ARG	2.5
1	A	412	TYR	2.5
1	B	134	GLY	2.5
1	A	463	PHE	2.5
1	B	164	HIS	2.4
1	A	154	GLY	2.4
1	A	133	ASP	2.4
1	A	149	ARG	2.3
1	A	205	PRO	2.3
1	C	215	GLU	2.3
1	B	132	MET	2.2
1	C	200	ARG	2.2
1	D	371	ASN	2.2
1	A	170	LYS	2.2
1	A	182	ALA	2.2
1	A	189	LYS	2.2
1	B	294	PHE	2.2
1	A	177	LEU	2.1
1	A	354	THR	2.1
1	A	516	THR	2.1
1	A	379	ARG	2.1
1	A	203	SER	2.1
1	A	432	ASN	2.1
1	C	346	PHE	2.1
1	B	425	ASN	2.1
1	B	201	LEU	2.0
1	A	186	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	A	803	6/6	0.92	0.35	10.33	58,59,64,66	0
2	ACX	B	801	66/66	0.90	0.28	4.31	55,90,101,107	0
2	ACX	D	801	66/66	0.78	0.34	3.24	87,123,135,139	0
3	GOL	D	804	6/6	0.96	0.14	1.33	48,51,53,57	0
2	ACX	C	801	66/66	0.93	0.19	1.10	53,77,86,89	0
2	ACX	A	802	66/66	0.89	0.22	0.95	67,90,106,113	0
2	ACX	C	802	66/66	0.89	0.21	0.74	73,92,103,106	0
3	GOL	B	802	6/6	0.97	0.17	0.52	45,51,58,62	0
2	ACX	D	802	66/66	0.90	0.23	0.47	55,83,94,102	0
2	ACX	A	801	66/66	0.87	0.19	0.40	74,94,101,104	0
3	GOL	B	803	6/6	0.79	0.17	0.26	70,74,75,76	0
2	ACX	C	803	66/66	0.93	0.21	0.23	65,92,100,102	0
2	ACX	D	803	66/66	0.94	0.16	-0.05	46,69,85,90	0
3	GOL	A	804	6/6	0.97	0.12	-0.33	44,47,52,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.