W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

May 4, 2016 – 08:24 PM EDT

|		
PDB ID	:	5E6Z
Title	:	Crystal structure of Ecoli Branching Enzyme with beta cyclodextrin
Authors	:	Feng, L.; Nosrati, M.; Geiger, J.H.
Deposited on	:	2015-10-11
Resolution	:	1.88 Å(reported)

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1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
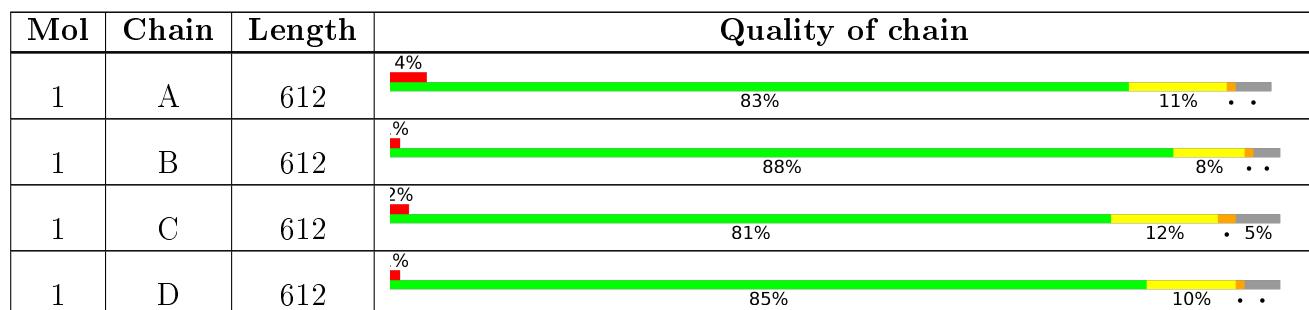
The reported resolution of this entry is 1.88 Å.

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	Percentile Ranks	Value
Rfree		0.245
Clashscore		4
Ramachandran outliers		0.6%
Sidechain outliers		5.4%
RSRZ outliers		1.9%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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 <=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	4% / 83% / 11% · ·
1	B	612	% / 88% / 8% · ·
1	C	612	2% / 81% / 12% · 5%
1	D	612	% / 85% / 10% · ·

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	BCD	B	801	-	-	-	X
2	BCD	C	802	-	-	-	X
3	GOL	A	803	-	-	-	X
3	GOL	C	803	-	-	-	X

2 Entry composition (i)
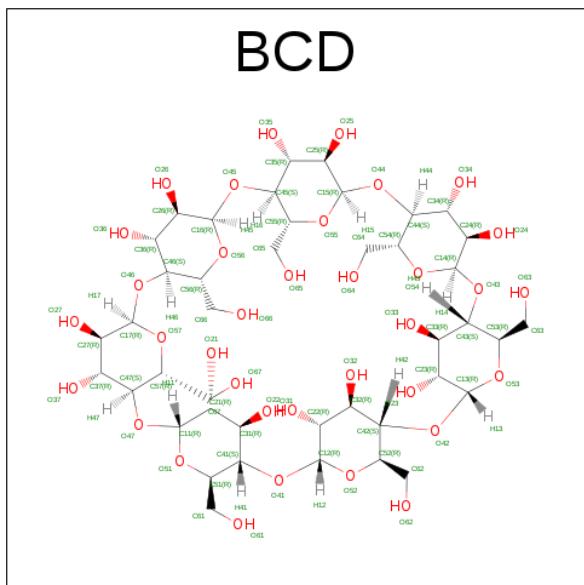
There are 4 unique types of molecules in this entry. The entry contains 21819 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	9	0
			4866	3117	859	874	16			
1	B	596	Total	C	N	O	S	0	8	0
			4953	3169	881	887	16			
1	C	582	Total	C	N	O	S	0	4	0
			4810	3082	852	861	15			
1	D	587	Total	C	N	O	S	0	4	0
			4849	3101	863	869	16			

- Molecule 2 is BETA-CYCLODEXTRIN (three-letter code: BCD) (formula: $C_{42}H_{70}O_{35}$).
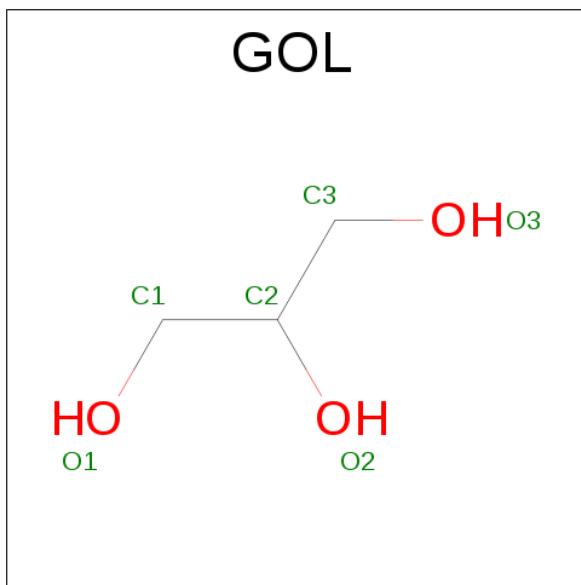
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			77	42	35		
2	A	1	Total	C	O	0	0
			77	42	35		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 77	C 42	O 35	0	0
2	C	1	Total 77	C 42	O 35	0	0
2	C	1	Total 77	C 42	O 35	0	0
2	D	1	Total 77	C 42	O 35	0	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
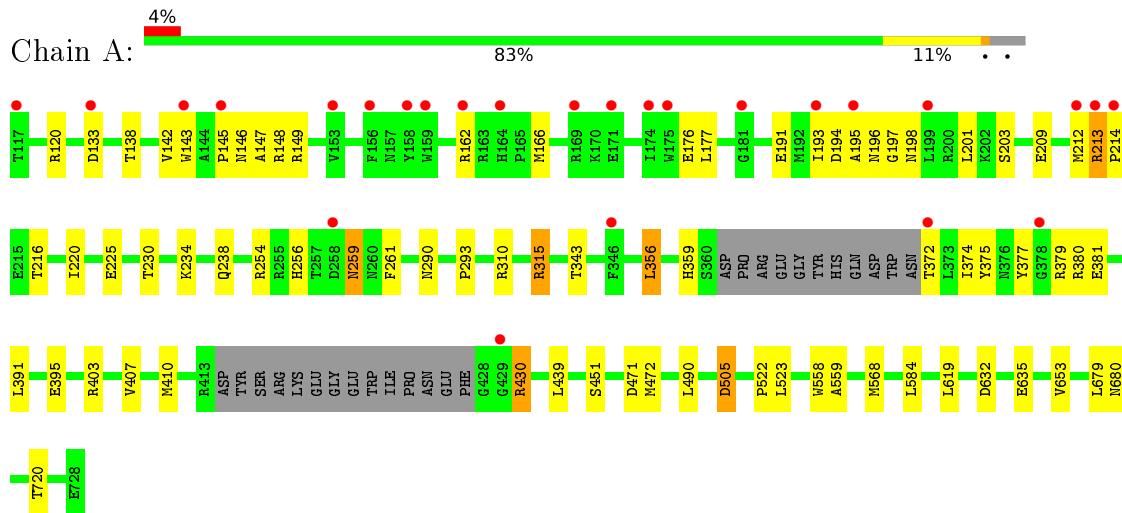
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	447	Total 447	O 447	0	0
4	B	615	Total 615	O 615	0	0
4	C	289	Total 289	O 289	0	0
4	D	486	Total 486	O 486	0	0
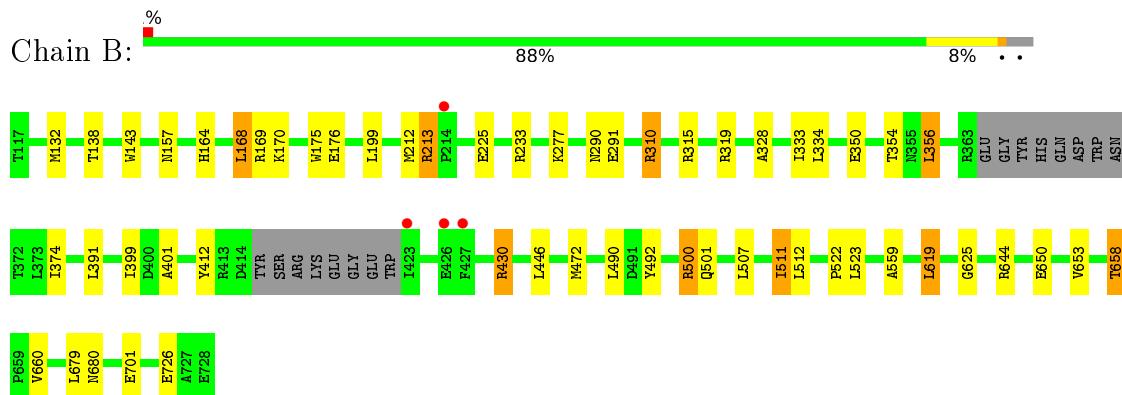
3 Residue-property plots ⓘ

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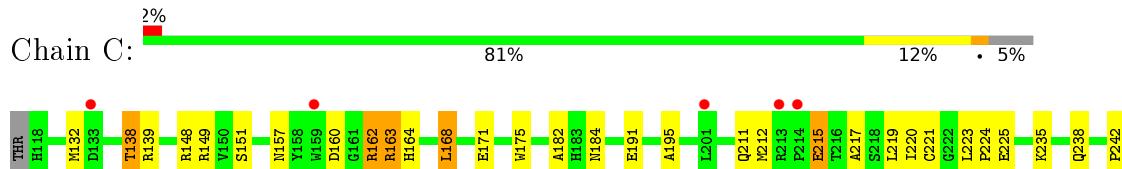
- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB
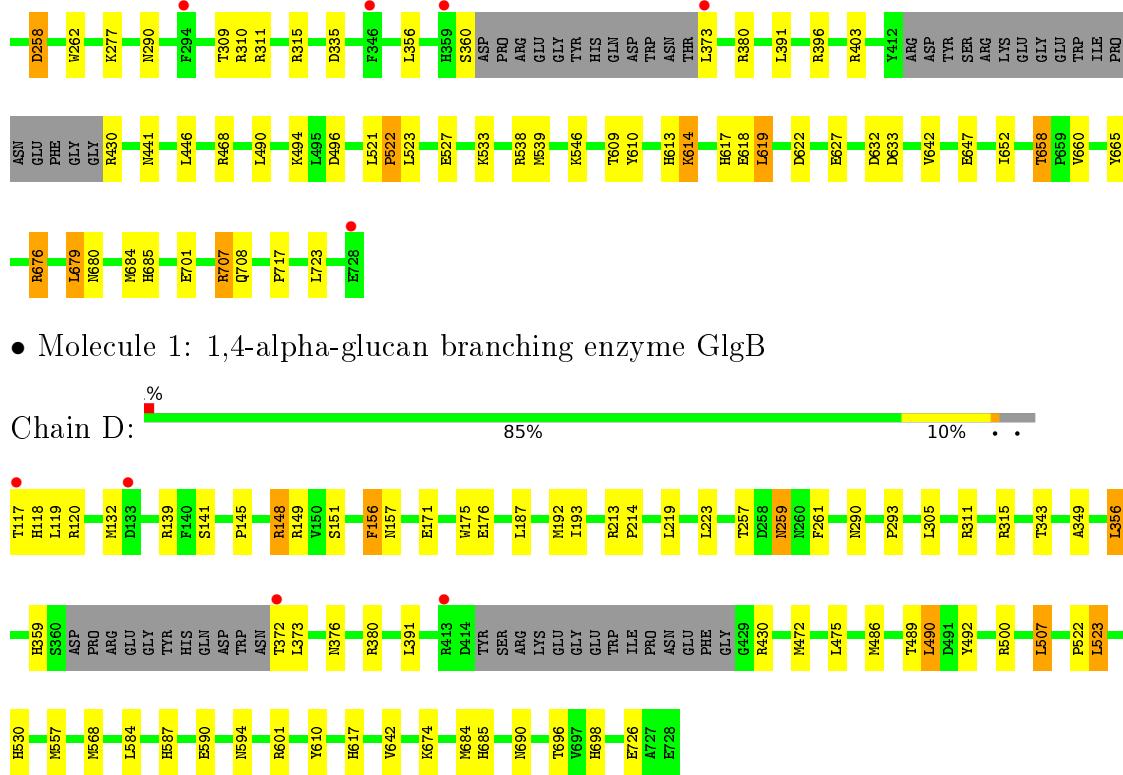
- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

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

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

Chain D:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.95Å 103.00Å 186.24Å 90.00° 91.57° 90.00°	Depositor
Resolution (Å)	44.93 – 1.88 44.93 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.93-1.88) 99.4 (44.93-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 1.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.206 , 0.249 0.203 , 0.245	Depositor DCC
R_{free} test set	28003 reflections (9.97%)	DCC
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.0	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.067 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21819	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.38	0/5040	0.55	0/6845
1	B	0.44	0/5128	0.60	2/6962 (0.0%)
1	C	0.32	0/4973	0.49	0/6755
1	D	0.38	0/5014	0.55	0/6807
All	All	0.38	0/20155	0.55	2/27369 (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	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	500	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	B	500	ARG	NE-CZ-NH2	-6.26	117.17	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	156	PHE	Peptide

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	4866	0	4604	39	0
1	B	4953	0	4700	28	0
1	C	4810	0	4547	49	0
1	D	4849	0	4597	35	0
2	A	154	0	140	2	0
2	B	77	0	70	1	0
2	C	154	0	140	1	0
2	D	77	0	70	1	0
3	A	12	0	16	0	0
3	B	12	0	16	0	0
3	C	6	0	8	0	0
3	D	12	0	16	0	0
4	A	447	0	0	9	1
4	B	615	0	0	7	1
4	C	289	0	0	9	0
4	D	486	0	0	7	1
All	All	21819	0	18924	150	2

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 (150) 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:403:ARG:NH1	4:A:902:HOH:O	2.11	0.84
1:B:658:THR:HG22	1:B:660:VAL:H	1.44	0.83
1:A:194:ASP:HB2	1:A:198:ASN:H	1.46	0.78
1:C:162[A]:ARG:NH1	4:C:902:HOH:O	2.16	0.78
1:D:151:SER:OG	4:D:901:HOH:O	2.02	0.76
1:A:149:ARG:HB3	1:A:193:ILE:HB	1.69	0.73
1:A:254:ARG:NH2	4:A:905:HOH:O	2.21	0.72
1:D:684:MET:H	1:D:690:ASN:HD22	1.35	0.72
1:D:132:MET:SD	1:D:139[A]:ARG:NH1	2.63	0.71
1:B:511:ILE:HB	4:B:1490:HOH:O	1.91	0.71
1:A:632[B]:ASP:OD1	4:A:901:HOH:O	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162[B]:ARG:NH2	4:C:905:HOH:O	2.24	0.70
1:A:256:HIS:HB2	1:A:259:ASN:HD21	1.58	0.69
1:A:259:ASN:HD22	1:A:261:PHE:H	1.41	0.69
1:C:658:THR:HG22	1:C:660:VAL:H	1.58	0.68
1:C:162[A]:ARG:HH11	1:C:162[A]:ARG:HB2	1.58	0.68
1:B:169:ARG:NH1	1:B:176:GLU:OE2	2.27	0.68
1:B:213[A]:ARG:HD3	1:B:213[A]:ARG:H	1.60	0.66
1:A:194:ASP:HB3	1:A:196:ASN:H	1.60	0.65
1:A:213:ARG:NH1	1:A:293:PRO:O	2.28	0.65
1:A:632[B]:ASP:OD1	4:A:903:HOH:O	2.15	0.64
1:C:609:THR:O	4:C:901:HOH:O	2.15	0.64
1:C:494:LYS:HD3	1:C:538:ARG:HG2	1.80	0.64
1:A:471:ASP:OD1	4:A:904:HOH:O	2.15	0.62
1:A:212:MET:HG2	1:A:310:ARG:HG2	1.82	0.62
1:D:492:TYR:CZ	1:D:500:ARG:HG2	2.36	0.60
1:D:684:MET:H	1:D:690:ASN:ND2	1.99	0.60
1:C:527:GLU:O	1:C:538:ARG:NH1	2.26	0.60
1:D:139[A]:ARG:NH2	1:D:176:GLU:OE1	2.35	0.60
2:D:801:BCD:H622	4:D:1071:HOH:O	2.01	0.59
1:A:234:LYS:NZ	1:A:451:SER:O	2.30	0.58
1:C:163:ARG:NH1	4:C:913:HOH:O	2.36	0.58
1:B:701:GLU:OE2	4:B:901:HOH:O	2.17	0.58
1:D:259:ASN:HB3	1:D:261:PHE:H	1.69	0.57
1:C:242:PRO:HD3	1:C:617:HIS:CE1	2.39	0.57
1:D:349:ALA:O	4:D:902:HOH:O	2.18	0.57
1:B:233:ARG:NH1	4:B:915:HOH:O	2.38	0.56
1:B:492:TYR:CZ	1:B:500:ARG:HG2	2.41	0.56
1:D:696:THR:OG1	1:D:726:GLU:OE1	2.21	0.55
1:D:343:THR:HG22	1:D:373:LEU:HD12	1.87	0.55
1:C:162[B]:ARG:NH1	4:C:903:HOH:O	2.17	0.55
1:B:319:ARG:NH1	4:B:914:HOH:O	2.38	0.54
1:A:149:ARG:NH1	1:A:191:GLU:OE2	2.41	0.54
1:A:120:ARG:NH1	1:A:395:GLU:OE2	2.41	0.53
1:C:627:GLU:OE1	1:C:707:ARG:NH2	2.41	0.53
1:B:143:TRP:CH2	1:B:356:LEU:HD22	2.42	0.53
1:B:212:MET:HG3	1:B:310:ARG:HD3	1.91	0.53
1:D:486:MET:O	1:D:490:LEU:HB2	2.10	0.52
1:C:139:ARG:HD3	4:C:933:HOH:O	2.10	0.52
1:C:539:MET:O	1:C:546:LYS:NZ	2.39	0.51
1:C:157:ASN:OD1	1:C:164:HIS:ND1	2.42	0.51
1:A:635[A]:GLU:H	1:A:635[A]:GLU:CD	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:GLU:HG2	4:B:1293:HOH:O	2.10	0.51
1:C:224:PRO:HG2	1:C:396:ARG:HB3	1.92	0.51
1:B:644:ARG:CG	1:B:650:GLU:HG2	2.42	0.49
1:A:679:LEU:HG	1:A:680:ASN:N	2.27	0.49
1:C:262:TRP:CH2	1:C:311:ARG:HD3	2.47	0.49
2:A:801:BCD:O31	2:A:801:BCD:O22	2.27	0.49
1:B:658:THR:CG2	1:B:660:VAL:H	2.20	0.49
1:C:676[A]:ARG:NH2	4:C:912:HOH:O	2.36	0.48
1:D:594:ASN:HB2	4:D:1235:HOH:O	2.13	0.48
1:A:356:LEU:O	1:A:379:ARG:NH1	2.46	0.48
1:C:138:THR:HG23	1:C:182:ALA:HB3	1.95	0.47
1:C:309:THR:OG1	1:C:311:ARG:HG3	2.14	0.47
1:B:501:GLN:NE2	4:B:921:HOH:O	2.41	0.47
1:C:309:THR:OG1	4:C:904:HOH:O	2.20	0.47
1:D:120:ARG:NH2	4:D:918:HOH:O	2.37	0.47
1:C:652:ILE:HB	1:C:723:LEU:HB2	1.96	0.47
1:D:148:ARG:HG3	1:D:193:ILE:HG22	1.95	0.47
1:A:143:TRP:CH2	1:A:356:LEU:HD22	2.50	0.47
1:C:717:PRO:HG3	2:C:802:BCD:H612	1.97	0.47
1:D:530:HIS:HE1	4:D:1344:HOH:O	1.98	0.47
1:B:212:MET:HG2	1:B:213[A]:ARG:NH1	2.30	0.47
1:D:617:HIS:HE1	4:D:1335:HOH:O	1.97	0.46
1:C:138:THR:HG21	1:C:220:ILE:HD13	1.97	0.46
1:B:213[B]:ARG:NH2	1:B:291:GLU:OE1	2.38	0.46
1:B:679:LEU:HG	1:B:680:ASN:N	2.30	0.46
1:B:277[A]:LYS:HD2	1:B:328:ALA:HB1	1.96	0.46
1:A:559:ALA:HB1	1:A:653:VAL:HG21	1.98	0.46
1:B:619:LEU:HB3	1:B:625:GLY:HA3	1.97	0.46
1:D:213:ARG:NH2	1:D:293:PRO:O	2.49	0.46
1:D:587:HIS:O	1:D:590:GLU:HB2	2.16	0.46
1:A:238:GLN:HG2	4:A:1324:HOH:O	2.16	0.46
1:C:149:ARG:NH2	1:C:191:GLU:OE2	2.37	0.46
1:C:619:LEU:HG	1:C:622:ASP:HB3	1.99	0.45
1:D:145:PRO:HD2	1:D:356:LEU:HD11	1.98	0.45
1:A:148:ARG:HH12	1:A:197:GLY:HA2	1.80	0.45
1:A:148:ARG:NH2	1:A:195:ALA:O	2.49	0.45
1:A:407:VAL:HA	1:A:410:MET:HE2	1.99	0.45
1:A:138:THR:HG21	1:A:220:ILE:HG21	1.98	0.45
1:A:356:LEU:HA	1:A:356:LEU:HD23	1.77	0.45
1:C:149:ARG:NH1	1:C:151:SER:OG	2.48	0.45
1:C:685:HIS:CE1	1:D:685:HIS:HD2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:HG2	1:A:430:ARG:H	1.49	0.45
1:D:359:HIS:CD2	1:D:376:ASN:HA	2.52	0.45
1:A:146:ASN:O	1:A:148:ARG:N	2.50	0.44
1:D:486:MET:HG2	1:D:490:LEU:HD22	1.98	0.44
1:A:261:PHE:CD2	2:A:802:BCD:H36	2.51	0.44
1:B:157:ASN:OD1	1:B:164:HIS:ND1	2.50	0.44
1:C:235:LYS:HA	1:C:238:GLN:HG3	1.98	0.44
1:C:258:ASP:N	1:C:258:ASP:OD1	2.43	0.44
1:C:335:ASP:OD1	1:C:403:ARG:HD3	2.18	0.44
1:D:213:ARG:HH22	1:D:311:ARG:NH1	2.16	0.44
1:C:168:LEU:HG	1:C:175:TRP:CE2	2.52	0.43
1:D:568:MET:HB2	1:D:584:LEU:HD11	1.99	0.43
1:C:633:ASP:OD2	1:C:665:TYR:OH	2.29	0.43
1:C:160:ASP:CG	1:C:162[A]:ARG:HG2	2.40	0.43
1:C:610:TYR:O	1:C:617:HIS:HD2	2.01	0.43
1:C:533:LYS:O	1:C:538:ARG:NH1	2.52	0.42
1:B:333:ILE:HG12	1:B:401:ALA:HB3	2.01	0.42
1:B:168:LEU:HG	1:B:175:TRP:CE2	2.54	0.42
1:C:211:GLN:HE21	1:C:217:ALA:H	1.65	0.42
1:C:613:HIS:HB2	4:C:901:HOH:O	2.19	0.42
1:C:614:LYS:O	1:C:618:GLU:HB2	2.19	0.42
1:D:489:THR:HG22	1:D:507:LEU:HD12	2.02	0.42
1:C:685:HIS:NE2	1:D:685:HIS:HD2	2.18	0.42
1:A:254:ARG:NE	4:A:952:HOH:O	2.53	0.42
1:B:334[B]:LEU:HG	1:B:399:ILE:HD12	2.00	0.42
1:C:521:LEU:HA	1:C:522:PRO:HD3	1.92	0.42
1:C:211:GLN:NE2	1:C:215:GLU:HB2	2.34	0.42
1:C:685:HIS:CD2	1:D:685:HIS:CD2	3.07	0.42
1:D:601:ARG:HD2	1:D:685:HIS:NE2	2.34	0.42
1:B:350:GLU:HA	1:B:354:THR:O	2.20	0.42
1:B:412:TYR:CE2	1:B:430:ARG:HD2	2.55	0.41
1:A:505:ASP:HB3	4:A:1284:HOH:O	2.19	0.41
1:A:230:THR:HB	4:A:1129:HOH:O	2.20	0.41
1:D:430:ARG:HB2	1:D:430:ARG:NH1	2.35	0.41
1:B:492:TYR:CE2	1:B:500:ARG:HG2	2.55	0.41
1:A:410:MET:HE1	1:A:439:LEU:HD21	2.02	0.41
1:C:685:HIS:CD2	1:D:685:HIS:HD2	2.39	0.41
1:A:145:PRO:HD2	1:A:356:LEU:HD21	2.03	0.41
1:A:568:MET:HB2	1:A:584:LEU:HD11	2.03	0.41
1:C:184:ASN:OD1	1:C:221:CYS:HA	2.21	0.41
1:C:632:ASP:N	1:C:632:ASP:OD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:610:TYR:O	1:D:617:HIS:HD2	2.03	0.41
1:C:679:LEU:HG	1:C:680:ASN:N	2.35	0.41
1:C:701:GLU:OE2	1:C:708:GLN:NE2	2.54	0.41
1:A:166:MET:HA	1:A:177:LEU:HB2	2.03	0.41
1:A:209:GLU:HG3	1:A:315:ARG:HB3	2.02	0.41
1:C:148:ARG:NH2	1:C:195:ALA:O	2.54	0.41
1:D:523:LEU:HD22	1:D:557:MET:SD	2.61	0.41
2:B:801:BCD:H672	4:B:1030:HOH:O	2.21	0.41
1:C:468:ARG:HD3	1:C:468:ARG:HA	1.90	0.41
1:B:559:ALA:HB1	1:B:653:VAL:HG21	2.03	0.40
1:D:141:SER:HA	1:D:175:TRP:O	2.21	0.40
1:A:375:TYR:HB2	1:A:377:TYR:CZ	2.56	0.40
1:A:381:GLU:N	1:A:381:GLU:OE2	2.50	0.40
1:D:674:LYS:HG2	1:D:698:HIS:CD2	2.55	0.40
1:D:684:MET:HB3	1:D:684:MET:HE3	1.88	0.40

All (2) 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)
4:D:1070:HOH:O	4:D:1328:HOH:O[2_655]	2.13	0.07
4:A:1291:HOH:O	4:B:1318:HOH:O[1_455]	2.17	0.03

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	589/612 (96%)	568 (96%)	16 (3%)	5 (1%)	24	10
1	B	598/612 (98%)	580 (97%)	17 (3%)	1 (0%)	52	40
1	C	580/612 (95%)	563 (97%)	15 (3%)	2 (0%)	46	33
1	D	585/612 (96%)	571 (98%)	9 (2%)	5 (1%)	21	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2352/2448 (96%)	2282 (97%)	57 (2%)	13 (1%)	30 16

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	PRO
1	D	259	ASN
1	A	133	ASP
1	A	147	ALA
1	A	216	THR
1	C	212	MET
1	D	156	PHE
1	D	157	ASN
1	D	522	PRO
1	A	522	PRO
1	B	522	PRO
1	C	522	PRO
1	D	214	PRO

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	504/521 (97%)	479 (95%)	25 (5%)	30 16
1	B	514/521 (99%)	489 (95%)	25 (5%)	31 16
1	C	496/521 (95%)	458 (92%)	38 (8%)	16 5
1	D	502/521 (96%)	477 (95%)	25 (5%)	30 16
All	All	2016/2084 (97%)	1903 (94%)	113 (6%)	27 12

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	VAL
1	A	162	ARG

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Mol	Chain	Res	Type
1	A	176	GLU
1	A	201	LEU
1	A	203	SER
1	A	213	ARG
1	A	225	GLU
1	A	259	ASN
1	A	290	ASN
1	A	315	ARG
1	A	343	THR
1	A	356	LEU
1	A	359	HIS
1	A	372	THR
1	A	374	ILE
1	A	380	ARG
1	A	391	LEU
1	A	430	ARG
1	A	472	MET
1	A	490	LEU
1	A	505	ASP
1	A	523	LEU
1	A	558	TRP
1	A	619	LEU
1	A	720	THR
1	B	132	MET
1	B	138	THR
1	B	168	LEU
1	B	170	LYS
1	B	199	LEU
1	B	213[A]	ARG
1	B	213[B]	ARG
1	B	225	GLU
1	B	290	ASN
1	B	310	ARG
1	B	315	ARG
1	B	356	LEU
1	B	374	ILE
1	B	391	LEU
1	B	430	ARG
1	B	446	LEU
1	B	472	MET
1	B	490	LEU
1	B	507	LEU

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Mol	Chain	Res	Type
1	B	511	ILE
1	B	512[A]	LEU
1	B	512[B]	LEU
1	B	523	LEU
1	B	619	LEU
1	B	658	THR
1	C	132	MET
1	C	138	THR
1	C	162[A]	ARG
1	C	162[B]	ARG
1	C	163	ARG
1	C	168	LEU
1	C	171	GLU
1	C	215	GLU
1	C	219	LEU
1	C	223	LEU
1	C	225	GLU
1	C	258	ASP
1	C	277	LYS
1	C	290	ASN
1	C	310	ARG
1	C	315	ARG
1	C	356	LEU
1	C	360	SER
1	C	373	LEU
1	C	380	ARG
1	C	391	LEU
1	C	430	ARG
1	C	441	ASN
1	C	446	LEU
1	C	490	LEU
1	C	496	ASP
1	C	523	LEU
1	C	614	LYS
1	C	619	LEU
1	C	642[A]	VAL
1	C	642[B]	VAL
1	C	647	GLU
1	C	658	THR
1	C	676[A]	ARG
1	C	676[B]	ARG
1	C	679	LEU

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Mol	Chain	Res	Type
1	C	684	MET
1	C	707	ARG
1	D	117	THR
1	D	118	HIS
1	D	119	LEU
1	D	148	ARG
1	D	149	ARG
1	D	171	GLU
1	D	187	LEU
1	D	192	MET
1	D	219	LEU
1	D	223	LEU
1	D	257	THR
1	D	290	ASN
1	D	305	LEU
1	D	315	ARG
1	D	356	LEU
1	D	372	THR
1	D	380	ARG
1	D	391	LEU
1	D	472	MET
1	D	475	LEU
1	D	490	LEU
1	D	507	LEU
1	D	523	LEU
1	D	642[A]	VAL
1	D	642[B]	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	ASN
1	A	501	GLN
1	A	617	HIS
1	C	157	ASN
1	C	211	GLN
1	C	441	ASN
1	C	617	HIS
1	D	617	HIS
1	D	685	HIS
1	D	690	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 carbohydrates in this entry.

5.6   Ligand geometry (i)

13 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	BCD	A	801	-	84,84,84	1.14	5 (5%)	126,126,126	1.68	10 (7%)
2	BCD	A	802	-	84,84,84	1.17	7 (8%)	126,126,126	1.62	11 (8%)
3	GOL	A	803	-	5,5,5	0.31	0	5,5,5	0.37	0
3	GOL	A	804	-	5,5,5	0.28	0	5,5,5	0.27	0
2	BCD	B	801	-	84,84,84	1.13	7 (8%)	126,126,126	1.63	14 (11%)
3	GOL	B	802	-	5,5,5	0.33	0	5,5,5	0.40	0
3	GOL	B	803	-	5,5,5	0.32	0	5,5,5	0.21	0
2	BCD	C	801	-	84,84,84	1.14	5 (5%)	126,126,126	1.71	14 (11%)
2	BCD	C	802	-	84,84,84	1.14	5 (5%)	126,126,126	1.77	14 (11%)
3	GOL	C	803	-	5,5,5	0.35	0	5,5,5	0.30	0
2	BCD	D	801	-	84,84,84	1.14	7 (8%)	126,126,126	1.73	15 (11%)
3	GOL	D	802	-	5,5,5	0.37	0	5,5,5	0.25	0
3	GOL	D	803	-	5,5,5	0.30	0	5,5,5	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BCD	A	801	-	-	0/42/182/182	0/0/8/8
2	BCD	A	802	-	-	0/42/182/182	0/0/8/8
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	BCD	B	801	-	-	0/42/182/182	0/0/8/8
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	BCD	C	801	-	-	0/42/182/182	0/0/8/8
2	BCD	C	802	-	-	0/42/182/182	0/0/8/8
3	GOL	C	803	-	-	0/4/4/4	0/0/0/0
2	BCD	D	801	-	-	0/42/182/182	0/0/8/8
3	GOL	D	802	-	-	0/4/4/4	0/0/0/0
3	GOL	D	803	-	-	0/4/4/4	0/0/0/0

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	BCD	O52-C12	-2.15	1.36	1.41
2	D	801	BCD	O43-C14	-2.06	1.36	1.41
2	B	801	BCD	O56-C16	2.01	1.47	1.41
2	D	801	BCD	O56-C16	2.01	1.47	1.41
2	A	802	BCD	O46-C17	2.02	1.47	1.41
2	A	802	BCD	O56-C16	2.10	1.47	1.41
2	C	801	BCD	O42-C13	2.31	1.48	1.41
2	D	801	BCD	O42-C13	2.33	1.48	1.41
2	B	801	BCD	O47-C11	2.33	1.48	1.41
2	D	801	BCD	O44-C44	2.33	1.49	1.43
2	A	802	BCD	O44-C44	2.37	1.49	1.43
2	C	802	BCD	O44-C44	2.41	1.49	1.43
2	A	801	BCD	O42-C13	2.41	1.48	1.41
2	A	801	BCD	O44-C44	2.41	1.49	1.43
2	B	801	BCD	O44-C44	2.44	1.50	1.43
2	C	801	BCD	O44-C44	2.46	1.50	1.43
2	B	801	BCD	O41-C12	2.53	1.48	1.41
2	C	802	BCD	O42-C13	2.55	1.48	1.41
2	A	802	BCD	O42-C13	2.58	1.48	1.41
2	C	802	BCD	O47-C11	2.58	1.48	1.41
2	B	801	BCD	O42-C13	2.70	1.49	1.41
2	D	801	BCD	O41-C12	2.76	1.49	1.41
2	C	802	BCD	O41-C12	2.77	1.49	1.41
2	C	801	BCD	O47-C11	2.78	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	BCD	O41-C12	2.78	1.49	1.41
2	A	801	BCD	O41-C12	2.86	1.49	1.41
2	A	802	BCD	O47-C11	2.88	1.49	1.41
2	C	801	BCD	O41-C12	2.96	1.49	1.41
2	A	801	BCD	O47-C11	2.96	1.49	1.41
2	D	801	BCD	O47-C11	3.01	1.49	1.41
2	C	801	BCD	O54-C14	3.75	1.51	1.41
2	B	801	BCD	O54-C14	3.79	1.51	1.41
2	C	802	BCD	O54-C14	3.84	1.51	1.41
2	A	802	BCD	O54-C14	3.93	1.51	1.41
2	D	801	BCD	O54-C14	3.94	1.51	1.41
2	A	801	BCD	O54-C14	3.99	1.52	1.41

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	BCD	C17-O46-C46	-3.98	107.42	118.00
2	C	802	BCD	C13-O42-C42	-3.45	108.81	118.00
2	B	801	BCD	C17-O46-C46	-3.41	108.93	118.00
2	A	801	BCD	C12-O41-C41	-3.37	109.05	118.00
2	D	801	BCD	C12-O41-C41	-3.36	109.07	118.00
2	D	801	BCD	C17-O46-C46	-3.28	109.28	118.00
2	C	801	BCD	C12-O41-C41	-3.27	109.32	118.00
2	A	802	BCD	C13-O42-C42	-3.26	109.34	118.00
2	A	801	BCD	C13-O42-C42	-3.21	109.46	118.00
2	C	802	BCD	C12-O41-C41	-3.03	109.94	118.00
2	D	801	BCD	C13-O42-C42	-3.01	109.99	118.00
2	C	802	BCD	C16-O45-C45	-3.01	110.00	118.00
2	C	801	BCD	C13-O42-C42	-3.01	110.00	118.00
2	D	801	BCD	C16-O45-C45	-2.98	110.08	118.00
2	B	801	BCD	C12-O41-C41	-2.86	110.41	118.00
2	C	802	BCD	C17-O46-C46	-2.84	110.46	118.00
2	C	801	BCD	C17-O46-C46	-2.80	110.55	118.00
2	B	801	BCD	C15-O44-C44	-2.80	110.56	118.00
2	D	801	BCD	C15-O44-C44	-2.77	110.64	118.00
2	C	801	BCD	C14-O43-C43	-2.70	110.83	118.00
2	A	801	BCD	C12-O52-C52	-2.58	108.67	113.74
2	A	801	BCD	C15-O55-C55	-2.58	108.69	113.74
2	C	802	BCD	C15-O44-C44	-2.56	111.19	118.00
2	A	802	BCD	C14-O43-C43	-2.56	111.20	118.00
2	C	801	BCD	C15-O44-C44	-2.54	111.25	118.00
2	A	802	BCD	C16-O45-C45	-2.51	111.33	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	BCD	C16-O45-C45	-2.45	111.49	118.00
2	D	801	BCD	C14-O43-C43	-2.43	111.54	118.00
2	A	802	BCD	C12-O41-C41	-2.36	111.72	118.00
2	A	801	BCD	C16-O45-C45	-2.33	111.79	118.00
2	C	802	BCD	O47-C11-O51	-2.32	104.64	110.69
2	B	801	BCD	C16-O56-C56	-2.32	109.20	113.74
2	C	801	BCD	C12-O52-C52	-2.30	109.23	113.74
2	B	801	BCD	C14-O43-C43	-2.27	111.97	118.00
2	C	801	BCD	C14-O54-C54	-2.27	109.29	113.74
2	B	801	BCD	O41-C12-O52	-2.25	104.83	110.69
2	A	802	BCD	C15-O55-C55	-2.23	109.36	113.74
2	C	802	BCD	C14-O54-C54	-2.22	109.38	113.74
2	A	802	BCD	C15-O44-C44	-2.22	112.09	118.00
2	D	801	BCD	C12-O52-C52	-2.21	109.42	113.74
2	B	801	BCD	C13-O42-C42	-2.17	112.24	118.00
2	A	802	BCD	C17-O46-C46	-2.16	112.26	118.00
2	C	801	BCD	O45-C16-O56	-2.16	105.06	110.69
2	C	801	BCD	C15-O55-C55	-2.13	109.56	113.74
2	D	801	BCD	C16-O56-C56	-2.13	109.56	113.74
2	C	801	BCD	C16-O56-C56	-2.12	109.58	113.74
2	A	802	BCD	C12-O52-C52	-2.11	109.60	113.74
2	C	802	BCD	C14-O43-C43	-2.10	112.41	118.00
2	B	801	BCD	C14-O54-C54	-2.09	109.64	113.74
2	C	802	BCD	C12-O52-C52	-2.04	109.74	113.74
2	C	802	BCD	C16-O56-C56	-2.02	109.77	113.74
2	C	802	BCD	C26-C36-C46	2.01	114.08	109.63
2	D	801	BCD	O53-C53-C43	2.04	114.12	109.78
2	A	801	BCD	O54-C54-C44	2.07	114.18	109.78
2	B	801	BCD	O54-C54-C44	2.07	114.20	109.78
2	B	801	BCD	O55-C55-C45	2.10	114.26	109.78
2	A	802	BCD	O53-C53-C43	2.10	114.27	109.78
2	C	801	BCD	O57-C17-C27	2.12	114.68	110.28
2	C	801	BCD	C25-C35-C45	2.13	114.33	109.63
2	D	801	BCD	O57-C17-C27	2.19	114.84	110.28
2	A	801	BCD	O57-C17-C27	2.29	115.05	110.28
2	D	801	BCD	C26-C36-C46	2.33	114.77	109.63
2	C	802	BCD	O53-C53-C43	2.38	114.85	109.78
2	A	802	BCD	O51-C11-C21	2.41	115.29	110.28
2	D	801	BCD	C11-C21-C31	2.42	114.78	109.98
2	A	801	BCD	O51-C11-C21	2.45	115.37	110.28
2	D	801	BCD	O54-C54-C44	2.68	115.50	109.78
2	C	802	BCD	O51-C11-C21	2.73	115.94	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	BCD	O57-C17-C27	2.76	116.02	110.28
2	D	801	BCD	O51-C11-C21	2.92	116.36	110.28
2	C	801	BCD	O51-C11-C21	3.32	117.19	110.28
2	B	801	BCD	O51-C11-C21	4.46	119.56	110.28
2	B	801	BCD	C11-O47-C47	12.67	151.69	118.00
2	A	802	BCD	C11-O47-C47	13.87	154.90	118.00
2	D	801	BCD	C11-O47-C47	14.01	155.26	118.00
2	A	801	BCD	C11-O47-C47	14.19	155.75	118.00
2	C	801	BCD	C11-O47-C47	14.50	156.58	118.00
2	C	802	BCD	C11-O47-C47	15.14	158.27	118.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	BCD	1	0
2	A	802	BCD	1	0
2	B	801	BCD	1	0
2	C	802	BCD	1	0
2	D	801	BCD	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.10	26 (4%)	38	40	10, 27, 86, 112	3 (0%)
1	B	596/612 (97%)	-0.23	4 (0%)	89	89	9, 22, 39, 60	7 (1%)
1	C	582/612 (95%)	-0.02	10 (1%)	73	75	22, 36, 52, 71	2 (0%)
1	D	587/612 (95%)	-0.14	4 (0%)	89	89	15, 27, 46, 68	1 (0%)
All	All	2352/2448 (96%)	-0.07	44 (1%)	70	72	9, 28, 58, 112	13 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	THR	4.9
1	A	212	MET	4.9
1	A	429	GLY	4.9
1	D	117	THR	4.1
1	C	346	PHE	4.0
1	A	193	ILE	3.9
1	A	214	PRO	3.7
1	A	346	PHE	3.6
1	C	201	LEU	3.6
1	A	372	THR	3.3
1	A	378	GLY	3.3
1	A	175	TRP	3.1
1	A	195	ALA	3.1
1	C	359	HIS	3.0
1	A	156	PHE	2.9
1	B	423	ILE	2.9
1	A	153	VAL	2.8
1	C	294	PHE	2.8
1	A	133	ASP	2.8
1	C	213	ARG	2.8
1	A	171	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	214	PRO	2.6
1	C	133	ASP	2.6
1	C	373	LEU	2.6
1	B	427	PHE	2.6
1	A	143	TRP	2.6
1	C	728	GLU	2.5
1	A	181	GLY	2.5
1	A	174	ILE	2.5
1	A	145	PRO	2.5
1	A	164	HIS	2.4
1	A	213	ARG	2.4
1	A	159	TRP	2.4
1	A	169	ARG	2.3
1	A	199	LEU	2.3
1	B	426	GLU	2.3
1	A	258	ASP	2.3
1	A	158	TYR	2.2
1	C	159	TRP	2.2
1	D	413	ARG	2.2
1	A	162	ARG	2.1
1	D	133	ASP	2.1
1	B	214	PRO	2.0
1	D	372	THR	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
2	BCD	C	802	77/77	0.80	0.19	7.26	45,73,84,88	0
2	BCD	B	801	77/77	0.89	0.16	3.45	21,55,74,78	0
3	GOL	C	803	6/6	0.92	0.17	2.58	44,48,51,53	0
3	GOL	A	803	6/6	0.93	0.12	2.35	24,25,41,44	0
2	BCD	C	801	77/77	0.79	0.25	1.94	41,66,87,90	0
2	BCD	A	802	77/77	0.83	0.19	1.69	40,54,64,69	0
3	GOL	B	803	6/6	0.89	0.16	1.50	36,44,48,49	0
2	BCD	D	801	77/77	0.89	0.16	1.00	25,53,73,80	0
2	BCD	A	801	77/77	0.91	0.12	0.56	22,46,68,74	0
3	GOL	D	802	6/6	0.95	0.10	-0.19	26,32,34,36	0
3	GOL	B	802	6/6	0.98	0.09	-0.68	16,20,21,27	0
3	GOL	A	804	6/6	0.98	0.08	-1.09	16,23,24,27	0
3	GOL	D	803	6/6	0.97	0.07	-2.89	25,28,33,35	0

6.5 Other polymers (i)

There are no such residues in this entry.