



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:15 pm BST

PDB ID : 2DFK
Title : Crystal structure of the CDC42-Collybistin II complex
Authors : Xiang, S.; Kim, E.Y.; Connelly, J.J.; Nassar, N.; Kirsch, J.; Winking, J.; Schwarz, G.; Schindelin, H.
Deposited on : 2006-03-02
Resolution : 2.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

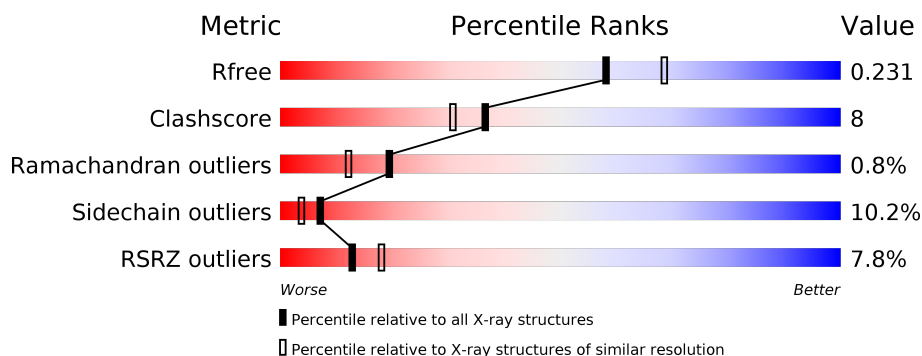
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	402	<div> <div>12%</div> <div> <div></div> <div>66%</div> <div>21%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	402	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>17%</div> <div>•</div> <div>12%</div> </div> </div>
2	B	194	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>5%</div> <div>•</div> </div> </div>
2	D	194	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>•</div> <div>•</div> <div>•</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	D	701	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9654 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 collybistin II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	1	0
			3084	1948	548	564	24			
1	C	353	Total	C	N	O	S	0	2	0
			3001	1895	532	552	22			

- Molecule 2 is a protein called cell division cycle 42 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	187	Total	C	N	O	S	0	2	0
			1468	943	238	278	9			
2	D	189	Total	C	N	O	S	0	1	0
			1474	945	240	280	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	CLONING ARTIFACT	UNP P60953
B	-1	SER	-	CLONING ARTIFACT	UNP P60953
B	0	HIS	-	CLONING ARTIFACT	UNP P60953
D	-2	GLY	-	CLONING ARTIFACT	UNP P60953
D	-1	SER	-	CLONING ARTIFACT	UNP P60953
D	0	HIS	-	CLONING ARTIFACT	UNP P60953

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

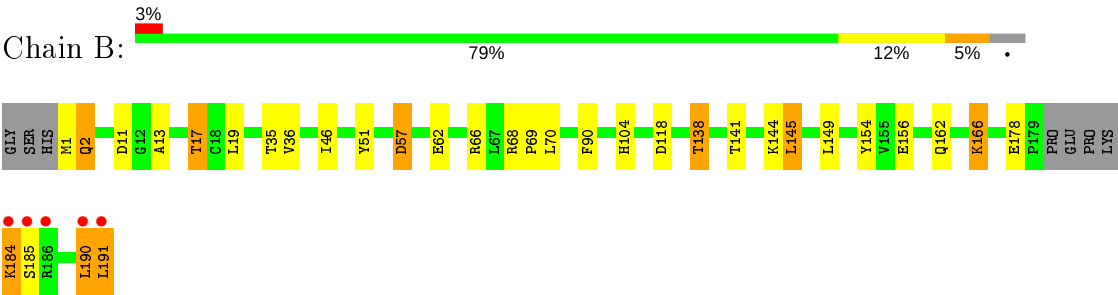
- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



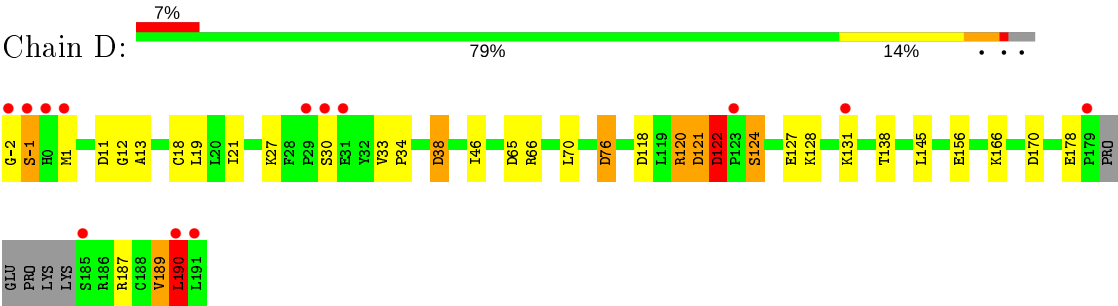
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	174	Total	O	0	0
			174	174		
5	B	91	Total	O	0	0
			91	91		
5	C	195	Total	O	0	0
			195	195		
5	D	121	Total	O	0	0
			121	121		



• Molecule 2: cell division cycle 42 isoform 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.96Å 147.50Å 167.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.67 – 2.15 45.57 – 2.11	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.67-2.15) 94.9 (45.57-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.180 , 0.229 0.185 , 0.231	Depositor DCC
R_{free} test set	3915 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9654	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	0.96	3/3149 (0.1%)	1.06	22/4223 (0.5%)
1	C	1.05	4/3070 (0.1%)	1.08	22/4118 (0.5%)
2	B	0.90	0/1506	0.94	4/2046 (0.2%)
2	D	1.05	0/1509	1.07	9/2051 (0.4%)
All	All	0.99	7/9234 (0.1%)	1.05	57/12438 (0.5%)

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
2	B	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	233	GLU	CD-OE2	7.79	1.34	1.25
1	A	202	GLU	CD-OE2	6.57	1.32	1.25
1	A	107	MET	SD-CE	-5.80	1.45	1.77
1	A	234	ARG	CG-CD	5.67	1.66	1.51
1	C	378	GLU	CD-OE1	5.38	1.31	1.25
1	C	235	LYS	CE-NZ	5.28	1.62	1.49
1	C	76	TYR	CE2-CZ	-5.17	1.31	1.38

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ARG	NE-CZ-NH1	12.99	126.80	120.30
1	A	104	ARG	NE-CZ-NH2	-9.59	115.50	120.30
2	D	122	ASP	CB-CG-OD2	9.30	126.67	118.30
1	C	242	ASP	CB-CG-OD2	9.14	126.53	118.30
1	A	51	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	C	237	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	A	296	LEU	CA-CB-CG	7.98	133.64	115.30
2	D	11	ASP	CB-CG-OD2	7.94	125.44	118.30
1	C	329	ASP	CB-CG-OD2	7.72	125.25	118.30
1	C	112	ASP	CB-CG-OD2	7.54	125.09	118.30
1	A	121	ASP	CB-CG-OD2	7.38	124.94	118.30
1	A	314	ASP	CB-CG-OD2	7.37	124.94	118.30
1	C	368	ARG	NE-CZ-NH2	-7.32	116.64	120.30
2	D	76	ASP	CB-CG-OD2	7.06	124.66	118.30
2	D	38	ASP	CB-CG-OD1	6.88	124.49	118.30
1	C	262	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	A	331	PHE	N-CA-C	6.82	129.42	111.00
1	A	112	ASP	CB-CG-OD2	6.76	124.38	118.30
2	D	19	LEU	CB-CG-CD1	-6.71	99.58	111.00
1	C	314	ASP	CB-CG-OD2	6.68	124.31	118.30
1	C	261	ASP	CB-CG-OD2	6.56	124.21	118.30
2	D	118	ASP	CB-CG-OD2	6.38	124.05	118.30
1	A	51	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	C	368	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	210	ASP	CB-CG-OD2	6.22	123.90	118.30
1	C	262	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	C	63	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	A	316	ASP	CB-CG-OD2	6.01	123.71	118.30
2	B	57	ASP	CB-CG-OD1	5.97	123.67	118.30
1	C	81	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	183	ASP	CB-CG-OD2	5.88	123.59	118.30
1	C	183	ASP	CB-CG-OD2	5.84	123.55	118.30
1	A	111	ARG	NE-CZ-NH1	5.83	123.22	120.30
2	D	121	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	120	ASP	CB-CG-OD2	5.82	123.53	118.30
1	A	377	ASP	CB-CG-OD2	5.81	123.53	118.30
1	C	365	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	C	63	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	316	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	365	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	322	ASP	CB-CG-OD2	5.59	123.33	118.30
2	D	120	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	330	ASP	CB-CG-OD2	5.47	123.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	190	LEU	N-CA-C	-5.45	96.28	111.00
1	A	253	ASP	CB-CG-OD2	5.37	123.13	118.30
2	B	19	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	261	ASP	CB-CG-OD2	5.36	123.12	118.30
1	C	296	LEU	CA-CB-CG	5.28	127.44	115.30
1	C	121	ASP	CB-CG-OD2	5.22	123.00	118.30
2	B	118	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	174	LEU	CB-CG-CD1	5.14	119.74	111.00
1	C	328	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	300	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	258	ASP	CB-CG-OD2	5.04	122.83	118.30
2	B	11	ASP	CB-CG-OD2	5.03	122.82	118.30
1	C	305	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	234	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	184	LYS	Peptide
1	C	346	THR	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	3084	0	3037	47	0
1	C	3001	0	2939	53	0
2	B	1468	0	1494	28	0
2	D	1474	0	1492	24	0
3	A	18	0	24	2	0
3	B	6	0	8	1	0
3	D	12	0	16	3	0
4	B	5	0	0	1	0
4	D	5	0	0	0	0
5	A	174	0	0	8	0
5	B	91	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	195	0	0	17	0
5	D	121	0	0	7	0
All	All	9654	0	9010	143	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 (143) 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:C:335:MET:CE	1:C:335:MET:SD	2.03	1.46
1:C:195:LYS:NZ	5:C:472:HOH:O	1.83	1.08
1:C:106:GLN:OE1	5:C:603:HOH:O	1.73	1.06
1:A:107:MET:SD	5:A:770:HOH:O	2.22	0.98
2:D:189:VAL:C	2:D:190:LEU:O	1.99	0.93
1:A:248:GLN:HE21	1:A:259:ILE:HG22	1.32	0.92
1:C:232:ASN:HD21	2:D:66:ARG:H	1.24	0.86
1:A:57:GLU:OE2	2:B:35:THR:HG22	1.77	0.85
2:D:166:LYS:HB2	5:D:764:HOH:O	1.77	0.85
1:C:235:LYS:NZ	1:C:239:GLU:OE1	2.11	0.84
1:C:195:LYS:HE2	5:D:822:HOH:O	1.80	0.81
1:A:64:HIS:O	1:A:68:HIS:CD2	2.33	0.81
2:B:104:HIS:ND1	2:B:191:LEU:HD21	1.98	0.79
2:B:191:LEU:O	2:B:191:LEU:HD22	1.83	0.78
1:C:335:MET:HB2	5:C:590:HOH:O	1.84	0.77
1:A:232:ASN:HD21	2:B:66:ARG:H	1.33	0.77
1:C:230:GLN:HE21	1:C:234:ARG:HH12	1.30	0.77
1:C:66:ILE:HD11	1:C:107:MET:HG2	1.67	0.76
1:C:335:MET:CB	5:C:590:HOH:O	2.34	0.75
2:D:21:ILE:HD13	2:D:34:PRO:HD2	1.69	0.74
1:C:235:LYS:NZ	5:C:518:HOH:O	2.19	0.74
1:A:259:ILE:HD11	1:A:290:PHE:CD2	2.24	0.73
1:C:106:GLN:NE2	5:C:605:HOH:O	2.01	0.72
1:A:175:GLN:HG2	1:A:177:MET:HE2	1.71	0.71
2:B:35:THR:HG23	2:B:36:VAL:HG23	1.74	0.70
2:D:12:GLY:O	2:D:13:ALA:HB3	1.91	0.70
1:C:133:GLU:OE2	5:C:594:HOH:O	2.09	0.69
2:B:62:GLU:HG3	5:B:764:HOH:O	1.91	0.69
1:A:64:HIS:O	1:A:68:HIS:HD2	1.75	0.69
2:D:122:ASP:C	2:D:122:ASP:OD1	2.31	0.68
2:B:166:LYS:HG3	5:B:734:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLN:NE2	1:A:259:ILE:HG22	2.08	0.68
2:B:2:GLN:HG3	2:B:51:TYR:CE2	2.29	0.68
1:C:192:LYS:NZ	1:C:199:GLN:HE22	1.92	0.67
2:B:104:HIS:CE1	2:B:191:LEU:HD21	2.30	0.66
2:D:18[A]:CYS:SG	2:D:33:VAL:HG11	2.37	0.64
1:C:230:GLN:NE2	1:C:234:ARG:HH12	1.96	0.64
2:D:189:VAL:O	2:D:190:LEU:O	2.15	0.64
3:D:605:GOL:H12	5:D:784:HOH:O	1.99	0.62
1:A:346:THR:HG22	1:A:347:GLU:H	1.65	0.61
1:A:215:ARG:HD3	3:A:602:GOL:H32	1.83	0.61
1:A:293:GLN:HE22	1:A:312:ARG:HH11	1.49	0.60
2:B:138:THR:HG21	5:B:749:HOH:O	2.00	0.60
1:C:148:HIS:CE1	5:C:552:HOH:O	2.53	0.60
2:D:138:THR:HG21	5:D:738:HOH:O	2.00	0.60
1:C:342:HIS:CE1	5:C:606:HOH:O	2.55	0.59
1:C:66:ILE:HD11	1:C:107:MET:CG	2.31	0.59
1:A:68:HIS:HE1	5:B:792:HOH:O	1.85	0.59
2:D:124:SER:O	2:D:127:GLU:HG2	2.03	0.59
2:D:76:ASP:OD1	2:D:187:ARG:HD2	2.02	0.59
2:D:18[A]:CYS:SG	5:D:768:HOH:O	2.57	0.58
1:A:259:ILE:CD1	1:A:290:PHE:CE2	2.87	0.57
2:B:166:LYS:HE3	5:B:734:HOH:O	2.03	0.57
1:C:327:ARG:NE	1:C:332:ASN:HD21	2.02	0.57
1:A:175:GLN:CG	1:A:177:MET:HE2	2.34	0.57
2:B:13:ALA:N	4:B:702:SO4:O1	2.38	0.57
1:A:259:ILE:HB	5:A:700:HOH:O	2.04	0.56
1:A:159:MET:HE2	5:A:771:HOH:O	2.05	0.56
1:A:149:LEU:HD23	2:B:70:LEU:CD2	2.35	0.56
1:C:62:GLU:OE2	5:C:605:HOH:O	2.18	0.56
1:C:192:LYS:HZ3	1:C:199:GLN:HE22	1.54	0.55
1:C:243:LYS:NZ	5:C:597:HOH:O	2.40	0.55
1:C:248:GLN:NE2	1:C:259:ILE:H	2.05	0.54
1:C:385:SER:H	1:C:388:GLN:HE21	1.52	0.54
1:C:335:MET:HA	1:C:335:MET:CE	2.37	0.54
1:A:293:GLN:HE21	1:A:312:ARG:HD3	1.73	0.54
1:A:270:GLY:HA3	5:A:676:HOH:O	2.08	0.54
1:A:264:SER:HB3	1:A:384:ILE:HG12	1.90	0.54
1:A:37:CYS:O	1:A:38:LEU:HD23	2.08	0.53
1:A:259:ILE:CD1	1:A:290:PHE:CD2	2.91	0.53
2:D:187:ARG:NH1	5:D:789:HOH:O	2.41	0.53
2:B:162:GLN:HE22	3:B:603:GOL:C3	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASP:CG	5:A:773:HOH:O	2.47	0.53
1:C:385:SER:H	1:C:388:GLN:NE2	2.07	0.53
1:A:351:LEU:HD13	1:A:353:PHE:CZ	2.43	0.52
2:B:104:HIS:ND1	2:B:191:LEU:CD2	2.72	0.52
1:C:235:LYS:HE3	2:D:70:LEU:HD21	1.90	0.52
2:B:154:TYR:OH	2:B:156:GLU:HG3	2.10	0.52
2:D:187:ARG:CZ	5:D:789:HOH:O	2.57	0.52
1:A:248:GLN:NE2	1:A:259:ILE:H	2.06	0.52
1:A:215:ARG:HD3	3:A:602:GOL:C3	2.40	0.52
1:C:149:LEU:HD21	5:C:420:HOH:O	2.10	0.52
1:C:236[B]:ARG:NH2	2:D:65:ASP:OD1	2.43	0.51
2:D:166:LYS:NZ	2:D:170:ASP:OD2	2.43	0.51
1:A:155:LEU:HD22	5:A:771:HOH:O	2.11	0.51
1:A:370:GLU:O	1:A:374:VAL:HG23	2.12	0.50
1:C:335:MET:HA	1:C:335:MET:HE3	1.93	0.50
1:A:346:THR:HG22	1:A:347:GLU:N	2.27	0.49
1:A:153:MET:HG2	2:B:190:LEU:HD22	1.95	0.49
2:B:13:ALA:HA	5:B:733:HOH:O	2.13	0.49
2:B:166:LYS:H	2:B:166:LYS:HE3	1.79	0.48
2:B:138:THR:HG22	2:B:141:THR:H	1.78	0.48
1:A:121:ASP:OD1	1:A:123:HIS:HD2	1.97	0.47
1:C:283[A]:GLN:NE2	5:C:516:HOH:O	2.47	0.47
1:A:241:ILE:HG22	1:A:392:ALA:HB2	1.96	0.47
2:B:191:LEU:C	2:B:191:LEU:HD22	2.36	0.47
1:C:268:TYR:OH	1:C:359:GLU:OE2	2.22	0.47
1:A:149:LEU:HD23	2:B:70:LEU:HD23	1.96	0.46
1:C:67:LYS:NZ	1:C:71:ASP:OD2	2.34	0.46
1:C:269:THR:HG21	1:C:288:PHE:CE2	2.51	0.46
2:D:38:ASP:H	3:D:605:GOL:H11	1.81	0.46
2:D:-2:GLY:O	2:D:-1:SER:CB	2.64	0.45
1:C:104:ARG:HA	1:C:107:MET:HE2	1.99	0.45
2:B:68:ARG:N	2:B:69:PRO:CD	2.79	0.45
1:A:80:CYS:HB3	1:A:92:LEU:HD21	1.98	0.45
1:C:269:THR:HG23	1:C:287:PHE:O	2.16	0.45
1:A:270:GLY:CA	5:A:676:HOH:O	2.64	0.44
1:A:291:ASP:O	1:A:292:HIS:HB2	2.17	0.44
2:B:46:ILE:O	2:B:46:ILE:HG23	2.17	0.44
1:C:303:ARG:NH2	1:C:306:ILE:HD11	2.32	0.44
1:A:149:LEU:HD23	2:B:70:LEU:HD22	1.99	0.44
2:B:145:LEU:HD22	2:B:149:LEU:HG	2.00	0.44
1:A:112:ASP:OD2	1:A:134:HIS:CE1	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ASP:OD1	1:A:314:ASP:C	2.56	0.43
1:C:112:ASP:HB3	5:C:594:HOH:O	2.18	0.43
1:A:230:GLN:NE2	5:A:688:HOH:O	2.52	0.43
1:C:232:ASN:ND2	2:D:66:ARG:H	2.04	0.43
2:B:90:PHE:CE2	2:B:145:LEU:HD12	2.53	0.43
1:C:346:THR:OG1	1:C:347:GLU:N	2.51	0.43
2:B:17:THR:HB	2:B:57:ASP:OD2	2.18	0.43
1:A:74:GLU:HA	1:A:74:GLU:OE2	2.19	0.43
1:C:376:GLU:HG2	5:C:467:HOH:O	2.19	0.42
2:D:18[A]:CYS:SG	2:D:33:VAL:CG1	3.06	0.42
2:D:-2:GLY:O	2:D:-1:SER:HB2	2.19	0.42
1:A:267:ILE:HD13	1:A:370:GLU:HB3	2.01	0.42
1:C:392:ALA:O	1:C:395:THR:HB	2.19	0.42
1:C:92:LEU:HD23	1:C:92:LEU:HA	1.87	0.42
1:A:175:GLN:HB3	1:A:177:MET:CE	2.50	0.42
1:C:335:MET:HB3	5:C:590:HOH:O	2.09	0.42
1:A:169:GLU:HA	1:A:169:GLU:OE2	2.20	0.42
1:C:327:ARG:NE	1:C:332:ASN:ND2	2.67	0.42
1:C:230:GLN:HE21	1:C:234:ARG:NH1	2.06	0.41
1:A:267:ILE:HD13	1:A:370:GLU:CB	2.49	0.41
1:C:293:GLN:NE2	5:C:493:HOH:O	2.53	0.41
1:C:233:GLU:OE1	1:C:236[B]:ARG:CZ	2.69	0.41
1:C:317:LYS:HE3	1:C:317:LYS:HB3	1.90	0.41
2:D:38:ASP:N	3:D:605:GOL:H11	2.36	0.41
1:C:328:ASP:OD1	1:C:340:LYS:NZ	2.41	0.41
1:C:335:MET:SD	1:C:353:PHE:CD2	3.14	0.40
2:D:12:GLY:O	2:D:13:ALA:CB	2.54	0.40
1:C:346:THR:HB	1:C:347:GLU:HG2	2.02	0.40
1:A:192:LYS:HD3	1:A:192:LYS:HA	1.76	0.40
1:C:323:ILE:HG21	1:C:340:LYS:HE2	2.03	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	364/402 (90%)	350 (96%)	11 (3%)	3 (1%)	19	12
1	C	353/402 (88%)	343 (97%)	9 (2%)	1 (0%)	41	37
2	B	185/194 (95%)	180 (97%)	3 (2%)	2 (1%)	14	8
2	D	186/194 (96%)	177 (95%)	6 (3%)	3 (2%)	9	4
All	All	1088/1192 (91%)	1050 (96%)	29 (3%)	9 (1%)	19	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331	PHE
1	A	400	SER
2	B	190	LEU
1	C	347	GLU
2	D	-1	SER
2	D	190	LEU
1	A	330	ASP
2	B	185	SER
2	D	189	VAL

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	334/367 (91%)	288 (86%)	46 (14%)	3	1
1	C	325/367 (89%)	293 (90%)	32 (10%)	8	4
2	B	169/173 (98%)	159 (94%)	10 (6%)	19	15
2	D	169/173 (98%)	155 (92%)	14 (8%)	11	6
All	All	997/1080 (92%)	895 (90%)	102 (10%)	7	4

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	CYS
1	A	39	CYS
1	A	42	ARG
1	A	77	LEU
1	A	84	ARG
1	A	89	ASP
1	A	123	HIS
1	A	149	LEU
1	A	157	LYS
1	A	160	LYS
1	A	166	HIS
1	A	174	LEU
1	A	209	GLN
1	A	233	GLU
1	A	234	ARG
1	A	238	LEU
1	A	242	ASP
1	A	266	LEU
1	A	274	TRP
1	A	281	ARG
1	A	289	LEU
1	A	296	LEU
1	A	325	ASP
1	A	333	VAL
1	A	334	SER
1	A	345	GLU
1	A	347	GLU
1	A	348	GLU
1	A	351	LEU
1	A	356	LYS
1	A	357	LEU
1	A	358	GLU
1	A	361	ILE
1	A	362	ARG
1	A	364	LEU
1	A	365	ARG
1	A	372	LYS
1	A	378	GLU
1	A	380	ILE
1	A	384	ILE
1	A	386	GLU
1	A	387	ASN
1	A	388	GLN

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Mol	Chain	Res	Type
1	A	390	ARG
1	A	391	GLN
1	A	394	MET
2	B	1	MET
2	B	2	GLN
2	B	17	THR
2	B	138	THR
2	B	144	LYS
2	B	145	LEU
2	B	166	LYS
2	B	178	GLU
2	B	184	LYS
2	B	191	LEU
1	C	46	ASN
1	C	66	ILE
1	C	77	LEU
1	C	149	LEU
1	C	153	MET
1	C	156	SER
1	C	166	HIS
1	C	176	GLN
1	C	233	GLU
1	C	237	ARG
1	C	242	ASP
1	C	265	GLU
1	C	266	LEU
1	C	274	TRP
1	C	282	ASN
1	C	283[A]	GLN
1	C	283[B]	GLN
1	C	289	LEU
1	C	296	LEU
1	C	301	LEU
1	C	302	ILE
1	C	329	ASP
1	C	333	VAL
1	C	335	MET
1	C	351	LEU
1	C	357	LEU
1	C	365	ARG
1	C	368	ARG
1	C	378	GLU

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Mol	Chain	Res	Type
1	C	394	MET
1	C	395	THR
1	C	397	ARG
2	D	1	MET
2	D	27	LYS
2	D	30	SER
2	D	46	ILE
2	D	120	ARG
2	D	121	ASP
2	D	122	ASP
2	D	124	SER
2	D	128	LYS
2	D	131	LYS
2	D	145	LEU
2	D	156	GLU
2	D	178	GLU
2	D	190	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	123	HIS
1	A	146	ASN
1	A	175	GLN
1	A	199	GLN
1	A	232	ASN
1	A	248	GLN
1	A	293	GLN
1	A	342	HIS
1	A	387	ASN
1	A	391	GLN
2	B	92	ASN
2	B	162	GLN
1	C	106	GLN
1	C	146	ASN
1	C	199	GLN
1	C	229	GLN
1	C	230	GLN
1	C	232	ASN
1	C	248	GLN
1	C	293	GLN

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Mol	Chain	Res	Type
1	C	332	ASN
1	C	388	GLN
2	D	92	ASN
2	D	132	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](#)

8 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	$\# Z > 2$
4	SO4	B	702	-	4,4,4	0.27	0	6,6,6	0.72	0
4	SO4	D	701	-	4,4,4	0.17	0	6,6,6	0.19	0
3	GOL	B	603	-	5,5,5	0.48	0	5,5,5	0.11	0
3	GOL	A	606	-	5,5,5	0.39	0	5,5,5	0.43	0
3	GOL	D	604	-	5,5,5	0.45	0	5,5,5	0.39	0
3	GOL	A	602	-	5,5,5	0.44	0	5,5,5	0.43	0
3	GOL	A	601	-	5,5,5	0.48	0	5,5,5	0.39	0
3	GOL	D	605	-	5,5,5	0.61	0	5,5,5	0.98	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	603	-	-	4/4/4/4	-
3	GOL	A	606	-	-	2/4/4/4	-
3	GOL	D	604	-	-	2/4/4/4	-
3	GOL	A	602	-	-	4/4/4/4	-
3	GOL	A	601	-	-	2/4/4/4	-
3	GOL	D	605	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	603	GOL	C1-C2-C3-O3
3	D	604	GOL	C1-C2-C3-O3
3	D	605	GOL	O1-C1-C2-O2
3	D	605	GOL	O1-C1-C2-C3
3	A	601	GOL	O2-C2-C3-O3
3	B	603	GOL	O1-C1-C2-C3
3	A	606	GOL	O1-C1-C2-C3
3	A	602	GOL	O1-C1-C2-C3
3	A	602	GOL	C1-C2-C3-O3
3	A	601	GOL	C1-C2-C3-O3
3	B	603	GOL	O1-C1-C2-O2
3	B	603	GOL	O2-C2-C3-O3
3	A	602	GOL	O2-C2-C3-O3
3	D	604	GOL	O2-C2-C3-O3
3	A	606	GOL	O1-C1-C2-O2
3	A	602	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	702	SO4	1	0
3	B	603	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	GOL	2	0
3	D	605	GOL	3	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	365/402 (90%)	0.67	50 (13%) 3 3	31, 56, 113, 141	0
1	C	353/402 (87%)	0.24	17 (4%) 30 39	31, 47, 77, 116	0
2	B	187/194 (96%)	0.02	5 (2%) 54 63	37, 49, 79, 99	0
2	D	189/194 (97%)	0.24	13 (6%) 16 23	31, 41, 77, 101	0
All	All	1094/1192 (91%)	0.34	85 (7%) 13 18	31, 48, 99, 141	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	400	SER	8.3
1	A	37	CYS	8.2
2	D	191	LEU	8.1
2	B	190	LEU	6.8
2	B	191	LEU	6.5
1	A	396	VAL	6.5
1	C	397	ARG	5.8
1	A	390	ARG	5.4
1	C	301	LEU	5.4
1	A	401	LYS	5.2
1	A	345	GLU	5.0
1	A	336	LYS	5.0
2	D	190	LEU	5.0
1	A	397	ARG	4.9
1	A	393	ALA	4.6
1	A	327	ARG	4.5
2	D	1	MET	4.5
2	D	-2	GLY	4.5
1	C	304	ARG	4.4
1	A	212	SER	4.2
2	D	0	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	357	LEU	4.1
1	C	302	ILE	4.1
1	A	398	LYS	3.8
1	C	306	ILE	3.7
1	A	358	GLU	3.7
1	C	396	VAL	3.6
1	A	378	GLU	3.6
2	D	-1	SER	3.5
1	A	335	MET	3.4
1	A	332	ASN	3.3
1	A	353	PHE	3.3
1	A	355	LYS	3.3
1	A	321	ILE	3.3
1	A	375	GLN	3.3
1	C	303	ARG	3.2
1	A	386	GLU	3.2
1	A	394	MET	3.2
1	A	324	GLU	3.1
1	A	242	ASP	3.1
2	D	29	PRO	3.1
2	D	185	SER	3.1
1	A	399	ALA	3.0
2	D	123	PRO	3.0
1	A	334	SER	3.0
1	A	381	GLY	3.0
1	A	391	GLN	3.0
2	B	184	LYS	3.0
2	B	185	SER	2.9
1	A	365	ARG	2.9
1	C	45	GLN	2.8
1	A	387	ASN	2.8
1	A	356	LYS	2.8
1	A	211	HIS	2.7
1	C	120	ASP	2.6
1	A	215	ARG	2.6
1	A	377	ASP	2.5
2	B	186	ARG	2.5
2	D	179	PRO	2.4
1	C	227	VAL	2.4
1	A	380	ILE	2.4
1	C	390	ARG	2.4
1	A	38	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	252	LEU	2.4
2	D	31	GLU	2.4
2	D	131	LYS	2.4
1	A	329	ASP	2.4
1	A	189	PRO	2.3
1	A	364	LEU	2.3
1	A	392	ALA	2.3
1	C	194	CYS	2.3
1	A	384	ILE	2.2
1	A	330	ASP	2.2
1	A	328	ASP	2.2
1	A	383	GLU	2.2
1	A	281	ARG	2.2
1	C	305	ASP	2.2
1	A	347	GLU	2.2
2	D	30	SER	2.2
1	C	324	GLU	2.1
1	C	394	MET	2.1
1	C	329	ASP	2.1
1	A	395	THR	2.1
1	A	371	ARG	2.0
1	A	333	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	602	6/6	0.35	0.39	134,135,135,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	D	604	6/6	0.40	0.27	115,116,116,116	0
3	GOL	A	601	6/6	0.46	0.31	81,91,92,93	0
3	GOL	B	603	6/6	0.62	0.33	121,122,122,123	0
4	SO4	D	701	5/5	0.67	0.49	170,170,171,171	0
3	GOL	A	606	6/6	0.71	0.33	120,122,123,123	0
3	GOL	D	605	6/6	0.81	0.22	72,76,77,78	0
4	SO4	B	702	5/5	0.93	0.27	91,91,96,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.