



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:33 AM UTC

PDB ID : 2DFK / pdb\_00002dfk  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

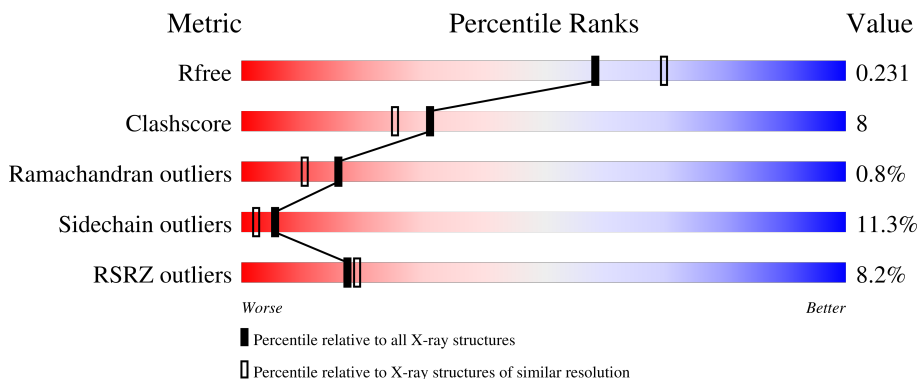
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	402	 11% 65% 20% 5% 9%
1	C	402	 5% 68% 17% .. 12%
2	B	194	 5% 78% 14% ...
2	D	194	 9% 78% 15% ...

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	365	3084	1948	548	564	24	0	1	0
1	C	353	3001	1895	532	552	22	0	2	0

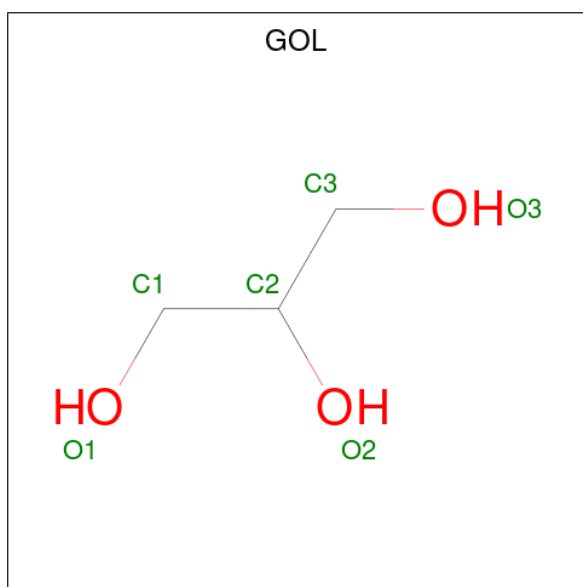
- Molecule 2 is a protein called cell division cycle 42 isoform 1.

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

There are 6 discrepancies between the modelled and reference sequences:

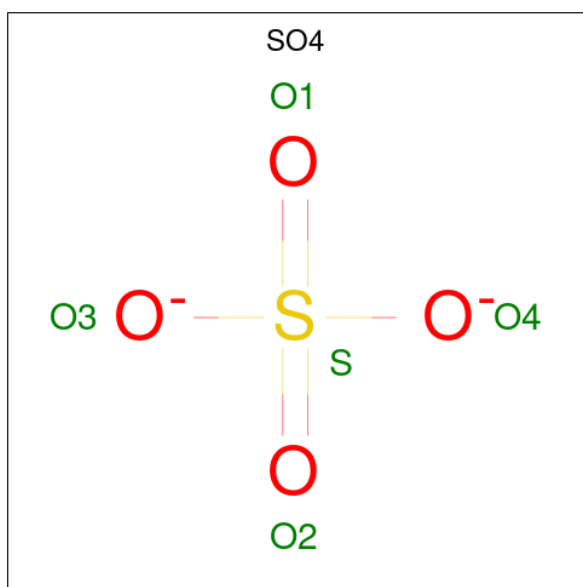
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	cloning artifact	UNP P60953
B	-1	SER	-	cloning artifact	UNP P60953
B	0	HIS	-	cloning artifact	UNP P60953
D	-2	GLY	-	cloning artifact	UNP P60953
D	-1	SER	-	cloning artifact	UNP P60953
D	0	HIS	-	cloning artifact	UNP P60953

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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 (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

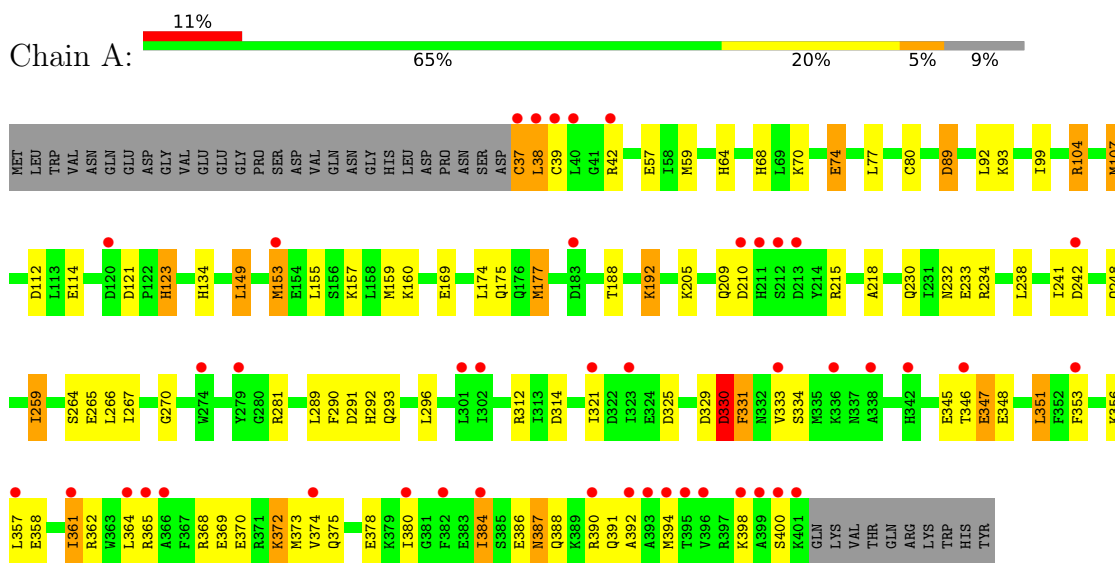
- Molecule 5 is water.

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

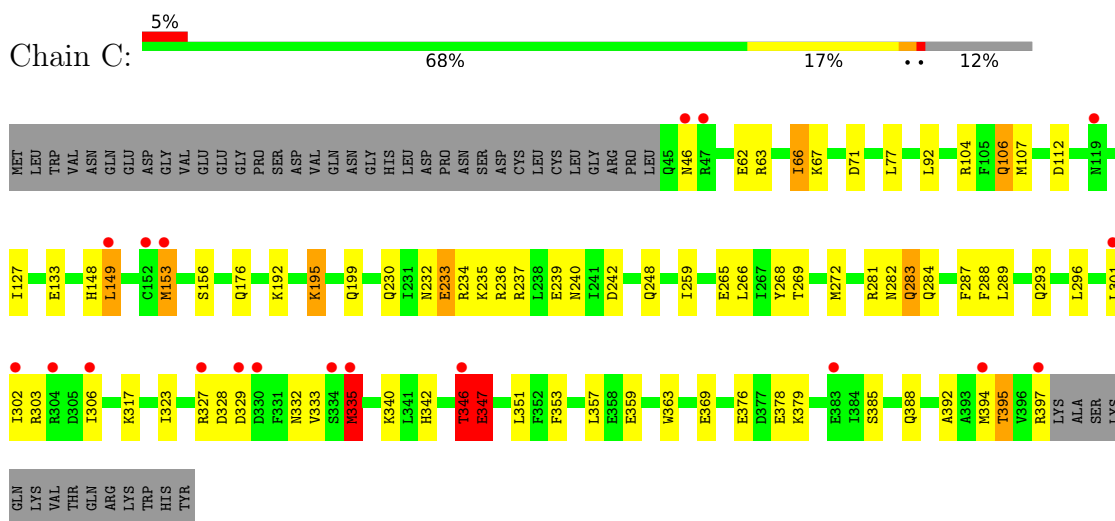
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

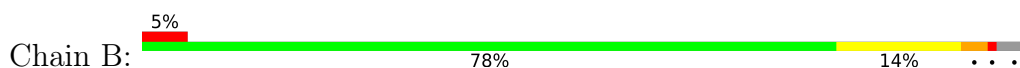
- Molecule 1: collybistin II

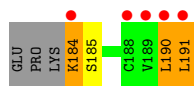
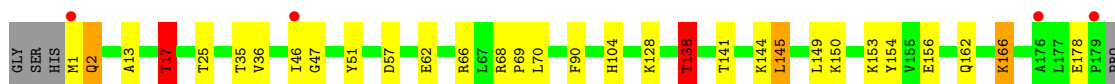


- Molecule 1: collybistin II

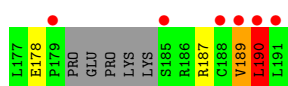
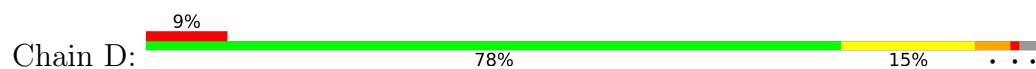


- Molecule 2: cell division cycle 42 isoform 1





● 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, $\alpha$ , $\beta$ , $\gamma$	57.96Å 147.50Å 167.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.67 – 2.15 47.67 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.67-2.15) 96.2 (47.67-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.12Å)	Xtrriage
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 (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtrriage
Anisotropy	0.094	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9654	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	1.23	12/3149 (0.4%)	1.11	6/4223 (0.1%)
1	C	1.29	6/3070 (0.2%)	1.12	2/4118 (0.0%)
2	B	1.16	1/1506 (0.1%)	1.09	5/2046 (0.2%)
2	D	1.31	3/1509 (0.2%)	1.18	5/2051 (0.2%)
All	All	1.25	22/9234 (0.2%)	1.12	18/12438 (0.1%)

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 (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	MET	SD-CE	-13.66	1.45	1.79
1	A	177	MET	SD-CE	-11.09	1.51	1.79
1	C	335	MET	SD-CE	9.71	2.03	1.79
2	D	98	VAL	CA-CB	-7.58	1.50	1.54
1	A	188	THR	C-O	-6.83	1.18	1.24
1	A	153	MET	SD-CE	6.70	1.96	1.79
1	A	361	ILE	CA-CB	6.49	1.61	1.54
1	C	63	ARG	C-O	-6.41	1.16	1.24
1	C	369	GLU	C-O	-6.14	1.17	1.24
2	D	1	MET	SD-CE	6.05	1.94	1.79
1	A	74	GLU	C-O	-5.84	1.16	1.24
2	D	45	MET	SD-CE	-5.74	1.65	1.79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	106	GLN	C-O	-5.67	1.17	1.24
1	A	373	MET	SD-CE	5.51	1.93	1.79
2	B	17	THR	CA-CB	5.48	1.62	1.53
1	A	107	MET	CG-SD	5.35	1.94	1.80
1	A	104	ARG	CD-NE	-5.32	1.38	1.46
1	A	218	ALA	CA-CB	5.28	1.61	1.53
1	C	153	MET	SD-CE	5.21	1.92	1.79
1	A	99	ILE	CA-CB	-5.18	1.47	1.54
1	A	70	LYS	C-O	-5.14	1.18	1.24
1	C	281	ARG	CA-C	-5.05	1.46	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	190	LEU	N-CA-C	-6.82	96.28	110.80
2	B	25	THR	CA-C-N	-6.81	113.81	123.20
2	B	25	THR	C-N-CA	-6.81	113.81	123.20
1	A	331	PHE	N-CA-C	6.58	129.42	111.00
1	A	330	ASP	CA-C-N	6.51	133.41	121.70
1	A	330	ASP	C-N-CA	6.51	133.41	121.70
1	C	127	ILE	N-CA-C	6.25	118.90	112.90
1	A	368	ARG	N-CA-C	-5.96	104.78	111.28
2	D	135	LYS	N-CA-C	5.91	113.54	108.22
2	D	12	GLY	CA-C-N	-5.90	114.46	124.31
2	D	12	GLY	C-N-CA	-5.90	114.46	124.31
2	D	12	GLY	N-CA-C	-5.79	104.67	112.14
2	B	153	LYS	N-CA-C	5.57	115.89	108.38
2	B	138	THR	N-CA-CB	-5.47	103.41	110.03
1	A	210	ASP	N-CA-C	5.32	119.48	113.15
1	A	104	ARG	NE-CZ-NH1	5.30	126.80	121.50
1	C	240	ASN	N-CA-C	5.24	119.77	113.17
2	B	47	GLY	N-CA-C	-5.20	106.25	114.10

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	51	0
1	C	3001	0	2939	53	0
2	B	1468	0	1494	28	0
2	D	1474	0	1492	25	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
5	C	195	0	0	16	0
5	D	121	0	0	7	0
All	All	9654	0	9010	148	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 (148) 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
2:D:189:VAL:C	2:D:190:LEU:O	1.99	0.98
1:A:107:MET:SD	5:A:770:HOH:O	2.22	0.98
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
1:C:335:MET:HE3	1:C:335:MET:HA	1.63	0.80
2:B:104:HIS:ND1	2:B:191:LEU:HD21	1.98	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:LEU:HD22	2:B:191:LEU:O	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
2:D:122:ASP:OD1	2:D:122:ASP:C	2.31	0.73
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
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:B:166:LYS:HG3	5:B:734:HOH:O	1.93	0.68
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:A:175:GLN:HG2	1:A:177:MET:HE2	1.75	0.67
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:67:LYS:NZ	1:C:71:ASP:OD2	2.34	0.59
1:C:66:ILE:HD11	1:C:107:MET:CG	2.31	0.59
1:C:272:MET:HE2	1:C:363:TRP:CE2	2.38	0.59
1:A:68:HIS:HE1	5:B:792:HOH:O	1.85	0.59
2:D:76:ASP:OD1	2:D:187:ARG:HD2	2.02	0.59
2:D:124:SER:O	2:D:127:GLU:HG2	2.03	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASP:CG	5:A:773:HOH:O	2.47	0.57
1:A:175:GLN:HB3	1:A:177:MET:HE3	1.86	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
2:B:13:ALA:N	4:B:702:SO4:O1	2.38	0.57
1:A:159:MET:HE2	5:A:771:HOH:O	2.05	0.56
1:A:259:ILE:HB	5:A:700:HOH:O	2.04	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: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:CE	1:C:335:MET:HA	2.37	0.54
1:A:293:GLN:HE21	1:A:312:ARG:HD3	1.73	0.54
1:A:264:SER:HB3	1:A:384:ILE:HG12	1.90	0.54
1:A:270:GLY:HA3	5:A:676:HOH:O	2.08	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
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:A:59:MET:HE1	1:A:114:GLU:HA	1.92	0.52
2:B:191:LEU:HD22	2:B:191:LEU:C	2.36	0.51
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: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:HE3	2:B:166:LYS:H	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ASP:OD1	1:A:314:ASP:C	2.56	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
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: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
2:B:68:ARG:N	2:B:69:PRO:CD	2.79	0.45
1:C:104:ARG:HA	1:C:107:MET:HE2	1.97	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: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
2:B:46:ILE:O	2:B:46:ILE:HG23	2.17	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:A:291:ASP:O	1:A:292:HIS:HB2	2.17	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:OE2	1:A:74:GLU:HA	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
1:A:267:ILE:HD13	1:A:370:GLU:HB3	2.01	0.42
1:C:92:LEU:HD23	1:C:92:LEU:HA	1.87	0.42
1:C:392:ALA:O	1:C:395:THR:HB	2.19	0.42
2:D:19:LEU:C	2:D:19:LEU:HD23	2.44	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:OE2	1:A:169:GLU:HA	2.20	0.42
1:C:327:ARG:NE	1:C:332:ASN:ND2	2.67	0.42
2:D:-2:GLY:O	2:D:-1:SER:HB2	2.19	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

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:LYS:HB3	1:C:317:LYS:HE3	1.90	0.41
2:D:38:ASP:N	3:D:605:GOL:H11	2.36	0.41
1:A:329:ASP:O	1:A:330:ASP:C	2.64	0.41
1:C:328:ASP:OD1	1:C:340:LYS:NZ	2.41	0.41
1:A:387:ASN:HD22	1:A:387:ASN:C	2.27	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:A:369:GLU:OE1	1:A:372:LYS:NZ	2.45	0.40
1:C:346:THR:HB	1:C:347:GLU:HG2	2.02	0.40
1:A:192:LYS:HA	1:A:192:LYS:HD3	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 [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	364/402 (90%)	350 (96%)	11 (3%)	3 (1%)	16 10
1	C	353/402 (88%)	343 (97%)	9 (2%)	1 (0%)	36 34
2	B	185/194 (95%)	180 (97%)	3 (2%)	2 (1%)	11 7
2	D	186/194 (96%)	177 (95%)	6 (3%)	3 (2%)	7 3
All	All	1088/1192 (91%)	1050 (96%)	29 (3%)	9 (1%)	16 10

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

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
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 [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	334/367 (91%)	281 (84%)	53 (16%)	2	1
1	C	325/367 (89%)	292 (90%)	33 (10%)	7	3
2	B	169/173 (98%)	157 (93%)	12 (7%)	13	8
2	D	169/173 (98%)	154 (91%)	15 (9%)	9	5
All	All	997/1080 (92%)	884 (89%)	113 (11%)	5	2

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

Mol	Chain	Res	Type
1	A	37	CYS
1	A	38	LEU
1	A	39	CYS
1	A	42	ARG
1	A	77	LEU
1	A	89	ASP
1	A	93	LYS
1	A	104	ARG
1	A	123	HIS
1	A	149	LEU
1	A	157	LYS
1	A	160	LYS
1	A	174	LEU
1	A	192	LYS
1	A	205	LYS
1	A	209	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	233	GLU
1	A	234	ARG
1	A	238	LEU
1	A	242	ASP
1	A	259	ILE
1	A	265	GLU
1	A	266	LEU
1	A	281	ARG
1	A	289	LEU
1	A	296	LEU
1	A	321	ILE
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	375	GLN
1	A	378	GLU
1	A	380	ILE
1	A	384	ILE
1	A	386	GLU
1	A	387	ASN
1	A	388	GLN
1	A	390	ARG
1	A	391	GLN
1	A	394	MET
1	A	398	LYS
2	B	1	MET
2	B	2	GLN
2	B	17	THR
2	B	128	LYS
2	B	138	THR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	144	LYS
2	B	145	LEU
2	B	150	LYS
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	176	GLN
1	C	195	LYS
1	C	233	GLU
1	C	237	ARG
1	C	242	ASP
1	C	265	GLU
1	C	266	LEU
1	C	282	ASN
1	C	283[A]	GLN
1	C	283[B]	GLN
1	C	284	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	346	THR
1	C	347	GLU
1	C	351	LEU
1	C	357	LEU
1	C	378	GLU
1	C	379	LYS
1	C	394	MET
1	C	395	THR
1	C	397	ARG
2	D	1	MET
2	D	30	SER

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	46	ILE
2	D	120	ARG
2	D	121	ASP
2	D	122	ASP
2	D	124	SER
2	D	126	ILE
2	D	128	LYS
2	D	131	LYS
2	D	145	LEU
2	D	156	GLU
2	D	166	LYS
2	D	178	GLU
2	D	190	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	68	HIS
1	A	119	ASN
1	A	123	HIS
1	A	147	ASN
1	A	175	GLN
1	A	199	GLN
1	A	226	ASN
1	A	230	GLN
1	A	232	ASN
1	A	248	GLN
1	A	284	GLN
1	A	293	GLN
1	A	337	ASN
1	A	342	HIS
1	A	387	ASN
1	A	391	GLN
2	B	92	ASN
2	B	162	GLN
1	C	49	GLN
1	C	106	GLN
1	C	165	GLN
1	C	199	GLN
1	C	230	GLN
1	C	232	ASN
1	C	248	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	293	GLN
1	C	332	ASN
1	C	375	GLN
1	C	388	GLN
2	D	61	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 oligosaccharides 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	0.28	0	6,6,6	0.71	0
3	GOL	A	606	-	5,5,5	0.39	0	5,5,5	0.47	0
3	GOL	D	605	-	5,5,5	0.63	0	5,5,5	1.03	0
4	SO4	D	701	-	4,4,4	0.27	0	6,6,6	0.18	0
3	GOL	A	601	-	5,5,5	0.50	0	5,5,5	0.40	0
3	GOL	B	603	-	5,5,5	0.49	0	5,5,5	0.12	0
3	GOL	A	602	-	5,5,5	0.44	0	5,5,5	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	D	604	-	5,5,5	0.46	0	5,5,5	0.40	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	A	606	-	-	2/4/4/4	-
3	GOL	D	605	-	-	2/4/4/4	-
3	GOL	A	601	-	-	2/4/4/4	-
3	GOL	B	603	-	-	4/4/4/4	-
3	GOL	A	602	-	-	4/4/4/4	-
3	GOL	D	604	-	-	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	A	601	GOL	C1-C2-C3-O3
3	A	602	GOL	O1-C1-C2-C3
3	A	602	GOL	C1-C2-C3-O3
3	A	606	GOL	O1-C1-C2-C3
3	B	603	GOL	O1-C1-C2-C3
3	A	602	GOL	O2-C2-C3-O3
3	B	603	GOL	O1-C1-C2-O2
3	B	603	GOL	O2-C2-C3-O3
3	D	604	GOL	O2-C2-C3-O3
3	A	602	GOL	O1-C1-C2-O2
3	A	606	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	D	605	GOL	3	0
3	B	603	GOL	1	0
3	A	602	GOL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	365/402 (90%)	0.76	44 (12%) 8 9	31, 56, 113, 141	1 (0%)
1	C	353/402 (87%)	0.44	19 (5%) 31 35	26, 47, 77, 116	2 (0%)
2	B	187/194 (96%)	0.38	9 (4%) 35 40	30, 49, 79, 99	2 (1%)
2	D	189/194 (97%)	0.36	18 (9%) 14 15	29, 41, 77, 101	1 (0%)
All	All	1094/1192 (91%)	0.52	90 (8%) 17 19	26, 48, 99, 141	6 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	190	LEU	5.7
2	B	191	LEU	5.6
2	D	191	LEU	5.4
1	A	399	ALA	5.2
2	D	179	PRO	4.7
1	A	346	THR	4.4
1	A	401	LYS	4.3
2	D	29	PRO	4.2
2	D	190	LEU	4.1
1	A	384	ILE	4.1
2	D	-2	GLY	4.0
1	A	353	PHE	3.8
2	D	1	MET	3.8
1	A	38	LEU	3.7
1	A	211	HIS	3.7
1	A	333	VAL	3.6
1	A	393	ALA	3.6
1	C	335	MET	3.5
1	C	302	ILE	3.5
1	A	212	SER	3.4
2	D	-1	SER	3.4

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	213	ASP	3.3
2	D	189	VAL	3.2
1	A	321	ILE	3.2
2	D	13	ALA	3.2
1	A	380	ILE	3.1
1	C	301	LEU	3.1
1	A	400	SER	3.1
2	D	0	HIS	3.1
1	C	397	ARG	3.0
1	A	361	ILE	2.9
1	A	336	LYS	2.9
2	B	1	MET	2.9
1	A	390	ARG	2.8
1	A	40	LEU	2.8
1	A	279	TYR	2.8
1	A	37	CYS	2.8
1	A	374	VAL	2.8
2	B	179	PRO	2.8
1	C	149	LEU	2.7
1	C	329	ASP	2.7
1	C	383	GLU	2.6
1	C	304	ARG	2.6
1	C	394	MET	2.6
1	A	342	HIS	2.6
1	A	398	LYS	2.6
2	D	121	ASP	2.6
1	C	306	ILE	2.6
1	A	42	ARG	2.6
2	D	30	SER	2.6
2	B	189	VAL	2.5
1	A	242	ASP	2.5
1	A	395	THR	2.5
1	C	330	ASP	2.5
1	A	301	LEU	2.5
1	A	396	VAL	2.4
1	A	323	ILE	2.4
1	A	39	CYS	2.4
1	C	327	ARG	2.4
1	A	366	ALA	2.4
1	A	392	ALA	2.4
2	B	176	ALA	2.4
1	A	382	PHE	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	153	MET	2.4
1	C	119	ASN	2.3
2	B	184	LYS	2.3
1	C	152	CYS	2.3
2	D	176	ALA	2.3
1	C	46	ASN	2.3
1	A	210	ASP	2.3
1	A	274	TRP	2.3
2	D	31	GLU	2.2
2	D	185	SER	2.2
1	A	365	ARG	2.2
2	B	188	CYS	2.2
2	D	188	CYS	2.2
1	A	183	ASP	2.2
1	A	364	LEU	2.1
1	A	153	MET	2.1
1	A	302	ILE	2.1
2	D	28	PHE	2.1
2	D	12	GLY	2.1
1	C	346	THR	2.1
1	A	357	LEU	2.1
1	A	394	MET	2.1
1	C	334	SER	2.1
1	C	47	ARG	2.0
2	B	46	ILE	2.0
1	A	338	ALA	2.0
1	A	120	ASP	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	B	702	5/5	0.73	0.18	91,91,96,98	0
3	GOL	D	604	6/6	0.75	0.19	115,116,116,116	0
3	GOL	A	602	6/6	0.75	0.28	134,135,135,136	0
3	GOL	B	603	6/6	0.76	0.22	121,122,122,123	0
3	GOL	A	601	6/6	0.78	0.23	81,91,92,93	0
3	GOL	A	606	6/6	0.87	0.20	120,122,123,123	0
4	SO4	D	701	5/5	0.87	0.22	170,170,171,171	0
3	GOL	D	605	6/6	0.93	0.15	72,76,77,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.