



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:05 pm GMT

PDB ID : 4F0K  
Title : UNACTIVATED RUBISCO with MAGNESIUM AND CARBON DIOXIDE BOUND  
Authors : Stec, B.  
Deposited on : 2012-05-04  
Resolution : 2.05 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

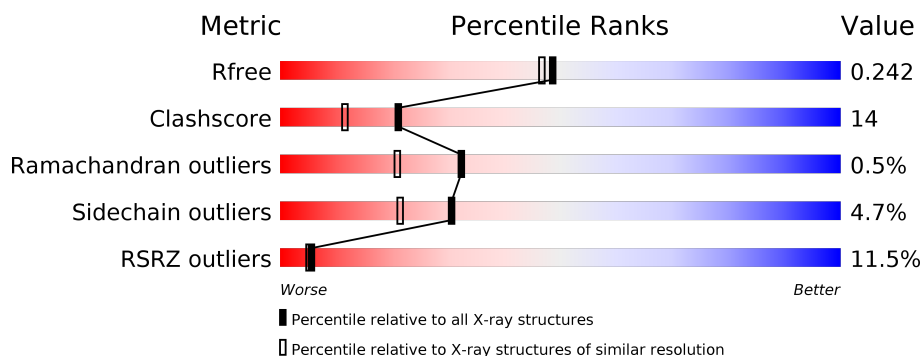
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	493	
2	B	138	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SNC	A	181	-	-	X	-
3	MG	A	501	-	-	-	X
4	CO2	A	502	-	-	-	X
5	GOL	B	903	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5094 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 Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	1	0
			3521	2247	612	642	20			

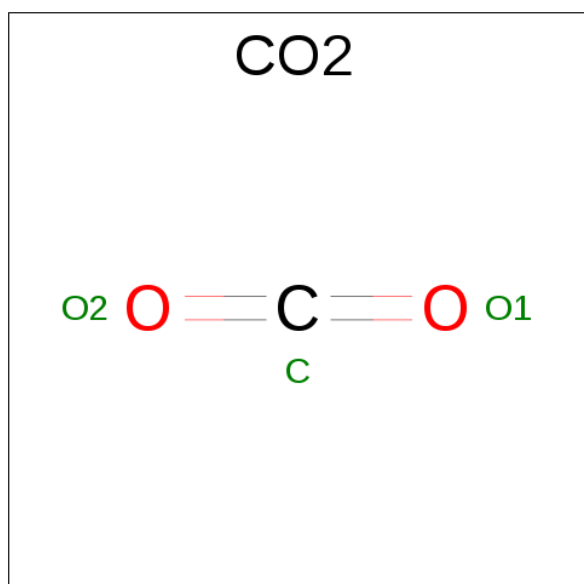
- Molecule 2 is a protein called Ribulose biphosphate carboxylase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	138	Total	C	N	O	S	0	0	0
			1145	738	191	212	4			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula:  $Cl$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

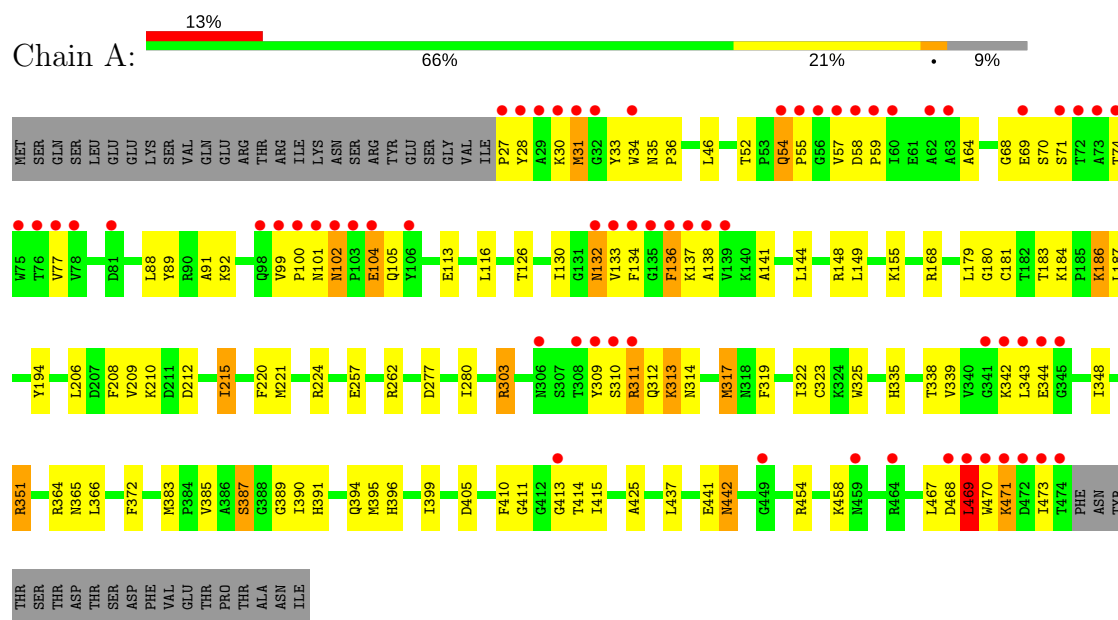
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	259	Total	O	0	0
			259	259		
7	B	146	Total	O	0	0
			146	146		

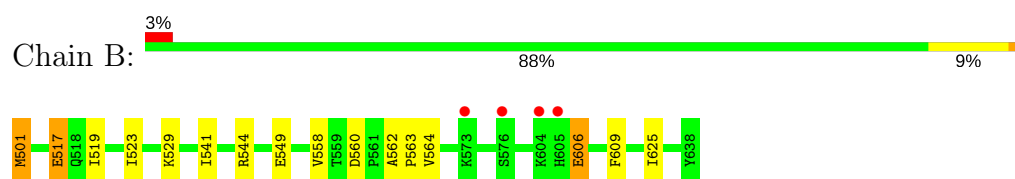
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Ribulose biphosphate carboxylase large chain



- Molecule 2: Ribulose biphosphate carboxylase small chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.14Å 136.14Å 121.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.23 – 2.05 43.05 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.9 (96.23-2.05) 97.9 (43.05-2.05)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.178 , 0.241 0.179 , 0.242	Depositor DCC
$R_{free}$ test set	1772 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.2	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5094	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CO2, SNC, CL

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	0.97	2/3580 (0.1%)	0.92	7/4844 (0.1%)
2	B	1.04	2/1174 (0.2%)	0.94	1/1583 (0.1%)
All	All	0.99	4/4754 (0.1%)	0.93	8/6427 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	517	GLU	CG-CD	6.09	1.61	1.51
1	A	155	LYS	CD-CE	5.43	1.64	1.51
1	A	257	GLU	CG-CD	5.23	1.59	1.51
2	B	606	GLU	CG-CD	5.08	1.59	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	A	351	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	262	ARG	NE-CZ-NH2	-7.61	116.50	120.30
2	B	544	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	A	405	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	168	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	215	ILE	CG1-CB-CG2	-5.04	100.30	111.40
1	A	383	MET	CG-SD-CE	5.03	108.25	100.20

There are no chirality outliers.

There are no planarity outliers.



## 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	3521	0	3512	113	1
2	B	1145	0	1135	14	0
3	A	1	0	0	0	0
4	A	3	0	0	0	0
5	A	6	0	8	1	0
5	B	12	0	16	2	0
6	B	1	0	0	0	0
7	A	259	0	0	15	1
7	B	146	0	0	3	0
All	All	5094	0	4671	128	1

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 14.

All (128) 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:215:ILE:HD11	1:A:221:MET:CE	1.64	1.25
1:A:215:ILE:HD11	1:A:221:MET:HE3	1.12	1.12
1:A:335:HIS:HB2	7:A:1001:HOH:O	1.63	0.99
1:A:313:LYS:HD3	1:A:313:LYS:H	1.31	0.94
1:A:215:ILE:CD1	1:A:221:MET:HE3	1.99	0.92
1:A:338:THR:HG22	1:A:343:LEU:HD12	1.60	0.83
1:A:33:TYR:CD1	1:A:68:GLY:HA2	2.16	0.81
1:A:27:PRO:HB2	1:A:30:LYS:HB3	1.64	0.80
1:A:215:ILE:HD11	1:A:221:MET:HE1	1.62	0.80
1:A:411:GLY:HA3	7:A:1106:HOH:O	1.83	0.79
2:B:562:ALA:HB3	2:B:563:PRO:CD	2.16	0.75
1:A:313:LYS:N	1:A:313:LYS:HD3	2.00	0.74
1:A:69:GLU:OE2	1:A:134:PHE:HB2	1.88	0.72
2:B:562:ALA:HB3	2:B:563:PRO:HD3	1.71	0.72
1:A:70:SER:HB3	1:A:133:VAL:HG13	1.70	0.72
2:B:549:GLU:OE2	7:B:1039:HOH:O	2.08	0.71
1:A:54:GLN:HG3	1:A:55:PRO:CD	2.21	0.69
1:A:132:ASN:ND2	1:A:132:ASN:H	1.90	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:SNC:CB	1:A:410:PHE:O	2.42	0.68
1:A:92:LYS:CD	7:A:1196:HOH:O	2.43	0.67
1:A:348:ILE:HG12	1:A:351:ARG:HH21	1.61	0.66
1:A:88:LEU:HD12	1:A:113:GLU:HG3	1.76	0.66
1:A:69:GLU:O	1:A:132:ASN:HB2	1.96	0.65
1:A:348:ILE:HG12	1:A:351:ARG:NH2	2.11	0.65
1:A:34:TRP:NE1	1:A:36:PRO:HD3	2.12	0.65
1:A:54:GLN:HG3	1:A:55:PRO:HD2	1.79	0.65
1:A:181:SNC:HB2	1:A:410:PHE:O	1.98	0.63
1:A:104:GLU:OE1	1:A:104:GLU:N	2.29	0.62
1:A:100:PRO:O	1:A:101:ASN:HB2	1.99	0.62
1:A:184:LYS:HB3	1:A:415:ILE:HG21	1.82	0.61
1:A:215:ILE:CD1	1:A:221:MET:CE	2.59	0.61
1:A:132:ASN:ND2	1:A:132:ASN:N	2.48	0.61
1:A:33:TYR:CE1	1:A:68:GLY:HA2	2.35	0.61
1:A:221:MET:HE1	7:A:1009:HOH:O	2.00	0.60
5:B:903:GOL:H32	7:B:1127:HOH:O	2.02	0.59
1:A:31:MET:HB2	1:A:33:TYR:CD2	2.38	0.59
1:A:136:PHE:CD1	1:A:136:PHE:N	2.69	0.59
1:A:27:PRO:O	1:A:31:MET:HG2	2.03	0.59
1:A:181:SNC:HB3	1:A:410:PHE:O	2.03	0.58
1:A:413:GLY:HA3	7:A:1216:HOH:O	2.02	0.58
1:A:209:VAL:HG12	1:A:210:LYS:N	2.18	0.58
1:A:313:LYS:CD	1:A:313:LYS:H	2.09	0.57
1:A:31:MET:HB2	1:A:33:TYR:HD2	1.70	0.57
1:A:391:HIS:HB2	1:A:470:TRP:CZ3	2.40	0.56
1:A:132:ASN:HA	1:A:134:PHE:CE2	2.41	0.55
1:A:52:THR:HB	1:A:141:ALA:HB3	1.89	0.55
1:A:58:ASP:OD1	1:A:59:PRO:HD2	2.07	0.55
1:A:92:LYS:HD2	7:A:1196:HOH:O	2.07	0.55
1:A:186:LYS:HD3	1:A:212:ASP:OD2	2.06	0.54
2:B:609:PHE:O	5:B:903:GOL:H11	2.08	0.54
1:A:314:ASN:HB3	5:A:503:GOL:O3	2.07	0.54
2:B:523:ILE:HD12	2:B:564:VAL:HG11	1.90	0.53
1:A:54:GLN:NE2	1:A:136:PHE:O	2.41	0.52
1:A:27:PRO:N	7:A:1153:HOH:O	2.42	0.52
1:A:454:ARG:NH1	7:A:1239:HOH:O	2.40	0.52
7:A:1217:HOH:O	2:B:625:ILE:HG23	2.09	0.52
1:A:27:PRO:CD	7:A:1153:HOH:O	2.57	0.52
1:A:364:ARG:HH22	1:A:366:LEU:HD11	1.74	0.52
1:A:180:GLY:HA2	1:A:208:PHE:O	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LYS:CD	1:A:389:GLY:HA3	2.40	0.51
1:A:468:ASP:O	1:A:471:LYS:HG3	2.10	0.51
1:A:184:LYS:HB2	1:A:415:ILE:HG13	1.92	0.51
2:B:562:ALA:CB	2:B:563:PRO:CD	2.83	0.51
1:A:57:VAL:HG11	1:A:138:ALA:HB1	1.92	0.51
1:A:224:ARG:HD2	7:A:1201:HOH:O	2.09	0.50
1:A:102:ASN:ND2	1:A:104:GLU:OE1	2.43	0.50
1:A:130:ILE:CG2	1:A:144:LEU:HD22	2.41	0.50
1:A:69:GLU:C	1:A:132:ASN:O	2.50	0.50
1:A:71:SER:CB	1:A:91:ALA:H	2.24	0.50
1:A:132:ASN:HD22	1:A:132:ASN:N	2.09	0.50
2:B:541:ILE:HG13	2:B:541:ILE:O	2.12	0.50
1:A:396:HIS:H	1:A:396:HIS:CD2	2.30	0.49
1:A:132:ASN:HA	1:A:134:PHE:HE2	1.77	0.49
1:A:70:SER:HB3	1:A:133:VAL:CG1	2.41	0.49
1:A:126:THR:HG22	1:A:325:TRP:CH2	2.47	0.49
1:A:187:LEU:HG	1:A:220:PHE:CZ	2.48	0.48
1:A:181:SNC:SG	1:A:206:LEU:CD1	3.01	0.48
1:A:317:MET:CE	1:A:322:ILE:HD11	2.44	0.48
1:A:148:ARG:HB2	1:A:372:PHE:CG	2.49	0.48
1:A:342:LYS:HD2	1:A:389:GLY:HA3	1.96	0.48
1:A:99:VAL:HG21	1:A:105:GLN:HB3	1.95	0.47
1:A:391:HIS:HB2	1:A:470:TRP:CE3	2.50	0.46
2:B:501:MET:O	2:B:606:GLU:HB3	2.16	0.46
1:A:468:ASP:O	1:A:469:LEU:C	2.54	0.46
1:A:184:LYS:HD3	1:A:184:LYS:HA	1.66	0.46
1:A:311:ARG:HG2	1:A:311:ARG:HH11	1.81	0.46
1:A:69:GLU:HB3	1:A:132:ASN:O	2.17	0.45
1:A:89:TYR:HA	1:A:116:LEU:HD21	1.98	0.45
1:A:342:LYS:HG3	1:A:389:GLY:HA3	1.98	0.45
7:A:1217:HOH:O	2:B:625:ILE:CG2	2.63	0.45
1:A:181:SNC:SG	1:A:206:LEU:HD11	2.57	0.45
2:B:529:LYS:NZ	7:B:1087:HOH:O	2.50	0.45
1:A:395:MET:O	1:A:399:ILE:HG12	2.16	0.45
1:A:130:ILE:HG23	1:A:144:LEU:HD22	1.98	0.44
1:A:215:ILE:HG23	1:A:215:ILE:O	2.16	0.44
1:A:277:ASP:O	1:A:280:ILE:HG12	2.17	0.44
1:A:390:ILE:HA	1:A:394:GLN:OE1	2.17	0.44
1:A:437:LEU:O	1:A:441:GLU:HG3	2.17	0.44
1:A:92:LYS:HD3	7:A:1196:HOH:O	2.12	0.44
1:A:309:TYR:O	1:A:312:GLN:NE2	2.51	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ASN:OD1	1:A:365:ASN:C	2.56	0.43
1:A:335:HIS:HE1	1:A:387:SER:H	1.66	0.43
1:A:54:GLN:HG3	1:A:55:PRO:HD3	2.00	0.43
1:A:338:THR:OG1	1:A:339:VAL:N	2.50	0.43
1:A:342:LYS:CG	1:A:389:GLY:HA3	2.49	0.43
1:A:319:PHE:CE2	1:A:323:CYS:SG	3.12	0.43
1:A:335:HIS:CE1	1:A:387:SER:H	2.36	0.43
1:A:209:VAL:CG1	1:A:210:LYS:N	2.82	0.43
1:A:57:VAL:HG21	1:A:138:ALA:HA	2.01	0.43
1:A:28:TYR:HB3	1:A:64:ALA:HB1	2.01	0.43
1:A:35:ASN:HA	1:A:36:PRO:HD2	1.87	0.43
1:A:467:LEU:HD23	1:A:467:LEU:HA	1.75	0.43
1:A:130:ILE:HD13	7:A:1074:HOH:O	2.18	0.42
2:B:529:LYS:HA	2:B:529:LYS:HD3	1.70	0.42
1:A:46:LEU:HB2	1:A:148:ARG:HB3	2.01	0.42
1:A:187:LEU:HG	1:A:220:PHE:HZ	1.83	0.42
1:A:303:ARG:O	1:A:303:ARG:HD3	2.20	0.42
1:A:183:THR:HG21	1:A:194:TYR:CZ	2.54	0.42
1:A:414:THR:HG23	1:A:425:ALA:N	2.34	0.42
2:B:517:GLU:CD	2:B:517:GLU:H	2.23	0.41
1:A:34:TRP:CD1	1:A:36:PRO:HD3	2.55	0.41
1:A:335:HIS:HA	1:A:385:VAL:HB	2.01	0.41
1:A:366:LEU:HG	7:A:1132:HOH:O	2.21	0.41
2:B:519:ILE:O	2:B:523:ILE:HG12	2.19	0.41
1:A:442:ASN:HA	1:A:442:ASN:HD22	1.60	0.41
1:A:179:LEU:HD22	1:A:410:PHE:HE2	1.85	0.41
1:A:126:THR:HG22	1:A:325:TRP:CZ3	2.56	0.41
1:A:391:HIS:N	1:A:394:GLN:OE1	2.40	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:VAL:O	7:A:1222:HOH:O[6_565]	2.10	0.10

## 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	445/493 (90%)	413 (93%)	29 (6%)	3 (1%)	25	14
2	B	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
All	All	581/631 (92%)	542 (93%)	36 (6%)	3 (0%)	32	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	ARG
1	A	473	ILE
1	A	469	LEU

### 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	359/401 (90%)	339 (94%)	20 (6%)	25	15
2	B	127/127 (100%)	124 (98%)	3 (2%)	54	48
All	All	486/528 (92%)	463 (95%)	23 (5%)	30	21

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	MET
1	A	54	GLN
1	A	74	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	102	ASN
1	A	104	GLU
1	A	132	ASN
1	A	136	PHE
1	A	137	LYS
1	A	149	LEU
1	A	186	LYS
1	A	303	ARG
1	A	310	SER
1	A	313	LYS
1	A	317	MET
1	A	344	GLU
1	A	387	SER
1	A	442	ASN
1	A	458	LYS
1	A	469	LEU
1	A	471	LYS
2	B	501	MET
2	B	558	VAL
2	B	560	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	216	ASN
1	A	302	HIS
1	A	306	ASN
1	A	312	GLN
1	A	314	ASN
1	A	335	HIS
1	A	396	HIS
1	A	442	ASN
2	B	545	ASN
2	B	601	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	SNC	A	181	1	4,7,8	0.59	0	1,7,9	1.88	0
1	SNC	A	460	1	4,7,8	0.84	0	1,7,9	1.05	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
1	SNC	A	181	1	-	0/0/6/8	0/0/0/0
1	SNC	A	460	1	-	0/0/6/8	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	181	SNC	5	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	CO2	A	502	-	2,2,2	1.33	0	1,1,1	0.12	0
5	GOL	A	503	-	5,5,5	0.37	0	5,5,5	0.43	0
5	GOL	B	902	-	5,5,5	0.53	0	5,5,5	0.86	0
5	GOL	B	903	-	5,5,5	0.87	0	5,5,5	1.68	2 (40%)

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
4	CO2	A	502	-	-	0/0/0/0	0/0/0/0
5	GOL	A	503	-	-	0/4/4/4	0/0/0/0
5	GOL	B	902	-	-	0/4/4/4	0/0/0/0
5	GOL	B	903	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	903	GOL	O2-C2-C3	2.24	119.43	108.84
5	B	903	GOL	O2-C2-C1	2.92	122.61	108.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	GOL	1	0
5	B	903	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	446/493 (90%)	0.70	63 (14%) 3 3	17, 32, 100, 129	0
2	B	138/138 (100%)	-0.20	4 (2%) 52 58	22, 30, 47, 57	0
All	All	584/631 (92%)	0.48	67 (11%) 5 5	17, 32, 92, 129	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	474	THR	21.0
1	A	470	TRP	9.2
1	A	134	PHE	8.8
1	A	77	VAL	7.8
1	A	472	ASP	7.5
1	A	76	THR	7.3
1	A	471	LYS	7.3
1	A	343	LEU	7.1
1	A	473	ILE	7.1
1	A	73	ALA	6.9
1	A	309	TYR	6.6
1	A	133	VAL	6.4
1	A	29	ALA	6.2
1	A	306	ASN	6.0
1	A	344	GLU	5.8
1	A	136	PHE	5.8
1	A	75	TRP	5.7
1	A	74	THR	5.4
1	A	27	PRO	5.4
1	A	31	MET	5.2
1	A	28	TYR	5.0
1	A	55	PRO	5.0
1	A	30	LYS	4.9
1	A	135	GLY	4.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	57	VAL	4.7
1	A	103	PRO	4.6
1	A	72	THR	4.5
1	A	56	GLY	4.4
1	A	342	LYS	4.4
1	A	132	ASN	4.3
1	A	308	THR	4.3
1	A	62	ALA	4.3
1	A	137	LYS	4.2
1	A	138	ALA	4.0
1	A	345	GLY	3.8
1	A	139	VAL	3.5
1	A	101	ASN	3.4
1	A	104	GLU	3.4
1	A	106	TYR	3.2
1	A	341	GLY	3.1
1	A	69	GLU	3.0
1	A	102	ASN	3.0
1	A	469	LEU	3.0
2	B	605	HIS	2.9
1	A	34	TRP	2.9
1	A	59	PRO	2.8
2	B	604	LYS	2.8
1	A	71	SER	2.7
1	A	310	SER	2.7
1	A	459	ASN	2.7
1	A	98	GLN	2.7
1	A	54	GLN	2.6
1	A	413	GLY	2.5
1	A	311	ARG	2.5
1	A	78	VAL	2.4
1	A	464	ARG	2.4
1	A	60	ILE	2.4
1	A	58	ASP	2.4
1	A	449	GLY	2.4
1	A	63	ALA	2.4
1	A	468	ASP	2.3
1	A	32	GLY	2.3
2	B	573	LYS	2.2
2	B	576	SER	2.2
1	A	99	VAL	2.1
1	A	100	PRO	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	81	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SNC	A	460	8/9	0.84	0.19	-	39,49,60,60	0
1	SNC	A	181	8/9	0.89	0.17	-	35,45,73,75	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CO2	A	502	3/3	0.71	0.39	8.19	65,65,66,67	0
3	MG	A	501	1/1	0.99	0.25	4.11	51,51,51,51	0
5	GOL	B	903	6/6	0.86	0.16	2.56	34,40,42,48	0
5	GOL	B	902	6/6	0.90	0.17	1.24	36,45,47,50	0
5	GOL	A	503	6/6	0.96	0.12	-	58,59,59,59	6
6	CL	B	901	1/1	0.96	0.40	-	64,64,64,64	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.