



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:23 PM UTC

PDB ID : 1WDD / pdb_00001wdd
Title : Crystal Structure of Activated Rice Rubisco Complexed with 2-Carboxyarabitol-1,5-bisphosphate
Authors : Mizohata, E.; Matsumura, H.; Ueno, T.; Ishida, H.; Inoue, T.; Makino, A.; Mae, T.; Kai, Y.
Deposited on : 2004-05-13
Resolution : 1.35 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 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)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

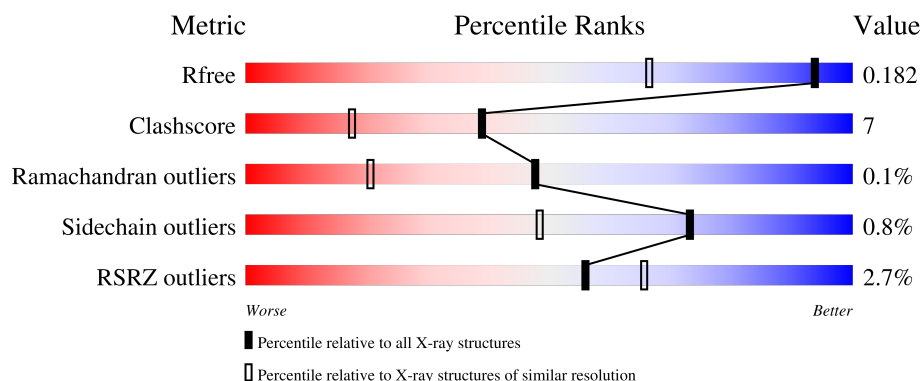
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	1216 (1.36-1.36)
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

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 ≥ 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	477	 2% 88% 8% . .
1	E	477	 % 87% 10% .
2	S	128	 7% 76% 16% . 5%
2	W	128	 5% 69% 26% . 5%

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
5	GOL	A	3015	-	-	X	-
5	GOL	E	3016	-	-	X	-
5	GOL	W	3007	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10448 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	465	Total	C	N	O	S	0	0	0
			3639	2311	639	669	20			
1	E	464	Total	C	N	O	S	0	0	0
			3632	2306	638	668	20			

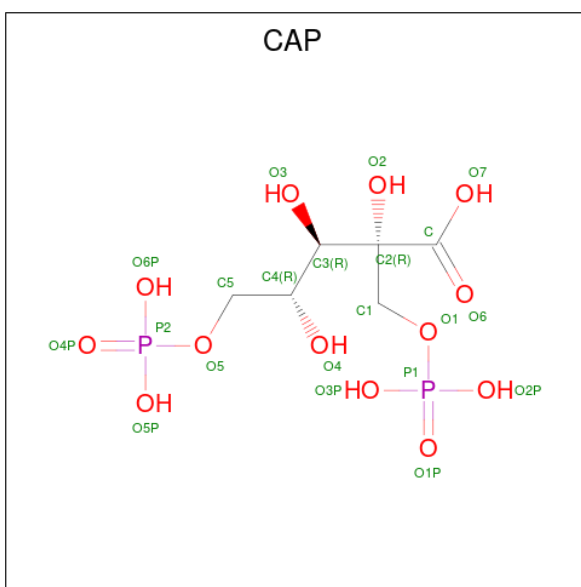
- Molecule 2 is a protein called Ribulose biphosphate carboxylase small chain C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	122	Total	C	N	O	S	0	0	0
			1016	672	163	175	6			
2	W	122	Total	C	N	O	S	0	0	0
			1016	672	163	175	6			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (CCD ID: CAP) (formula: C₆H₁₄O₁₃P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 21	C 6	O 13	P 2	0	0
4	E	1	Total 21	C 6	O 13	P 2	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

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

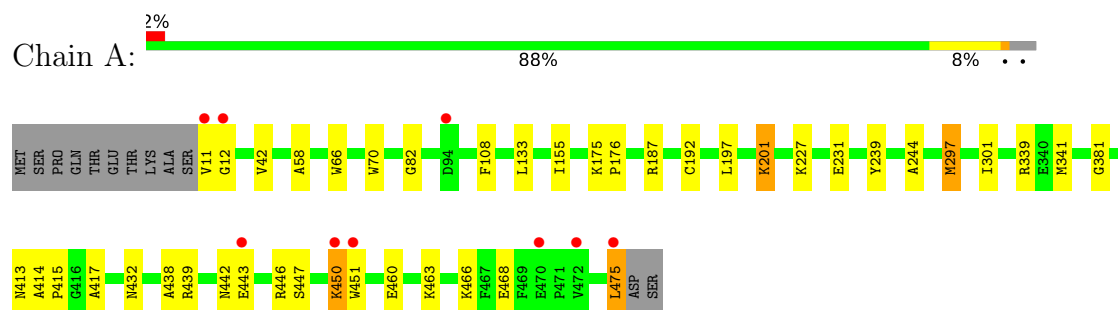
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	402	Total	O	0	0
			402	402		
6	S	120	Total	O	0	0
			120	120		
6	E	366	Total	O	0	0
			366	366		
6	W	111	Total	O	0	0
			111	111		

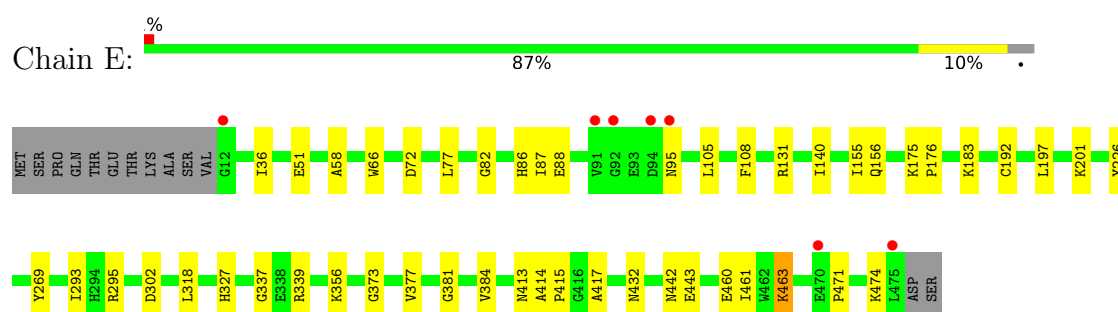
3 Residue-property plots [i](#)

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.

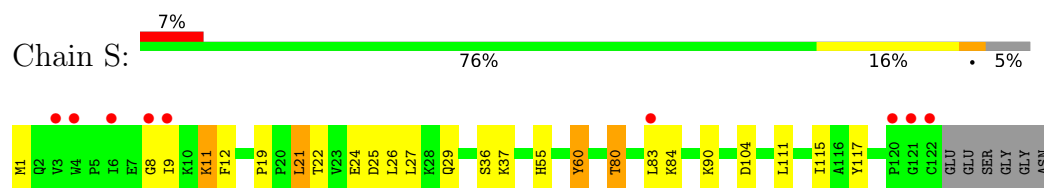
- Molecule 1: Ribulose biphosphate carboxylase large chain



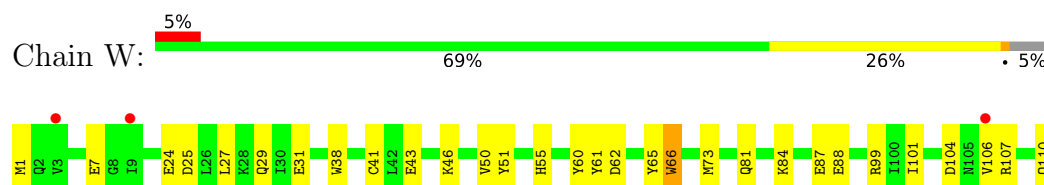
- Molecule 1: Ribulose biphosphate carboxylase large chain



- Molecule 2: Ribulose biphosphate carboxylase small chain C



- Molecule 2: Ribulose biphosphate carboxylase small chain C



•	•	•
P120	G121	C122
GLU	GLU	SER
		GLY
		GLY
		ASN

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	111.71Å 111.71Å 196.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.32 – 1.35 22.32 – 1.35	Depositor EDS
% Data completeness (in resolution range)	98.3 (22.32-1.35) 98.4 (22.32-1.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 1.36Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.160 , 0.182 0.161 , 0.182	Depositor DCC
R_{free} test set	12745 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10448	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CAP, KCX, MME, GOL, MG

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	1.15	4/3717 (0.1%)	1.17	5/5035 (0.1%)
1	E	1.15	3/3710 (0.1%)	1.19	10/5025 (0.2%)
2	S	0.95	0/1039	1.10	1/1410 (0.1%)
2	W	1.04	1/1039 (0.1%)	1.19	4/1410 (0.3%)
All	All	1.12	8/9505 (0.1%)	1.17	20/12880 (0.2%)

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
2	S	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	112	ILE	CA-CB	7.01	1.62	1.55
1	E	461	ILE	CA-CB	6.86	1.63	1.54
1	A	301	ILE	CA-CB	6.35	1.63	1.54
1	A	297	MET	CG-SD	6.12	1.96	1.80
1	E	58	ALA	CA-CB	5.87	1.62	1.53
1	A	58	ALA	CA-CB	5.86	1.62	1.53
1	E	140	ILE	CA-C	5.79	1.57	1.53
1	A	244	ALA	CA-CB	5.09	1.62	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	119	PRO	CA-C-N	-8.29	111.47	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	119	PRO	C-N-CA	-8.29	111.47	119.76
1	E	339	ARG	N-CA-C	8.24	119.88	111.07
1	E	413	ASN	N-CA-C	7.56	119.60	111.36
1	A	413	ASN	N-CA-C	6.89	118.58	111.14
1	E	155	ILE	N-CA-C	6.67	117.36	110.36
1	E	82	GLY	N-CA-C	-6.60	103.13	112.37
2	W	121	GLY	N-CA-C	-6.15	105.00	115.08
1	E	269	TYR	N-CA-C	6.10	118.89	111.82
1	A	339	ARG	N-CA-C	6.08	118.41	111.11
1	A	155	ILE	N-CA-C	5.98	116.45	110.23
1	A	82	GLY	N-CA-C	-5.92	104.08	112.37
1	A	108	PHE	N-CA-C	5.43	118.34	109.59
2	S	11	LYS	N-CA-C	5.39	118.06	109.81
1	E	302	ASP	N-CA-C	5.37	119.81	112.88
2	W	66	TRP	N-CA-C	-5.36	102.24	109.95
1	E	463	LYS	CA-C-N	-5.29	114.19	122.65
1	E	463	LYS	C-N-CA	-5.29	114.19	122.65
1	E	384	VAL	N-CA-C	5.21	116.56	110.62
1	E	140	ILE	N-CA-C	-5.07	102.53	107.55

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	S	60	TYR	Sidechain

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	3639	0	3554	37	0
1	E	3632	0	3545	34	0
2	S	1016	0	1020	23	0
2	W	1016	0	1020	33	2
3	A	1	0	0	0	0
3	E	1	0	0	0	0
4	A	21	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	21	0	7	0	0
5	A	42	0	56	7	0
5	E	48	0	64	12	0
5	W	12	0	16	10	0
6	A	402	0	0	5	2
6	E	366	0	0	12	4
6	S	120	0	0	3	1
6	W	111	0	0	4	1
All	All	10448	0	9289	126	6

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 7.

All (126) 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)
2:W:104:ASP:OD1	2:W:106:VAL:HG22	1.59	1.00
1:A:443:GLU:HG3	6:A:3143:HOH:O	1.73	0.88
1:E:356:LYS:NZ	6:E:3356:HOH:O	2.06	0.87
1:E:95:ASN:ND2	6:E:3315:HOH:O	2.09	0.85
5:A:3001:GOL:H12	6:A:3407:HOH:O	1.75	0.84
1:A:432:ASN:HD22	2:S:29:GLN:HE22	1.26	0.84
2:W:87:GLU:HG3	6:W:865:HOH:O	1.75	0.83
1:E:373:GLY:H	5:E:3016:GOL:C1	1.92	0.82
1:A:475:LEU:H	1:A:475:LEU:HD12	1.45	0.82
1:E:432:ASN:HD22	2:W:29:GLN:HE22	1.25	0.81
2:W:84:LYS:HE3	2:W:88:GLU:HG2	1.62	0.81
1:E:373:GLY:H	5:E:3016:GOL:H11	1.48	0.79
1:A:450:LYS:N	1:A:450:LYS:HD2	1.97	0.79
2:W:25:ASP:OD2	6:W:935:HOH:O	2.03	0.76
1:A:450:LYS:HD2	1:A:450:LYS:H	1.49	0.76
1:A:438:ALA:HB3	1:A:439:ARG:HH21	1.51	0.76
2:W:99:ARG:HH21	5:W:3007:GOL:H31	1.53	0.73
2:W:84:LYS:NZ	2:W:88:GLU:OE1	2.15	0.73
1:E:183:LYS:HE3	6:E:3112:HOH:O	1.87	0.73
1:A:11:VAL:HG12	1:A:12:GLY:N	2.04	0.72
1:E:443:GLU:HG3	6:E:3161:HOH:O	1.88	0.71
2:S:25:ASP:OD2	6:S:192:HOH:O	2.10	0.70
1:A:446:ARG:C	1:A:450:LYS:HZ2	2.01	0.68
5:A:3001:GOL:C1	6:A:3407:HOH:O	2.38	0.68
1:E:156:GLN:OE1	5:E:3016:GOL:H12	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:3002:GOL:O1	6:E:3375:HOH:O	2.10	0.65
2:W:84:LYS:HE3	2:W:88:GLU:CG	2.25	0.65
1:A:466:LYS:HG3	1:A:468:GLU:HG3	1.79	0.65
1:A:451:TRP:CD2	2:S:19:PRO:HG3	2.31	0.65
2:S:80:THR:HA	2:S:83:LEU:HD12	1.78	0.65
1:A:466:LYS:HD2	6:A:3149:HOH:O	1.96	0.64
1:E:295:ARG:HH12	5:E:3014:GOL:H31	1.63	0.64
1:A:70:TRP:HA	5:A:3012:GOL:H32	1.79	0.63
5:E:3009:GOL:H12	6:E:3366:HOH:O	1.98	0.63
1:E:460:GLU:CG	6:E:3374:HOH:O	2.47	0.62
2:W:43:GLU:OE2	5:W:3007:GOL:H12	2.01	0.61
2:S:84:LYS:HE3	6:S:223:HOH:O	2.01	0.61
1:E:460:GLU:HG3	6:E:3374:HOH:O	2.01	0.61
1:E:131:ARG:HD2	6:E:3377:HOH:O	2.01	0.60
2:S:12:PHE:HB3	2:S:115:ILE:HG13	1.83	0.60
2:W:99:ARG:HH21	5:W:3007:GOL:C3	2.15	0.60
1:A:42:VAL:HG22	1:A:133:LEU:CD1	2.33	0.59
2:S:12:PHE:CB	2:S:115:ILE:HG13	2.33	0.59
1:E:460:GLU:CD	6:E:3374:HOH:O	2.44	0.59
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.83	0.59
1:E:373:GLY:N	5:E:3016:GOL:H11	2.16	0.59
2:S:21:LEU:HD23	2:S:26:LEU:HD23	1.84	0.59
1:A:11:VAL:CG1	1:A:12:GLY:N	2.66	0.58
2:W:50:VAL:CG2	2:W:61:TYR:HB3	2.34	0.58
1:E:156:GLN:OE1	5:E:3016:GOL:C1	2.53	0.56
2:S:9:ILE:HG22	2:S:11:LYS:HE2	1.88	0.55
2:W:43:GLU:OE1	5:W:3007:GOL:H31	2.08	0.54
2:S:27:LEU:HG	2:S:83:LEU:HD11	1.88	0.54
2:S:22:THR:OG1	2:S:24:GLU:HG3	2.08	0.53
2:W:27:LEU:O	2:W:31:GLU:HG3	2.09	0.53
2:W:101:ILE:C	2:W:101:ILE:HD12	2.33	0.53
1:A:187:ARG:HH22	5:A:3015:GOL:H11	1.74	0.53
2:W:110:GLN:OE1	5:W:3007:GOL:H11	2.09	0.52
1:A:11:VAL:CG1	1:A:12:GLY:H	2.23	0.52
2:W:50:VAL:HG23	2:W:62:ASP:O	2.10	0.51
2:W:66:TRP:H	5:W:3007:GOL:C3	2.24	0.51
1:A:192:CYS:HB3	1:A:197:LEU:HD12	1.92	0.51
2:S:90:LYS:HE3	2:S:117:TYR:CD1	2.44	0.51
1:A:460:GLU:OE2	1:A:463:LYS:NZ	2.35	0.51
1:E:197:LEU:HG	1:E:417:ALA:HB1	1.91	0.51
2:W:65:TYR:HA	5:W:3007:GOL:H32	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:73:MET:CE	2:W:81:GLN:HE21	2.24	0.51
2:W:41:CYS:HB3	2:W:101:ILE:HD11	1.93	0.50
2:W:66:TRP:H	5:W:3007:GOL:H32	1.77	0.50
2:W:106:VAL:HG23	2:W:107:ARG:N	2.26	0.50
2:S:8:GLY:O	2:S:9:ILE:HD13	2.12	0.49
2:S:9:ILE:HG22	2:S:9:ILE:O	2.13	0.49
1:A:187:ARG:HH22	5:A:3015:GOL:C1	2.26	0.48
1:A:450:LYS:H	1:A:450:LYS:CD	2.20	0.48
2:W:38:TRP:CE2	2:W:111:LEU:HD12	2.49	0.48
1:A:438:ALA:CB	1:A:439:ARG:HH21	2.24	0.48
2:S:104:ASP:HB2	2:S:111:LEU:CD1	2.44	0.47
1:A:447:SER:O	1:A:450:LYS:HD3	2.15	0.47
1:E:295:ARG:HH12	5:E:3014:GOL:C3	2.28	0.47
2:W:106:VAL:CG2	6:W:749:HOH:O	2.63	0.47
1:A:475:LEU:HD12	1:A:475:LEU:N	2.22	0.47
2:W:50:VAL:HG22	2:W:51:TYR:N	2.29	0.47
1:A:11:VAL:HG12	1:A:12:GLY:H	1.74	0.47
1:A:175:LYS:HA	1:A:176:PRO:C	2.40	0.46
1:A:187:ARG:NH2	5:A:3015:GOL:C1	2.79	0.46
2:S:21:LEU:HD23	2:S:26:LEU:CD2	2.46	0.46
1:A:381:GLY:HA2	1:E:66:TRP:CD1	2.51	0.46
1:E:86:HIS:HE1	1:E:88:GLU:OE1	1.99	0.46
2:W:43:GLU:CD	5:W:3007:GOL:H12	2.41	0.46
2:W:50:VAL:HG23	2:W:61:TYR:HB3	1.98	0.45
2:W:106:VAL:HG21	6:W:749:HOH:O	2.16	0.45
2:S:60:TYR:C	2:S:60:TYR:CD1	2.95	0.45
1:E:226:TYR:O	5:E:3009:GOL:O1	2.31	0.45
2:W:73:MET:HE1	2:W:81:GLN:HG2	1.98	0.45
1:A:197:LEU:HG	1:A:417:ALA:HB1	1.99	0.45
2:W:73:MET:HE2	2:W:81:GLN:HE21	1.82	0.45
2:S:27:LEU:CD1	2:S:83:LEU:HD11	2.47	0.44
1:A:442:ASN:O	1:A:446:ARG:HG3	2.18	0.44
1:E:327:HIS:HA	1:E:377:VAL:HB	1.99	0.44
1:A:187:ARG:NH1	6:A:3271:HOH:O	2.50	0.43
1:E:36:ILE:HD12	1:E:108:PHE:CE2	2.54	0.43
1:A:201:KCX:HB2	1:A:239:TYR:CD2	2.54	0.43
2:W:99:ARG:NH2	5:W:3007:GOL:C3	2.80	0.43
1:E:51:GLU:HA	1:E:87:ILE:CD1	2.49	0.42
1:E:192:CYS:HB3	1:E:197:LEU:HD12	2.00	0.42
1:E:105:LEU:HB3	5:E:3002:GOL:H32	2.01	0.42
2:W:60:TYR:CD1	2:W:60:TYR:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:12:PHE:HB3	2:S:115:ILE:CG1	2.49	0.42
2:S:84:LYS:CE	6:S:223:HOH:O	2.65	0.42
1:E:72:ASP:HB2	5:E:3013:GOL:H12	2.02	0.42
1:E:460:GLU:OE1	1:E:463:LYS:NZ	2.47	0.42
1:A:187:ARG:NH2	5:A:3015:GOL:H12	2.35	0.41
2:S:104:ASP:HB2	2:S:111:LEU:HD12	2.01	0.41
2:S:36:SER:O	2:S:37:LYS:HB2	2.20	0.41
1:A:66:TRP:CD1	1:E:381:GLY:HA2	2.56	0.41
1:E:175:LYS:HA	1:E:176:PRO:C	2.45	0.41
2:W:38:TRP:NE1	2:W:111:LEU:HD12	2.35	0.41
2:S:90:LYS:HG2	2:S:117:TYR:CG	2.56	0.41
1:A:414:ALA:HB3	1:A:415:PRO:HD3	2.03	0.40
1:A:447:SER:HA	1:A:450:LYS:NZ	2.36	0.40
1:E:293:ILE:HG13	1:E:318:LEU:HD21	2.03	0.40
1:E:471:PRO:O	1:E:474:LYS:HE2	2.21	0.40
1:A:227:LYS:O	1:A:231:GLU:HG3	2.21	0.40
1:A:341:MET:CG	1:A:475:LEU:HG	2.52	0.40
1:E:131:ARG:CD	6:E:3377:HOH:O	2.67	0.40
1:E:442:ASN:ND2	6:E:3379:HOH:O	2.54	0.40

All (6) 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)
2:W:7:GLU:OE1	2:W:46:LYS:NZ[4_565]	1.91	0.29
6:A:3321:HOH:O	6:E:3375:HOH:O[4_565]	1.94	0.26
6:E:3249:HOH:O	6:E:3352:HOH:O[4_565]	2.02	0.18
2:W:24:GLU:OE2	6:S:192:HOH:O[6_555]	2.08	0.12
6:E:3320:HOH:O	6:W:693:HOH:O[4_565]	2.10	0.10
6:A:3266:HOH:O	6:E:3363:HOH:O[3_555]	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	462/477 (97%)	448 (97%)	14 (3%)	0	100	100
1	E	461/477 (97%)	447 (97%)	13 (3%)	1 (0%)	43	19
2	S	120/128 (94%)	115 (96%)	5 (4%)	0	100	100
2	W	120/128 (94%)	114 (95%)	6 (5%)	0	100	100
All	All	1163/1210 (96%)	1124 (97%)	38 (3%)	1 (0%)	48	20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	337	GLY

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	374/385 (97%)	371 (99%)	3 (1%)	73	48
1	E	373/385 (97%)	372 (100%)	1 (0%)	86	72
2	S	109/113 (96%)	106 (97%)	3 (3%)	38	9
2	W	109/113 (96%)	108 (99%)	1 (1%)	70	44
All	All	965/996 (97%)	957 (99%)	8 (1%)	73	48

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	MET
1	A	450	LYS
1	A	475	LEU
2	S	21	LEU
2	S	55	HIS
2	S	80	THR
1	E	77	LEU
2	W	55	HIS

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

Mol	Chain	Res	Type
1	A	401	GLN
2	S	29	GLN
2	S	54	ASN
1	E	86	HIS
1	E	95	ASN
1	E	304	GLN
1	E	401	GLN
1	E	442	ASN
2	W	2	GLN
2	W	29	GLN
2	W	54	ASN
2	W	81	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	KCX	E	201	3,1	10,11,12	1.62	2 (20%)	6,12,14	1.74	2 (33%)
1	KCX	A	201	3,1	10,11,12	1.53	1 (10%)	6,12,14	1.58	2 (33%)
2	MME	S	1	2	7,8,9	2.00	1 (14%)	5,8,10	1.45	1 (20%)
2	MME	W	1	2	7,8,9	1.99	1 (14%)	5,8,10	1.51	1 (20%)

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	KCX	E	201	3,1	-	0/9/10/12	-
1	KCX	A	201	3,1	-	0/9/10/12	-
2	MME	S	1	2	-	2/5/8/10	-
2	MME	W	1	2	-	1/5/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	1	MME	CM-N	-5.17	1.33	1.46
2	W	1	MME	CM-N	-5.06	1.34	1.46
1	A	201	KCX	OQ1-CX	4.16	1.29	1.21
1	E	201	KCX	OQ1-CX	3.56	1.28	1.21
1	E	201	KCX	CE-NZ	2.45	1.51	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	201	KCX	OQ1-CX-NZ	-3.64	119.38	124.92
1	A	201	KCX	OQ1-CX-NZ	-3.12	120.17	124.92
2	W	1	MME	CM-N-CA	2.92	122.42	113.70
2	S	1	MME	CM-N-CA	2.73	121.85	113.70
1	A	201	KCX	CE-NZ-CX	2.17	125.67	121.98
1	E	201	KCX	CE-NZ-CX	2.08	125.51	121.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	S	1	MME	CB-CG-SD-CE
2	W	1	MME	CB-CG-SD-CE
2	S	1	MME	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	201	KCX	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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
5	GOL	W	3007	-	5,5,5	1.03	0	5,5,5	0.33	0
5	GOL	A	3001	-	5,5,5	1.63	1 (20%)	5,5,5	1.20	1 (20%)
5	GOL	E	3014	-	5,5,5	1.24	1 (20%)	5,5,5	0.81	0
5	GOL	A	3006	-	5,5,5	0.89	0	5,5,5	0.37	0
5	GOL	A	3015	-	5,5,5	1.21	1 (20%)	5,5,5	0.27	0
5	GOL	E	3005	-	5,5,5	1.06	0	5,5,5	0.46	0
5	GOL	E	3003	-	5,5,5	2.22	1 (20%)	5,5,5	0.99	1 (20%)
5	GOL	E	3013	-	5,5,5	0.93	0	5,5,5	0.52	0
5	GOL	E	3011	-	5,5,5	1.45	1 (20%)	5,5,5	0.39	0
5	GOL	A	3010	-	5,5,5	1.04	0	5,5,5	0.52	0
5	GOL	E	3016	-	5,5,5	1.27	0	5,5,5	0.76	0
5	GOL	E	3009	-	5,5,5	1.02	0	5,5,5	1.06	0
4	CAP	A	1001	3	18,20,20	0.88	0	23,31,31	1.53	4 (17%)
5	GOL	A	3017	-	5,5,5	0.74	0	5,5,5	0.29	0
4	CAP	E	2001	3	18,20,20	1.04	2 (11%)	23,31,31	1.39	3 (13%)
5	GOL	A	3012	-	5,5,5	0.91	0	5,5,5	0.35	0
5	GOL	W	3008	-	5,5,5	1.15	0	5,5,5	0.39	0
5	GOL	E	3002	-	5,5,5	1.18	0	5,5,5	1.08	0
5	GOL	A	3004	-	5,5,5	1.39	1 (20%)	5,5,5	0.47	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
5	GOL	W	3007	-	-	4/4/4/4	-
5	GOL	A	3001	-	-	2/4/4/4	-
5	GOL	E	3014	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	3006	-	-	3/4/4/4	-
5	GOL	A	3015	-	-	4/4/4/4	-
5	GOL	E	3005	-	-	2/4/4/4	-
5	GOL	E	3003	-	-	0/4/4/4	-
5	GOL	E	3013	-	-	0/4/4/4	-
5	GOL	E	3011	-	-	0/4/4/4	-
5	GOL	A	3010	-	-	2/4/4/4	-
5	GOL	E	3016	-	-	2/4/4/4	-
5	GOL	E	3009	-	-	4/4/4/4	-
4	CAP	A	1001	3	-	11/29/29/29	-
5	GOL	A	3017	-	-	0/4/4/4	-
4	CAP	E	2001	3	-	10/29/29/29	-
5	GOL	A	3012	-	-	0/4/4/4	-
5	GOL	W	3008	-	-	4/4/4/4	-
5	GOL	E	3002	-	-	2/4/4/4	-
5	GOL	A	3004	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	3003	GOL	O3-C3	4.26	1.60	1.42
5	A	3001	GOL	C3-C2	-2.95	1.40	1.51
5	E	3011	GOL	O3-C3	2.74	1.53	1.42
5	A	3004	GOL	O3-C3	2.39	1.52	1.42
5	E	3014	GOL	O3-C3	2.38	1.52	1.42
4	E	2001	CAP	C2-C	-2.37	1.51	1.53
5	A	3015	GOL	C3-C2	-2.10	1.43	1.51
4	E	2001	CAP	O6-C	2.03	1.28	1.22

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	CAP	O7-C-C2	4.56	121.70	114.06
4	E	2001	CAP	O7-C-C2	4.07	120.88	114.06
4	A	1001	CAP	O6-C-C2	-3.01	116.71	122.32
4	E	2001	CAP	O6-C-C2	-2.46	117.74	122.32
4	A	1001	CAP	C2-C3-C4	2.28	118.58	114.03
4	E	2001	CAP	C2-C3-C4	2.10	118.22	114.03
5	E	3003	GOL	C3-C2-C1	2.10	119.49	111.80
5	A	3001	GOL	C3-C2-C1	-2.08	104.15	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	CAP	O4-C4-C3	-2.01	104.76	108.78

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	CAP	O7-C-C2-C1
4	A	1001	CAP	O6-C-C2-O2
4	A	1001	CAP	C2-C3-C4-O4
4	A	1001	CAP	O3-C3-C4-O4
4	E	2001	CAP	O7-C-C2-C1
4	E	2001	CAP	O6-C-C2-O2
4	E	2001	CAP	C2-C3-C4-O4
4	E	2001	CAP	O3-C3-C4-O4
5	A	3015	GOL	O1-C1-C2-O2
5	A	3015	GOL	O1-C1-C2-C3
5	E	3002	GOL	O1-C1-C2-C3
5	E	3009	GOL	O1-C1-C2-C3
5	E	3014	GOL	O1-C1-C2-C3
5	E	3014	GOL	C1-C2-C3-O3
5	W	3007	GOL	O2-C2-C3-O3
5	W	3008	GOL	C1-C2-C3-O3
5	A	3006	GOL	C1-C2-C3-O3
5	A	3010	GOL	C1-C2-C3-O3
5	A	3015	GOL	C1-C2-C3-O3
5	E	3005	GOL	C1-C2-C3-O3
5	E	3009	GOL	C1-C2-C3-O3
5	E	3016	GOL	C1-C2-C3-O3
5	W	3007	GOL	O1-C1-C2-C3
5	W	3007	GOL	C1-C2-C3-O3
5	W	3008	GOL	O1-C1-C2-C3
5	E	3002	GOL	O1-C1-C2-O2
5	E	3005	GOL	O2-C2-C3-O3
5	E	3009	GOL	O1-C1-C2-O2
5	E	3009	GOL	O2-C2-C3-O3
5	E	3014	GOL	O1-C1-C2-O2
5	E	3014	GOL	O2-C2-C3-O3
5	A	3010	GOL	O2-C2-C3-O3
5	W	3008	GOL	O2-C2-C3-O3
4	A	1001	CAP	O7-C-C2-O2
4	E	2001	CAP	O7-C-C2-O2
4	A	1001	CAP	O6-C-C2-C1

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Mol	Chain	Res	Type	Atoms
5	W	3008	GOL	O1-C1-C2-O2
5	A	3015	GOL	O2-C2-C3-O3
5	E	3016	GOL	O2-C2-C3-O3
5	W	3007	GOL	O1-C1-C2-O2
5	A	3001	GOL	C1-C2-C3-O3
4	E	2001	CAP	O6-C-C2-C1
5	A	3001	GOL	O2-C2-C3-O3
4	A	1001	CAP	O2-C2-C3-C4
4	E	2001	CAP	O2-C2-C3-C4
4	A	1001	CAP	O7-C-C2-C3
4	E	2001	CAP	O7-C-C2-C3
5	A	3006	GOL	O1-C1-C2-C3
5	A	3006	GOL	O1-C1-C2-O2
4	A	1001	CAP	O6-C-C2-C3
4	E	2001	CAP	O6-C-C2-C3
4	A	1001	CAP	O3-C3-C4-C5
4	A	1001	CAP	C2-C3-C4-C5
4	E	2001	CAP	C2-C3-C4-C5

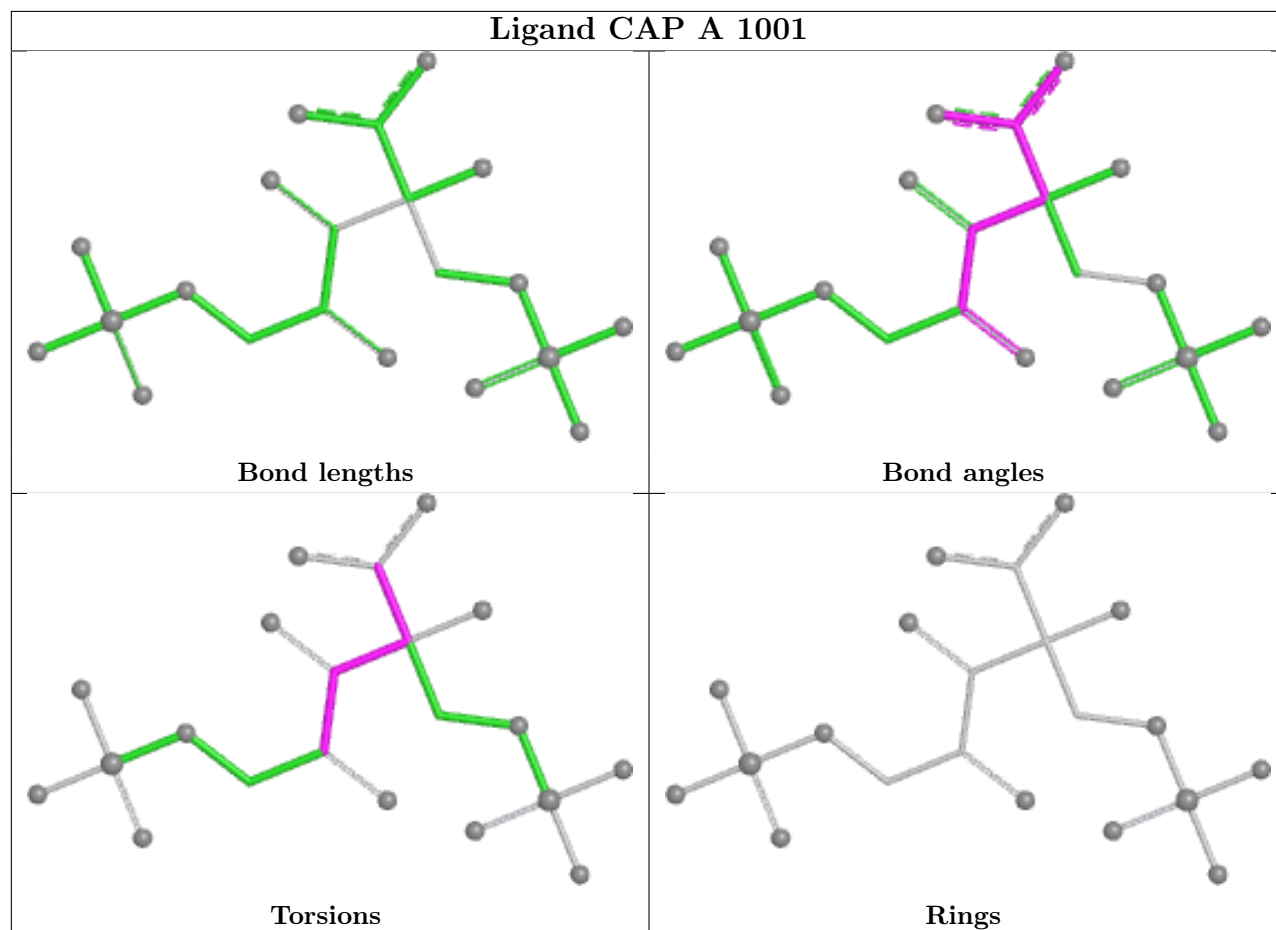
There are no ring outliers.

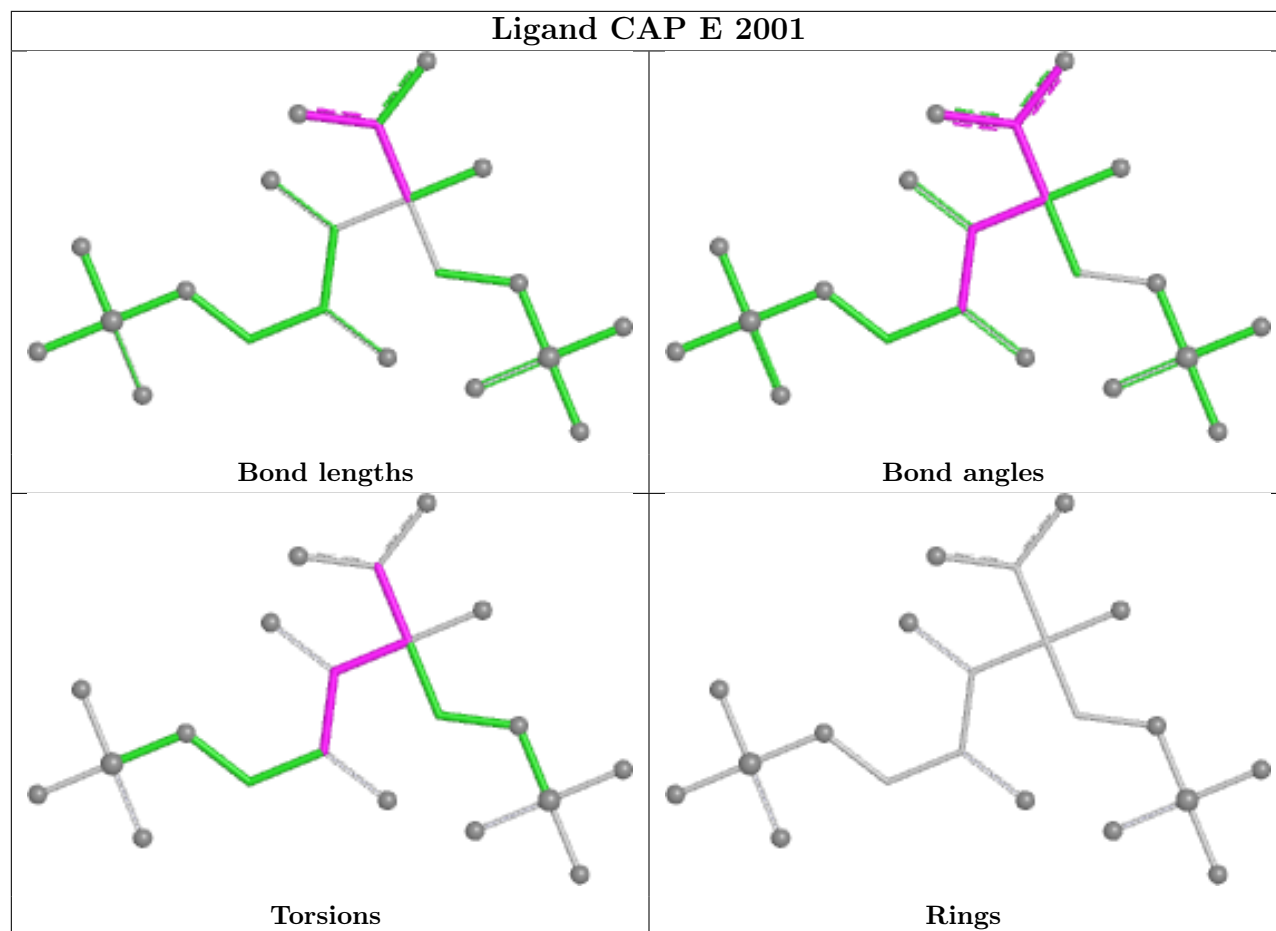
9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	W	3007	GOL	10	0
5	A	3001	GOL	2	0
5	E	3014	GOL	2	0
5	A	3015	GOL	4	0
5	E	3013	GOL	1	0
5	E	3016	GOL	5	0
5	E	3009	GOL	2	0
5	A	3012	GOL	1	0
5	E	3002	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	464/477 (97%)	-0.38	9 (1%) 66 76	11, 16, 31, 46	0
1	E	463/477 (97%)	-0.39	7 (1%) 72 81	11, 15, 30, 49	0
2	S	121/128 (94%)	0.55	9 (7%) 20 28	13, 26, 40, 63	0
2	W	121/128 (94%)	0.40	6 (4%) 34 44	13, 25, 37, 66	0
All	All	1169/1210 (96%)	-0.20	31 (2%) 56 65	11, 17, 35, 66	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	475	LEU	6.8
2	W	121	GLY	4.8
2	W	122	CYS	4.7
1	A	11	VAL	4.4
1	A	451	TRP	4.2
2	S	9	ILE	3.7
1	E	475	LEU	3.7
2	S	120	PRO	3.5
2	S	8	GLY	3.4
2	S	121	GLY	3.4
1	E	92	GLY	3.3
1	E	91	VAL	3.2
2	S	122	CYS	3.0
2	W	120	PRO	3.0
1	E	94	ASP	2.9
2	S	6	ILE	2.8
2	W	9	ILE	2.8
2	S	83	LEU	2.8
2	S	3	VAL	2.7
2	W	3	VAL	2.7
1	E	12	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	470	GLU	2.5
2	S	4	TRP	2.4
1	A	450	LYS	2.4
1	A	443	GLU	2.4
1	E	470	GLU	2.4
1	A	472	VAL	2.3
1	E	95	ASN	2.2
2	W	106	VAL	2.1
1	A	12	GLY	2.0
1	A	94	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. 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
2	MME	S	1	9/10	0.87	0.13	36,40,47,48	0
2	MME	W	1	9/10	0.88	0.13	35,38,44,45	0
1	KCX	E	201	12/13	0.99	0.04	12,13,14,14	0
1	KCX	A	201	12/13	0.99	0.02	11,12,13,13	0

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, 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
5	GOL	E	3009	6/6	0.77	0.15	39,41,43,43	0
5	GOL	E	3014	6/6	0.79	0.15	32,37,40,40	0
5	GOL	A	3012	6/6	0.80	0.16	49,51,52,53	0
5	GOL	E	3013	6/6	0.82	0.14	43,49,49,49	0

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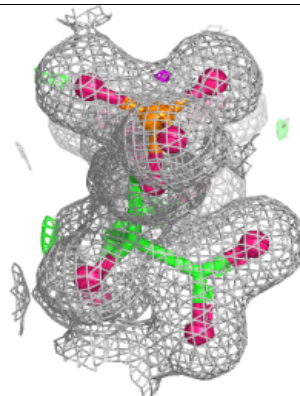
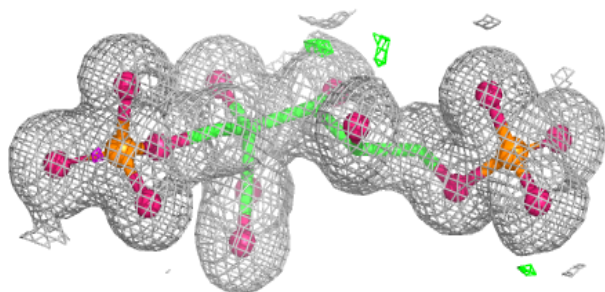
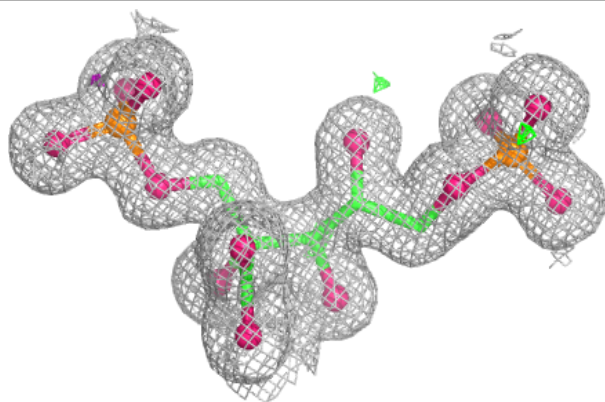
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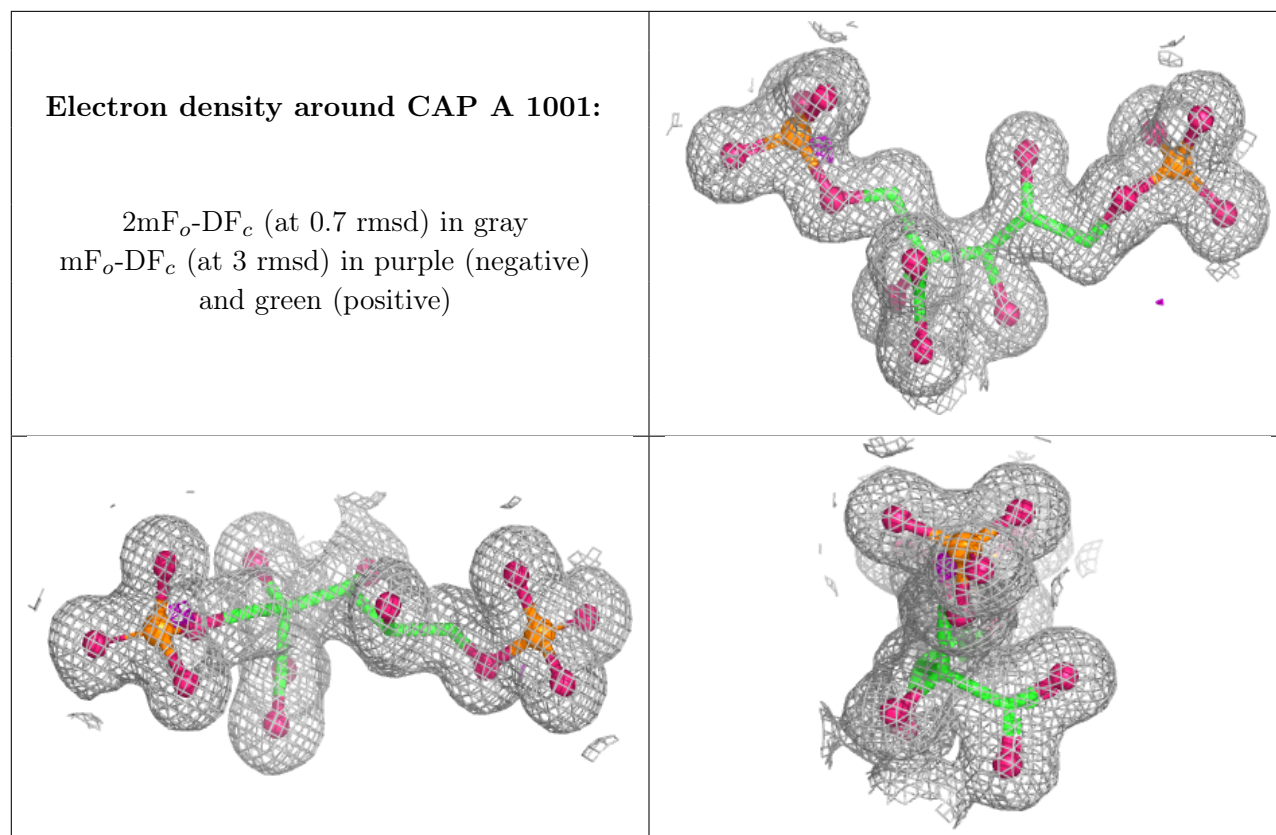
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	3010	6/6	0.82	0.12	43,45,46,47	0
5	GOL	E	3016	6/6	0.84	0.12	32,41,41,44	0
5	GOL	W	3008	6/6	0.84	0.12	41,47,48,51	0
5	GOL	A	3015	6/6	0.86	0.12	30,37,40,45	0
5	GOL	A	3001	6/6	0.87	0.10	28,32,37,39	0
5	GOL	A	3004	6/6	0.87	0.11	26,27,32,34	0
5	GOL	E	3002	6/6	0.88	0.11	30,34,35,38	0
5	GOL	W	3007	6/6	0.89	0.10	23,33,34,39	0
5	GOL	A	3017	6/6	0.89	0.10	32,42,45,46	0
5	GOL	E	3011	6/6	0.90	0.10	27,28,32,35	0
5	GOL	A	3006	6/6	0.91	0.10	26,37,39,45	0
5	GOL	E	3003	6/6	0.94	0.08	17,20,22,24	0
5	GOL	E	3005	6/6	0.95	0.07	24,33,35,40	0
4	CAP	E	2001	21/21	0.99	0.03	13,14,16,18	0
4	CAP	A	1001	21/21	0.99	0.03	13,14,15,18	0
3	MG	E	2476	1/1	1.00	0.01	12,12,12,12	0
3	MG	A	1476	1/1	1.00	0.03	13,13,13,13	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CAP E 2001:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.