



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 05:59 am BST

PDB ID : 1PT8
Title : Crystal structure of the yfdW gene product of E. coli, in complex with oxalate and acetyl-CoA
Authors : Gruez, A.; Roig-Zamboni, V.; Valencia, C.; Campanacci, V.; Cambillau, C.
Deposited on : 2003-06-23
Resolution : 2.20 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
buster-report : 1.1.7 (2018)
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

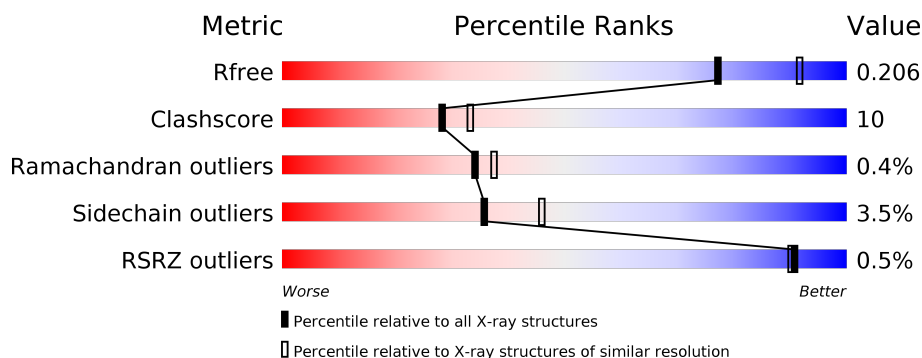
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	437	
1	B	437	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7044 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 Hypothetical protein yfdW.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	4	0	0
			3224	2045	550	611	18			
1	B	415	Total	C	N	O	S	0	0	0
			3216	2040	549	610	17			

There are 42 discrepancies between the modelled and reference sequences:

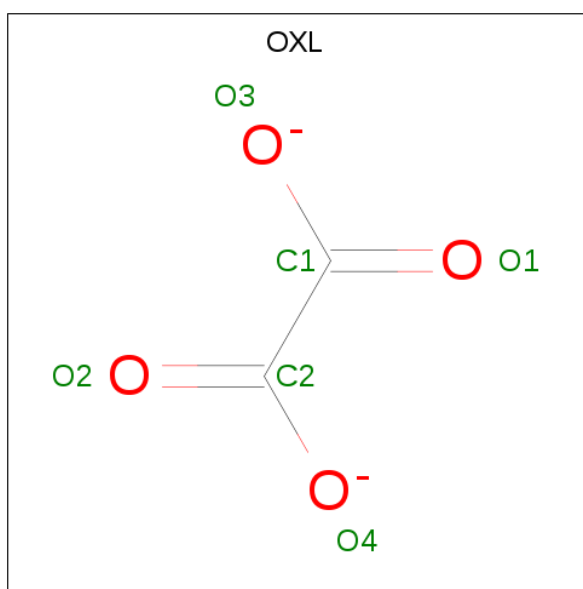
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	SER	-	CLONING ARTIFACT	UNP P69902
A	-19	TYR	-	CLONING ARTIFACT	UNP P69902
A	-18	TYR	-	CLONING ARTIFACT	UNP P69902
A	-17	HIS	-	EXPRESSION TAG	UNP P69902
A	-16	HIS	-	EXPRESSION TAG	UNP P69902
A	-15	HIS	-	EXPRESSION TAG	UNP P69902
A	-14	HIS	-	EXPRESSION TAG	UNP P69902
A	-13	HIS	-	EXPRESSION TAG	UNP P69902
A	-12	HIS	-	EXPRESSION TAG	UNP P69902
A	-11	LEU	-	CLONING ARTIFACT	UNP P69902
A	-10	GLU	-	CLONING ARTIFACT	UNP P69902
A	-9	SER	-	CLONING ARTIFACT	UNP P69902
A	-8	THR	-	CLONING ARTIFACT	UNP P69902
A	-7	SER	-	CLONING ARTIFACT	UNP P69902
A	-6	LEU	-	CLONING ARTIFACT	UNP P69902
A	-5	TYR	-	CLONING ARTIFACT	UNP P69902
A	-4	LYS	-	CLONING ARTIFACT	UNP P69902
A	-3	LYS	-	CLONING ARTIFACT	UNP P69902
A	-2	ALA	-	CLONING ARTIFACT	UNP P69902
A	-1	GLY	-	CLONING ARTIFACT	UNP P69902
A	0	LEU	-	CLONING ARTIFACT	UNP P69902
B	-20	SER	-	CLONING ARTIFACT	UNP P69902
B	-19	TYR	-	CLONING ARTIFACT	UNP P69902
B	-18	TYR	-	CLONING ARTIFACT	UNP P69902
B	-17	HIS	-	EXPRESSION TAG	UNP P69902

Continued on next page...

Continued from previous page...

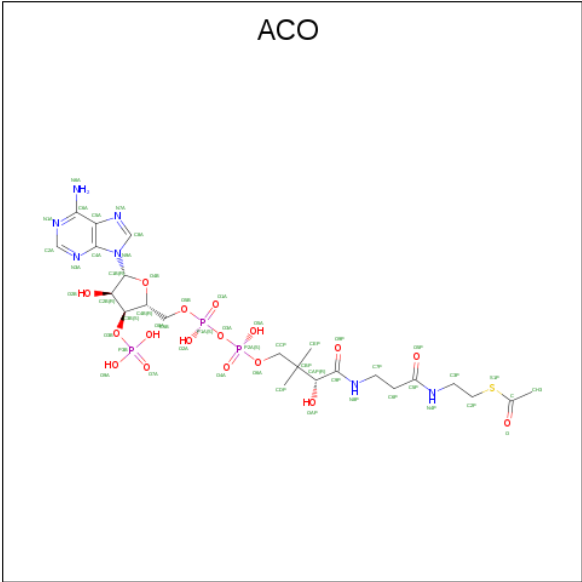
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	EXPRESSION TAG	UNP P69902
B	-15	HIS	-	EXPRESSION TAG	UNP P69902
B	-14	HIS	-	EXPRESSION TAG	UNP P69902
B	-13	HIS	-	EXPRESSION TAG	UNP P69902
B	-12	HIS	-	EXPRESSION TAG	UNP P69902
B	-11	LEU	-	CLONING ARTIFACT	UNP P69902
B	-10	GLU	-	CLONING ARTIFACT	UNP P69902
B	-9	SER	-	CLONING ARTIFACT	UNP P69902
B	-8	THR	-	CLONING ARTIFACT	UNP P69902
B	-7	SER	-	CLONING ARTIFACT	UNP P69902
B	-6	LEU	-	CLONING ARTIFACT	UNP P69902
B	-5	TYR	-	CLONING ARTIFACT	UNP P69902
B	-4	LYS	-	CLONING ARTIFACT	UNP P69902
B	-3	LYS	-	CLONING ARTIFACT	UNP P69902
B	-2	ALA	-	CLONING ARTIFACT	UNP P69902
B	-1	GLY	-	CLONING ARTIFACT	UNP P69902
B	0	LEU	-	CLONING ARTIFACT	UNP P69902

- Molecule 2 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	2	4		
2	B	1	Total	C	O	0	0
			6	2	4		

- Molecule 3 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	2	1
			54	25	7	18	3	1		
3	B	1	Total	C	N	O	P	S	2	1
			54	25	7	18	3	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

Continued on next page...

Continued from previous page...

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

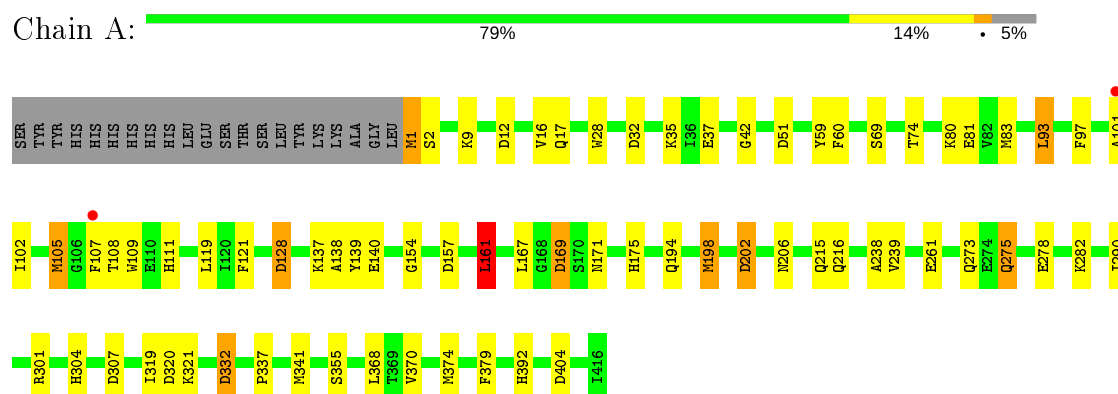
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	231	Total	O	0	0
			231	231		
5	B	223	Total	O	0	0
			223	223		

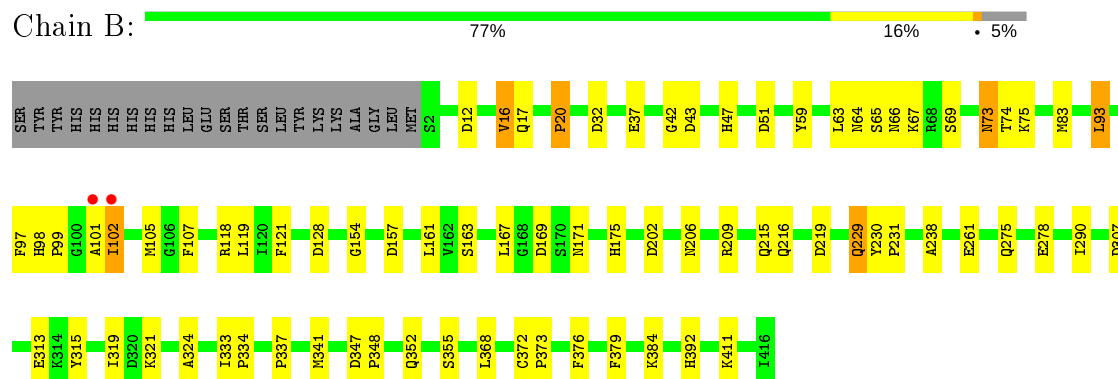
3 Residue-property plots [i](#)

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: Hypothetical protein yfdW



- Molecule 1: Hypothetical protein yfdW



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	146.79Å 146.79Å 129.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.54 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.20) 98.8 (19.54-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.57 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.181 , 0.204 0.183 , 0.206	Depositor DCC
R_{free} test set	6647 reflections (8.37%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.682	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.459 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7044	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: OXL, GOL, ACO

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	0.74	0/3300	0.87	16/4479 (0.4%)
1	B	0.76	1/3292 (0.0%)	0.85	12/4469 (0.3%)
All	All	0.75	1/6592 (0.0%)	0.86	28/8948 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	20	PRO	N-CD	11.52	1.64	1.47

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	ARG	NE-CZ-NH2	-10.17	115.22	120.30
1	A	161	LEU	CB-CG-CD1	-7.28	98.62	111.00
1	A	404	ASP	CB-CG-OD2	7.28	124.85	118.30
1	B	219	ASP	CB-CG-OD2	7.02	124.61	118.30
1	B	43	ASP	CB-CG-OD2	6.99	124.59	118.30
1	B	51	ASP	CB-CG-OD2	6.67	124.30	118.30
1	A	128	ASP	CB-CG-OD2	6.46	124.12	118.30
1	B	347	ASP	CB-CG-OD2	6.27	123.95	118.30
1	A	51	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	157	ASP	CB-CG-OD2	6.06	123.75	118.30
1	B	128	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	118	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	A	1	MET	CG-SD-CE	5.73	109.37	100.20
1	B	105	MET	CG-SD-CE	5.68	109.29	100.20
1	A	105	MET	CG-SD-CE	5.67	109.28	100.20
1	A	198	MET	CG-SD-CE	5.66	109.25	100.20
1	A	169	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	161	LEU	CA-CB-CG	5.60	128.18	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	202	ASP	CB-CG-OD2	5.45	123.21	118.30
1	A	332	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	32	ASP	CB-CG-OD2	5.30	123.08	118.30
1	B	12	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	202	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	161	LEU	CB-CG-CD2	5.24	119.91	111.00
1	B	307	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	307	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	157	ASP	CB-CG-OD2	5.10	122.89	118.30

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	3224	0	3171	66	3
1	B	3216	0	3159	75	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
3	A	54	0	6	2	0
3	B	54	0	6	3	0
4	A	18	0	24	2	0
4	B	12	0	16	0	0
5	A	231	0	0	9	0
5	B	223	0	0	3	3
All	All	7044	0	6382	124	3

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 10.

All (124) 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:161:LEU:HD12	1:B:161:LEU:CD2	1.94	0.98
1:A:175:HIS:HE1	1:A:206:ASN:HD22	1.17	0.92
1:A:161:LEU:CD1	1:B:161:LEU:HD23	2.01	0.91
1:A:161:LEU:CD1	1:B:161:LEU:CD2	2.49	0.90
1:B:83:MET:HE3	1:B:107:PHE:HD1	1.34	0.90
1:B:83:MET:CE	1:B:107:PHE:CD1	2.59	0.85
1:A:69:SER:H	1:A:392:HIS:HD2	1.23	0.83
1:B:229:GLN:H	1:B:229:GLN:HE21	1.25	0.81
1:B:69:SER:H	1:B:392:HIS:HD2	1.26	0.81
1:A:12:ASP:OD2	5:A:1118:HOH:O	1.97	0.81
1:B:355:SER:OG	5:B:1115:HOH:O	1.98	0.80
1:B:74:THR:HB	1:B:83:MET:HE1	1.62	0.80
1:B:83:MET:HE3	1:B:107:PHE:CD1	2.17	0.80
1:A:161:LEU:HD12	1:B:161:LEU:HD21	1.64	0.79
1:A:169:ASP:OD2	3:A:751[B]:ACO:C	2.30	0.79
1:A:167:LEU:HD21	1:B:167:LEU:HD21	1.66	0.77
1:B:83:MET:CE	1:B:107:PHE:HD1	1.98	0.76
1:B:17:GLN:H	3:B:752[B]:ACO:C	2.00	0.75
1:A:69:SER:H	1:A:392:HIS:CD2	2.06	0.74
1:B:69:SER:H	1:B:392:HIS:CD2	2.07	0.72
1:A:368:LEU:H	1:B:216:GLN:HE22	1.38	0.72
1:A:102:ILE:O	5:A:1131:HOH:O	2.07	0.71
1:B:83:MET:HE2	1:B:107:PHE:CE1	2.27	0.70
1:B:315:TYR:OH	1:B:319:ILE:CD1	2.42	0.68
1:A:273:GLN:HG2	1:A:275:GLN:HE21	1.58	0.67
1:A:93:LEU:HD22	1:A:121:PHE:CD1	2.29	0.67
1:A:108:THR:O	1:A:111:HIS:N	2.26	0.67
1:A:216:GLN:HE22	1:B:368:LEU:H	1.43	0.67
1:A:368:LEU:H	1:B:216:GLN:NE2	1.94	0.66
1:A:107:PHE:O	5:A:1132:HOH:O	2.14	0.66
1:B:315:TYR:CZ	1:B:319:ILE:CD1	2.80	0.65
1:A:17:GLN:H	3:A:751[A]:ACO:C	2.10	0.65
1:A:175:HIS:HE1	1:A:206:ASN:ND2	1.94	0.65
1:B:66:ASN:HD21	1:B:384:LYS:H	1.44	0.64
1:B:16:VAL:O	1:B:20:PRO:HG2	1.98	0.64
1:A:93:LEU:HD22	1:A:121:PHE:CE1	2.33	0.64
1:A:161:LEU:HD11	1:B:161:LEU:CD2	2.27	0.64
1:B:229:GLN:H	1:B:229:GLN:NE2	1.96	0.63
1:B:315:TYR:CZ	1:B:319:ILE:HD13	2.33	0.63
1:B:73:ASN:HD22	1:B:75:LYS:H	1.46	0.63
1:A:278:GLU:HG2	1:A:282:LYS:HE3	1.81	0.62
1:B:66:ASN:ND2	1:B:384:LYS:H	1.97	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:HIS:HE1	1:B:206:ASN:OD1	1.83	0.62
1:A:216:GLN:NE2	1:B:368:LEU:H	1.98	0.62
1:B:319:ILE:CD1	1:B:324:ALA:HA	2.29	0.62
1:B:97:PHE:HB3	1:B:101:ALA:HB3	1.83	0.61
1:B:315:TYR:OH	1:B:319:ILE:HD13	2.00	0.60
1:B:83:MET:CE	1:B:107:PHE:CE1	2.86	0.58
1:B:163:SER:OG	5:B:1119:HOH:O	2.17	0.58
1:A:278:GLU:HG3	1:A:290:ILE:HD13	1.86	0.56
1:B:83:MET:HE2	1:B:107:PHE:HE1	1.71	0.56
1:A:161:LEU:HD12	1:B:161:LEU:HD23	1.68	0.55
1:B:319:ILE:HD11	1:B:324:ALA:HA	1.87	0.55
1:A:9:LYS:HE3	5:A:922:HOH:O	2.06	0.55
1:B:93:LEU:HD22	1:B:121:PHE:CE1	2.41	0.55
1:A:175:HIS:CE1	1:A:206:ASN:HD22	2.09	0.54
1:A:215:GLN:HE21	1:B:341:MET:HB2	1.72	0.54
1:A:355:SER:OG	5:A:1128:HOH:O	2.19	0.54
1:A:171:ASN:O	1:A:175:HIS:HD2	1.91	0.53
1:B:315:TYR:CZ	1:B:319:ILE:HD11	2.42	0.53
1:B:102:ILE:HG22	5:B:976:HOH:O	2.08	0.53
1:A:154:GLY:HA2	1:B:161:LEU:HD21	1.89	0.53
1:A:161:LEU:HD11	1:B:161:LEU:HD23	1.85	0.53
1:B:206:ASN:HD21	1:B:209:ARG:HH11	1.55	0.52
1:A:37:GLU:HB3	1:A:42:GLY:HA2	1.92	0.52
1:A:161:LEU:HD11	1:B:154:GLY:HA2	1.92	0.51
1:B:98:HIS:HD2	1:B:99:PRO:O	1.94	0.51
1:A:97:PHE:HB3	1:A:101:ALA:HB3	1.94	0.50
1:B:83:MET:SD	1:B:107:PHE:CD1	3.04	0.49
1:A:28:TRP:O	4:A:901:GOL:H11	2.13	0.49
1:B:37:GLU:HB3	1:B:42:GLY:HA2	1.94	0.49
1:B:73:ASN:C	1:B:73:ASN:HD22	2.13	0.49
1:A:9:LYS:HE2	5:A:1101:HOH:O	2.12	0.49
1:B:17:GLN:HG3	1:B:63:LEU:HD11	1.94	0.49
1:B:319:ILE:HD12	1:B:324:ALA:HA	1.94	0.49
1:B:73:ASN:ND2	1:B:75:LYS:H	2.09	0.48
1:A:1:MET:HA	1:A:2:SER:HB2	1.95	0.48
1:B:169:ASP:OD2	3:B:752[A]:ACO:C	2.62	0.47
1:B:215:GLN:HE22	1:B:238:ALA:HA	1.80	0.47
1:A:341:MET:HB2	1:B:215:GLN:HE21	1.79	0.47
1:A:215:GLN:HE22	1:A:238:ALA:HA	1.80	0.47
1:B:206:ASN:ND2	1:B:209:ARG:HH11	2.12	0.46
1:B:64:ASN:HD22	1:B:67:LYS:HD2	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:THR:O	1:A:109:TRP:C	2.53	0.46
1:A:93:LEU:HD22	1:A:121:PHE:HD1	1.80	0.46
1:A:9:LYS:HB2	5:A:1101:HOH:O	2.17	0.45
1:A:273:GLN:HG2	1:A:275:GLN:NE2	2.28	0.44
1:A:1:MET:HA	1:A:2:SER:CB	2.48	0.44
1:A:74:THR:O	1:A:80:LYS:HG3	2.17	0.44
1:B:348:PRO:O	1:B:352:GLN:HG3	2.17	0.44
1:B:321:LYS:HG3	1:B:337:PRO:HB3	2.00	0.43
1:A:304:HIS:HD2	5:A:1030:HOH:O	2.01	0.43
1:B:93:LEU:HD22	1:B:121:PHE:CD1	2.53	0.42
1:A:198:MET:HE1	1:A:202:ASP:HB3	2.01	0.42
1:B:171:ASN:O	1:B:175:HIS:HD2	2.03	0.42
1:A:215:GLN:HE22	1:A:239:VAL:H	1.67	0.42
1:A:275:GLN:NE2	1:A:275:GLN:H	2.18	0.42
1:B:65:SER:HB3	1:B:66:ASN:HD22	1.85	0.42
1:A:83:MET:SD	1:A:105:MET:HE3	2.61	0.41
1:A:275:GLN:CD	1:A:275:GLN:H	2.23	0.41
1:A:194:GLN:OE1	1:B:376:PHE:HB3	2.21	0.41
1:B:97:PHE:HB3	1:B:101:ALA:CB	2.50	0.41
1:A:321:LYS:HG3	1:A:337:PRO:HB3	2.03	0.41
1:A:370:VAL:HG11	1:B:206:ASN:HA	2.02	0.41
1:B:333:ILE:HA	1:B:334:PRO:HD3	1.97	0.41
1:A:278:GLU:CG	1:A:282:LYS:HE3	2.48	0.41
1:A:28:TRP:O	4:A:901:GOL:C1	2.69	0.40
1:A:107:PHE:HB2	5:A:1135:HOH:O	2.20	0.40
1:B:278:GLU:HG3	1:B:290:ILE:HD13	2.03	0.40
1:B:319:ILE:CD1	1:B:324:ALA:CA	2.99	0.40
1:B:372:CYS:HA	1:B:373:PRO:HD3	1.93	0.40
1:B:230:TYR:HA	1:B:231:PRO:HA	1.89	0.40
1:A:35:LYS:HE2	1:A:60:PHE:HE2	1.86	0.40
1:B:97:PHE:CB	1:B:101:ALA:HB3	2.50	0.40

All (3) 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:81:GLU:OE2	5:B:924:HOH:O[4_675]	0.83	1.37
1:A:81:GLU:CD	5:B:924:HOH:O[4_675]	1.23	0.97
1:A:81:GLU:CG	5:B:924:HOH:O[4_675]	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	414/437 (95%)	402 (97%)	10 (2%)	2 (0%)	29	31
1	B	413/437 (94%)	405 (98%)	7 (2%)	1 (0%)	47	55
All	All	827/874 (95%)	807 (98%)	17 (2%)	3 (0%)	34	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	140	GLU
1	B	16	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	342/361 (95%)	330 (96%)	12 (4%)	36	46
1	B	341/361 (94%)	329 (96%)	12 (4%)	36	46
All	All	683/722 (95%)	659 (96%)	24 (4%)	36	46

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	TYR
1	A	93	LEU
1	A	119	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	128	ASP
1	A	161	LEU
1	A	261	GLU
1	A	275	GLN
1	A	319	ILE
1	A	320	ASP
1	A	332	ASP
1	A	374	MET
1	A	379	PHE
1	B	47	HIS
1	B	59	TYR
1	B	73	ASN
1	B	93	LEU
1	B	102	ILE
1	B	119	LEU
1	B	229	GLN
1	B	261	GLU
1	B	275	GLN
1	B	313	GLU
1	B	379	PHE
1	B	411	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	48	GLN
1	A	175	HIS
1	A	201	GLN
1	A	215	GLN
1	A	216	GLN
1	A	275	GLN
1	A	276	ASN
1	A	302	GLN
1	A	304	HIS
1	A	392	HIS
1	B	48	GLN
1	B	64	ASN
1	B	66	ASN
1	B	73	ASN
1	B	98	HIS
1	B	175	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	201	GLN
1	B	206	ASN
1	B	215	GLN
1	B	216	GLN
1	B	229	GLN
1	B	273	GLN
1	B	302	GLN
1	B	392	HIS
1	B	398	GLN
1	B	412	GLN
1	B	413	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](#)

11 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
3	ACO	B	752[A]	-	45,53,53	1.23	6 (13%)	56,79,79	1.13	5 (8%)
3	ACO	A	751[B]	1	45,53,53	1.38	7 (15%)	56,79,79	1.44	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	903	-	5,5,5	0.62	0	5,5,5	0.49	0
3	ACO	B	752[B]	1	45,53,53	1.14	6 (13%)	56,79,79	1.24	8 (14%)
4	GOL	A	901	-	5,5,5	0.46	0	5,5,5	0.59	0
4	GOL	A	902	-	5,5,5	0.36	0	5,5,5	0.64	0
4	GOL	A	904	-	5,5,5	0.47	0	5,5,5	0.23	0
2	OXL	B	801	-	0,5,5	0.00	-	0,6,6	0.00	-
4	GOL	B	905	-	5,5,5	0.40	0	5,5,5	0.66	0
3	ACO	A	751[A]	1	45,53,53	1.38	7 (15%)	56,79,79	1.40	9 (16%)
2	OXL	A	802	-	0,5,5	0.00	-	0,6,6	0.00	-

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	ACO	B	752[A]	-	-	13/47/67/67	0/3/3/3
3	ACO	A	751[B]	1	-	10/47/67/67	0/3/3/3
4	GOL	B	903	-	-	2/4/4/4	-
3	ACO	B	752[B]	1	-	11/47/67/67	0/3/3/3
4	GOL	A	901	-	-	2/4/4/4	-
4	GOL	A	902	-	-	0/4/4/4	-
4	GOL	A	904	-	-	2/4/4/4	-
2	OXL	B	801	-	-	0/0/4/4	-
4	GOL	B	905	-	-	0/4/4/4	-
3	ACO	A	751[A]	1	-	11/47/67/67	0/3/3/3
2	OXL	A	802	-	-	0/0/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	751[A]	ACO	CH3-C	5.48	1.72	1.50
3	A	751[B]	ACO	CH3-C	5.41	1.72	1.50
3	B	752[A]	ACO	CH3-C	3.39	1.64	1.50
3	B	752[A]	ACO	O4B-C1B	2.72	1.44	1.41
3	B	752[B]	ACO	O4B-C1B	2.72	1.44	1.41
3	B	752[A]	ACO	P3B-O7A	2.59	1.58	1.50
3	B	752[B]	ACO	P3B-O7A	2.59	1.58	1.50
3	B	752[A]	ACO	C2A-N3A	2.57	1.36	1.32
3	B	752[B]	ACO	C2A-N3A	2.57	1.36	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	751[B]	ACO	P3B-O7A	2.55	1.58	1.50
3	A	751[A]	ACO	P3B-O7A	2.55	1.58	1.50
3	A	751[B]	ACO	O4B-C1B	2.45	1.44	1.41
3	A	751[A]	ACO	O4B-C1B	2.45	1.44	1.41
3	A	751[B]	ACO	P3B-O3B	2.33	1.63	1.59
3	A	751[A]	ACO	P3B-O3B	2.33	1.63	1.59
3	A	751[B]	ACO	P1A-O1A	2.32	1.59	1.50
3	A	751[A]	ACO	P1A-O1A	2.32	1.59	1.50
3	A	751[B]	ACO	C2A-N3A	2.31	1.35	1.32
3	A	751[A]	ACO	C2A-N3A	2.31	1.35	1.32
3	B	752[A]	ACO	P1A-O1A	2.17	1.58	1.50
3	B	752[B]	ACO	P1A-O1A	2.17	1.58	1.50
3	B	752[A]	ACO	P2A-O4A	2.15	1.58	1.50
3	B	752[B]	ACO	P2A-O4A	2.15	1.58	1.50
3	B	752[B]	ACO	C-S1P	-2.04	1.63	1.75
3	A	751[B]	ACO	C8A-N7A	2.03	1.38	1.34
3	A	751[A]	ACO	C8A-N7A	2.03	1.38	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	752[A]	ACO	O4B-C1B-C2B	-3.79	101.39	106.93
3	B	752[B]	ACO	O4B-C1B-C2B	-3.79	101.39	106.93
3	A	751[B]	ACO	C1B-N9A-C4A	-3.72	120.10	126.64
3	A	751[A]	ACO	C1B-N9A-C4A	-3.72	120.10	126.64
3	A	751[B]	ACO	N3A-C2A-N1A	-3.64	122.99	128.68
3	A	751[A]	ACO	N3A-C2A-N1A	-3.64	122.99	128.68
3	A	751[B]	ACO	O4B-C1B-C2B	-3.54	101.75	106.93
3	A	751[A]	ACO	O4B-C1B-C2B	-3.54	101.75	106.93
3	B	752[A]	ACO	C1B-N9A-C4A	-3.53	120.43	126.64
3	B	752[B]	ACO	C1B-N9A-C4A	-3.53	120.43	126.64
3	A	751[B]	ACO	O-C-CH3	-3.40	109.11	123.07
3	B	752[A]	ACO	N3A-C2A-N1A	-3.40	123.36	128.68
3	B	752[B]	ACO	N3A-C2A-N1A	-3.40	123.36	128.68
3	A	751[B]	ACO	C6P-C5P-N4P	3.40	122.14	116.42
3	A	751[A]	ACO	C6P-C5P-N4P	3.40	122.14	116.42
3	B	752[B]	ACO	O-C-CH3	-3.08	110.43	123.07
3	A	751[B]	ACO	CDP-CBP-CAP	2.66	113.43	108.82
3	A	751[A]	ACO	CDP-CBP-CAP	2.66	113.43	108.82
3	A	751[B]	ACO	O5P-C5P-C6P	-2.41	117.60	122.02
3	A	751[A]	ACO	O5P-C5P-C6P	-2.41	117.60	122.02
3	B	752[B]	ACO	O-C-S1P	2.22	132.45	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	752[A]	ACO	N6A-C6A-N1A	2.18	123.11	118.57
3	B	752[B]	ACO	N6A-C6A-N1A	2.18	123.11	118.57
3	B	752[B]	ACO	C2P-S1P-C	2.10	112.74	101.68
3	A	751[A]	ACO	O-C-CH3	-2.05	114.64	123.07
3	A	751[B]	ACO	C2A-N1A-C6A	2.04	122.25	118.75
3	A	751[A]	ACO	C2A-N1A-C6A	2.04	122.25	118.75
3	A	751[B]	ACO	P2A-O3A-P1A	-2.03	125.84	132.83
3	A	751[A]	ACO	P2A-O3A-P1A	-2.03	125.84	132.83
3	B	752[A]	ACO	P2A-O3A-P1A	-2.03	125.88	132.83
3	B	752[B]	ACO	P2A-O3A-P1A	-2.03	125.88	132.83

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	752[A]	ACO	C5B-O5B-P1A-O1A
3	B	752[A]	ACO	C5B-O5B-P1A-O3A
3	B	752[A]	ACO	CCP-O6A-P2A-O4A
3	B	752[A]	ACO	CCP-O6A-P2A-O5A
3	B	752[A]	ACO	C5P-C6P-C7P-N8P
3	B	752[A]	ACO	C3P-C2P-S1P-C
3	A	751[B]	ACO	C5B-O5B-P1A-O1A
3	A	751[B]	ACO	C5B-O5B-P1A-O3A
3	A	751[B]	ACO	CCP-O6A-P2A-O4A
3	A	751[B]	ACO	CCP-O6A-P2A-O5A
3	A	751[B]	ACO	C6P-C5P-N4P-C3P
3	A	751[B]	ACO	O5P-C5P-N4P-C3P
3	A	751[B]	ACO	C3P-C2P-S1P-C
3	B	752[B]	ACO	C5B-O5B-P1A-O1A
3	B	752[B]	ACO	C5B-O5B-P1A-O3A
3	B	752[B]	ACO	CCP-O6A-P2A-O4A
3	B	752[B]	ACO	CCP-O6A-P2A-O5A
3	B	752[B]	ACO	C5P-C6P-C7P-N8P
3	B	752[B]	ACO	C3P-C2P-S1P-C
4	A	901	GOL	C1-C2-C3-O3
4	A	904	GOL	C1-C2-C3-O3
3	A	751[A]	ACO	C5B-O5B-P1A-O1A
3	A	751[A]	ACO	C5B-O5B-P1A-O3A
3	A	751[A]	ACO	CCP-O6A-P2A-O4A
3	A	751[A]	ACO	CCP-O6A-P2A-O5A
3	A	751[A]	ACO	C6P-C5P-N4P-C3P
3	A	751[A]	ACO	O5P-C5P-N4P-C3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	903	GOL	O1-C1-C2-C3
4	A	901	GOL	O2-C2-C3-O3
4	A	904	GOL	O2-C2-C3-O3
3	A	751[A]	ACO	O-C-S1P-C2P
3	B	752[A]	ACO	P1A-O3A-P2A-O6A
3	A	751[B]	ACO	P1A-O3A-P2A-O6A
3	B	752[B]	ACO	P1A-O3A-P2A-O6A
3	A	751[A]	ACO	P1A-O3A-P2A-O6A
3	B	752[A]	ACO	C3B-O3B-P3B-O9A
3	A	751[B]	ACO	C3B-O3B-P3B-O9A
3	A	751[B]	ACO	CCP-O6A-P2A-O3A
3	B	752[B]	ACO	C3B-O3B-P3B-O9A
3	A	751[A]	ACO	C3B-O3B-P3B-O9A
3	A	751[A]	ACO	CCP-O6A-P2A-O3A
3	B	752[A]	ACO	O-C-S1P-C2P
3	B	752[A]	ACO	CH3-C-S1P-C2P
3	B	752[A]	ACO	CDP-CBP-CCP-O6A
3	B	752[B]	ACO	CDP-CBP-CCP-O6A
3	B	752[A]	ACO	CCP-O6A-P2A-O3A
3	B	752[B]	ACO	CCP-O6A-P2A-O3A
3	B	752[A]	ACO	C5B-O5B-P1A-O2A
3	B	752[B]	ACO	C5B-O5B-P1A-O2A
4	B	903	GOL	O1-C1-C2-O2
3	A	751[A]	ACO	CH3-C-S1P-C2P

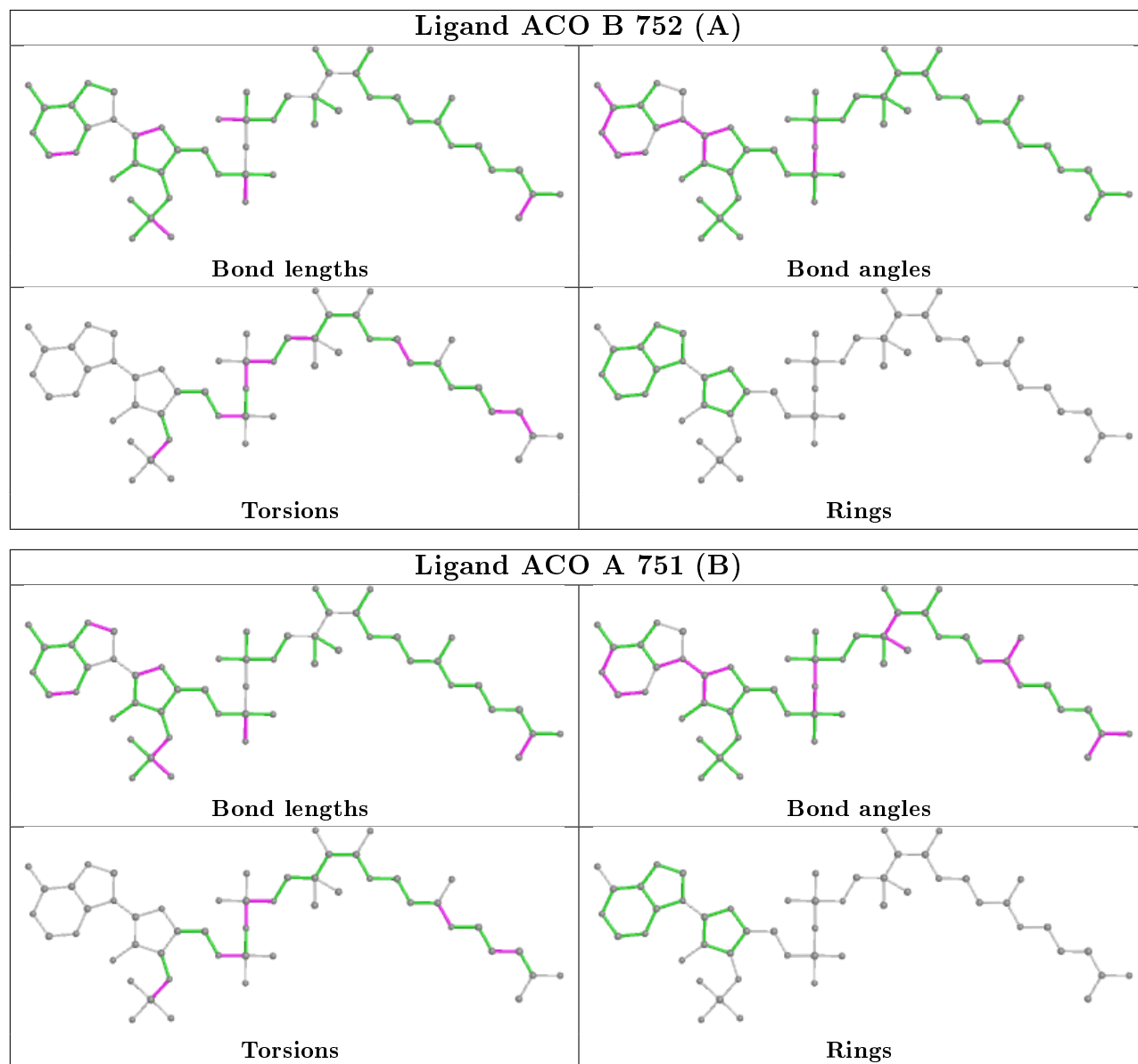
There are no ring outliers.

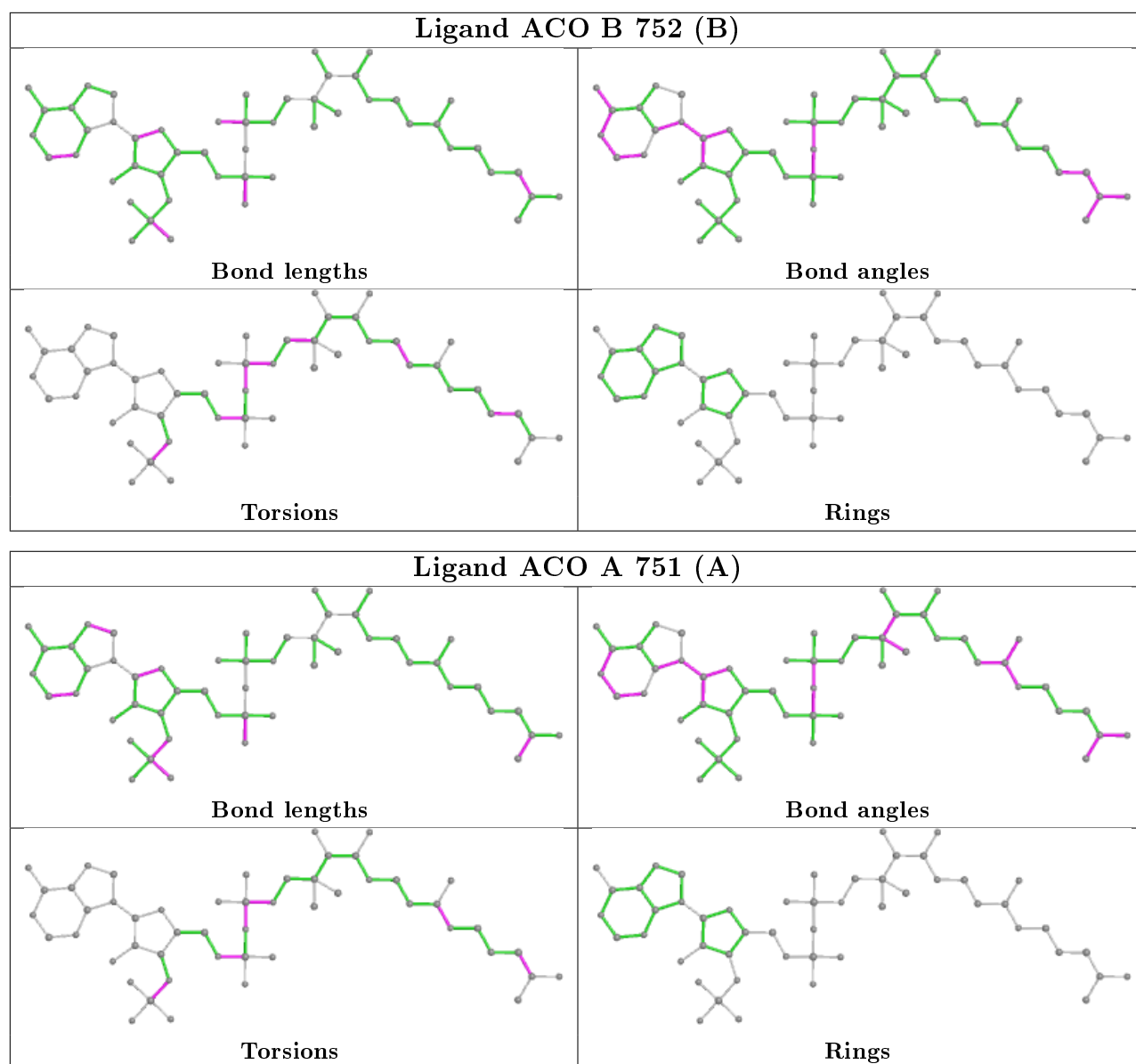
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	752[A]	ACO	1	0
3	A	751[B]	ACO	1	0
3	B	752[B]	ACO	2	0
4	A	901	GOL	2	0
3	A	751[A]	ACO	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	416/437 (95%)	-0.69	2 (0%) 91 90	31, 38, 55, 63	16 (3%)
1	B	415/437 (94%)	-0.70	2 (0%) 91 90	30, 38, 55, 61	11 (2%)
All	All	831/874 (95%)	-0.70	4 (0%) 91 90	30, 38, 55, 63	27 (3%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	ALA	4.1
1	A	101	ALA	3.4
1	B	102	ILE	2.7
1	A	107	PHE	2.1

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
2	OXL	B	801	6/6	0.71	0.21	76,78,79,80	0

Continued on next page...

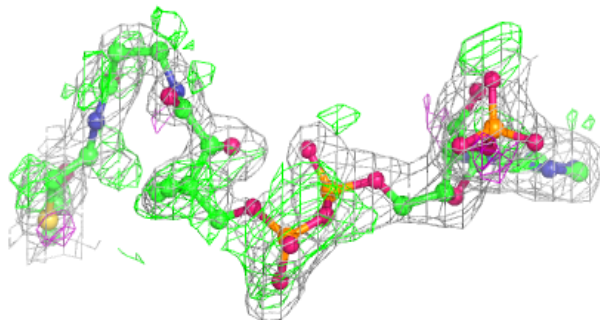
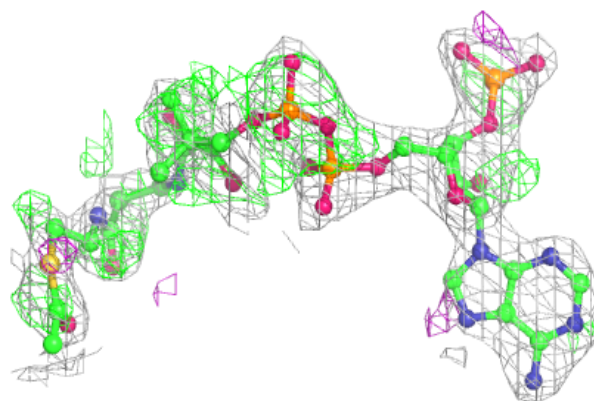
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	OXL	A	802	6/6	0.72	0.26	85,86,86,87	0
3	ACO	B	752[B]	51/51	0.82	0.20	32,39,55,57	51
3	ACO	B	752[A]	51/51	0.82	0.20	32,39,55,57	51
3	ACO	A	751[A]	51/51	0.82	0.21	27,39,50,61	51
3	ACO	A	751[B]	51/51	0.82	0.21	27,39,50,61	51
4	GOL	B	903	6/6	0.85	0.21	65,69,74,76	0
4	GOL	B	905	6/6	0.86	0.19	47,60,62,65	0
4	GOL	A	901	6/6	0.90	0.18	51,63,66,68	0
4	GOL	A	902	6/6	0.90	0.12	55,56,58,61	0
4	GOL	A	904	6/6	0.95	0.11	53,64,66,67	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.

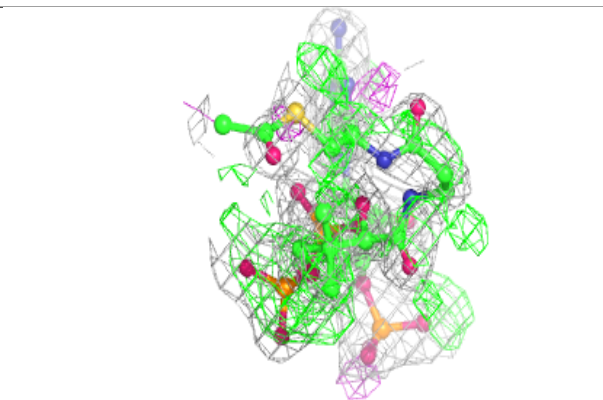
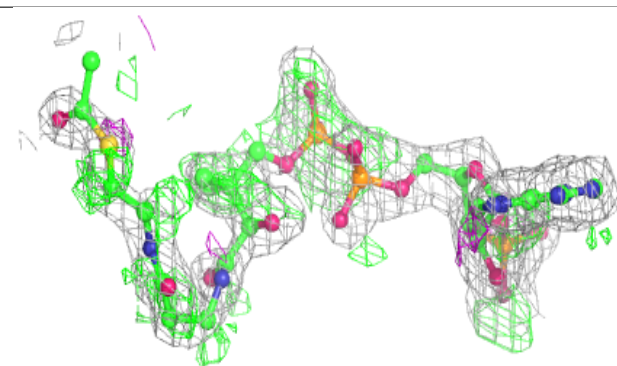
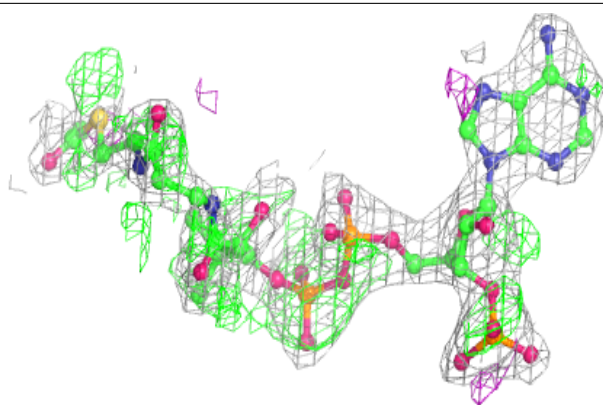
Electron density around ACO B 752 (B):

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

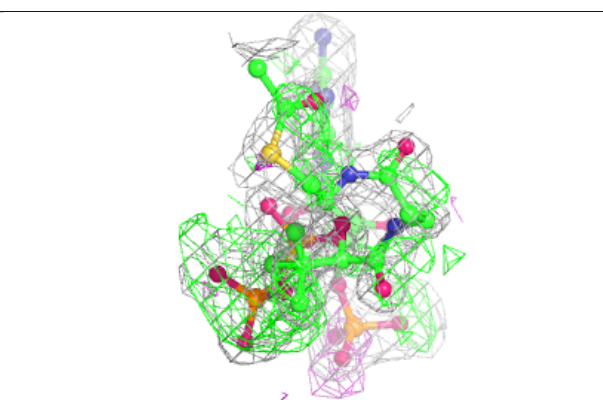
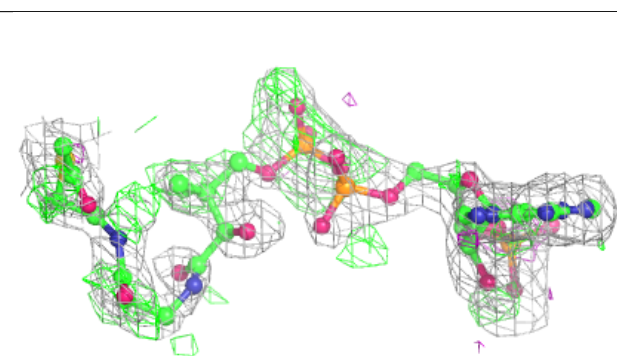
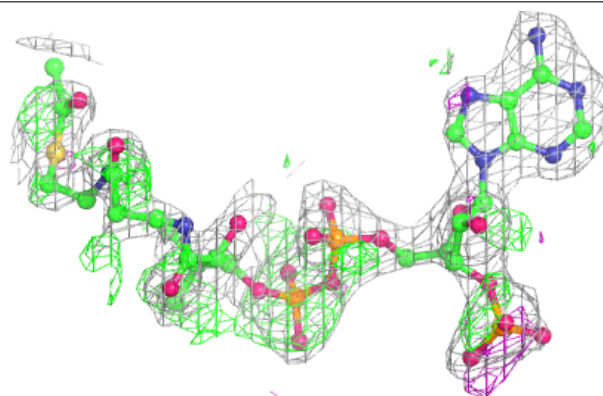


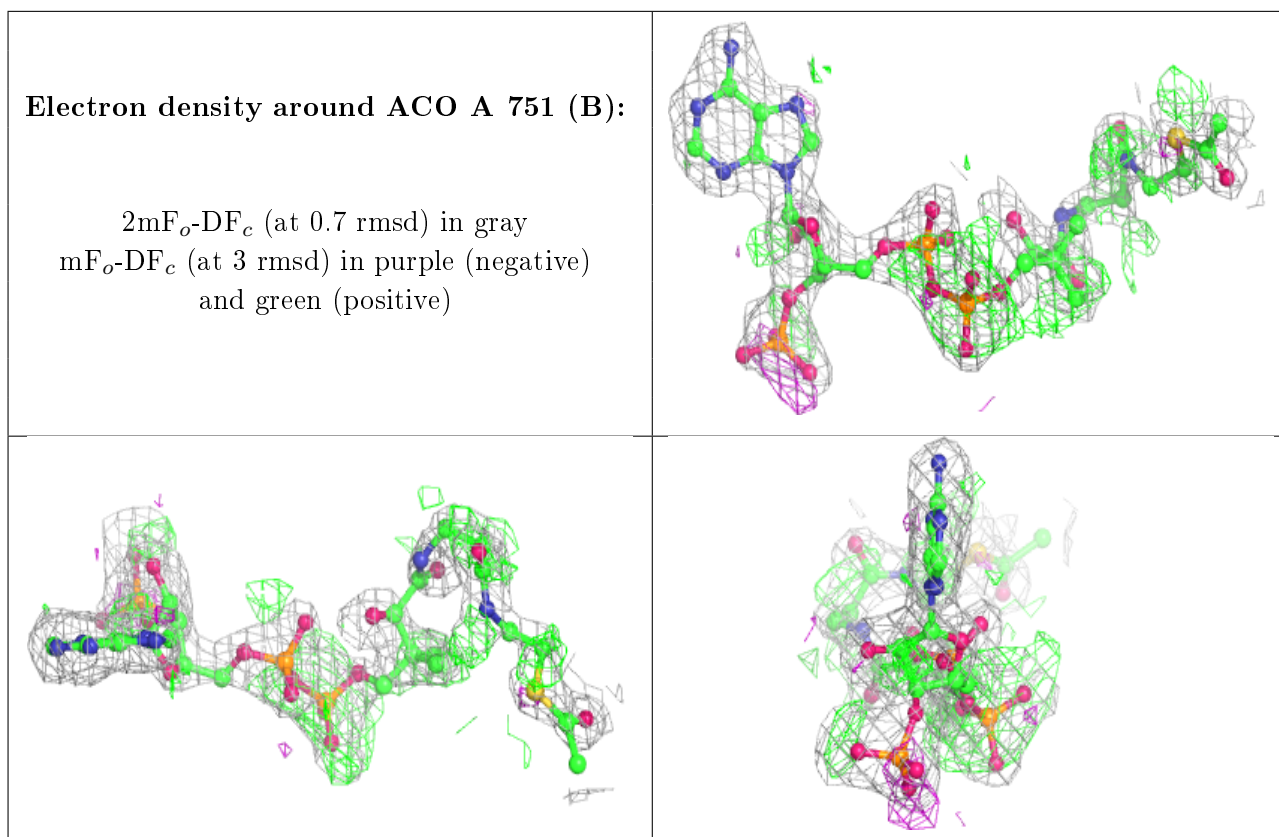
Electron density around ACO B 752 (A):

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

**Electron density around ACO A 751 (A):**

$2mF_o-DF_c$ (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.